

# Nonequilibrium Many-Body Quantum Dynamics

Lea F. Santos

September 15, 2026



# Contents

|          |                                                                           |          |
|----------|---------------------------------------------------------------------------|----------|
| <b>1</b> | <b>Introduction</b>                                                       | <b>1</b> |
| 1.0.1    | Lattice many-body systems . . . . .                                       | 1        |
| 1.0.2    | Quantum simulators: experimental developments . . . . .                   | 2        |
| 1.0.3    | Theoretical developments and open questions . . . . .                     | 4        |
| 1.0.4    | Theoretical and computational challenges of many-body systems . . .       | 5        |
| <b>2</b> | <b>Random Matrix Theory</b>                                               | <b>7</b> |
| 2.1      | Wigner’s approach to nuclear spectra . . . . .                            | 7        |
| 2.2      | Gaussian ensembles and symmetries . . . . .                               | 9        |
| 2.2.1    | Gaussian Orthogonal Ensemble (GOE) . . . . .                              | 12       |
| 2.2.2    | Gaussian Unitary Ensemble (GUE) . . . . .                                 | 13       |
| 2.2.3    | Gaussian Symplectic Ensemble (GSE) . . . . .                              | 14       |
| 2.3      | Density of states and global spectral properties . . . . .                | 15       |
| 2.4      | Level statistics: Short-range correlations . . . . .                      | 17       |
| 2.4.1    | Distribution of the spacings between neighboring levels, $P(s)$ . . . . . | 17       |
| 2.4.2    | Interpolation: Brody distribution . . . . .                               | 24       |
| 2.4.3    | Interpolation: Izrailev distribution . . . . .                            | 25       |
| 2.4.4    | Ratio of consecutive level spacings . . . . .                             | 25       |
| 2.4.5    | Random matrix theory and quantum chaos . . . . .                          | 27       |
| 2.4.6    | Examples of Classical Chaotic Systems in Everyday Life . . . . .          | 28       |
| 2.5      | Level statistics: Short- and long-range correlations . . . . .            | 29       |
| 2.5.1    | Level number variance and rigidity . . . . .                              | 29       |
| 2.5.2    | Spectral form factor . . . . .                                            | 30       |
| 2.6      | Eigenvectors and Participation Ratios . . . . .                           | 31       |
| 2.6.1    | Derivation of the participation ratio of GOE eigenvectors . . . . .       | 33       |
| 2.7      | The role of interactions: 2x2 matrices . . . . .                          | 36       |
| 2.7.1    | Level splitting, avoided crossing, and mixing . . . . .                   | 36       |
| 2.7.2    | Eigenvectors . . . . .                                                    | 37       |
| 2.7.3    | Wigner surmise: 2x2 Gaussian random matrices . . . . .                    | 38       |
| 2.8      | Fractality and multifractality of eigenstates . . . . .                   | 39       |
| 2.8.1    | Rényi Participation Entropies . . . . .                                   | 41       |
| 2.9      | Wigner band random matrices . . . . .                                     | 42       |
| 2.10     | Rosenzweig-Porter ensemble . . . . .                                      | 43       |
| 2.11     | Powerlaw banded random matrices . . . . .                                 | 45       |
| 2.12     | Assignment 01: Random Matrices . . . . .                                  | 46       |

|          |                                                                           |            |
|----------|---------------------------------------------------------------------------|------------|
| <b>3</b> | <b>Physical Models: Spin-1/2 Chains and Beyond</b>                        | <b>51</b>  |
| 3.1      | Spin-1/2 chain: Hamiltonian matrix . . . . .                              | 52         |
| 3.2      | Symmetries . . . . .                                                      | 57         |
| 3.2.1    | Conservation of total magnetization along the $z$ -direction . . . . .    | 57         |
| 3.2.2    | Reflection symmetry and parity conservation . . . . .                     | 60         |
| 3.2.3    | Global spin-flip symmetry . . . . .                                       | 63         |
| 3.2.4    | Spatial translation invariance . . . . .                                  | 64         |
| 3.3      | Integrability and Chaos in Spin-1/2 Models . . . . .                      | 67         |
| 3.4      | Eigenstates and Basis Choices . . . . .                                   | 69         |
| 3.5      | Mappings of the XXZ chain . . . . .                                       | 72         |
| 3.5.1    | Jordan–Wigner mapping to spinless fermions . . . . .                      | 72         |
| 3.5.2    | Holstein–Primakoff mapping to bosons . . . . .                            | 76         |
| 3.5.3    | Interaction and the role of basis . . . . .                               | 77         |
| 3.6      | Bipartite entanglement: Concepts and measures . . . . .                   | 78         |
| 3.6.1    | Reduced density matrix . . . . .                                          | 79         |
| 3.6.2    | Entanglement entropy . . . . .                                            | 82         |
| 3.7      | Assignment 02: Spectrum and Level Statistics of Spin-1/2 Chains . . . . . | 84         |
| 3.8      | Tools for Spin Hamiltonians . . . . .                                     | 87         |
| 3.8.1    | QuTiP . . . . .                                                           | 89         |
| 3.8.2    | QuSpin . . . . .                                                          | 90         |
| 3.9      | Beyond Spin-1/2 Models . . . . .                                          | 96         |
| 3.9.1    | Spin-1 Heisenberg XXZ chain . . . . .                                     | 96         |
| 3.9.2    | Bose–Hubbard model . . . . .                                              | 98         |
| <b>4</b> | <b>Thermalization</b>                                                     | <b>99</b>  |
| 4.1      | Eigenstate Thermalization Hypothesis . . . . .                            | 101        |
| 4.2      | Diagonal ETH . . . . .                                                    | 103        |
| 4.2.1    | Diagonal ETH is automatic in full random matrix models . . . . .          | 103        |
| 4.2.2    | Diagonal ETH is subtler in physical Hamiltonians than GOE . . . . .       | 104        |
| 4.3      | Off-diagonal ETH . . . . .                                                | 105        |
| 4.4      | Assignment 03: Thermalization . . . . .                                   | 105        |
| <b>5</b> | <b>Quench Dynamics</b>                                                    | <b>107</b> |
| 5.1      | Survival probability . . . . .                                            | 107        |
| 5.1.1    | Local density of states (LDOS) . . . . .                                  | 108        |
| 5.2      | Short-Time Behavior and Saturation . . . . .                              | 109        |
| 5.2.1    | Survival Probability: Bessel decay . . . . .                              | 110        |
| 5.2.2    | Survival Probability: Gaussian Decay . . . . .                            | 110        |
| 5.2.3    | Survival Probability: Exponential Decay . . . . .                         | 112        |
| 5.2.4    | Survival Probability: Cosine-squared behavior . . . . .                   | 113        |
| 5.2.5    | Saturation of the survival probability . . . . .                          | 115        |
| 5.3      | Assignment 04: Survival Probability . . . . .                             | 116        |
| 5.4      | Other Observables . . . . .                                               | 118        |
| 5.4.1    | Loschmidt echo . . . . .                                                  | 118        |
| 5.4.2    | Expectation values of local observables . . . . .                         | 119        |

|          |                                                                             |            |
|----------|-----------------------------------------------------------------------------|------------|
| 5.4.3    | Correlations in space . . . . .                                             | 119        |
| 5.4.4    | Correlations in time . . . . .                                              | 120        |
| 5.4.5    | Entanglement entropy . . . . .                                              | 121        |
| 5.4.6    | Participation ratio and Shannon/Participation entropy . . . . .             | 122        |
| 5.4.7    | Out-of-time-ordered correlators (OTOCs) . . . . .                           | 126        |
| 5.4.8    | Fidelity out-of-time-ordered correlators (FOTOCs) . . . . .                 | 128        |
| 5.4.9    | Momentum distribution in bosonic systems . . . . .                          | 129        |
| 5.5      | Transport in 1D spin models . . . . .                                       | 130        |
| 5.5.1    | Why the current operator appears: continuity equation . . . . .             | 130        |
| 5.5.2    | A useful commutator identity . . . . .                                      | 130        |
| 5.5.3    | Current operator for the nearest-neighbor XX model . . . . .                | 130        |
| 5.5.4    | Current operator for the nearest-neighbor XXZ model . . . . .               | 131        |
| 5.5.5    | Current operator for the XXZ model with second-neighbor couplings . . . . . | 132        |
| 5.5.6    | Total current . . . . .                                                     | 132        |
| 5.5.7    | How transport is characterized . . . . .                                    | 133        |
| 5.5.8    | Method 1: spreading of a local excitation . . . . .                         | 133        |
| 5.5.9    | Method 2: current autocorrelation and the Green–Kubo approach . . . . .     | 135        |
| 5.5.10   | Which method is best for numerical analysis of spin models? . . . . .       | 137        |
| 5.5.11   | Typical expectations for common models . . . . .                            | 137        |
| 5.6      | Temporal Fluctuations . . . . .                                             | 137        |
| <b>6</b> | <b>Many-body localization and multifractality</b>                           | <b>139</b> |
| 6.1      | Many-Body Localization . . . . .                                            | 139        |
| 6.2      | Multifractality . . . . .                                                   | 139        |
| <b>7</b> | <b>Floquet systems</b>                                                      | <b>141</b> |
| 7.1      | Floquet theorem and Floquet states . . . . .                                | 141        |
| 7.2      | Floquet operator . . . . .                                                  | 143        |
| 7.2.1    | Stroboscopic evolution . . . . .                                            | 143        |
| 7.2.2    | Floquet modes and quasienergies . . . . .                                   | 144        |
| 7.2.3    | Floquet Hamiltonian . . . . .                                               | 145        |
| 7.2.4    | Practical recipe to compute quasienergies . . . . .                         | 147        |
| 7.2.5    | Using quasienergies to diagnose chaos . . . . .                             | 149        |
| 7.3      | Example 1: Piecewise constant drive (spin chain) . . . . .                  | 154        |
| 7.3.1    | Symmetry considerations . . . . .                                           | 155        |
| 7.3.2    | Average Hamiltonian and Magnus Expansion . . . . .                          | 155        |
| 7.3.3    | Level statistics . . . . .                                                  | 156        |
| 7.3.4    | Prethermalization . . . . .                                                 | 156        |
| 7.3.5    | Heating and the infinite-temperature state . . . . .                        | 157        |
| 7.4      | Trotter decomposition and Trotter–Suzuki approximation . . . . .            | 159        |
| 7.4.1    | Second-order (symmetric) Trotter–Suzuki decomposition . . . . .             | 161        |
| 7.4.2    | Higher-order decompositions . . . . .                                       | 162        |
| 7.4.3    | Practical remarks . . . . .                                                 | 164        |
| 7.5      | Example 2: Continuously driven two-level system . . . . .                   | 164        |
| 7.5.1    | Time discretization . . . . .                                               | 164        |

|          |                                                            |            |
|----------|------------------------------------------------------------|------------|
| 7.5.2    | Left endpoint: First-order accurate . . . . .              | 165        |
| 7.5.3    | Midpoint: Second-order accurate . . . . .                  | 166        |
| 7.5.4    | Symmetrized Trotter-Suzuki decomposition . . . . .         | 167        |
| 7.5.5    | Exact evaluation of each time step . . . . .               | 168        |
| 7.6      | Assignment: Floquet Systems . . . . .                      | 170        |
| 7.6.1    | Illustrations of the solutions . . . . .                   | 175        |
| <b>8</b> | <b>Open Quantum Systems</b>                                | <b>179</b> |
| 8.1      | Density matrices for pure and mixed states . . . . .       | 179        |
| 8.2      | Purity . . . . .                                           | 180        |
| 8.3      | Lindblad master equation . . . . .                         | 181        |
| 8.4      | Properties of the Lindblad equation . . . . .              | 183        |
| 8.4.1    | Continuous-time . . . . .                                  | 183        |
| 8.4.2    | Markovian . . . . .                                        | 183        |
| 8.4.3    | Trace preserving: Normalization . . . . .                  | 183        |
| 8.4.4    | Completely positive . . . . .                              | 183        |
| 8.5      | Unitary evolution: Closed system . . . . .                 | 185        |
| 8.5.1    | Von Neumann equation for density matrices . . . . .        | 185        |
| 8.6      | Open systems and reduced density matrices . . . . .        | 186        |
| 8.7      | Vectorization of the density matrix . . . . .              | 188        |
| 8.7.1    | Vectorization identity . . . . .                           | 189        |
| 8.7.2    | Vectorization identity for the Lindblad equation . . . . . | 190        |
| 8.7.3    | Spectral properties of the Lindbladian . . . . .           | 191        |
| 8.7.4    | Steady states and long-time behavior . . . . .             | 194        |
| 8.8      | Example 1: One qubit with one jump operator . . . . .      | 196        |
| 8.9      | Example 2: Two-level atom with decay . . . . .             | 203        |
| 8.10     | Spectrum of the Lindbladian . . . . .                      | 205        |
| 8.11     | Assignment: Open Quantum Systems . . . . .                 | 211        |
| 8.11.1   | Sketches of the solutions . . . . .                        | 217        |
| 8.12     | Derivation of the Lindblad equation . . . . .              | 219        |
| <b>9</b> | <b>Ideas for projects and practice questions:</b>          | <b>227</b> |
| 9.1      | Ideas for Projects . . . . .                               | 227        |
| 9.2      | Practice Questions . . . . .                               | 228        |
| 9.2.1    | Chapter 2 – Random Matrix Theory . . . . .                 | 228        |

# Chapter 1

## Introduction

Many-body quantum systems refer to quantum systems composed of many particles, where interactions give rise to collective behaviors that have no counterpart at the level of single particles or ensembles of many noninteracting particles. These behaviors include many-body quantum chaos, thermalization under purely unitary dynamics, many-body localization, and complex nonequilibrium dynamics. A particularly important playground is provided by *lattice systems*, where bosons, fermions, or spins reside on the sites of a discrete graph and interact locally (or quasi-locally). Lattice models are central both as effective theories of real materials and as the actual Hamiltonians for many quantum-simulation platforms.

### 1.0.1 Lattice many-body systems

Representative examples of lattice many-body systems include:

- Quantum spin models such as the Heisenberg and Ising families,

$$\hat{H}_{\text{XXZ}} = J \sum_{\langle i,j \rangle} \left( \hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \Delta \hat{S}_i^z \hat{S}_j^z \right) + \sum_i \mathbf{h}_i \cdot \hat{\mathbf{S}}_i, \quad (1.1)$$

which serve as paradigms for magnetism, integrability, many-body quantum chaos, and many-body localization.

- The Bose–Hubbard model, capturing the competition between kinetic delocalization and onsite interactions,

$$\hat{H}_{\text{BH}} = -J \sum_{\langle i,j \rangle} \left( \hat{b}_i^\dagger \hat{b}_j + \text{h.c.} \right) + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) + \sum_i V_i \hat{n}_i, \quad (1.2)$$

which exhibits, e.g., the superfluid–Mott transition.

- The Fermi–Hubbard model,

$$\hat{H}_{\text{FH}} = -t \sum_{\langle i,j \rangle, \sigma} \left( \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{h.c.} \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}, \quad (1.3)$$

widely used to discuss antiferromagnetism, Mott physics, and connections to unconventional superconductivity.

Lattice locality constrains the structure of dynamics and entanglement, enabling scalable numerical approaches such as matrix product states (tensor train).

### 1.0.2 Quantum simulators: experimental developments

The modern surge of interest in lattice many-body systems is inseparable from the rise of *quantum simulation*: the idea that a controllable quantum device can emulate another quantum system that is difficult to study using classical quantum computers. Generic many-body quantum dynamics is exponentially hard to simulate on classical computers, motivating the use of quantum hardware and quantum simulators [1–4].

In practice, lattice Hamiltonians are realized in several major quantum-simulation platforms:

- **NMR Platforms.** Nuclear magnetic resonance (NMR) systems constitute one of the earliest and most versatile platforms for quantum simulation of many-body dynamics. In these experiments, nuclear spins embedded in molecules or solid-state crystals play the role of qubits, while radio-frequency (RF) pulses provide high-fidelity coherent control. Typical experiments monitor collective observables such as the magnetization  $M(t) = \langle \sum_i I_i^z \rangle$  or multi-quantum coherence spectra. These measurements enable direct studies of fundamental dynamical phenomena, including quantum transport and spin diffusion in long-range interacting networks; Loschmidt echoes and reversibility under engineered sign reversal of  $H_{\text{NMR}}$ ; growth of operator complexity and out-of-time-ordered correlators; prethermalization, many-body localization, and Floquet engineering.
- **Ultracold atoms in optical lattices.** Neutral atoms loaded into standing-wave potentials realize Hubbard-type models with tunable tunneling, interactions (via Feshbach resonances), and dimensionality. Comprehensive reviews cover equilibrium and dynamical many-body physics with ultracold gases [5] and the toolbox for optical-lattice quantum simulation [6].
- **Rydberg-atom arrays.** Individually programmable neutral-atom arrays with strong, tunable Rydberg interactions naturally implement Ising-type and constrained spin models on configurable lattices, enabling studies of quantum magnetism, dynamics, and exotic phases [7].
- **Trapped ions.** Internal states of ions encode the structure of the presentation of the presentation of effective spins, with long-range spin–spin couplings mediated by collective phonon modes. This platform offers high-fidelity control, flexible interaction graphs, and direct access to spin dynamics [8].
- **Superconducting circuits.** Lithographically fabricated qubits and resonators implement lattice models of interacting spins and bosons (including driven-dissipative settings), with fast gates and nonequilibrium control [9].

Additional important platforms include polar molecules and hybrid architectures. Across platforms, experimental capabilities now commonly include single-site resolution (in many

neutral-atom settings), programmable geometries, tailored disorder, and time-dependent control, making lattice models a primary experimental language.

**NOTE:**

All Rydberg-atom arrays use cold atoms, but not all cold-atom experiments use Rydberg atoms. Rydberg-atom arrays are a subset of cold-atom experiments, but they are conceptually and operationally distinct from traditional cold-atom lattice experiments. They address different Hamiltonians, control knobs, and questions, which is why the literature treats them as a separate platform.

**Traditional cold atoms in optical lattices:** Cold-atom experiments employ neutral atoms cooled to ultralow temperatures, typically in the nanokelvin to microkelvin range, where quantum effects dominate the dynamics. These atoms are loaded into *optical lattices*\* – periodic potentials created by the interference of counterpropagating laser beams – forming highly controllable realizations of lattice systems. In this setting, atoms are mobile and can tunnel coherently between neighboring lattice sites, giving rise to effective lattice Hamiltonians with tunable parameters.

Optical-lattice cold-atom systems naturally realize paradigmatic models of strongly correlated quantum matter, most notably the Bose–Hubbard, Fermi–Hubbard and spin models. These platforms have enabled the experimental observation and characterization of fundamental many-body phenomena, including the superfluid–Mott insulator transition, quantum magnetism arising from superexchange processes, transport in interacting systems, and thermalization dynamics in isolated quantum matter.

Interactions are predominantly short-ranged, consisting of on-site interactions with strength  $U$  and, in certain regimes, effective nearest-neighbor couplings mediated by superexchange. These systems are highly scalable, routinely involving thousands to millions of atoms, and thus provide access to the thermodynamic limit. The relevant many-body dynamics typically unfolds on relatively slow timescales

\**Optical Lattices:* Optical lattices are periodic potentials created by the interference of counterpropagating laser beams [10]. The standing wave produces an intensity pattern  $V(x) \propto \sin^2(kx)$ , which acts as a crystal-like lattice for neutral atoms. Properties:

- Global structure: the lattice extends over the whole atomic cloud.
- Identical sites: translationally invariant (up to trapping and disorder).
- Tunneling allowed: atoms can hop between neighboring sites.

**Rydberg-atom arrays:** Rydberg-atom arrays are built from neutral atoms that are trapped individually in tightly focused *optical tweezers*\*\*, allowing for deterministic preparation and precise spatial control of each atom. The atoms are coherently laser-excited from their electronic ground states to highly excited Rydberg states\*\*\*, characterized by large principal quantum numbers. These Rydberg states exhibit exaggerated atomic properties, most notably strong electric dipole moments, which give rise to large and controllable interatomic

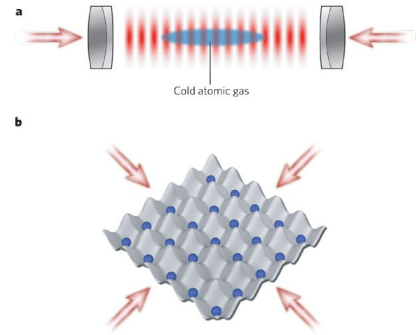


Figure 1.1: Cold atoms in optical lattices.

interactions.

In Rydberg-atom arrays, the relevant low-energy degrees of freedom are typically encoded in two internal atomic states, corresponding to the electronic ground state and a selected Rydberg state. This mapping naturally realizes effective spin-1/2 models, where interactions between atoms are mediated by strong Rydberg–Rydberg couplings. The resulting Hamiltonians are often of Ising type, featuring long-range interactions whose strength and spatial profile can be tuned by laser parameters and atomic spacing. A defining phenomenon is the Rydberg blockade, which suppresses simultaneous excitation of nearby atoms and leads to constrained many-body dynamics and reduced effective Hilbert spaces.

A key distinction of Rydberg-atom arrays is that the atoms are effectively pinned to their trapping sites, and particle tunneling is absent. Interactions are strong, long-ranged, and highly tunable, enabling access to regimes that are difficult to realize in other platforms. The geometry of the array is fully programmable, allowing the implementation of arbitrary lattice structures and interaction graphs. Owing to the large interaction strengths and optical control, coherent many-body dynamics typically occurs on fast timescales, often in the microsecond range, making Rydberg-atom arrays particularly well suited for studies of nonequilibrium dynamics, quantum chaos, and analog quantum simulation.

**\*\*Optical Tweezers:** Optical tweezers are tightly focused laser beams that trap individual atoms at specific positions. Each tweezer is an independent potential well. Properties:

- Local control: each atom is trapped and addressed individually.
- Pinned atoms: no tunneling between sites.
- Reconfigurable geometry: arbitrary graphs, not just periodic lattices.
- Single-atom resolution: preparation, control, and readout site by site.

**\*\*\*Rydberg states:** In an atom, electrons occupy discrete energy levels labeled by the principal quantum number  $n = 1, 2, 3, \dots$ . A Rydberg state is an electronic state with very large  $n$ , typically  $n \sim 20 - 100$  (sometimes even higher), so one electron is promoted far from the nucleus and the atom becomes huge in size. Rydberg atoms strongly interact with each other. Using optical tweezers we can place atoms in arbitrary 1D/2D geometries, turn lasers on/off locally, realize programmable Hamiltonians in real time.

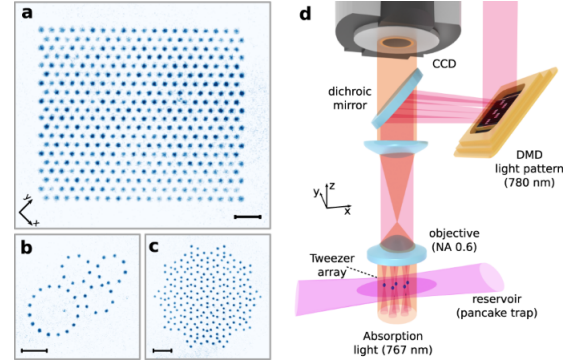


Figure 1.2: Optical tweezer.

### 1.0.3 Theoretical developments and open questions

Historically, lattice many-body physics was driven by equilibrium questions: classification of phases, universality at critical points, and quasiparticle descriptions where applicable. Over the last two decades, emphasis has expanded dramatically toward *dynamics* and *information-theoretic* viewpoints. Key themes include:

- **Thermalization and ergodicity:** when and how isolated lattice systems approach equilibrium, the role of conservation laws and integrability, and the emergence of hydrodynamics.

- **Many-body localization (MBL):** the persistence (or breakdown) of localization and memory of initial conditions in interacting disordered lattices, and its implications for entanglement growth and transport.
- **Floquet and driven matter:** prethermalization, dynamical stabilization of phases, time crystalline behavior, and heating mechanisms in periodically driven lattices.
- **Open lattice systems:** comparison with the level statistics of non-Hermitian random matrices, competition between coherent many-body evolution and measurement/dissipation.

Despite striking progress, many foundational questions remain open, especially in regimes where strong interactions, high dimensions, disorder, and long-time dynamics meet. A non-exhaustive list of active frontiers includes:

- **Thermalization versus localization in large lattices:** establishing the stability (or instability) of MBL beyond one dimension, clarifying long-time dynamics and the timescales for equilibration, performing finite-size scaling, and identifying robust experimental diagnostics.
- **Universal nonequilibrium behavior:** understanding prethermal regimes, emergent hydrodynamics, operator spreading, and the fate of quasiparticles near integrability-breaking perturbations.
- **Quantum critical dynamics:** characterizing out-of-equilibrium scaling near quantum phase transitions, including Kibble–Zurek physics.
- **Quantum advantage in analog simulators:** developing reliable methods to certify that a programmable lattice simulator implements the intended model in parameter regimes beyond classical tractability.
- **Interplay of coherence, dissipation, and measurement:** engineering dissipative dynamics for state preparation and exploring measurement-induced transitions and entanglement phases in monitored lattice systems.

These questions lie at the intersection of condensed-matter physics, atomic, molecular, and optical (AMO) physics, and quantum information science, where lattice models provide experimentally controllable testbeds for entanglement growth, information scrambling, thermalization, and localization in interacting quantum matter.

#### 1.0.4 Theoretical and computational challenges of many-body systems

The theoretical description of generic many-body quantum systems poses a major challenge, as typically they cannot be solved analytically. At the same time, the exponential growth of their Hilbert space renders the direct simulation on classical computers intractable. Addressing this challenge has motivated three complementary research directions.

First, the development of quantum simulators and quantum computers aims to provide experimental platforms capable of emulating many-body quantum dynamics beyond classical computational limits. This effort is intrinsically intertwined with theory: while quantum hardware is needed to study complex many-body systems, a deeper theoretical understanding of many-body dynamics is simultaneously required to control, benchmark, and optimize these quantum devices. A catch-22!

Second, substantial effort is devoted to the development of more efficient numerical algorithms for classical computers. These approaches exploit physical structure, such as locality, symmetries, and constraints to extend the reach of classical simulations beyond brute-force methods.

Third, analytical and semi-analytical approaches seek to extract universal insights through approximations. In this context, random matrix theory plays a central role. By modeling complex Hamiltonians as matrices with statistically distributed elements that respect fundamental symmetries, random matrix ensembles capture universal features of many-body quantum systems, such as spectral correlations, without relying on microscopic details. We start our discussion with these matrices.

# Chapter 2

## Random Matrix Theory

Random matrix theory (RMT) originated in mathematics in the early twentieth century, well before its physical significance was recognized. Early contributions can be traced to the work of statisticians and mathematicians such as Wishart.

A decisive turning point occurred in the 1950s through the work of Eugene Wigner, who employed random matrices in nuclear physics. He was motivated by the complexity of the spectra of heavy atomic nuclei, which resisted descriptions in terms of detailed microscopic nuclear models, so he proposed a statistical approach. Rather than attempting to model the precise interactions among nucleons, he suggested replacing the nuclear Hamiltonian by a large matrix whose entries were random variables, constrained only by the fundamental symmetries of the physical system.

This idea marked the birth of random matrix theory as a tool in physics. Wigner's insight was that spectral properties of complex quantum systems should be universal, depending primarily on symmetry rather than on microscopic details. His work laid the foundation for a statistical description of quantum spectra and introduced concepts that would later become central to quantum chaos.

### 2.1 Wigner's approach to nuclear spectra

In Wigner's model, the Hamiltonian of a complex nucleus is represented by a large real symmetric matrix (which reflects the time-reversal symmetry of the nuclei he was studying), where the elements are independent Gaussian random variables. In fact, in Wigner's statistical description of nuclei, one considers an *ensemble* of random Hamiltonian matrices.

For systems with time-reversal symmetry satisfying  $\mathcal{T}^2 = +1$ , a basis can be chosen in which each Hamiltonian of the ensemble is represented by a real symmetric matrix,

$$H = H^T.$$

The independent entries of such a matrix are the diagonal elements  $H_{ii}$  and one set of off-diagonal elements  $H_{ij}$  with  $i < j$ .

A probability density  $P(H)$  is introduced on the space of real symmetric matrices, where  $P(H)$  specifies how likely it is to obtain a particular matrix  $H$  when a matrix is randomly drawn from the ensemble.

An important principle in constructing the ensemble is that no particular orthonormal basis should be preferred. In other words, if we represent the same Hamiltonian in a different orthonormal basis,

$$H \rightarrow H' = OHO^T,$$

where  $O$  is an orthogonal matrix, the probability assigned to the matrix should not change:

$$P(H') = P(H).$$

This property is known as *orthogonal invariance*.

We therefore look for quantities constructed from  $H$  that are unchanged under an orthogonal change of basis. A simple example is

$$\text{Tr}(H^2).$$

Indeed,

$$\text{Tr}[(OHO^T)^2] = \text{Tr}(OH^2O^T) = \text{Tr}(H^2).$$

Thus, a probability distribution that depends on  $H$  through  $\text{Tr}(H^2)$  does not privilege any particular orthonormal basis.

There are many possible basis-invariant probability distributions. A particularly simple choice is the Gaussian form

$$P(H) \propto \exp[-a \text{Tr}(H^2)],$$

where  $a > 0$  sets the overall scale of the matrix elements. But we could think of other possibilities, such as  $P(H) \propto e^{-a[\text{Tr}(H^2)]^2}$  or some more general function,  $P(H) = F(\text{Tr}(H^2))$ . However, the Gaussian Orthogonal Ensemble introduces an additional assumption: the independent matrix elements are statistically independent. This means that their joint probability distribution must factorize into probability distributions for the individual independent matrix elements. The combination of this statistical independence with orthogonal invariance singles out a Gaussian distribution.

For a real symmetric matrix,  $H_{ij} = H_{ji}$ , and

$$\text{Tr}(H^2) = \sum_{i,j} H_{ij}H_{ji} = \sum_{i,j} H_{ij}^2.$$

Since the off-diagonal elements appear twice in the double sum,

$$\text{Tr}(H^2) = \sum_i H_{ii}^2 + 2 \sum_{i<j} H_{ij}^2.$$

Consequently,

$$P(H) \propto \exp \left[ -a \sum_i H_{ii}^2 - 2a \sum_{i<j} H_{ij}^2 \right],$$

or, equivalently,

$$P(H) \propto \prod_i e^{-aH_{ii}^2} \prod_{i<j} e^{-2aH_{ij}^2}.$$

The probability density therefore factorizes into separate Gaussian distributions for all the independent matrix elements. Comparing these factors with the probability density of a Gaussian random variable,

$$p(x) \propto \exp \left[ -\frac{x^2}{2\sigma^2} \right],$$

we find

$$\text{Var}(H_{ii}) = \frac{1}{2a}, \quad \text{Var}(H_{ij}) = \frac{1}{4a}, \quad i \neq j,$$

and hence

$$\boxed{\text{Var}(H_{ii}) = 2 \text{Var}(H_{ij})}.$$

Thus, Gaussianity is not imposed by the requirement of basis invariance. Rather, the Gaussian distribution is a particularly simple choice that combines orthogonal invariance with statistical independence of the independent matrix elements. Other, non-Gaussian orthogonally invariant ensembles can also be constructed, and many of them exhibit the same universal spectral statistics.

Wigner focused in particular on the statistical properties of level spacings, that is, the differences between neighboring eigenvalues. One of his most influential results was the observation that the probability distribution of nearest-neighbor level spacings exhibits *level repulsion*: the probability of finding two nearby levels close together vanishes as a power law as the spacing goes to zero. To make these ideas quantitative, Wigner introduced what is now known as the *Wigner surmise*, an approximate formula for the level-spacing distribution derived from  $2 \times 2$  random matrices. Despite its simplicity, the Wigner surmise captures the essential universal features of large random matrices and remains a cornerstone of RMT.

## 2.2 Gaussian ensembles and symmetries

In random matrix theory, one considers *ensembles* of random matrices in order to study the statistical properties of their spectra and eigenstates. The choice of ensemble is dictated by the symmetries of the physical system under consideration. In random-matrix descriptions of quantum systems, time-reversal symmetry plays a central role in determining the appropriate universality class, while the classical Gaussian ensembles are characterized by invariance under basis transformations in Hilbert space (sometimes referred to as rotational invariance in Hilbert space).

---

**(i) Time-reversal invariance.** A Hamiltonian is time-reversal invariant when the dynamics looks the same if the direction of time is reversed. Classically, reversing time,  $t \rightarrow -t$ , leaves positions unchanged but reverses quantities associated with motion, such as momentum and angular momentum,

$$\mathbf{r} \rightarrow \mathbf{r}, \quad \mathbf{p} \rightarrow -\mathbf{p}, \quad \mathbf{L} \rightarrow -\mathbf{L}.$$

For example, the Hamiltonian of a particle in a potential,

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}),$$

is invariant under time reversal because it depends on  $\mathbf{p}$  only through  $\mathbf{p}^2$ . By contrast, a charged particle in a fixed magnetic field is generally not time-reversal invariant, since time reversal reverses the particle's motion but not the externally imposed magnetic field.

In quantum mechanics, time reversal is represented by an *antiunitary* operator  $T$ . Unlike an ordinary unitary symmetry, an antiunitary operator complex conjugates numerical coefficients:

$$T(c_1|\psi_1\rangle + c_2|\psi_2\rangle) = c_1^*T|\psi_1\rangle + c_2^*T|\psi_2\rangle.$$

The complex conjugation is essential because the Schrödinger equation contains the imaginary unit  $i$ . Under  $t \rightarrow -t$ , consistency of

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$$

requires  $i \rightarrow -i$ , which is precisely what an antiunitary transformation accomplishes. Time-reversal invariance is therefore expressed as

$$THT^{-1} = H.$$

For a spinless particle, in the position representation, time reversal is simply complex conjugation,  $T = K$ . Indeed, since  $\mathbf{p} = -i\hbar\nabla$ , complex conjugation gives

$$K\mathbf{p}K^{-1} = -\mathbf{p},$$

while leaving  $\mathbf{r}$  unchanged. The condition  $THT^{-1} = H$  then becomes

$$H^* = H.$$

Since a Hamiltonian is also Hermitian,  $H^\dagger = H$ , it can in this basis be represented by a real symmetric matrix.

This connection is precisely why the Gaussian orthogonal ensemble (GOE) describes quantum systems with time-reversal symmetry of the type  $T^2 = +1$ . A GOE matrix is, by definition, a real symmetric matrix. Because it is real,

$$KHK^{-1} = H^* = H,$$

so every GOE matrix is invariant under the antiunitary operation  $T = K$ , with  $T^2 = K^2 = +1$ . Conversely, a generic chaotic Hamiltonian possessing an antiunitary symmetry with  $T^2 = +1$  can be represented in a basis in which it is real symmetric, and its spectral fluctuations are therefore expected to follow GOE statistics.

The relevant antiunitary symmetry need not always be the physical time-reversal operator in its simplest form. This point is particularly important for spin-1/2 many-body systems. Although the physical time-reversal operator for a single spin-1/2 satisfies  $T^2 = -1$ , many spin Hamiltonians possess another antiunitary symmetry that squares to  $+1$ , or can simply be represented by a real matrix in an appropriate basis. Such systems belong to the orthogonal symmetry class and, when quantum chaotic, exhibit GOE spectral statistics.

---

(ii) **Rotational invariance in Hilbert space.** In random-matrix theory, the term “rotational invariance” does not refer to rotations in physical space. It is a statistical symmetry of an ensemble rather than a property of an individual Hamiltonian. It refers to the invariance of a statistical description (the ensemble probability measure) under changes of orthonormal basis in Hilbert space. An ensemble is said to be rotationally invariant if its probability distribution remains unchanged under basis transformations,

$$H \rightarrow UHU^\dagger,$$

where  $U$  belongs to the appropriate symmetry group. This invariance implies that no basis in Hilbert space is preferred and ensures that statistical properties depend only on basis-independent quantities, such as eigenvalues and spectral correlations.

For example, consider the Gaussian orthogonal ensemble (GOE), whose elements are real symmetric matrices. An orthogonal change of basis transforms a matrix according to

$$H \longrightarrow H' = OHO^T, \quad O^T O = \mathbb{I}.$$

The GOE is rotationally invariant because

$$P(H') = P(H)$$

for every orthogonal matrix  $O$ . Thus, no orthonormal basis is statistically preferred by the ensemble.

This property can be seen directly from the Gaussian probability distribution,

$$P(H) \propto \exp \left[ -a \operatorname{Tr}(H^2) \right].$$

Under an orthogonal transformation,

$$\operatorname{Tr} [(OHO^T)^2] = \operatorname{Tr} (OH^2O^T) = \operatorname{Tr}(H^2),$$

and therefore the probability assigned to  $H$  is unchanged. More generally, quantities such as  $\operatorname{Tr}(H^n)$  are invariant under a change of basis and depend only on the eigenvalues of  $H$ .

The name “rotational invariance” arises because an orthogonal transformation can be viewed geometrically as a rotation (or reflection) of the coordinate axes used to represent vectors in a real Hilbert space. Changing these axes changes the matrix elements of  $H$ , but it does not change the statistical probability of obtaining that matrix from the GOE. In this sense, the ensemble has no preferred direction, or equivalently no preferred basis, in Hilbert space.

The corresponding invariance depends on the random-matrix ensemble. For the GOE,

$$H \longrightarrow OHO^T, \quad O \in O(N),$$

whereas for the Gaussian unitary ensemble (GUE),

$$H \longrightarrow UHU^\dagger, \quad U \in U(N).$$

Both are therefore rotationally invariant ensembles, with “rotation” understood in the generalized sense of an orthogonal or unitary change of basis in Hilbert space.

Dyson classified random matrix ensembles according to these symmetries, leading to the three classical Gaussian ensembles: the Gaussian Orthogonal Ensemble (GOE), the Gaussian Unitary Ensemble (GUE), and the Gaussian Symplectic Ensemble (GSE). These ensembles are characterized by the Dyson index  $\beta = 1, 2, 4$ , respectively, which governs the strength of level repulsion.

### 2.2.1 Gaussian Orthogonal Ensemble (GOE)

GOE random matrices are real symmetric matrices  $H = H^T$ . The GOE ensemble describes Hamiltonians that are time-reversal invariant and whose probability distribution is invariant under orthogonal (rotational) changes of basis,  $H \mapsto OHO^T$ . We often choose

$$\boxed{\mathbb{E}[H_{ii}] = \mathbb{E}[H_{ij}] = 0, \quad \text{Var}(H_{ii}) = 2, \quad \text{Var}(H_{ij}) = 1.} \quad (2.1)$$

A standard way to generate a matrix drawn from the GOE ensemble is to first construct an  $N \times N$  real random matrix  $M$  with independent and identically distributed (*i.i.d.*) Gaussian entries

$$M_{ij} \text{ independent,} \quad \mathbb{E}[M_{ij}] = \mu = 0, \quad \text{Var}(M_{ij}) = \sigma^2 = 1.$$

The GOE matrix is then obtained by symmetrization,

$$H = \frac{M + M^T}{\sqrt{2}}, \quad (2.2)$$

which ensures that  $H$  is real and symmetric.

*Diagonal entries:*

For  $i = j$ ,

$$H_{ii} = \frac{M_{ii} + M_{ii}}{\sqrt{2}} = \sqrt{2}M_{ii},$$

and therefore

$$\mathbb{E}[H_{ii}] = \sqrt{2}\mu = 0, \quad \text{Var}(H_{ii}) = 2\sigma^2 = 2. \quad (2.3)$$

*Off-diagonal entries:*

For  $i \neq j$ ,

$$H_{ij} = \frac{M_{ij} + M_{ji}}{\sqrt{2}}, \quad \text{with } M_{ij} \text{ and } M_{ji} \text{ independent.}$$

Hence

$$\mathbb{E}[H_{ij}] = \frac{\mathbb{E}[M_{ij}] + \mathbb{E}[M_{ji}]}{\sqrt{2}} = \frac{\mu + \mu}{\sqrt{2}} = \sqrt{2}\mu, \quad (2.4)$$

and

$$\text{Var}(H_{ij}) = \text{Var}\left(\frac{M_{ij} + M_{ji}}{\sqrt{2}}\right) = \frac{1}{2}(\text{Var}(M_{ij}) + \text{Var}(M_{ji})) = \frac{1}{2}(\sigma^2 + \sigma^2) = \sigma^2. \quad (2.5)$$

So for  $i \neq j$ ,

$$\mathbb{E}[H_{ij}] = \mu = 0, \quad \text{Var}(H_{ij}) = \sigma^2 = 1. \quad (2.6)$$

The diagonal has twice the variance of an off-diagonal entry. This choice makes the distribution invariant under orthogonal changes of basis  $H \mapsto OHO^T$  with  $O \in O(N)$ .

**NOTE:** There are other possibilities when generating the matrices. If we use, for example,

$$H = \frac{M + M^T}{2}, \quad (2.7)$$

we get

$$\mathbb{E}[H_{ij}] = 0, \quad \text{for } i = j, i \neq j \quad \text{Var}(H_{ii}) = 1 \quad \text{and} \quad \text{Var}(H_{ij}) = \frac{1}{2} \quad \text{for } i \neq j. \quad (2.8)$$

### 2.2.2 Gaussian Unitary Ensemble (GUE)

GUE random matrices are complex Hermitian matrices  $H = H^\dagger$ . The diagonal entries are real (not complex), because Hermiticity forces  $H_{ii} = H_{ii}^*$ , and the off-diagonal entries are complex. The GUE ensemble describes Hamiltonians that break time-reversal symmetry and whose probability distribution is invariant under unitary (rotational) changes of basis,  $H \mapsto UHU^\dagger$  with  $U \in U(N)$ . We often choose

$$\boxed{\mathbb{E}[H_{ii}] = \mathbb{E}[H_{ij}] = 0, \quad \text{Var}(H_{ii}) = 1, \quad \text{Var}(H_{ij}) = \mathbb{E}[|H_{ij}|^2] = 1.} \quad (2.9)$$

---

**NOTE:** For a complex random variable  $z = x + iy$ , the variance is defined as

$$\text{Var}(z) = \mathbb{E}[|z - \mathbb{E}[z]|^2].$$

This is the natural extension of the variance of a real random variable, since variance measures the average squared distance from the mean. For a complex number, the distance in the complex plane is given by its absolute value. Thus, if  $\mathbb{E}[x] = \mathbb{E}[y] = 0$ , so that  $\mathbb{E}[z] = 0$ , then

$$\text{Var}(z) = \mathbb{E}[|z|^2] = \mathbb{E}[x^2 + y^2] = \text{Var}(x) + \text{Var}(y).$$


---

1) We can construct the GUE matrix using real diagonal elements,

$$H_{ii} \sim \mathcal{N}(0, \sigma^2) \quad (\text{real}),$$

and off diagonal elements for  $i < j$  as

$$M_{ij} = X_{ij} + iY_{ij}, \quad X_{ij}, Y_{ij} \sim \mathcal{N}\left(0, \frac{\sigma^2}{2}\right),$$

then setting  $H_{ji} = H_{ij}^*$ .

2) Another convenient construction begins with an  $N \times N$  complex matrix  $M$  whose entries are independent complex Gaussians (notice that the variance is now  $\sigma^2 = 1$  for all elements, which is different from what we did above),

$$M_{ij} = X_{ij} + iY_{ij}, \quad X_{ij}, Y_{ij} \text{ i.i.d. } \mathcal{N}(0, 1).$$

The GUE matrix is obtained by Hermitian symmetrization,

$$H = \frac{M + M^\dagger}{2}. \quad (2.10)$$

*Diagonal entries:*

For  $i = j$ , the elements are **real** Gaussians

$$H_{ii} = \frac{M_{ii} + M_{ii}^*}{2} = \text{Re}(M_{ii}) = X_{ii},$$

so

$$\mathbb{E}[H_{ii}] = 0, \quad \text{Var}(H_{ii}) = 1. \quad (2.11)$$

*Off-diagonal entries:*

For  $i \neq j$ ,

$$H_{ij} = \frac{M_{ij} + M_{ji}^*}{2},$$

where  $M_{ij}$  and  $M_{ji}$  are independent complex Gaussians. Writing  $M_{ij} = X_{ij} + iY_{ij}$  and  $M_{ji} = X_{ji} + iY_{ji}$  gives

$$H_{ij} = \frac{X_{ij} + X_{ji}}{2} + i \frac{Y_{ij} - Y_{ji}}{2}.$$

Hence

$$\mathbb{E}[H_{ij}] = 0, \quad (2.12)$$

and

$$\text{Var}[H_{ij}] = \mathbb{E}[|H_{ij}|^2] = \text{Var}\left(\frac{X_{ij} + X_{ji}}{2}\right) + \text{Var}\left(\frac{Y_{ij} - Y_{ji}}{2}\right) = \left(\frac{1+1}{4}\right) + \left(\frac{1+1}{4}\right) = 1. \quad (2.13)$$

### 2.2.3 Gaussian Symplectic Ensemble (GSE)

*We will not study this ensemble.* The GSE describes time-reversal invariant systems with  $\mathcal{T}^2 = -1$  (Kramers degeneracy) and is most conveniently represented as a  $2N \times 2N$  complex Hermitian matrix with a symplectic constraint. A standard construction is to write

$$H = \begin{pmatrix} A & B \\ -B^* & A^* \end{pmatrix}, \quad A = A^\dagger, \quad B = B^T, \quad (2.14)$$

where  $A$  is an  $N \times N$  complex Hermitian matrix and  $B$  is an  $N \times N$  complex symmetric matrix. The block structure (2.14) is equivalent to *quaternion self-duality* and ensures invariance under symplectic basis transformations (the unitary symplectic group).

## 2.3 Density of states and global spectral properties

A fundamental spectral quantity is the density of states (DOS),

$$\rho(E) = \frac{1}{N} \left\langle \sum_n \delta(E - E_n) \right\rangle, \quad (2.15)$$

where  $\{E_n\}$  are the eigenvalues of the random matrix,  $\langle \cdots \rangle$  denotes ensemble averaging, and  $1/N$  ensure that the DOS is normalized to integrate to unity, that is

$$\int \rho(E) dE = 1.$$

In practice, for a discrete spectrum, this normalization means that the total area of the histogram used to approximate  $\rho(E)$  is 1. How is this obtained?

When constructing a histogram to approximate the density of states, we proceed as follows.

(i) We analyze the range of energies in the spectrum and choose a reasonable bin size, such that all energies are covered. The bin size should be neither too small (leading to noisy statistics) nor too large (washing out spectral structure).

(ii) We count the number of energy levels  $n_k$  that fall within each bin  $k$ . Attention: To obtain a *density of states*, the histogram must be plotted as a *density*, that is, with bin heights

$$h_k = \frac{n_k}{(\text{bin size})}$$

The area of this density histogram is then

$$\sum_k h_k \times (\text{bin size}) = \sum_k n_k = N,$$

which corresponds to the unnormalized density of states  $D(E)$ . If one divides the unnormalized density histogram  $D(E)$  by  $N$ , one obtains the normalized density of states,  $\rho(E)$ , whose total area is equal to one.

For large  $N$ ,  $\rho(E)$ , converges to the **Wigner semicircle law** with  $N$ -dependent support,

$$\rho(E) = \frac{1}{2\pi N\sigma^2} \sqrt{4N\sigma^2 - E^2}, \quad |E| \leq 2\sqrt{N}\sigma, \quad (2.16)$$

and  $\rho(E) = 0$  outside this interval. In the limit of large matrix dimension  $N$ , the average DOS of all three Gaussian ensembles (GOE, GUE, and GSE) converges to the same universal form

*Remark (standard scaling):* To obtain an  $N$ -independent semicircle support  $[-2\sigma, 2\sigma]$ , one rescales the entries. Taking the GOE as an example, the typical off-diagonal second moment becomes of order  $1/N$ , namely

$$\mathbb{E}[H_{ij}^2] \sim \frac{\sigma^2}{N} \quad (i \neq j).$$

For example, start from an  $N \times N$  real matrix  $M$  with i.i.d. Gaussian entries

$$M_{ij} \text{ independent, } \quad M_{ij} \sim \mathcal{N}(0, \sigma^2).$$

Defining the symmetric matrix  $H = \frac{M+M^T}{\sqrt{2}}$ , we arrive at Eq. (2.8) for  $i \neq j$ . But rescaling by  $1/\sqrt{N}$ ,

$$\tilde{H} = \frac{1}{\sqrt{N}} H = \frac{M + M^T}{\sqrt{2N}}, \quad (2.17)$$

we get

$$\text{Var}(\tilde{H}_{ii}) = \frac{1}{N} \text{Var}(H_{ii}) = \frac{2\sigma^2}{N} \quad \text{and} \quad \text{Var}(\tilde{H}_{ij}) = \frac{1}{N} \text{Var}(H_{ij}) = \frac{\sigma^2}{N} \quad \text{for } i \neq j.$$

With this normalization, the empirical density of states converges as  $N \rightarrow \infty$  to the Wigner semicircle law

$$\rho(E) = \frac{1}{2\pi\sigma^2} \sqrt{4\sigma^2 - E^2}, \quad |E| \leq 2\sigma, \quad (2.18)$$

and  $\rho(E) = 0$  otherwise. Therefore, choosing  $\sigma = 1$  sets the spectral support to  $E \in [-2, 2]$ . The unnormalized density of states is

$$D(E) = \frac{N}{2\pi\sigma^2} \sqrt{4\sigma^2 - E^2}, \quad |E| \leq 2\sigma, \quad (2.19)$$

Equation (2.16) and Eq.(2.18) are the same for all three Gaussian ensembles. The fact that the DOS is identical for GOE, GUE, and GSE reflects the universality of global spectral properties. For the Gaussian ensembles, the matrices are normalized so that the variance  $\langle |H_{ij}|^2 \rangle$  is the same, independently of the symmetry class. This fixes the overall width of the spectrum, since the second moment of the DOS is related to

$$\frac{1}{N} \langle \text{Tr}(H^2) \rangle.$$

More generally, the shape of the DOS is determined by all of its moments,

$$\mu_k = \frac{1}{N} \langle \text{Tr}(H^k) \rangle = \int dE E^k \rho(E).$$

In the limit of large matrix dimension  $N$ , the leading contributions to these moments are the same for GOE, GUE, and GSE: the odd moments vanish, while the even moments are those of the Wigner semicircle distribution. Differences associated with the symmetry class, characterized by the Dyson index  $\beta = 1, 2, 4$ , contribute only to subleading finite- $N$  corrections to these global moments. Consequently, GOE, GUE, and GSE have the same semicircular DOS in the large- $N$  limit. The symmetry class becomes important instead for correlations between eigenvalues, and therefore for local spectral quantities such as the level-spacing distribution, where the different ensembles exhibit different degrees of level repulsion.

## 2.4 Level statistics: Short-range correlations

A main feature of random matrices is that their eigenvalues are correlated. This means that they repel each other, degeneracies are avoided. We say that the spectrum is rigid. A remarkable feature of the full random matrices from Gaussian ensembles is the universality of their spectral correlations. These correlations depend only on the symmetry class, not on the detailed form of the probability distribution. This universality underlies the broad applicability of random matrix theory, from nuclear physics and quantum chaos to mesoscopic systems, condensed matter physics, and beyond.

There are different ways to determine the degree of repulsion. One is by analyzing the distribution  $P$  of the spacings  $s$  between neighboring levels,  $s_n = E_{n+1} - E_n$ . This option requires unfolding the spectrum, as explained below. Another option is by studying the ratio of consecutive spacings

$$\tilde{r}_n = \frac{\min(s_n, s_{n-1})}{\max(s_n, s_{n-1})}, \quad n = 2, \dots, N-1, \quad (2.20)$$

so that  $0 \leq \tilde{r}_n \leq 1$ . One then studies the distribution  $P(r)$  or its mean  $\langle r \rangle$ . This second alternative does not require unfolding.

Either  $P(s)$  or  $P(r)$  only detects correlations among neighboring levels, that is, short-range correlations. A more complete analysis of the spectrum is gained by analyzing quantities that capture also long-range correlations, such as the level number variance, rigidity, and spectral form factor.

### 2.4.1 Distribution of the spacings between neighboring levels, $P(s)$

**Why unfolding is needed:** In general, the density of states (DOS) is energy dependent, so spacings in the middle of the spectrum differ systematically from spacings near the edges. Unfolding removes this slow variation by mapping the “raw” eigenvalues into unfolded energies,  $E \mapsto \xi$ , so that the mean density of states of  $\{\xi_n\}$  is 1. Two methods for unfolding the spectrum are described below.

#### Method 1: “Quick” local rescaling in small windows

1. Order the spectrum  $\{E_n\}$  increasingly:  $E_1 \leq E_2 \leq \dots \leq E_N$ .
2. Discard a fraction of levels at both edges (e.g. 10%) to avoid strong edge fluctuations.
3. Partition the remaining spectrum into small windows of  $(m+1)$  consecutive levels. A common choice is  $(m+1) \sim 11$ , which contains  $m = 10$  spacings.
4. In window  $k$ , containing  $E_{k+1}, E_{k+2}, \dots, E_{k+11}$ , define the spacings

$$s_1 = E_{k+2} - E_{k+1}, \dots, s_{10} = E_{k+11} - E_{k+10}.$$

5. Compute the local mean spacing in that window,

$$\bar{s}_k = \frac{s_1 + \dots + s_{10}}{10} = \frac{E_{k+11} - E_{k+1}}{10}. \quad (2.21)$$

6. Define locally unfolded spacings by rescaling each spacing in the window:

$$\tilde{s}_j = \frac{s_j}{\bar{s}_k}, \quad j = 1, \dots, 10, \quad (2.22)$$

so that the mean spacing of the rescaled set is 1 by construction.

**NOTE:** The unnormalized density of states at an energy  $E$ , denoted by  $D(E)$ , is defined as the number of energy levels per unit energy. Operationally, it can be estimated as

$$D(E) = \frac{\text{number of levels in a small energy window } [E, E + \delta E]}{\text{energy interval } \delta E}.$$

The mean level spacing at energy  $E$ , denoted by  $\Delta(E)$ , is defined as the typical distance between consecutive levels in the same window, and can be estimated as

$$\Delta(E) = \frac{\text{energy interval } \delta E}{\text{number of levels in a small energy window } [E, E + \delta E]}.$$

Therefore, the mean level spacing is approximately the inverse of the unnormalized density of states,

$$\Delta(E) \approx 1/D(E).$$

This is why the method above ensures that the mean level spacing is locally equal to 1.

The “quick” method is often sufficient when one is mainly interested in short-range correlations such as  $P(s)$ .

## Method 2: Staircase unfolding via a smooth fit

**Staircase function.** Given a discrete spectrum  $\{E_n\}_{n=1}^N$  (sorted in increasing order), define the staircase function (integrated density of states)

$$\eta(E) \equiv \#\{E_n \leq E\} = \sum_{n=1}^N \Theta(E - E_n), \quad (2.23)$$

which counts the number of levels up to energy  $E$ . It is customary to decompose  $\eta(E)$  into a smooth (secular) part and a fluctuating part,

$$\eta(E) = \xi(E) + \eta_{\text{fl}}(E), \quad (2.24)$$

where  $\xi(E)$  is a smooth, monotonically increasing approximation to the mean integrated density of states, and  $\eta_{\text{fl}}(E)$  contains the oscillatory fluctuations.

**Unfolded levels.** The unfolding procedure consists of a monotonic change of variables,

$$E \mapsto \xi(E), \quad (2.25)$$

under which the original energy levels  $E_n$  are mapped onto the unfolded levels

$$\xi_n \equiv \xi(E_n), \quad n = 1, 2, \dots, N. \quad (2.26)$$

This choice ensures that the *local mean level spacing* becomes unity. This can be understood as follows:

(i) If the spectrum is very dense, we may regard  $\eta(E)$  as approximately continuous. Its derivative is then  $\frac{d\eta}{dE}$  = number of levels per unit energy, which is precisely the definition of the unnormalized density of states  $D(E)$ . When we split  $\eta(E) = \xi(E) + \eta_{\text{fl}}(E)$ , the fluctuating part oscillates around zero and has zero average slope, so the mean density of states is given by the derivative of the smooth part  $\overline{D}(E) = \frac{d\xi}{dE}$ .

(ii) As already explained above, the local mean level spacing is inversely proportional to the smooth density of states,  $\Delta(E) \simeq 1/\overline{D}(E)$ . To see this, consider a small energy interval  $[E, E + \delta E]$  over which the smooth density of states  $\overline{D}(E)$  varies negligibly. Since  $\overline{D}(E)$  gives the mean number of levels per unit energy, the expected number of levels in this interval is approximately  $\delta N \simeq \overline{D}(E) \delta E$ . If  $\Delta(E)$  denotes the local mean spacing between consecutive levels near energy  $E$ , then an interval of width  $\Delta(E)$  contains, on average, approximately one level. Therefore,  $\overline{D}(E) \Delta(E) \simeq 1$ , and hence

$$\Delta(E) \simeq \frac{1}{\overline{D}(E)}. \quad (2.27)$$

(iii) We can now show explicitly that the unfolding procedure produces a spectrum with unit local mean level spacing. Consider the Taylor expansion of the smooth function  $\xi(E)$  around  $E_n$ ,

$$\xi(E) = \xi(E_n) + \xi'(E_n)(E - E_n) + \frac{1}{2} \xi''(E_n)(E - E_n)^2 + \cdots. \quad (2.28)$$

Evaluating this expression at the neighboring level  $E_{n+1}$  gives

$$\xi(E_{n+1}) - \xi(E_n) = \xi'(E_n)(E_{n+1} - E_n) + \frac{1}{2} \xi''(E_n)(E_{n+1} - E_n)^2 + \cdots. \quad (2.29)$$

Since  $E_n$  and  $E_{n+1}$  are neighboring levels, their separation is much smaller than the energy scale over which the smooth density of states changes appreciably. Hence,  $\xi(E)$  is approximately linear between  $E_n$  and  $E_{n+1}$ , and the higher-order terms in the Taylor expansion can be neglected. Therefore,

$$\xi_{n+1} - \xi_n \simeq \xi'(E_n)(E_{n+1} - E_n). \quad (2.30)$$

Taking a local spectral average around  $E_n$ , or equivalently an ensemble average at fixed energy, we obtain

$$\langle \xi_{n+1} - \xi_n \rangle \simeq \xi'(E_n) \langle E_{n+1} - E_n \rangle, \quad (2.31)$$

where  $\xi'(E_n)$  can be taken outside the average because it is a slowly varying deterministic function compared with the fluctuating spacing.

From (i),

$$\xi'(E_n) = \overline{D}(E_n), \quad (2.32)$$

while from (ii), the local mean level spacing is

$$\langle E_{n+1} - E_n \rangle \simeq \Delta(E_n) \simeq \frac{1}{\overline{D}(E_n)}. \quad (2.33)$$

Substituting these results into Eq. (2.31) gives

$$\boxed{\langle \xi_{n+1} - \xi_n \rangle \simeq \overline{D}(E_n) \frac{1}{\overline{D}(E_n)} = 1.} \quad (2.34)$$

**Fluctuations** While  $\xi(E)$  is, by construction, a smooth and monotonically increasing function,  $\eta_{\text{fl}}(E)$  describes the fluctuations of the spectral staircase around its smooth part and is not, in general, monotonic. Importantly, unfolding removes the smooth variation of the density of states but does *not* remove the spectral fluctuations.

To see this explicitly, evaluate the decomposition

$$\eta(E) = \xi(E) + \eta_{\text{fl}}(E) \quad (2.35)$$

at an eigenvalue  $E_n$ . Since  $\eta(E_n) = n$ , we obtain

$$n = \xi(E_n) + \eta_{\text{fl}}(E_n), \quad (2.36)$$

and therefore

$$\boxed{\xi_n \equiv \xi(E_n) = n - \eta_{\text{fl}}(E_n).} \quad (2.37)$$

Thus, the fluctuations of the original spectrum are encoded in the deviations of the unfolded levels  $\xi_n$  from the uniformly spaced “picket-fence” spectrum  $\xi_n = n$ . Indeed, in the absence of such fluctuations, one would have  $\xi_n = n$  and every unfolded nearest-neighbor spacing would be exactly equal to one.

More explicitly, defining the unfolded nearest-neighbor spacing as

$$s_n \equiv \xi_{n+1} - \xi_n, \quad (2.38)$$

we find

$$s_n = [n + 1 - \eta_{\text{fl}}(E_{n+1})] - [n - \eta_{\text{fl}}(E_n)] = 1 - [\eta_{\text{fl}}(E_{n+1}) - \eta_{\text{fl}}(E_n)]. \quad (2.39)$$

Therefore, unfolding removes the smooth energy dependence of the mean level spacing while retaining the level-to-level fluctuations. The spacing statistics of the unfolded spectrum probe these fluctuations in units for which the local mean spacing is equal to one.

**How to obtain the smooth function  $\xi(E)$ .** Common approaches include:

1. **Analytic mean DOS (preferred when available).** If a theoretical unnormalized density of states  $D(E)$  is known, define

$$\xi(E) = \int_{-\infty}^E D(E') dE'. \quad (2.40)$$

In the explicit case of the random matrices, where the unnormalized DOS is in Eq. (2.19), we have

$$\xi(E) = \int_{E_{\min}}^E D(E') dE' = \int_{-2\sigma}^E \frac{N}{2\pi\sigma^2} \sqrt{4\sigma^2 - E'^2} dE'.$$

The unfolded levels will be  $\xi_n = \xi(E_n)$ . When computing the spacings, discard the levels at the edges.

2. **Polynomial (or spline) fit to the staircase.** Fit the staircase  $\eta(E)$  by a smooth monotonic function  $\xi(E)$ , e.g.

$$\xi(E) \approx \sum_{k=0}^p a_k E^k \quad (\text{or use a spline / low-pass smoothing}), \quad (2.41)$$

and then set  $\xi_n = \xi(E_n)$ .

Because  $\eta(E)$  is a step function, one typically fits either: (i) the points  $(E_n, n)$  directly, or (ii) a smoothed version of  $\eta(E)$  obtained by convolution with a narrow kernel.

**Choosing the polynomial order.** There is no universal “best” polynomial degree  $p$ ; it depends on how rapidly the mean density varies across your chosen energy window and on the number of levels. The guiding principle is:

Choose  $p$  large enough to capture the secular variation of the DOS, but small enough that the fit does not track fluctuations on the scale of the mean spacing.

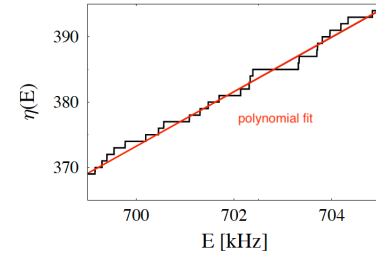


Figure 2.1: Staircase function.

Practical recommendations:

- Work in the **bulk** of the spectrum (avoid edges where the DOS changes rapidly).
- Use a **low** order polynomial or a spline with strong smoothing. Typical choices in the literature for global unfolding are  $p \sim 3-8$ , but the optimal value depends on the dataset size and the DOS curvature.
- Check robustness: compute statistics (e.g.,  $P(s)$ ,  $\Sigma^2(L)$ ,  $\Delta_3(L)$ ) for several reasonable  $p$  and verify that conclusions are stable.
- Avoid overfitting: if  $p$  is too large,  $\xi(E)$  begins to absorb genuine spectral correlations, artificially driving spacing distributions toward Poisson.

**Summary.** Unfolding is the mapping  $E \mapsto \xi(E)$  using the smooth part of the staircase. The unfolded levels  $\xi_n = \xi(E_n)$  have unit mean spacing, enabling universal comparisons. The fluctuations are not ignored; they appear in the deviations  $\xi_n - n = -\eta_{\text{fl}}(E_n)$  and hence in spacing and correlation statistics.

### Correlations and symmetry class:

The strength of level repulsion changes according to the symmetry class: GOE, GUE, and GSE.

**Nearest-neighbor level spacing distribution:  $P(s)$**

• **GOE:** The nearest-neighbor level spacing distribution for the GOE is well approximated by the Wigner surmise,

$$P_{\text{GOE}}(s) = \frac{\pi}{2} s \exp\left(-\frac{\pi}{4}s^2\right), \quad (2.42)$$

which exhibits linear level repulsion,

$$P(s) \sim s \quad \text{for } s \rightarrow 0,$$

therefore the notation  $\beta = 1$ .

• **GUE:** The Wigner surmise for the GUE level-spacing distribution is

$$P_{\text{GUE}}(s) = \frac{32}{\pi^2} s^2 \exp\left(-\frac{4}{\pi}s^2\right), \quad (2.43)$$

corresponding to quadratic level repulsion,

$$P(s) \sim s^2 \quad \text{for } s \rightarrow 0$$

therefore the notation  $\beta = 2$ .

**Intuition :** An intuition for why level repulsion is stronger for GUE than for GOE can be obtained by considering  $2 \times 2$  random matrices. The key point is that more independent parameters must simultaneously vanish for two eigenvalues to become degenerate in GUE than in GOE. For GOE, consider the real symmetric matrix

$$H_{\text{GOE}} = \begin{pmatrix} a & b \\ b & d \end{pmatrix}.$$

The separation between its two eigenvalues is

$$\Delta E = \sqrt{(a-d)^2 + 4b^2}.$$

For the two eigenvalues to become degenerate,  $\Delta E = 0$ , which requires

$$a - d = 0, \quad b = 0.$$

Thus, two independent real quantities must simultaneously vanish for an exact degeneracy to occur. For GUE, the off-diagonal matrix element is complex, and the corresponding Hermitian matrix can be written as

$$H_{\text{GUE}} = \begin{pmatrix} a & b + ic \\ b - ic & d \end{pmatrix}.$$

The separation between its eigenvalues is now

$$\Delta E = \sqrt{(a-d)^2 + 4b^2 + 4c^2}.$$

Therefore, an exact degeneracy requires

$$a - d = 0, \quad b = 0, \quad c = 0.$$

In this case, three independent real quantities must simultaneously vanish. This is less likely than satisfying the two conditions required for GOE. Consequently, it is more difficult for two eigenvalues to approach each other in GUE, providing an intuitive explanation for why level repulsion is stronger in GUE than in GOE.

- **GSE:** The Wigner surmise for the GSE is

$$P_{\text{GSE}}(s) = \frac{2^{18}}{3^6 \pi^3} s^4 \exp\left(-\frac{64}{9\pi} s^2\right), \quad (2.44)$$

which exhibits quartic level repulsion,

$$P(s) \sim s^4 \quad \text{for } s \rightarrow 0,$$

therefore the notation  $\beta = 4$ .

**Uncorrelated levels:** For uncorrelated energy levels, such as those corresponding to a random matrix with only diagonal elements, the level spacing distribution follows a Poisson distribution

$$P_{\text{Poisson}}(s) = e^{-s}.$$

---

**Poisson level-spacing distribution.** After unfolding, the smooth unnormalized density of states is equal to one,  $\overline{D}_{\text{unf}}(\xi) = 1$ , which is equivalent to saying that the local mean level spacing is unity,  $\langle s \rangle = 1$ . Suppose now that the unfolded eigenvalues are uncorrelated. In this case, the presence of a level at one position does not influence the probability of finding other levels nearby. The unfolded eigenvalues can therefore be modeled as randomly and independently distributed points along the energy axis, with constant mean density

$$\overline{D}_{\text{unf}} = 1. \quad (2.45)$$

Such a random set of points is described by a Poisson point process.

For a Poisson point process with constant mean density  $\overline{D}_{\text{unf}}$ , the probability of finding exactly  $k$  levels in an interval of length  $s$  is

$$P_k(s) = \frac{(\overline{D}_{\text{unf}} s)^k}{k!} e^{-\overline{D}_{\text{unf}} s}. \quad (2.46)$$

Since unfolding gives  $\overline{D}_{\text{unf}} = 1$ , this becomes

$$P_k(s) = \frac{s^k}{k!} e^{-s}. \quad (2.47)$$

We can now derive the nearest-neighbor level-spacing distribution. Suppose that there is an unfolded eigenvalue at  $\xi$ , and let  $S$  denote the distance from this level to the next one. The condition

$$S > s \quad (2.48)$$

means that the interval  $(\xi, \xi + s)$  contains no eigenvalues. Therefore, the probability that the nearest-neighbor spacing is larger than  $s$  is equal to the probability of finding zero levels in an interval of length  $s$ ,

$$\Pr(S > s) = P_0(s). \quad (2.49)$$

Setting  $k = 0$  in the Poisson distribution gives

$$P_0(s) = e^{-s}, \quad (2.50)$$

and hence

$$\Pr(S > s) = e^{-s}. \quad (2.51)$$

The nearest-neighbor spacing probability density, which we denote by  $P(s)$ , is obtained from the probability that  $S$  exceeds  $s$ ,

$$P(s) = -\frac{d}{ds} \Pr(S > s). \quad (2.52)$$

It follows that

$$\boxed{P_{\text{Poisson}}(s) = e^{-s}, \quad s \geq 0.} \quad (2.53)$$

The distribution is normalized,

$$\int_0^\infty P_{\text{Poisson}}(s) ds = \int_0^\infty e^{-s} ds = 1, \quad (2.54)$$

and its mean is

$$\langle s \rangle = \int_0^\infty s P_{\text{Poisson}}(s) ds$$

$\int_0^\infty s e^{-s} ds = 1$ , (2.55) as required for an unfolded spectrum.

Notice also that

$$P_{\text{Poisson}}(0) = 1. \quad (2.56)$$

Thus, very small spacings are not suppressed. Two neighboring eigenvalues can come arbitrarily close to each other with nonzero probability. This is a direct consequence of the absence of correlations between the levels and contrasts with the level repulsion found in random-matrix ensembles such as the GOE, for which  $P(s) \rightarrow 0$  as  $s \rightarrow 0$ .

---

## 2.4.2 Interpolation: Brody distribution

Real systems can lie between the two extremes, Poisson or Wigner-Dyson distribution. A widely used phenomenological interpolation is the **Brody distribution**,

$$P_B(s; \beta) = (\beta + 1) b(\beta) s^\beta \exp[-b(\beta) s^{\beta+1}], \quad 0 \leq \beta \leq 1, \quad (2.57)$$

where

$$b(\beta) = \left[ \Gamma\left(\frac{\beta + 2}{\beta + 1}\right) \right]^{\beta+1}. \quad (2.58)$$

and the parameter  $\beta$  quantifies the degree of chaoticity:

- $\beta = 0$ : the Poisson limit (integrable).
- $\beta = 1$ : Wigner-like behavior characteristic of GOE (chaotic).
- $0 < \beta < 1$ : intermediate level repulsion, describing a crossover from regular to chaotic dynamics.

The Brody form is phenomenological and does not follow from a controlled theory of mixed systems. Nevertheless, the Brody parameter  $\beta$  is widely used as a simple quantitative indicator of the transition from Poisson to GOE Wigner–Dyson statistics.

### 2.4.3 Interpolation: Izrailev distribution

Unlike the Brody distribution, which is restricted to  $0 \leq \beta \leq 1$ , the Izrailev distribution provides a phenomenological description over a broader range of level-repulsion strengths, including those characteristic of the GOE, GUE, and GSE symmetry classes. The **Izrailev distribution** is given by

$$P_1(s; \beta) = A s^\beta \exp \left[ -\frac{\pi^2}{16} \beta s^2 - \left( B - \frac{\pi}{4} \beta \right) s \right], \quad 0 \leq \beta \leq 4, \quad (2.59)$$

where the constants  $A$  and  $B$  are determined by imposing normalization and unit mean level spacing,

$$\int_0^\infty P_1(s; \beta) ds = 1, \quad \int_0^\infty s P_1(s; \beta) ds = 1. \quad (2.60)$$

The parameter  $\beta$  controls the strength of level repulsion, since

$$P_1(s; \beta) \propto s^\beta \quad \text{for } s \rightarrow 0. \quad (2.61)$$

The characteristic values of the level-repulsion exponent are

$$\beta = 0 \quad (\text{Poisson}), \quad \beta = 1 \quad (\text{GOE}), \quad \beta = 2 \quad (\text{GUE}), \quad \beta = 4 \quad (\text{GSE}). \quad (2.62)$$

### 2.4.4 Ratio of consecutive level spacings

The statistics of ratio of consecutive levels probes short-range correlations and is insensitive to the local density of states, making it particularly robust when the unfolding procedure is uncertain. There are two ratios that have been studied in the literature, the unsymmetrized ratio

$$r_n = \frac{s_n}{s_{n-1}} \in (0, \infty)$$

and the symmetrized ratio

$$\tilde{r}_n = \min \left( r_n, \frac{1}{r_n} \right) \in [0, 1]$$

Nowadays,  $\tilde{r}$  is the preferred one, because the distribution is less noisy, since  $\tilde{r} \in [0, 1]$ .

---

**NOTE:**

$$\tilde{r}_n = \min \left( r_n, \frac{1}{r_n} \right) = \frac{\min(s_n, s_{n-1})}{\max(s_n, s_{n-1})}.$$

This can be shown as follows,

$$\tilde{r}_n = \min \left( r_n, \frac{1}{r_n} \right) = \min \left( \frac{s_n}{s_{n-1}}, \frac{s_{n-1}}{s_n} \right).$$

Consider the two possible cases. If  $s_n \leq s_{n-1}$ , then

$$\frac{s_n}{s_{n-1}} \leq 1, \quad \frac{s_{n-1}}{s_n} \geq 1,$$

and hence

$$\tilde{r}_n = \frac{s_n}{s_{n-1}} = \frac{\min(s_n, s_{n-1})}{\max(s_n, s_{n-1})}.$$

If instead  $s_n > s_{n-1}$ , then

$$\frac{s_n}{s_{n-1}} > 1, \quad \frac{s_{n-1}}{s_n} < 1,$$

and therefore

$$\tilde{r}_n = \frac{s_{n-1}}{s_n} = \frac{\min(s_n, s_{n-1})}{\max(s_n, s_{n-1})}.$$

Thus, the two definitions are equivalent:

$$\boxed{\tilde{r}_n = \min\left(r_n, \frac{1}{r_n}\right) = \frac{\min(s_n, s_{n-1})}{\max(s_n, s_{n-1})}.$$

For the three classical Gaussian ensembles with Dyson index  $\beta = 1$  (GOE),  $\beta = 2$  (GUE), and  $\beta = 4$  (GSE), the distribution of the ratio of consecutive level spacings is well approximated by the following closed expressions.

For the unsymmetrized ratio, the Wigner-like surmise for the Gaussian ensembles is

$$P_\beta(r) = C_\beta \frac{(r + r^2)^\beta}{(1 + r + r^2)^{1+\frac{3}{2}\beta}}, \quad r \in (0, \infty), \quad (2.63)$$

where  $\beta = 1, 2, 4$  correspond to the GOE, GUE, and GSE, respectively.

For the symmetrized ratio, the probability distribution becomes

$$\tilde{P}_\beta(\tilde{r}) = 2P_\beta(\tilde{r}) = 2C_\beta \frac{(\tilde{r} + \tilde{r}^2)^\beta}{(1 + \tilde{r} + \tilde{r}^2)^{1+\frac{3}{2}\beta}}, \quad 0 \leq \tilde{r} \leq 1. \quad (2.64)$$

The normalization constants are

$$C_1 = \frac{27}{8}, \quad C_2 = \frac{81\sqrt{3}}{4\pi}, \quad C_4 = \frac{729\sqrt{3}}{4\pi}. \quad (2.65)$$

Notice that while  $P_\beta(r)$  is a distribution from  $r = 0$  to  $r \rightarrow \infty$ , exhibiting true tails, similar to  $P_\beta(s)$ , the distribution  $P_\beta(\tilde{r})$  only goes from  $\tilde{r} = 0$  to  $\tilde{r} = 1$ . When studying  $P_\beta(\tilde{r})$ , the interest is only in capturing whether there is the presence or absence of level repulsion, there is no interest in the tails.

Explicitly,

- **GOE** ( $\beta = 1$ ):

$$P_{\text{GOE}}(\tilde{r}) = \frac{27}{4} \frac{\tilde{r} + \tilde{r}^2}{(1 + \tilde{r} + \tilde{r}^2)^{5/2}} \quad \text{and} \quad \langle \tilde{r} \rangle_{\text{GOE}} \approx 0.535898. \quad (2.66)$$

- **GUE** ( $\beta = 2$ ):

$$P_{\text{GUE}}(\tilde{r}) = \frac{81\sqrt{3}}{2\pi} \frac{(\tilde{r} + \tilde{r}^2)^2}{(1 + \tilde{r} + \tilde{r}^2)^4} \quad \text{and} \quad \langle \tilde{r} \rangle_{\text{GUE}} \approx 0.602658. \quad (2.67)$$

- **GSE** ( $\beta = 4$ ):

$$P_{\text{GSE}}(\tilde{r}) = \frac{729\sqrt{3}}{2\pi} \frac{(\tilde{r} + \tilde{r}^2)^4}{(1 + \tilde{r} + \tilde{r}^2)^7} \quad \text{and} \quad \langle \tilde{r} \rangle_{\text{GSE}} \approx 0.676168. \quad (2.68)$$

The mean values provided above are often used as practical indicators of the symmetry class of a spectrum without constructing the full distribution.

**Uncorrelated levels:** For uncorrelated energy levels, such as those corresponding to a random matrix with only diagonal elements, the level spacings follow Poisson statistics. The corresponding distribution of spacing ratios is

$$P_{\text{Poisson}}(\tilde{r}) = \frac{2}{(1 + \tilde{r})^2} \quad \text{and} \quad \langle \tilde{r} \rangle_{\text{Poisson}} = 2 \ln 2 - 1 \approx 0.38629.$$

### 2.4.5 Random matrix theory and quantum chaos

Long after Wigner used random matrices as a statistical model for the spectra of heavy nuclei in 1950's, random matrix theory emerged in 1980's as a central framework for understanding the quantum signatures of classically chaotic dynamics, what became known as *quantum chaos*. A striking correspondence was uncovered between classical chaos and random-matrix spectral statistics, first revealed in seminal studies of quantum billiards. These works demonstrated that systems with chaotic classical motion exhibit level correlations consistent with Wigner–Dyson distributions, whereas integrable systems display Poisson statistics, establishing spectral fluctuations as a robust diagnostic of the underlying classical dynamics.

#### Classical billiards: regular vs chaotic motion

A billiard consists of a point particle moving freely inside a domain and undergoing specular reflections at the boundary. The nature of the classical trajectories depends on the geometry:

- **Integrable billiards** (rectangle, circle, ellipse): there exist sufficient constants of motion to confine trajectories to invariant tori; motion is quasi-periodic and predictable.
- **Chaotic billiards** (Sinai billiard, Bunimovich stadium): trajectories exhibit exponential sensitivity to initial conditions, ergodicity, and mixing.

#### Quantum spectra

Quantization of the billiards revealed that

- **Integrable systems: Poisson statistics** For systems whose classical limit is integrable, quantization conditions associated with different actions are essentially independent. As a result the unfolded levels behave as uncorrelated points and the nearest-neighbor spacing distribution is

$$P_{\text{P}}(s) = e^{-s}. \quad (2.69)$$

There is *no level repulsion*:  $P_{\text{P}}(s \rightarrow 0) = 1$ .

- **Chaotic systems: Wigner–Dyson statistics** For classically chaotic systems the spectral fluctuations become universal and are well described by random-matrix theory (RMT) according to the symmetries of the Hamiltonian. The GOE, GUE, and GSE spacing distributions are given, respectively, by Eqs. (2.42)–(2.44). They all imply *level repulsion*, which is a hallmark of quantum chaos.

The connection between level repulsion and classical chaos – first established in quantum billiards – was subsequently extended to other systems with few degrees of freedom. For many-body systems, however, a direct classical analysis is often intractable due to the high-dimensional phase space, and in some cases it is not even well defined. This is the case, for example, of spin-1/2 models, which are intrinsically quantum systems with no clear classical limit. In such situations, one typically refers to many-body quantum systems that exhibit Wigner–Dyson level statistics as *quantum chaotic systems*. Remarkably, systems as diverse as atomic nuclei, spin-1/2 models, Bose–Hubbard lattices, and quantum billiards all display the same universal level repulsion predicted by random matrix theory.

### 2.4.6 Examples of Classical Chaotic Systems in Everyday Life

Classical chaos refers to deterministic dynamics that exhibit strong sensitivity to initial conditions, leading to long-term unpredictability despite being governed by well-defined equations of motion. Such behavior is ubiquitous in systems of practical relevance:

- **Weather and climate:** Atmospheric dynamics, governed by nonlinear fluid equations, are chaotic, which explains the intrinsic limits of weather prediction.
- **Double pendulum:** A simple mechanical system of two coupled pendula exhibits chaotic motion, where arbitrarily small changes in initial conditions lead to drastically different trajectories.
- **Traffic flow:** Interacting vehicles form a nonlinear dynamical system in which small perturbations can amplify into stop-and-go waves, producing spontaneous traffic jams without external causes.
- **Turbulence:** Fluid flows at high Reynolds number display chaotic dynamics, characterized by complex vortex interactions and strong unpredictability, with major implications for aerodynamics and climate modeling.
- **Biological rhythms:** The electrical activity of the human heart is governed by nonlinear oscillatory dynamics, and certain cardiac arrhythmias are associated with chaotic regimes.
- **Population dynamics:** Simple discrete-time models such as the logistic map,

$$x_{n+1} = rx_n(1 - x_n), \quad (2.70)$$

exhibit chaos for appropriate parameters, with applications in ecology and epidemiology.

- **Power grids:** Networks of coupled generators behave as nonlinear oscillators, where chaotic instabilities can lead to cascading failures and large-scale blackouts.

These examples illustrate that chaos is not an exotic phenomenon but a fundamental feature of many natural and engineered systems.

## 2.5 Level statistics: Short- and long-range correlations

To probe both short- and long-range spectral correlations, instead of just short-range correlations as accomplished with  $P(s)$  and  $P(r)$ , we employ the level number variance, spectral rigidity, and the spectral form factor.

### 2.5.1 Level number variance and rigidity

The level number variance and rigidity are complementary to the nearest-neighbor statistics. They probe correlations on scales much larger than the mean spacing, both short- and long-range correlations, and are essential for distinguishing chaotic spectra from integrable or mixed cases. The analysis of these quantities require proper unfolding of the energy levels via the staircase function. These quantities

*Level-number variance*  $\Sigma^2(\ell)$ . Let  $\{\xi_n\}$  be the unfolded spectrum with unit mean density. Consider an interval of length  $\ell$  on the unfolded axis and denote by  $\tilde{\eta}(\ell)$  the number of *unfolded* levels inside this interval. The level-number variance is defined as

$$\Sigma^2(\ell) = \langle \tilde{\eta}(\ell, \xi)^2 \rangle - \langle \tilde{\eta}(\ell, \xi) \rangle^2, \quad (2.71)$$

where the average is taken over different interval  $[\xi_s, \xi_s + \ell]$  starting at different positions  $\xi_s$  and/or over disorder realizations. For uncorrelated (Poisson) levels one has  $\Sigma^2(\ell) = \ell$ , while random-matrix spectra exhibit strong suppression of fluctuations.  $\Sigma^2(\ell)$  exhibits a logarithmic growth for random matrices, reflecting strong level repulsion and spectral rigidity.

*Spectral rigidity*  $\Delta_3(\ell)$ . The Dyson-Mehta rigidity measures how well the staircase function can be approximated by a straight line inside an interval of length  $\ell$ . For an interval centered at  $E$ ,

$$\Delta_3(\ell) = \frac{1}{\ell} \min_{A, B} \int_{\xi_s}^{\xi_s + \ell} [\tilde{\eta}(\xi) - A\xi - B]^2 d\xi, \quad (2.72)$$

where  $\eta(\varepsilon)$  is the unfolded staircase function and the minimization is performed over all linear functions  $A\varepsilon + B$ . The quantity  $\Delta_3(\ell)$  probes correlations on long energy scales; for Poisson spectra  $\Delta_3(\ell) = \ell/15$ , while random matrices give a much slower (logarithmic) growth. Smaller values correspond to more rigid spectra.

- **GOE** ( $\beta = 1$ ):

$$\Sigma_{\text{GOE}}^2(\ell) \simeq \frac{2}{\pi^2} \left[ \ln(2\pi\ell) + \gamma + 1 - \frac{\pi^2}{8} \right], \quad (2.73)$$

$$\Delta_3^{\text{GOE}}(\ell) \simeq \frac{1}{\pi^2} \left[ \ln(2\pi\ell) + \gamma - \frac{5}{4} \right], \quad (2.74)$$

where  $\gamma \simeq 0.5772$  is Euler's constant.

- **GUE** ( $\beta = 2$ ):

$$\Sigma_{\text{GUE}}^2(\ell) \simeq \frac{1}{\pi^2} [\ln(2\pi\ell) + \gamma + 1], \quad (2.75)$$

$$\Delta_3^{\text{GUE}}(\ell) \simeq \frac{1}{2\pi^2} \left[ \ln(2\pi\ell) + \gamma - \frac{3}{2} \right]. \quad (2.76)$$

- **GSE** ( $\beta = 4$ ):

$$\Sigma_{\text{GSE}}^2(\ell) \simeq \frac{1}{2\pi^2} \left[ \ln(4\pi\ell) + \gamma + 1 - \frac{\pi^2}{8} \right], \quad (2.77)$$

$$\Delta_3^{\text{GSE}}(\ell) \simeq \frac{1}{4\pi^2} \left[ \ln(4\pi\ell) + \gamma - \frac{5}{4} \right]. \quad (2.78)$$

## 2.5.2 Spectral form factor

The two-point spectral form factor is defined as [11],

$$\text{SFF}(t) = \frac{1}{D^2} \left\langle \sum_{m,n} e^{i(E_m - E_n)t} \right\rangle, \quad (2.79)$$

where  $\hbar = 1$ ,  $N$  is the dimension of the Hilbert space,  $E_n$  represents the eigenvalues of the system, and  $\langle \cdot \rangle$  indicates an ensemble average.

For large random matrices from the Gaussian orthogonal ensemble (GOE), we have

$$\text{SFF}(t) \simeq \frac{\mathcal{J}_1^2(2\Gamma t)}{(\Gamma t)^2} - \frac{1}{D} b_2 \left( \frac{\Gamma t}{2D} \right) + \frac{1}{D}, \quad (2.80)$$

where  $\mathcal{J}_1(t)$  is the Bessel function of the first kind,  $\Gamma$  is the width of the semicircular density of states, and  $b_2(t)$  is the two-level form factor [11],

$$b_2(t) = \begin{cases} 1 - 2t + t \ln(1 + 2t), & t \leq 1, \\ t \ln \left( \frac{2t + 1}{2t - 1} \right) - 1, & t > 1. \end{cases} \quad (2.81)$$

In Fig. 2.2, we show the spectral form factor averaged over an ensemble of GOE random matrices. The first term in Eq. (2.80) represents the slope in the slope-dip-ramp-plateau structure. The slope exhibits oscillations characteristic of the Bessel function, whose envelope decays as a powerlaw  $\propto t^{-3}$ , as seen in Fig. 2.2.

The dip in Fig. 2.2 happens at  $t_{\text{dip}} = (12/\pi)^{1/4}$  and corresponds to the minimum value of the spectral form factor,  $\text{SFF}(t_{\text{dip}}) \approx 2/D$ . The dip is followed by the ramp, which is the region below the saturation value (plateau) at  $1/D$ . The beginning of the ramp and its end at the Heisenberg time,  $t_{\text{H}}$ , are marked with vertical lines in Fig. 2.2. The interval where  $\text{SFF}(t)$  is below the plateau corresponds to the correlation hole.

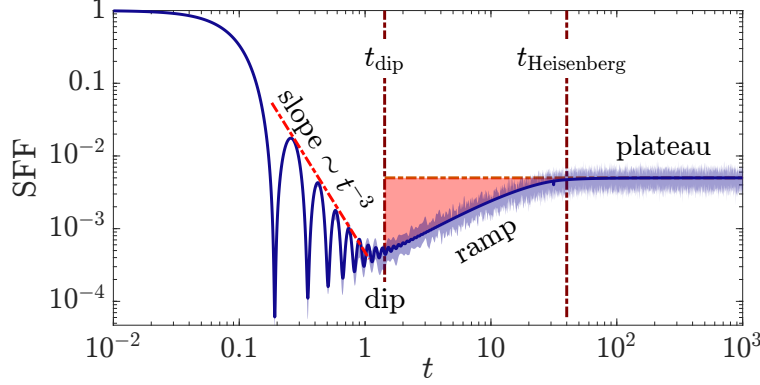


Figure 2.2: Slope-dip-ramp-plateau structure (correlation hole) of the spectral form factor obtained with an ensemble of 100 GOE random matrices of dimension  $D = 200$ . The elements of the matrices have  $\langle H_{ij} \rangle = 0$ ,  $\langle H_{ij}^2 \rangle = 1/2$  for  $i \neq j$ , and  $\langle H_{ii}^2 \rangle = 1$ , so that  $\Gamma \sim \sqrt{D/2}$ . The dark solid line is the analytical expression in Eq. (2.80) and the shaded curve is the average over the ensemble. Vertical dashed lines mark the beginning and the end of the ramp.

It is also common to work with the unfolded spectrum  $\{\xi_n\}$  and variances rescaled by the size of the matrix, and then define the spectral form factor as

$$K(t) = \frac{1}{N^2} \left\langle \left| \sum_{n=1}^N e^{-i\xi_n t} \right|^2 \right\rangle = \frac{1}{N^2} \left\langle \sum_{m,n=1}^N e^{-i(\xi_m - \xi_n)t} \right\rangle, \quad t \in \mathbb{R}. \quad (2.82)$$

## 2.6 Eigenvectors and Participation Ratios

Consider an eigenstate (eigenvector)  $|\alpha\rangle = \sum_{n=1}^N C_n^\alpha |n\rangle$  expanded in a fixed orthonormal basis  $\{|n\rangle\}$ , with normalization

$$\sum_{n=1}^N |C_n^\alpha|^2 = 1. \quad (2.83)$$

**Participation Ratio:** The inverse participation ratio (IPR) and participation ratio (PR) are

$$\text{IPR}_\alpha = \sum_{n=1}^N |C_n^\alpha|^4, \quad \text{PR}_\alpha = \frac{1}{\text{IPR}_\alpha} = \frac{1}{\sum_{n=1}^N |C_n^\alpha|^4}. \quad (2.84)$$

The participation ratio satisfies

$$1 \leq \text{PR}_\alpha \leq N. \quad (2.85)$$

The minimum value,

$$\text{PR}_\alpha = 1, \quad (2.86)$$

is obtained when the eigenstate coincides with a single basis state. For example, if  $|C_1^\alpha|^2 = 1$  and  $|C_n^\alpha|^2 = 0$  for  $n \neq 1$ , then

$$\text{IPR}_\alpha = 1, \quad \text{PR}_\alpha = 1. \quad (2.87)$$

Thus,  $\text{PR}_\alpha = 1$  corresponds to a state that is completely localized in the chosen basis.

The maximum value,

$$\text{PR}_\alpha = N, \quad (2.88)$$

is obtained when the eigenstate is uniformly distributed over all  $N$  basis states,

$$|C_n^\alpha|^2 = \frac{1}{N}, \quad n = 1, \dots, N. \quad (2.89)$$

In this case,

$$\text{IPR}_\alpha = \sum_{n=1}^N \frac{1}{N^2} = \frac{1}{N}, \quad \text{PR}_\alpha = N. \quad (2.90)$$

Thus, the PR provides an estimate of the number of basis states over which an eigenstate is significantly spread. For example, a state distributed with approximately equal weights over  $M$  basis states has  $\text{PR}_\alpha \simeq M$ .

For full random matrices (GOE/GUE), the eigenvectors are random vectors distributed uniformly on the corresponding unit sphere (real for GOE, complex for GUE). For the GOE, the components of the eigenvectors are real Gaussian random variables subject to the normalization constraint. For the GUE, the components of the eigenvectors are complex Gaussian random variables under the normalization constraint. All eigenstates  $\alpha$  are statistically equivalent, and  $\text{PR}_\alpha$  has (for large  $N$ ) the same typical value for every  $\alpha$ .

$$\boxed{\text{PR}_{\text{GOE}} = \frac{N+2}{3} \sim \frac{N}{3}, \quad \text{PR}_{\text{GUE}} = \frac{N+1}{2} \sim \frac{N}{2}.} \quad (2.91)$$

Another commonly used measure of the degree of delocalization of an eigenstate in a given basis is the **Shannon entropy**,

$$\text{Sh}_\alpha = - \sum_{n=1}^N |C_n^\alpha|^2 \ln |C_n^\alpha|^2. \quad (2.92)$$

Like the participation ratio, the Shannon entropy measures how broadly the eigenstate is spread over the basis states. If the eigenstate coincides with a single basis vector, for example  $|C_1^\alpha|^2 = 1$  and all other coefficients vanish, then

$$\text{Sh}_\alpha = 0. \quad (2.93)$$

At the opposite extreme, if the eigenstate is uniformly spread over all  $N$  basis states, so that  $|C_n^\alpha|^2 = 1/N$  for every  $n$ , then

$$\text{Sh}_\alpha = \ln N, \quad (2.94)$$

which is the maximum possible value.

For random eigenvectors, the coefficients are not all exactly equal to  $1/\sqrt{N}$ , but fluctuate according to the statistics of the corresponding random-matrix ensemble. The ensemble-averaged Shannon entropies are

$$\boxed{\langle \text{Sh} \rangle_{\text{GOE}} = \psi\left(\frac{N}{2} + 1\right) - \psi\left(\frac{3}{2}\right), \quad \langle \text{Sh} \rangle_{\text{GUE}} = \psi(N + 1) - \psi(2),} \quad (2.95)$$

where  $\psi(x) = d \ln \Gamma(x)/dx$  is the digamma function.

For large  $N$ , these expressions become

$$\langle \text{Sh} \rangle_{\text{GOE}} \simeq \ln N + \gamma + \ln 2 - 2 \simeq \ln(0.482, N), \quad (2.96)$$

and

$$\langle \text{Sh} \rangle_{\text{GUE}} \simeq \ln N + \gamma - 1 \simeq \ln(0.655, N), \quad (2.97)$$

where  $\gamma \simeq 0.5772$  is the Euler–Mascheroni constant.

Thus, both the participation ratio and the Shannon entropy quantify eigenstate delocalization in the chosen basis. For random-matrix eigenvectors, both indicate that the eigenstates are extended over a number of basis states proportional to the Hilbert-space dimension  $N$ , although the precise values depend on whether the eigenvectors are real (GOE) or complex (GUE).

### 2.6.1 Derivation of the participation ratio of GOE eigenvectors

A key fact from random-matrix theory is that *GOE eigenvectors are uniformly distributed on the real unit sphere  $S^{N-1}$*  (equivalently, the eigenvector matrix is Haar-distributed in  $O(N)$ ). Therefore, the statistics of the components of a GOE eigenvector in any fixed basis are the same as those of a random real unit vector.

The following derivation is **WRONG**, but it gives an idea of the result. The **CORRECT** derivation is below. The idea of this **WRONG** derivation is to see the components of the eigenstates as real random numbers with mean 0 and variance  $1/N$ . This is **WRONG**, because the components are NOT independent, but correlated through the normalization condition.

Let  $x$  be a Gaussian random variable with mean 0 and variance  $\sigma^2 = 1/N$ :

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right). \quad (2.98)$$

By definition, the fourth moment is

$$\mathbb{E}[x^4] = \int_{-\infty}^{\infty} x^4 p(x) dx = \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} x^4 \exp\left(-\frac{x^2}{2\sigma^2}\right) dx. \quad (2.99)$$

To evaluate the integral, perform the change of variables

$$y = \frac{x}{\sigma}, \quad x = \sigma y, \quad dx = \sigma dy. \quad (2.100)$$

Then

$$\mathbb{E}[x^4] = \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} (\sigma y)^4 e^{-y^2/2} \sigma dy \quad (2.101)$$

$$= \frac{\sigma^5}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} y^4 e^{-y^2/2} dy \quad (2.102)$$

$$= \frac{\sigma^4}{\sqrt{2\pi}} \int_{-\infty}^{\infty} y^4 e^{-y^2/2} dy. \quad (2.103)$$

The remaining integral is a standard Gaussian integral:

$$\int_{-\infty}^{\infty} y^4 e^{-y^2/2} dy = 3\sqrt{2\pi}. \quad (2.104)$$

Therefore,

$$\mathbb{E}[x^4] = 3\sigma^4. \quad (2.105)$$

Finally, if the variance is  $\sigma^2 = 1/N$ , then

$$\boxed{\mathbb{E}[x^4] = \frac{3}{N^2} \quad \text{so} \quad \mathbb{E}\left[\sum_{i=1}^N |x_i|^4\right] = N\mathbb{E}[x^4] = \frac{3}{N}.} \quad (2.106)$$

$\Rightarrow$  **CORRECT DERIVATON:**

### Gaussian construction of a random unit vector

Let  $x_i \sim \mathcal{N}(0, 1)$  be i.i.d. real Gaussians and define

$$c_i = \frac{x_i}{\sqrt{\sum_{j=1}^N x_j^2}}. \quad (2.107)$$

Then  $\sum_i c_i^2 = 1$  and the vector  $\mathbf{c}$  is uniformly distributed on  $S^{N-1}$ .

We want  $\mathbb{E}[\text{IPR}]$ . By symmetry,

$$\mathbb{E}[\text{IPR}] = \mathbb{E}\left[\sum_{i=1}^N c_i^4\right] = N \mathbb{E}[c_1^4]. \quad (2.108)$$

Let

$$S = \sum_{j=1}^N x_j^2, \quad c_1^2 = \frac{x_1^2}{S}. \quad (2.109)$$

Write

$$u = x_1^2, \quad v = \sum_{j=2}^N x_j^2, \quad \Rightarrow \quad S = u + v, \quad (2.110)$$

so that

$$c_1^4 = \left(\frac{u}{u+v}\right)^2. \quad (2.111)$$

The ratio  $u/(u+v)$  follows a Beta distribution

$$T = \frac{u}{u+v} \sim \text{Beta}\left(\frac{1}{2}, \frac{N-1}{2}\right)$$

**Why the Beta parameters are  $a = \frac{1}{2}$  and  $b = \frac{N-1}{2}$**

Because  $x_1 \sim \mathcal{N}(0, 1)$ , its square  $u = x_1^2$  follows a chi-square distribution with one degree of freedom:

$$u \sim \chi_1^2. \quad (2.112)$$

Likewise,  $v = \sum_{j=2}^N x_j^2$  is the sum of  $(N-1)$  independent squared standard Gaussians, hence

$$v \sim \chi_{N-1}^2. \quad (2.113)$$

Moreover,  $u$  and  $v$  are independent since they depend on disjoint sets of independent Gaussians. This explains the Beta parameters: each chi-square degree of freedom contributes one “half” in the Beta shape parameters.

**Compute  $\mathbb{E}[c_1^4]$  and  $\mathbb{E}[\text{IPR}]$**

Since  $c_1^4 = T^2$ , we need  $\mathbb{E}[T^2]$ . For  $T \sim \text{Beta}(a, b)$ , the second moment is

$$\mathbb{E}[T^2] = \frac{a(a+1)}{(a+b)(a+b+1)}. \quad (2.114)$$

With  $a = \frac{1}{2}$ ,  $b = \frac{N-1}{2}$ , we have  $a+b = \frac{N}{2}$ , hence

$$\mathbb{E}[c_1^4] = \mathbb{E}[T^2] = \frac{\left(\frac{1}{2}\right)\left(\frac{3}{2}\right)}{\left(\frac{N}{2}\right)\left(\frac{N}{2}+1\right)} = \frac{\frac{3}{4}}{\frac{N(N+2)}{4}} = \frac{3}{N(N+2)}. \quad (2.115)$$

Therefore

$$\mathbb{E}[\text{IPR}] = N \mathbb{E}[c_1^4] = N \cdot \frac{3}{N(N+2)} = \frac{3}{N+2}. \quad (2.116)$$

A commonly quoted GOE estimate for the participation ratio uses

$$\text{PR} \approx \frac{1}{\mathbb{E}[\text{IPR}]}, \quad (2.117)$$

which yields

$$\boxed{\text{PR} \approx \frac{N+2}{3}}. \quad (2.118)$$

### Remark

Strictly speaking,  $\mathbb{E}[1/\text{IPR}] \neq 1/\mathbb{E}[\text{IPR}]$  in general. However, for large  $N$  the IPR is sharply concentrated around its mean for random vectors, and the estimate above captures the correct scaling and the standard GOE prefactor.

## 2.7 The role of interactions: 2x2 matrices

One of the most transparent ways to understand how interactions mix states and split energy levels is to analyze a  $2 \times 2$  Hamiltonian. Despite its simplicity, this minimal model captures the essential physics of level repulsion and provides the building block for random matrix theory.

Consider two basis states  $|1\rangle$  and  $|2\rangle$  with bare energies  $E_1$  and  $E_2$ . In the absence of interactions, the Hamiltonian is diagonal,

$$H_0 = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix}. \quad (2.119)$$

The eigenvalues are trivially  $E_1$  and  $E_2$ , and the eigenstates coincide with the basis states. If  $E_1 = E_2$ , the spectrum is degenerate, and there is no mechanism that lifts this degeneracy.

Now introduce an interaction that couples the two states. This is done by adding off-diagonal elements. The most general Hermitian  $2 \times 2$  Hamiltonian can now be written as

$$H = \begin{pmatrix} E_1 & V \\ V^* & E_2 \end{pmatrix}, \quad (2.120)$$

where  $V$  is the interaction matrix element. For time-reversal invariant systems,  $V$  can be taken real, while in the absence of time-reversal symmetry it may be complex.

The eigenvalues are obtained by solving

$$\det(H - EI) = 0,$$

which yields

$$E_{\pm} = \frac{E_1 + E_2}{2} \pm \sqrt{\left(\frac{E_1 - E_2}{2}\right)^2 + |V|^2}. \quad (2.121)$$

Defining

$$\bar{E} = \frac{E_1 + E_2}{2}, \quad \delta = \frac{E_1 - E_2}{2}, \quad (2.122)$$

we can write

$$E_{\pm} = \bar{E} \pm \sqrt{\delta^2 + |V|^2}. \quad (2.123)$$

### 2.7.1 Level splitting, avoided crossing, and mixing

If  $E_1 = E_2 \equiv E_0$ , the interaction immediately lifts the degeneracy,

$$E_{\pm} = E_0 \pm |V|, \quad (2.124)$$

producing a level splitting

$$\Delta = 2|V|. \quad (2.125)$$

Thus, even an infinitesimal coupling removes exact degeneracies.

If  $E_1 \neq E_2$ , the interaction shifts the levels and prevents them from crossing when an external parameter is introduced that changes the diagonal terms, such as a magnetic field, interaction anisotropy, lattice depth, onsite disorder. This phenomenon is known as an *avoided crossing*.

### 2.7.2 Eigenvectors

The interaction not only splits the eigenvalues but also mixes the eigenstates. Writing in Eq. (2.120)

$$V = |V|e^{i\phi}, \quad (2.126)$$

a convenient orthonormal choice of eigenvectors is

$$|\psi_+\rangle = \cos\theta |1\rangle + e^{i\phi} \sin\theta |2\rangle, \quad |\psi_-\rangle = -\sin\theta |1\rangle + e^{i\phi} \cos\theta |2\rangle, \quad (2.127)$$

which automatically ensures  $\langle\psi_+|\psi_+\rangle = \langle\psi_-|\psi_-\rangle = 1$  and  $\langle\psi_+|\psi_-\rangle = 0$ .

Define the unitary change-of-basis matrix  $U(\theta, \phi)$  by collecting the new basis vectors as linear combinations of the old basis:

$$\begin{pmatrix} |\psi_+\rangle \\ |\psi_-\rangle \end{pmatrix} = U^\dagger(\theta, \phi) \begin{pmatrix} |1\rangle \\ |2\rangle \end{pmatrix}. \quad (2.128)$$

This means that

$$U^\dagger(\theta, \phi) = \begin{pmatrix} \cos\theta & e^{i\phi} \sin\theta \\ -\sin\theta & e^{i\phi} \cos\theta \end{pmatrix}, \quad U(\theta, \phi) = \begin{pmatrix} \cos\theta & -\sin\theta \\ e^{-i\phi} \sin\theta & e^{-i\phi} \cos\theta \end{pmatrix}, \quad (2.129)$$

and  $U^\dagger U = \mathbb{I}$ .

This means that

$$H'_{\{|\psi_+\rangle, |\psi_-\rangle\}} = U^\dagger H_{\{|1\rangle, |2\rangle\}} U,$$

is

$$\begin{pmatrix} \bar{E} + \sqrt{\delta^2 + |V|^2} & 0 \\ 0 & \bar{E} - \sqrt{\delta^2 + |V|^2} \end{pmatrix} = U^\dagger(\theta, \phi) \begin{pmatrix} E_1 & V \\ V^* & E_2 \end{pmatrix} U(\theta, \phi), \quad (2.130)$$

and equivalently,

$$\begin{aligned} \begin{pmatrix} \bar{E} + \sqrt{\delta^2 + |V|^2} & 0 \\ 0 & \bar{E} - \sqrt{\delta^2 + |V|^2} \end{pmatrix} &= \begin{pmatrix} \cos\theta & e^{i\phi} \sin\theta \\ -\sin\theta & e^{i\phi} \cos\theta \end{pmatrix} \begin{pmatrix} E_1 & V \\ V^* & E_2 \end{pmatrix} \begin{pmatrix} \cos\theta & -\sin\theta \\ e^{-i\phi} \sin\theta & e^{-i\phi} \cos\theta \end{pmatrix} = \\ &= \begin{pmatrix} \cos\theta & e^{i\phi} \sin\theta \\ -\sin\theta & e^{i\phi} \cos\theta \end{pmatrix} \begin{pmatrix} E_1 \cos\theta + V e^{-i\phi} \sin\theta & -E_1 \sin\theta + V e^{-i\phi} \cos\theta \\ V^* \cos\theta + E_2 e^{-i\phi} \sin\theta & -V^* \sin\theta + E_2 e^{-i\phi} \cos\theta \end{pmatrix}. \end{aligned}$$

This implies that

$$H'_{12} = \delta \sin(2\theta) + |V| \cos(2\theta) = 0 \quad \implies \quad \tan(2\theta) = -\frac{|V|}{\delta}, \quad (2.131)$$

so the mixing angle  $\theta$  satisfies

$$\tan(2\theta) = \frac{2|V|}{E_2 - E_1}. \quad (2.132)$$

Several regimes are worth highlighting:

- For  $|V| \ll |E_1 - E_2|$ , the mixing angle is small, and each eigenstate is dominated by a single basis state.
- For  $|V| \gg |E_1 - E_2|$ , the mixing is strong, and the eigenstates become nearly equal superpositions of  $|1\rangle$  and  $|2\rangle$ .
- At exact resonance ( $E_1 = E_2$ ), the eigenstates have equal contributions from each basis vector  $|i\rangle$  and  $\theta = \pi/4$ .

### 2.7.3 Wigner surmise: 2x2 Gaussian random matrices

The  $2 \times 2$  model provides a microscopic explanation for *level repulsion* in random matrix theory.

#### 1. The $2 \times 2$ GOE ensemble

Consider a real symmetric matrix

$$H = \begin{pmatrix} E_1 & V \\ V & E_2 \end{pmatrix}, \quad (2.133)$$

where the independent entries are Gaussian distributed. A convenient GOE parametrization (equivalent after unfolding to any other) is

$$E_1, E_2 \sim \mathcal{N}(0, \sigma^2), \quad V \sim \mathcal{N}\left(0, \frac{\sigma^2}{2}\right), \quad (2.134)$$

all independent.

#### 2. Eigenvalue spacing

According to Eq. (2.123), where now  $V = V^*$ , the level spacing is

$$\Delta \equiv E_+ - E_- = 2\sqrt{x^2 + y^2}, \quad (2.135)$$

where we defined

$$x = \frac{E_1 - E_2}{2}, \quad y = V. \quad (2.136)$$

Because  $E_1$  and  $E_2$  are independent  $\mathcal{N}(0, \sigma^2)$ ,

$$x = \frac{E_1 - E_2}{2} \sim \mathcal{N}\left(0, \frac{\sigma^2}{2}\right), \quad y \sim \mathcal{N}\left(0, \frac{\sigma^2}{2}\right), \quad (2.137)$$

and  $x$  and  $y$  are independent and identically distributed (i.i.d.).

#### 3. Distribution of $r = \sqrt{x^2 + y^2}$

The joint density of  $(x, y)$  is isotropic,

$$p(x, y) = p(x)p(y) = \frac{1}{2\pi\alpha^2} \exp\left(-\frac{x^2 + y^2}{2\alpha^2}\right), \quad \alpha^2 = \frac{\sigma^2}{2}. \quad (2.138)$$

In polar coordinates  $(x, y) = (r \cos \theta, r \sin \theta)$  with Jacobian  $J = r$ ,

$$p(r, \theta) = p(x, y)J = \frac{1}{\pi\sigma^2} e^{-r^2/\sigma^2} r, \quad (2.139)$$

where  $J$  is the Jacobian,

$$J = \left| \frac{\partial(x, y)}{\partial(r, \theta)} \right| = \left| \begin{pmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} \end{pmatrix} \right| = \left| \begin{pmatrix} \cos \theta & -r \sin \theta \\ \sin \theta & r \cos \theta \end{pmatrix} \right| = r.$$

Integrating over  $\theta \in [0, 2\pi)$  gives the Rayleigh distribution for  $r$ ,

$$p_r(r) = \frac{2r}{\sigma^2} \exp\left(-\frac{r^2}{\sigma^2}\right), \quad r \geq 0. \quad (2.140)$$

#### 4. Distribution of the spacing $\Delta$

Since  $\Delta = 2r$ , we use  $r = \Delta/2$  and  $dr = d\Delta/2$ :

$$p_\Delta(\Delta) = p_r(r) \left| \frac{dr}{d\Delta} \right| = p_r(\Delta/2) \frac{1}{2} = \frac{1}{2} \frac{2(\Delta/2)}{\sigma^2} \exp\left(-\frac{(\Delta/2)^2}{\sigma^2}\right) = \frac{\Delta}{2\sigma^2} \exp\left(-\frac{\Delta^2}{4\sigma^2}\right), \quad \Delta \geq 0. \quad (2.141)$$

This already shows *level repulsion*:  $p_\Delta(\Delta) \propto \Delta$  for  $\Delta \rightarrow 0$ .

#### 5. Unfolding to unit mean spacing

The Wigner surmise is written for unfolded spacings  $s = \Delta/\langle\Delta\rangle$  with mean 1, and

$$\langle\Delta\rangle = \int_0^\infty \frac{\Delta^2}{2\sigma^2} \exp\left(-\frac{\Delta^2}{4\sigma^2}\right) d\Delta = \sigma\sqrt{\pi}, \quad (2.142)$$

so

$$s = \frac{\Delta}{\sigma\sqrt{\pi}}, \quad \Delta = s\sigma\sqrt{\pi}. \quad (2.143)$$

Using  $p_s(s) = p_\Delta(\Delta) d\Delta/ds$  with  $d\Delta/ds = \sigma\sqrt{\pi}$ ,

$$\begin{aligned} p_s(s) &= \left[ \frac{\Delta}{2\sigma^2} e^{-\Delta^2/(4\sigma^2)} \right] \sigma\sqrt{\pi} \\ &= \frac{\pi}{2} s \exp\left(-\frac{\pi}{4} s^2\right). \end{aligned} \quad (2.144)$$

#### 6. Wigner surmise for the GOE

We obtain the celebrated result

$$\boxed{P_{\text{GOE}}(s) = \frac{\pi}{2} s \exp\left(-\frac{\pi}{4} s^2\right), \quad s \geq 0,} \quad (2.145)$$

known as the *Wigner surmise*. Although derived exactly for  $2 \times 2$  GOE matrices, it provides an excellent approximation to the nearest-neighbor spacing distribution of large GOE ensembles once the spectrum is unfolded.

## 2.8 Fractality and multifractality of eigenstates

The participation ratio provides information about how many basis states significantly contribute to an eigenstate. A more detailed characterization is obtained from the **generalized inverse participation ratios**. Consider an eigenstate

$$|\alpha\rangle = \sum_{n=1}^N C_n^\alpha |n\rangle, \quad \sum_{n=1}^N |C_n^\alpha|^2 = 1. \quad (2.146)$$

The generalized inverse participation ratio of order  $q$  is defined as

$$\text{IPR}_q^{(\alpha)} = \sum_{n=1}^N |C_n^\alpha|^{2q}. \quad (2.147)$$

For  $q = 2$ , this reduces to the usual inverse participation ratio,

$$\text{IPR}_2^{(\alpha)} = \sum_{n=1}^N |C_n^\alpha|^4. \quad (2.148)$$

Different values of  $q$  emphasize different parts of the wave function. For  $q > 1$ , the generalized IPR is increasingly dominated by basis states with large amplitudes, whereas smaller values of  $q$  give relatively more weight to components with small amplitudes.

The fractal properties of an eigenstate are obtained from the scaling of  $\text{IPR}_q$  with the Hilbert-space dimension  $N$ ,

$$\boxed{\text{IPR}_q \propto N^{-(q-1)D_q}}, \quad (2.149)$$

where  $D_q$  is called the **generalized fractal dimension**.

Taking the logarithm gives

$$\ln \text{IPR}_q = -(q-1)D_q \ln N + \text{const.} \quad (2.150)$$

Therefore,  $D_q$  can be obtained numerically by computing  $\text{IPR}_q$  for several system sizes and performing a linear fit of  $\ln \text{IPR}_q$  versus  $\ln N$ . If the slope of this fit is  $m_q$ , then

$$D_q = -\frac{m_q}{q-1}. \quad (2.151)$$

The physical meaning of  $D_q$  can be understood from three limiting cases.

- **Fully delocalized state:** If the state spreads over a finite fraction of all  $N$  basis states, then typically

$$|C_n^\alpha|^2 \sim \frac{1}{N}, \quad (2.152)$$

and therefore

$$\text{IPR}_q \sim N \left( \frac{1}{N} \right)^q = N^{-(q-1)}. \quad (2.153)$$

Comparing with Eq. (2.149) gives

$$\boxed{D_q = 1 \text{ (fully delocalized/ergodic)}}. \quad (2.154)$$

- **Localized state:** If the state has significant weight on only a finite number of basis states, independent of  $N$ , then  $\text{IPR}_q$  approaches a nonzero constant as  $N$  increases. Hence

$$\boxed{D_q = 0 \text{ (localized)}}. \quad (2.155)$$

- **Fractal extended state:** If

$$\boxed{0 < D_q < 1 \text{ (fractal)}}, \quad (2.156)$$

the eigenstate is extended, because the number of significantly occupied basis states grows with  $N$ , but it occupies only a vanishing fraction of the full Hilbert space. For example, for  $q = 2$ ,

$$\text{PR}_2 \sim N^{D_2}, \quad (2.157)$$

so when  $0 < D_2 < 1$ , the effective number of basis states participating in the eigenstate grows with  $N$ , but more slowly than the full Hilbert-space dimension. Thus the state is neither fully localized nor fully ergodic: it is **nonergodically extended** or **fractal**.

A state is called **multifractal** when a single fractal dimension is not sufficient to characterize its structure. In that case, different moments of the wave-function amplitudes scale with different exponents, so that

$$\boxed{0 < D_q < 1 \text{ and } D_q \text{ depends nontrivially on } q \text{ (multifractal)}} \quad (2.158)$$

### 2.8.1 Rényi Participation Entropies

Consider an eigenstate expanded in an orthonormal basis,

$$|\psi_\alpha\rangle = \sum_{n=1}^N C_n^{(\alpha)} |n\rangle, \quad \sum_{n=1}^N |C_n^{(\alpha)}|^2 = 1,$$

where  $N$  is the dimension of the Hilbert space. The Rényi participation entropy of order  $q$  is defined as

$$S_q^{(\alpha)} = \frac{1}{1-q} \ln \left[ \sum_{n=1}^N |C_n^{(\alpha)}|^{2q} \right], \quad q > 0, \quad q \neq 1.$$

For  $q = 1$ , the Rényi entropy is defined by taking the limit  $q \rightarrow 1$ , which gives the Shannon (or information) entropy,

$$S_1^{(\alpha)} = - \sum_{n=1}^N |C_n^{(\alpha)}|^2 \ln |C_n^{(\alpha)}|^2.$$

The Rényi participation entropies are directly related to the generalized inverse participation ratios. For  $q \neq 1$ ,

$$\boxed{S_q^{(\alpha)} = \frac{1}{1-q} \ln \text{IPR}_q^{(\alpha)}}.$$

For example, for  $q = 2$ ,

$$S_2^{(\alpha)} = -\ln(\text{IPR}) = \ln(\text{PR}).$$

The connection with multifractality follows from the scaling of the generalized participation ratios with the Hilbert-space dimension,  $\text{IPR}_q \propto N^{-(q-1)D_q}$ . Using the definition of the Rényi participation entropy, we obtain

$$\boxed{S_q \sim D_q \ln N}.$$

Thus, the generalized fractal dimension can be extracted from the scaling of the Rényi participation entropy as

$$D_q = \lim_{N \rightarrow \infty} \frac{S_q}{\ln N}.$$

For a fully delocalized state,  $D_q = 1$ , and therefore

$$S_q \sim \ln N.$$

## 2.9 Wigner band random matrices

In his pioneering work on the spectra of heavy nuclei, Wigner introduced random matrices as a statistical model for complex many-body Hamiltonians. Full random matrices, however, assume equal coupling between all basis states, an assumption that is physically unrealistic for systems governed by local interactions. In real many-body systems, interactions are not completely structureless: few-body operators can connect only configurations that differ by limited particle rearrangements, while matrix elements linking states far apart in energy or configuration space are strongly suppressed.

To incorporate this notion of *locality*, Wigner proposed **band random matrices** (BRM): matrices whose nonzero entries are concentrated near the main diagonal within a finite bandwidth  $b \ll N$ . For an  $N \times N$  matrix  $H$ , the structure is schematically

$$H_{ij} \neq 0 \quad \text{only if} \quad |i - j| \lesssim b,$$

while elements outside this band are zero or negligibly small. This contrasts with the full Gaussian ensembles, where all matrix elements are statistically equivalent and long-range couplings are allowed with equal strength.

By varying the bandwidth  $b$  one can interpolate between:

- nearly diagonal matrices ( $b \sim 1$ ), corresponding to weak mixing and almost integrable behavior;
- full random matrices ( $b \sim N$ ), corresponding to complete chaotic mixing and standard Wigner–Dyson statistics.

Thus BRM provided one of the earliest models to study how spectral statistics evolve from Poisson-like to GOE-like as the effective coupling range increases.

**NOTE:** Wigner’s original construction was not Gaussian, but had the following features

- The diagonal elements increase monotonically, representing unperturbed energies,

$$H_{ii} = i, \quad i = 1, \dots, N,$$

or more generally  $H_{ii} \propto i$ .

- Off-diagonal elements within a finite bandwidth  $b$  have fixed magnitude but random sign,

$$H_{ij} = \begin{cases} \pm 1, & |i - j| \leq b, \\ 0, & |i - j| > b, \end{cases}$$

with the signs chosen at random under the symmetry constraint  $H_{ij} = H_{ji}$ .

This model already contained the essential physical idea: the Hamiltonian is not fully random but has a *local structure in energy space*.

Chirikov, Casati, and Izrailev replaced the fixed-magnitude entries of Wigner's original model by Gaussian-distributed random numbers, leading to the now standard form

$$H_{ij} = \begin{cases} \text{Gaussian random variable with variance } \sigma^2(|i - j|), & |i - j| \leq b, \\ 0, & |i - j| > b. \end{cases}$$

Often  $\sigma^2(r)$  is taken constant inside the band or decaying with  $r$ .

## 2.10 Rosenzweig-Porter ensemble

The Rosenzweig–Porter ensemble (RPE) was originally introduced to describe the transition between regular and chaotic spectral statistics in complex atomic spectra. A commonly used generalized version of the real-symmetric RPE is defined by an  $N \times N$  random matrix whose elements are independent Gaussian random variables, subject to  $H_{ij} = H_{ji}$ , with

$$\langle H_{ij}^2 \rangle = \begin{cases} 1, & i = j, \\ \frac{1}{2N^\gamma}, & i \neq j, \end{cases} \quad (2.159)$$

where  $\gamma$  controls the strength of the off-diagonal couplings.

The model may be viewed as a diagonal random matrix perturbed by a GOE-like random matrix,

$$H = H_0 + N^{-\gamma/2}V, \quad (2.160)$$

where

$$(H_0)_{ii} \sim \mathcal{N}(0, 1) \quad (2.161)$$

and, for example, the off-diagonal elements of  $V$  satisfy

$$V_{ij} \sim \mathcal{N}(0, 1/2), \quad i < j. \quad (2.162)$$

Thus, the typical off-diagonal matrix element scales as

$$|H_{ij}|_{\text{typ}} \sim N^{-\gamma/2}. \quad (2.163)$$

The parameter  $\gamma$  controls the competition between the random diagonal energies and the off-diagonal hybridization. In the large- $N$  limit, the generalized RPE exhibits three regimes:

- $\gamma < 1$ : an **ergodic extended phase**. The eigenstates spread over an extensive fraction of the Hilbert space, with participation ratio scaling as

$$\text{PR} \sim N.$$

- $1 < \gamma < 2$ : a **nonergodic extended (fractal) phase**. The eigenstates extend over a number of basis states that diverges with  $N$ , but this number is subextensive:

$$\text{PR} \sim N^{D_2}, \quad 0 < D_2 < 1.$$

For the standard generalized RPE,

$$D_2 = 2 - \gamma,$$

and, in general,

$$\boxed{D_q = 2 - \gamma}, \quad \text{for } q \geq 1/2.$$

Because  $D_q$  is independent of  $q$ , the eigenstates are fractal, but not multifractal.

- $\gamma > 2$ : a **localized phase**. The eigenstates occupy only a finite number of basis states in the large- $N$  limit, so that

$$\text{PR} \sim O(1).$$

The transition from ergodic to non-ergodic extended ( $\gamma = 1$ ) can be determined from spacing arguments. The second transition point, from non-ergodic extended to localized ( $\gamma = 2$ ) has been done analytically, but it is more involved.

One can get an idea of why  $\gamma = 1$  marks the transition from ergodic to non-ergodic extended by comparing the mean level spacing of  $H_0$  with the typical off-diagonal element of  $\lambda V$ .

**Mean level spacing of  $H_0$ .** Since the  $N$  diagonal energies occupy an interval of  $O(1)$  width, the typical spacing between ordered consecutive levels is

$$\Delta \sim \frac{1}{N}. \quad (2.164)$$

**Typical coupling.** A typical off-diagonal matrix element of the perturbation  $\lambda V$  is

$$t \sim \lambda |V_{ij}| \sim N^{-\gamma/2} N^{-1/2} = N^{-(1+\gamma)/2}. \quad (2.165)$$

**Golden-rule width and the  $\gamma = 1$  criterion.** The relevant quantity controlling hybridization is the Fermi–Golden–Rule spreading width,

$$\Gamma \sim 2\pi \sum_j |H_{ij}|^2 \delta(E_i - E_j), \quad (2.166)$$

where the typical value of  $|H_{ij}|^2 \sim t^2$  and  $\delta(E_i - E_j) \sim 1/\Delta$ , so

$$\Gamma \sim \frac{t^2}{\Delta}$$

Using the scalings above,

$$\Gamma \sim \frac{N^{-(1+\gamma)}}{1/N} = N^{-\gamma}. \quad (2.167)$$

Ergodicity (strong overlap of many nearby levels) requires that the width exceed the mean spacing,

$$\Gamma \gg \Delta \iff N^{-\gamma} \gg \frac{1}{N} \iff \gamma < 1. \quad (2.168)$$

Thus  $\gamma = 1$  marks the transition from an ergodic regime ( $\gamma < 1$ ) to a non-ergodic extended regime ( $\gamma > 1$ ), where levels do not overlap strongly on the mean-spacing scale even though eigenstates can remain extended for  $1 < \gamma < 2$ .

## 2.11 Powerlaw banded random matrices

In the powerlaw banded random matrices (PBRM) ensemble the elements of the matrices are Gaussian random numbers with  $\langle H_{ij} \rangle = 0$  and variance

$$\langle H_{ij}^2 \rangle = \begin{cases} 1, & i = j, \\ \frac{1}{(1 + |i - j|^{2\alpha})}, & i \neq j, \end{cases} \quad (2.169)$$

where  $\alpha \in (0, \infty)$  is a control parameter. The ensemble has two limiting cases: if  $\alpha \rightarrow 0$ , we obtain the GOE model, and if  $\alpha \rightarrow \infty$ , we have a tridiagonal matrix. The model shows a phase transition determined by the value of  $\alpha$ . For  $\alpha < 1$ , the system is in the chaotic (delocalized) regime, while for  $\alpha > 1$ , the system is in the localized regime.

Therefore,

- If  $\alpha < 1$ , the eigenstates are extended.
- If  $\alpha > 1$ , the eigenstates are localized.
- The case  $\alpha = 1$  produces critical, multifractal eigenstates. Thus, the Anderson-type localization transition occurs at

$$\boxed{\alpha_c = 1}. \quad (2.170)$$

## 2.12 Assignment 01: Random Matrices

Use matrices of dimension  $N = 1000$  (or larger) and average over at least 5 independent random-matrix realizations. All Gaussian random variables should have mean  $\mu = 0$ . The variance depends on the ensemble under consideration and on whether you choose to work with the  $N$ -dependent ( $\sigma^2$ ) or  $N$ -independent ( $\sigma^2/N$ ) spectral scaling, as discussed in the notes.

1. **GOE: Density of states.** Compute the normalized density of states  $\rho(E)$  numerically and compare it with the Wigner semicircle law. Show the numerical and analytical results, Eq. (2.16), on the same plot.
2. **GOE: Nearest-neighbor level-spacing distribution.** Compute the nearest-neighbor level-spacing distribution  $P(s)$  using the two unfolding procedures discussed in the notes: (i) the “quick” local-rescaling method and (ii) the staircase-function method. Show the results obtained with both methods on the same plot and compare them with the GOE Wigner surmise in Eq. (2.42).
3. **GOE: Ratio of consecutive level spacings.** Compute the average symmetrized ratio  $\langle \tilde{r} \rangle$ . The average should include both the different values of  $\tilde{r}_n$  within each realization and the average over independent random-matrix realizations. Compare your numerical result with the analytical GOE value given in the notes.
4. **GOE: Level-number variance.** Compute the level-number variance  $\Sigma^2(\ell)$  using the unfolded spectrum obtained with the staircase-function method. Plot your numerical results together with the analytical GOE prediction in Eq. (2.73).
5. **GOE: Spectral form factor.** Compute and plot the spectral form factor as defined in Eq. (2.79). For this definition, no unfolding is required. Show results for both  $N = 1000$  and  $N = 2000$ . Since the spectral form factor can exhibit substantial fluctuations, increase the number of random-matrix realizations if necessary to obtain a sufficiently smooth ensemble average.
6. **GOE: Eigenvector delocalization.** For a single GOE realization, compute the participation ratio  $\text{PR}_\alpha$  of every eigenstate and plot  $\text{PR}_\alpha$  as a function of its corresponding eigenvalue  $E_\alpha$ . On the same plot, show the analytical GOE prediction for the typical participation ratio given in the notes.
7. **GUE.** Repeat items (1)–(6) for the Gaussian Unitary Ensemble (GUE), using the corresponding GUE analytical predictions whenever applicable.
8. **Rosenzweig–Porter ensemble: Spectral statistics.** For the Rosenzweig–Porter ensemble, investigate the evolution of the nearest-neighbor level-spacing distribution as the parameter  $\gamma$  is varied. For each value of  $\gamma$ , fit the numerical  $P(s)$  with the Brody distribution in Eq. (2.57) and extract the Brody parameter  $\beta$ . Plot the resulting  $\beta$  as a function of  $\gamma$ . Choose a range of  $\gamma$  to reveal the crossover between Wigner–Dyson-like and Poisson-like spectral statistics.

9. **Rosenzweig–Porter ensemble: Eigenvector delocalization.** For a single realization of the Rosenzweig–Porter ensemble, compute the participation ratio  $\text{PR}_\alpha$  of every eigenstate. On the same figure, plot  $\text{PR}_\alpha$  versus the corresponding eigenvalue  $E_\alpha$  for

$$\gamma = 0.5, \quad \gamma = 1.0, \quad \gamma = 1.5. \quad (2.171)$$

Compare the three cases. What do you observe about the degree of delocalization of the eigenstates as  $\gamma$  increases? Explain your results using the different regimes of the Rosenzweig–Porter ensemble discussed in the notes.

10. **Power-law banded random matrices: Spectral statistics.** For the power-law banded random-matrix ensemble, investigate the evolution of the nearest-neighbor level-spacing distribution as the exponent  $\alpha$  is varied. For each value of  $\alpha$ , fit the numerical  $P(s)$  with the Brody distribution in Eq. (2.57) and extract  $\beta$ . Plot the resulting  $\beta$  as a function of  $\alpha$ . Choose a range of  $\alpha$  to reveal the evolution between Wigner–Dyson-like and Poisson-like spectral statistics.
11. **Power-law banded random matrices: Multifractality.** Study the fractal properties of the eigenstates of the power-law banded random-matrix (PBRM) ensemble for

$$\alpha = 0, \quad \alpha = 1, \quad \alpha = 10. \quad (2.172)$$

For each value of  $\alpha$ , compute the generalized inverse participation ratios

$$\text{IPR}_q^{(\alpha')} = \sum_{n=1}^N |C_n^{\alpha'}|^{2q}, \quad (2.173)$$

for several values of  $q$  and several matrix dimensions  $N$  (depending on what your computer can handle, try, for example, various sizes with  $500 \leq N \leq 5000$ ). To minimize edge effects, use *eigenstates from a window around the center of the spectrum* (for example, 10% or 20% of the eigenstates closest to the spectrum center) and average  $\text{IPR}_q$  over these eigenstates and over independent random-matrix realizations.

For each fixed value of  $q$ , determine the generalized fractal dimension  $D_q$  from the finite-size scaling

$$\langle \text{IPR}_q \rangle \propto N^{-(q-1)D_q}, \quad (2.174)$$

using

$$\ln \langle \text{IPR}_q \rangle = -(q-1)D_q \ln N + \text{const.} \quad (2.175)$$

Thus, perform a linear fit of  $\ln \langle \text{IPR}_q \rangle$  versus  $\ln N$ . If the fitted slope is  $m_q$ , extract

$$D_q = -\frac{m_q}{q-1}. \quad (2.176)$$

Plot  $D_q$  as a function of  $q$  for  $\alpha = 0$ ,  $\alpha = 1$ , and  $\alpha = 10$  on the same figure. Use, for example,

$$q = 0.5, 1.5, 2.0, 2.5, 3.0 \text{ (or more points in between these ones)} \quad (2.177)$$

Compare the three cases. Which states are ergodically extended, localized, or multifractal? How can you distinguish a multifractal state from a simple fractal state from the dependence of  $D_q$  on  $q$ ?

How the plots should look like...

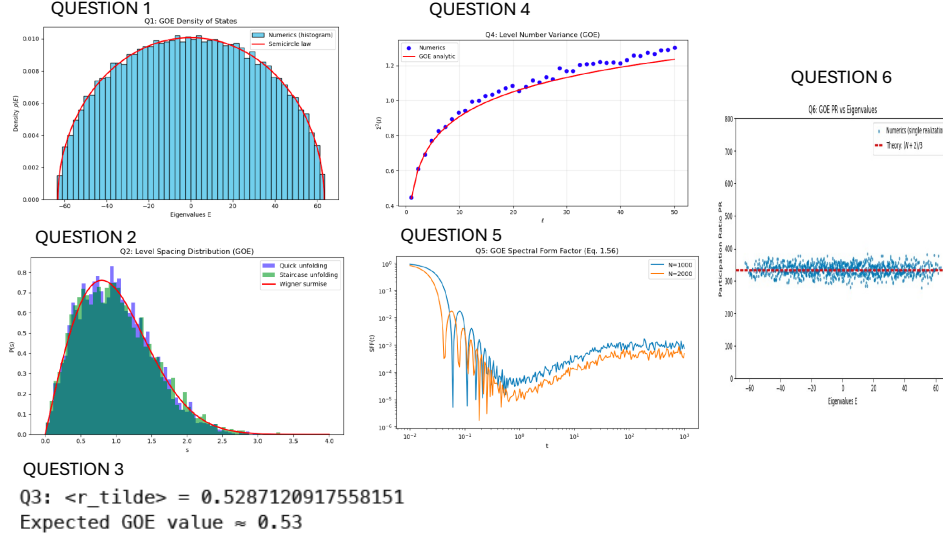


Figure 2.3: Questions 1-6

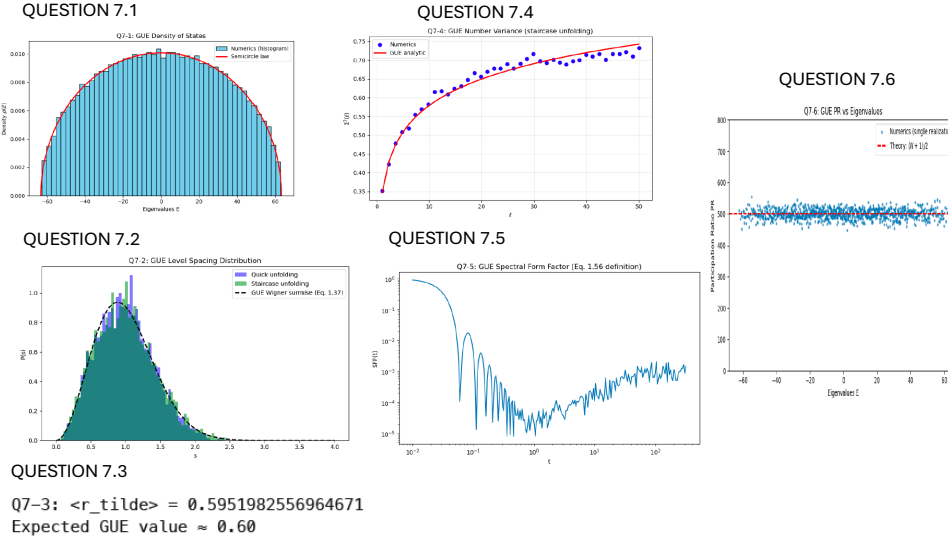
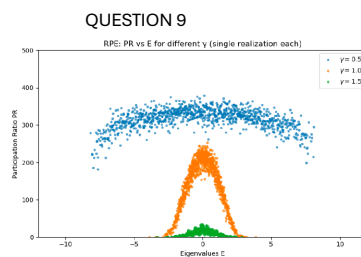
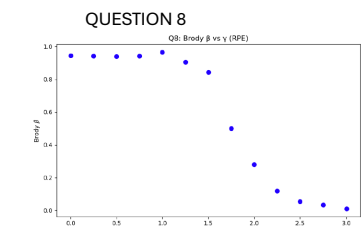


Figure 2.4: Question 7.

## Rosenzweig-Porter ensemble



## Power-law banded random matrices

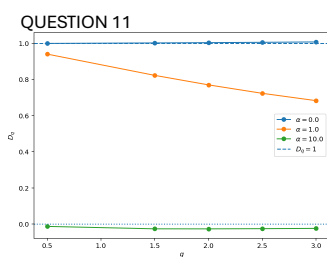
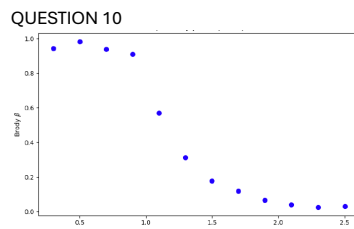
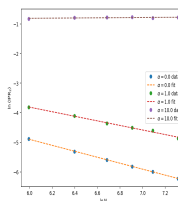
Example of scaling analysis for  $PR_2$ 

Figure 2.5: Questions 8-11.



# Chapter 3

## Physical Models: Spin-1/2 Chains and Beyond

Magnetism has fascinated humankind since antiquity, with early observations recorded in ancient China and Greece, but it was only with the advent of quantum mechanics and the discovery of electron spin that a microscopic understanding of magnetic phenomena became possible. Of particular relevance for us are the insulating magnetic solids, where the electrons are localized on atomic sites, so the system cannot conduct electricity, but their spins interact via exchange. In these systems, magnetism can be viewed as arising from a *lattice* of localized atomic or ionic magnetic moments. The total magnetic moment of each atom or ion originates mostly from the spins of electrons in partially filled shells. Interactions between these localized spins give rise to a wide range of collective phenomena with macroscopic manifestations, such as ferromagnetism, where spins align parallel to each other, and antiferromagnetism, where neighboring spins tend to orient in opposite directions. The dominant microscopic mechanism responsible for such ordering is the exchange interaction between the spins, which was introduced by Heisenberg and Dirac in the late 1920s and has a purely quantum-mechanical origin. This interaction arises from the interplay between Coulomb repulsion and the Pauli exclusion principle, and it is typically strong and short-ranged.

Spin-1/2 models occupy a central position in the theory of quantum many-body systems. Despite their apparent simplicity, these models capture a remarkably rich variety of physical phenomena, ranging from quantum phase transitions to integrability, quantum chaos, thermalization, quantum scars, and many-body localization. They provide some of the most paradigmatic and extensively studied examples of strongly correlated quantum systems, and serve as indispensable testbeds for both analytical and numerical methods in condensed matter physics, atomic and molecular physics, and statistical mechanics. They also play a fundamental role in quantum information science, since a spin-1/2 corresponds to a two-level quantum system and therefore serves as a natural physical model of a qubit, with spin chains providing minimal platforms for studying quantum computation and quantum information dynamics.

**Spin-1/2 Model**

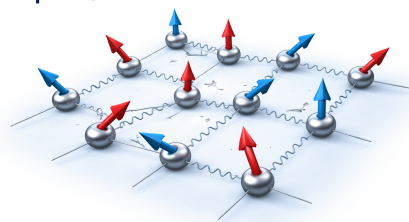


Figure 3.1: Illustration of a two-dimensional (2D) spin-1/2 system.

Our focus will be on spin-1/2 chains, which are systems of localized two-level degrees of freedom arranged on a one-dimensional (1D) lattice, where each site hosts a quantum spin operator  $\mathbf{S}_j = (S_j^x, S_j^y, S_j^z)$ . These degrees of freedom naturally arise as effective descriptions of a wide range of physical systems. In magnetic insulators, as mentioned above, they model the spin degrees of freedom of electrons localized on atomic sites and coupled via exchange interactions. In cold-atom and trapped-ion platforms, the spins-1/2 emerge as effective pseudospins encoded in internal atomic states, with interactions engineered through laser-induced couplings. In superconducting circuits, they describe qubits interacting through tunable couplers, providing a direct physical realization of spin chains in the context of quantum computation and simulation.

Even though the Hilbert space of spin-1/2 chains grows exponentially with the system size  $L$ , that is  $N = 2^L$ , this size is still smaller than other lattice systems, as those described by larger spins or Hubbard models. This allows for large-scale numerical simulations using exact diagonalization and tensor network methods, making them ideal platforms for testing fundamental concepts such as the eigenstate thermalization hypothesis (ETH) and the emergence of hydrodynamics.

The enduring importance of one-dimensional spin-1/2 models thus stems from a unique combination of features: conceptual simplicity, analytical tractability in special limits, experimental realizability, and extraordinary richness of physical behavior. They represent a bridge between exactly solvable models and generic interacting quantum systems, making them a cornerstone of modern research on quantum many-body dynamics and complexity.

### 3.1 Spin-1/2 chain: Hamiltonian matrix

The description of a system composed of a single spin-1/2 requires the use of the spin operators  $\hat{S}^{x,y,z} = \hat{\sigma}^{x,y,z}/2$ , where we set  $\hbar = 1$  and

$$\hat{\sigma}^x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}^y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{\sigma}^z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

are the Pauli matrices. The quantum state of the spin is represented by a two-component vector, known as the spinor. This state is commonly written in terms of basis vectors corresponding to the eigenstates of  $\hat{S}^z$ , which are the spin pointing up in the  $z$  direction  $|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$  and the down-spin  $|\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ . The eigenvalue associated with  $|\uparrow\rangle$  is  $+1/2$  and that of  $|\downarrow\rangle$  is  $-1/2$ , which justifies referring to the first as the **excitation**. The operators  $\hat{S}^x$  and  $\hat{S}^y$  flip the up- or down-spin according to

$$\hat{S}^x |\uparrow\rangle = \frac{1}{2} |\downarrow\rangle \quad \text{since} \quad \sigma_x |\uparrow\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |\downarrow\rangle.$$

Therefore,

$$\begin{aligned} \hat{S}^x |\uparrow\rangle &= \frac{1}{2} |\downarrow\rangle & \hat{S}^x |\downarrow\rangle &= \frac{1}{2} |\uparrow\rangle \\ \hat{S}^y |\uparrow\rangle &= \frac{i}{2} |\downarrow\rangle & \hat{S}^y |\downarrow\rangle &= \frac{-i}{2} |\uparrow\rangle. \end{aligned}$$


---

**Attention!** As written above, when studying spins-1/2, it is common to use as basis, the eigenstates of  $\hat{\sigma}^z$ ,

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

The labels  $|0\rangle$  and  $|1\rangle$  for these two states of a spin-1/2 system are also often used, but these labels are a matter of **convention**.

In quantum information and quantum computing, a common convention is

$$|\uparrow\rangle = |0\rangle, \quad |\downarrow\rangle = |1\rangle,$$

for which  $|0\rangle$  and  $|1\rangle$  are, respectively, the eigenstates of  $\sigma_z$  with eigenvalues  $+1$  and  $-1$ . Accordingly,  $|0\rangle$  lies at the north pole of the Bloch sphere (the zero polar angle of a vector pointing up in the Bloch sphere;  $+z$  direction), while  $|1\rangle$  lies at the south pole.

In condensed-matter physics and statistical mechanics, however, spin-1/2 degrees of freedom are often mapped onto occupation numbers. If  $|0\rangle$  denotes an empty site and  $|1\rangle$  an occupied site, one may choose to associate occupation with the spin up and thus higher energy (eigenvalue  $+1$ ), leading to

$$|\downarrow\rangle = |0\rangle, \quad |\uparrow\rangle = |1\rangle.$$

**This is the convention used in these notes!**

---

Let us consider a chain composed of  $L$  coupled spins-1/2 and analyze a generic class of Hamiltonians of the form

$$\hat{H} = \sum_{j=1}^L h_j \hat{S}_j^z + \sum_{j < k} \left[ J_x \hat{S}_j^x \hat{S}_k^x + J_y \hat{S}_j^y \hat{S}_k^y + J_z \hat{S}_j^z \hat{S}_k^z \right], \quad (3.1)$$

where the operators  $\hat{S}_j^{x,y,z}$  act only on the spin placed on site  $j$ ,  $J_{x,y,z}$  are the strengths of each term, and  $h_j$  is the local magnetic (longitudinal) field at site  $j$ , which determines the local Zeeman splitting between the two spin states. The choices of parameters and the range of the couplings between spins give rise to a variety of extensively studied models, including the following ones:

- **Ising model (nearest-neighbor):**

$$\hat{H}_{\text{Ising}} = \sum_{j=1}^{L-1} J_z \hat{S}_j^z \hat{S}_{j+1}^z + h \sum_{j=1}^L \hat{S}_j^z. \quad (3.2)$$

- **XX model (nearest-neighbor):**

$$\hat{H}_{\text{XX}} = \sum_{j=1}^{L-1} J \left( \hat{S}_j^x \hat{S}_{j+1}^x + \hat{S}_j^y \hat{S}_{j+1}^y \right). \quad (3.3)$$

- **XY model (nearest-neighbor):**

$$\hat{H}_{\text{XY}} = \sum_{j=1}^{L-1} \left( J_x \hat{S}_j^x \hat{S}_{j+1}^x + J_y \hat{S}_j^y \hat{S}_{j+1}^y \right). \quad (3.4)$$

- **XYZ Heisenberg model (nearest-neighbor):**

$$\hat{H}_{\text{XYZ}} = \sum_{j=1}^{L-1} \left( J_x \hat{S}_j^x \hat{S}_{j+1}^x + J_y \hat{S}_j^y \hat{S}_{j+1}^y + J_z \hat{S}_j^z \hat{S}_{j+1}^z \right). \quad (3.5)$$

- **XXZ Heisenberg model (nearest-neighbor):**

$$\hat{H}_{\text{XXZ}} = \sum_{j=1}^{L-1} \left( J \hat{S}_j^x \hat{S}_{j+1}^x + J \hat{S}_j^y \hat{S}_{j+1}^y + J \Delta \hat{S}_j^z \hat{S}_{j+1}^z \right). \quad (3.6)$$

- **Disordered XXZ model (nearest-neighbor):**

$$\hat{H}_{\text{XXZ}}^{\text{dis}} = \sum_{j=1}^{L-1} \left( J \hat{S}_j^x \hat{S}_{j+1}^x + J \hat{S}_j^y \hat{S}_{j+1}^y + J \Delta \hat{S}_j^z \hat{S}_{j+1}^z \right) + \sum_{j=1}^L h_j \hat{S}_j^z, \quad (3.7)$$

where  $h_j$  are random local fields, typically drawn from a uniform distribution  $h_j \in [-W, W]$ .

- **$J_1$ - $J_2$  XXZ model (nearest and next-nearest neighbors):**

$$\begin{aligned} \hat{H}_{J_1-J_2} &= \sum_{j=1}^{L-1} \left( J_1 \hat{S}_j^x \hat{S}_{j+1}^x + J_1 \hat{S}_j^y \hat{S}_{j+1}^y + J_1 \Delta_1 \hat{S}_j^z \hat{S}_{j+1}^z \right) \\ &+ \sum_{j=1}^{L-2} \left( J_2 \hat{S}_j^x \hat{S}_{j+2}^x + J_2 \hat{S}_j^y \hat{S}_{j+2}^y + J_2 \Delta_2 \hat{S}_j^z \hat{S}_{j+2}^z \right). \end{aligned} \quad (3.8)$$

In addition to the examples above, relaxing the nearest- and second-nearest-neighbor constraint leads to long-range interacting models, which typically display enhanced chaos and faster information scrambling.

We begin by studying the XXZ model with nearest-neighbor couplings and open boundary conditions,

$$\hat{H} = \sum_{n=1}^{L-1} \left[ J \left( \hat{S}_n^x \hat{S}_{n+1}^x + \hat{S}_n^y \hat{S}_{n+1}^y \right) + J_z \hat{S}_n^z \hat{S}_{n+1}^z \right], \quad (3.9)$$

where  $J$  is the strength of the flip-flop term  $\hat{S}_n^x \hat{S}_{n+1}^x + \hat{S}_n^y \hat{S}_{n+1}^y$ ,  $J_z$  is the strength of the Ising interaction  $\hat{S}_n^z \hat{S}_{n+1}^z$ , and the ratio  $\Delta = J_z/J$  is the anisotropy parameter. Notice that the term  $h \sum_{j=1}^L \hat{S}_j^z$ , which appeared in Eq. (3.1), is often omitted either because it commutes

with the Hamiltonian [as in the case of Eq. (3.9)] or has no further consequences. We come back to this point in EXERCISE 1.2.1.

The model is isotropic when  $\Delta = 1$ , in which case it is known as the XXX model, and it is anisotropic when  $\Delta \neq 1$ , usually referred to as the XXZ model. A natural basis choice for writing the Hamiltonian matrix is the set of  $2^L$  states where the spin on each site is either pointing up or down, such as  $|\downarrow_1 \uparrow_2 \uparrow_3 \dots \downarrow_L\rangle$ . In quantum information, these states are known as quantum computational basis vectors. They can also be referred to as site-basis vectors or product states. However, for any of these terms to be unambiguous, one should specify that we refer to spin pointing up or down *in the  $z$ -direction*.

The Ising interaction contributes to the diagonal part of the Hamiltonian matrix written in the site-basis. It causes a pair of adjacent parallel spins to have different energy from a pair of anti-parallel spins, because

$$J_z \hat{S}_n^z \hat{S}_{n+1}^z |\uparrow_n \uparrow_{n+1}\rangle = +\frac{J_z}{4} |\uparrow_n \uparrow_{n+1}\rangle, \quad (3.10)$$

while

$$J_z \hat{S}_n^z \hat{S}_{n+1}^z |\uparrow_n \downarrow_{n+1}\rangle = -\frac{J_z}{4} |\uparrow_n \downarrow_{n+1}\rangle. \quad (3.11)$$

A Hamiltonian containing only the Ising interaction,  $\hat{H}_{zz} = J_z \hat{S}_n^z \hat{S}_{n+1}^z$ , constitutes the Ising model in Eq. (3.2). As one can infer from Eqs. (3.10) and (3.11), the ground state of this model depends on the sign of the interaction strength; it is ferromagnetic, with all spins aligned in the same direction, when  $J_z < 0$ , and it shows an antiferromagnetic arrangement with antiparallel neighboring spins when  $J_z > 0$ .

The flip-flop (exchange) term in Hamiltonian (3.9) interchanges the position of neighboring up and down spins according to

$$J(\hat{S}_n^x \hat{S}_{n+1}^x + \hat{S}_n^y \hat{S}_{n+1}^y) |\uparrow_n \downarrow_{n+1}\rangle = \frac{J}{4} (\hat{\sigma}_n^x \hat{\sigma}_{n+1}^x + \hat{\sigma}_n^y \hat{\sigma}_{n+1}^y) |\uparrow_n \downarrow_{n+1}\rangle = \frac{J}{2} |\downarrow_n \uparrow_{n+1}\rangle.$$

This term is also commonly written with raising

$$\hat{S}^+ = \hat{S}^x + i\hat{S}^y = \frac{\hat{\sigma}^x + i\hat{\sigma}^y}{2} = \hat{\sigma}^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

and lowering

$$\hat{S}^- = \hat{S}^x - i\hat{S}^y = \frac{\hat{\sigma}^x - i\hat{\sigma}^y}{2} = \hat{\sigma}^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

operators, so

$$\frac{J}{2} (\hat{S}_n^+ \hat{S}_{n+1}^- + \hat{S}_{n+1}^+ \hat{S}_n^-) |\uparrow_n \downarrow_{n+1}\rangle = \frac{J}{2} (\hat{\sigma}_n^+ \hat{\sigma}_{n+1}^- + \hat{\sigma}_{n+1}^+ \hat{\sigma}_n^-) |\uparrow_n \downarrow_{n+1}\rangle = \frac{J}{2} |\downarrow_n \uparrow_{n+1}\rangle.$$

[**Note** that  $\hat{S}^{x,y,z} = \sigma^{x,y,z}/2$ , but there is not factor of 2 in  $\hat{S}^\pm = \sigma^\pm$ . ] The flip-flop term therefore couples site-basis vectors that differ only by the orientation of the spins in two adjacent sites, swapping the position of neighboring up and down spins. To be more precise, it couples the state  $|\uparrow\downarrow\rangle$  with the state  $|\downarrow\uparrow\rangle$ , but not the state  $|\uparrow\uparrow\rangle$  with the state  $|\downarrow\downarrow\rangle$ . In

| Index        | Binary | Spin state                                         | $H_{ii}$                     |
|--------------|--------|----------------------------------------------------|------------------------------|
| $ 1\rangle$  | 0000   | $ \downarrow\downarrow\downarrow\downarrow\rangle$ | $H_{1,1} = 3J_z/4$           |
| $ 2\rangle$  | 1000   | $ \uparrow\downarrow\downarrow\downarrow\rangle$   | $H_{2,2} = \frac{1}{4}J_z$   |
| $ 3\rangle$  | 0100   | $ \downarrow\uparrow\downarrow\downarrow\rangle$   | $-\frac{1}{4}J_z$            |
| $ 4\rangle$  | 0010   | $ \downarrow\downarrow\uparrow\downarrow\rangle$   | $-\frac{1}{4}J_z$            |
| $ 5\rangle$  | 0001   | $ \downarrow\downarrow\downarrow\uparrow\rangle$   | $\frac{1}{4}J_z$             |
| $ 6\rangle$  | 1100   | $ \uparrow\uparrow\downarrow\downarrow\rangle$     | $\frac{1}{4}J_z$             |
| $ 7\rangle$  | 1010   | $ \uparrow\downarrow\uparrow\downarrow\rangle$     | $-\frac{3}{4}J_z$            |
| $ 8\rangle$  | 1001   | $ \uparrow\downarrow\downarrow\uparrow\rangle$     | $-\frac{1}{4}J_z$            |
| $ 9\rangle$  | 0110   | $ \downarrow\uparrow\uparrow\downarrow\rangle$     | $-\frac{1}{4}J_z$            |
| $ 10\rangle$ | 0101   | $ \downarrow\uparrow\downarrow\uparrow\rangle$     | $-\frac{3}{4}J_z$            |
| $ 11\rangle$ | 0011   | $ \downarrow\downarrow\uparrow\uparrow\rangle$     | $\frac{1}{4}J_z$             |
| $ 12\rangle$ | 1110   | $ \uparrow\uparrow\uparrow\downarrow\rangle$       | $\frac{1}{4}J_z$             |
| $ 13\rangle$ | 1101   | $ \uparrow\uparrow\downarrow\uparrow\rangle$       | $-\frac{1}{4}J_z$            |
| $ 14\rangle$ | 1011   | $ \uparrow\downarrow\uparrow\uparrow\rangle$       | $-\frac{1}{4}J_z$            |
| $ 15\rangle$ | 0111   | $ \downarrow\uparrow\uparrow\uparrow\rangle$       | $\frac{1}{4}J_z$             |
| $ 16\rangle$ | 1111   | $ \uparrow\uparrow\uparrow\uparrow\rangle$         | $H_{16,16} = \frac{3}{4}J_z$ |

Table 3.1: Basis ordering grouped by total magnetization and diagonal matrix elements  $H_{ii} = \langle i | J_z \sum_{n=1}^3 S_n^z S_{n+1}^z | i \rangle$  for the XXZ chain with open boundary conditions.

the site-basis, it constitutes the off-diagonal elements of the Hamiltonian matrix. This term plays a key role in the evolution of the system by moving the excitations through the chain.

In the case of open boundary conditions (open chain), as in Eq. (3.9), where the sum goes from site  $n = 1$  to site  $L - 1$ , an excitation on site 1 can move only to site 2 and from site  $L$  to  $L - 1$ . The scenario of a ring (closed chain), where an excitation on site  $L$  can also move to site 1 corresponds to closed boundary conditions.

The Hamiltonian matrix for the case with  $L = 4$  and open boundary conditions, using the basis vectors in the order in Table 3.1 is given by

$$\left( \begin{array}{c|cccc|cccc|cccc|cccc|c}
 \frac{3J\Delta}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 \hline
 0 & +\frac{J\Delta}{4} & \frac{J}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & \frac{J}{2} & -\frac{J\Delta}{4} & \frac{J}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & \frac{J}{2} & -\frac{J\Delta}{4} & \frac{J}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & +\frac{J}{2} & +\frac{J\Delta}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 \hline
 0 & 0 & 0 & 0 & 0 & +\frac{J\Delta}{4} & \frac{J}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & \frac{J}{2} & -\frac{3J\Delta}{4} & \frac{J}{2} & \frac{J}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & \frac{J}{2} & -\frac{J\Delta}{4} & 0 & \frac{J}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & \frac{J}{2} & 0 & -\frac{J\Delta}{4} & \frac{J}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{J}{2} & \frac{J}{2} & -\frac{3J\Delta}{4} & \frac{J}{2} & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{J}{2} & \frac{J\Delta}{4} & 0 & 0 & 0 & 0 & 0 \\
 \hline
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & +\frac{J\Delta}{4} & \frac{J}{2} & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{J}{2} & -\frac{J\Delta}{4} & \frac{J}{2} & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{J}{2} & -\frac{J\Delta}{4} & \frac{J}{2} & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{J}{2} & +\frac{J\Delta}{4} & 0 \\
 \hline
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{3J\Delta}{4}
 \end{array} \right) \quad (3.12)$$

The matrix above is block diagonal. It shows the following structure

$$H = \begin{pmatrix} \boxed{H^{(0)}} & 0 & 0 & 0 & 0 \\ 0 & \boxed{H^{(1)}} & 0 & 0 & 0 \\ 0 & 0 & \boxed{H^{(2)}} & 0 & 0 \\ 0 & 0 & 0 & \boxed{H^{(3)}} & 0 \\ 0 & 0 & 0 & 0 & \boxed{H^{(4)}} \end{pmatrix} \quad (3.13)$$

with block dimensions

$$\dim H^{(0)} = 1, \quad \dim H^{(1)} = 4, \quad \dim H^{(2)} = 6, \quad \dim H^{(3)} = 4, \quad \dim H^{(4)} = 1.$$

The block-diagonal structure is preserved for both open and periodic boundary conditions. In the latter case, the diagonal elements are modified and additional off-diagonal terms appear, but only within each block. Let us take as an example the block  $H^{(2)}$  and the basis  $|\uparrow\uparrow\downarrow\downarrow\rangle$ . The corresponding diagonal element for the open chain is  $J_z/4$ , while for the periodic chain, it is 0. In the open chain,  $|\uparrow\uparrow\downarrow\downarrow\rangle$  couples only with the state  $|\uparrow\downarrow\uparrow\downarrow\rangle$ , while in the periodic case it also couples with  $|\downarrow\uparrow\downarrow\uparrow\rangle$ .

## 3.2 Symmetries

Operators that commute with the Hamiltonian play a fundamental role in quantum mechanics. They possess two important properties: (i) their eigenstates can be chosen to be simultaneous eigenstates of the Hamiltonian [12], and (ii) provided they have no explicit time dependence, they represent physical observables that are conserved in time. The latter property follows from the Heisenberg equation of motion for the expectation value,

$$\frac{d\langle\hat{O}\rangle}{dt} = \frac{i}{\hbar}\langle[\hat{H}, \hat{O}]\rangle \quad \text{so that} \quad [\hat{H}, \hat{O}] = 0 \quad \implies \quad \frac{d\langle\hat{O}\rangle}{dt} = 0,$$

and the observable  $\hat{O}$  is a constant of motion.

A systematic way to identify such conserved quantities is by analyzing the symmetries of the system. According to Noether's theorem, every continuous symmetry of the Hamiltonian is associated with a conserved quantity. For example, invariance of  $\hat{H}$  under spatial translations leads to conservation of linear momentum, invariance under time translations implies conservation of total energy, and rotational invariance leads to conservation of angular momentum.

### 3.2.1 Conservation of total magnetization along the $z$ -direction

The block structure of the matrix shown in Eq. (3.13) is a direct consequence of an underlying symmetry. In particular, the Hamiltonian commutes with the total spin operator in the  $z$ -direction,

$$\hat{S}^z = \sum_{n=1}^L \hat{S}_n^z, \quad [\hat{H}, \hat{S}^z] = 0.$$

You can check this by verifying that

$$[\hat{S}_n^x \hat{S}_{n+1}^x + \hat{S}_n^y \hat{S}_{n+1}^y, \hat{S}_n^z + \hat{S}_{n+1}^z] = 0$$

The commutation  $[\hat{H}, \hat{\mathcal{S}}^z] = 0$  means that the system is invariant under rotations around the  $z$ -axis, or equivalently, that the total magnetization in the  $z$ -axis direction,  $\hat{\mathcal{S}}^z$ , is a conserved quantity. As a result, the Hilbert space decomposes into independent invariant subspaces (or symmetry sectors), each characterized by a fixed number  $n \in [0, L]$  of up-spins. Consequently, although the full Hilbert space of a system with  $L$  sites has dimension  $2^L$ , the Hamiltonian matrix is composed of  $L + 1$  independent blocks, each of dimension

$$D_n = \binom{L}{n}.$$

This allows one to diagonalize the Hamiltonian separately within each magnetization sector, leading to a substantial reduction in computational cost. For even  $L$  the largest subspace has  $n = L/2$ , which has the maximal dimension

$$D_{L/2} = \binom{L}{L/2} = \frac{L!}{(L/2)!^2}.$$

A consequence of this symmetry is that if the initial state contains  $n$  up-spins, then all states participating in its time evolution must belong to the same magnetization sector, that is, they must have the same number of up-spins. Equivalently, the eigenvalue of the operator  $\hat{\mathcal{S}}^z$  associated with the initial state is conserved throughout the dynamics. In other words, the system cannot evolve into states with different total magnetization.

However, the XXZ Hamiltonian may possess additional symmetries, which lead to further decompositions of the Hilbert space and are discussed next.

**EXERCISE 1.2.1:** Build the Hamiltonian matrix in Eq. (3.9) with open boundary conditions for a chain of  $L = 5$  sites, restricted to the sector with 2 up-spins and 3 down-spins. This corresponds to the magnetization sector with total spin in the  $z$ -direction  $\mathcal{S}^z = -1/2$ . Consider  $J = 1$  and  $J_z = 0.5$ . Verify whether you obtain the following eigenvalues:

$$\begin{aligned} E_1 &= -1.62637, & E_2 &= -1.01814, & E_3 &= -0.564255, & E_4 &= -0.539431, \\ E_5 &= -0.147165, & E_6 &= 0.133361, & E_7 &= 0.329082, & E_8 &= 0.5, \\ E_9 &= 0.781947, & E_{10} &= 1.15098 \end{aligned} \quad (3.14)$$

Using the basis vectors in the following order,

$$\begin{aligned}
|1\rangle &= |11000\rangle, \\
|2\rangle &= |10100\rangle, \\
|3\rangle &= |10010\rangle, \\
|4\rangle &= |10001\rangle, \\
|5\rangle &= |01100\rangle, \\
|6\rangle &= |01010\rangle, \\
|7\rangle &= |01001\rangle, \\
|8\rangle &= |00110\rangle, \\
|9\rangle &= |00101\rangle, \\
|10\rangle &= |00011\rangle.
\end{aligned}$$

your matrix should be

$$H = \begin{pmatrix} 0.25 & 0.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.5 & -0.25 & 0.5 & 0 & 0.5 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.5 & -0.25 & 0.5 & 0 & 0.5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.5 & 0 & 0 & 0 & 0.5 & 0 & 0 & 0 \\ 0 & 0.5 & 0 & 0 & 0 & 0.5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.5 & 0 & 0.5 & -0.5 & 0.5 & 0.5 & 0 & 0 \\ 0 & 0 & 0 & 0.5 & 0 & 0.5 & -0.25 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.5 & 0 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.5 & 0.5 & -0.25 & 0.5 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.5 & 0.25 \end{pmatrix}. \quad (3.15)$$

### Diagonal Elements:

Determining the diagonal elements of the Hamiltonian matrix coming from the Ising interaction is straightforward: one simply counts the number of pairs of adjacent parallel spins and adjacent anti-parallel spins in each basis state. Each parallel (anti-parallel) pair contributes  $+J_z/4$  ( $-J_z/4$ ) to the diagonal energy.

### Onsite Energies:

If the Hamiltonian contains the term

$$\hat{H}_z = \sum_{j=1}^L h_j \hat{S}_j^z,$$

it also contributes to the diagonal elements of the Hamiltonian matrix in the computational basis. The amplitude  $h_j$  represents the local Zeeman splitting of spin  $j$ , as induced by a static magnetic field applied in the  $z$ -direction at that site. Note, however, that if  $h_j = h$ , corresponding to a homogeneous (clean) chain, this term contributes the same energy shift

to all basis states within a fixed  $\mathcal{S}^z$  sector. In the particular example of this exercise, we can see that

$$\langle 1|\hat{H}_z|1\rangle = \langle 2|\hat{H}_z|2\rangle = \dots = \langle 10|\hat{H}_z|10\rangle = -h/2.$$

Since this amounts to a uniform shift of all diagonal elements, it simply adds a constant to the spectrum and can therefore be disregarded, as it does not affect energy differences or the dynamics within the sector.

### Off-Diagonal Elements:

The off-diagonal elements are slightly more subtle. They arise from the exchange terms and are obtained by comparing pairs of basis states. Whenever two basis vectors differ only by the configuration of **two neighboring** sites, with a local pattern  $\uparrow\downarrow$  in one state and  $\downarrow\uparrow$  in the other, the corresponding matrix element is equal to  $J/2$ . All other off-diagonal elements vanish.

### 3.2.2 Reflection symmetry and parity conservation

Hamiltonian (3.9) is invariant under spatial reflection of the chain, which leads to conservation of parity. In other words, the Hamiltonian commutes with the parity (or reflection) operator,  $[\hat{H}, \hat{\Pi}]$  where the parity operator is defined as

$$\hat{\Pi} = \begin{cases} \hat{\mathcal{P}}_{1,L} \hat{\mathcal{P}}_{2,L-1} \dots \hat{\mathcal{P}}_{\frac{L}{2}, \frac{L+2}{2}} & \text{for } L = \text{even} \\ \hat{\mathcal{P}}_{1,L} \hat{\mathcal{P}}_{2,L-1} \dots \hat{\mathcal{P}}_{\frac{L-1}{2}, \frac{L+3}{2}} & \text{for } L = \text{odd} \end{cases}$$

and

$$\hat{\mathcal{P}}_{i,j} = \frac{1}{2}(\hat{\sigma}_i^x \hat{\sigma}_j^x + \hat{\sigma}_i^y \hat{\sigma}_j^y + \hat{\sigma}_i^z \hat{\sigma}_j^z + \mathbb{1})$$

is the permutation (swap) operator that exchanges the spin states at sites  $i$  and  $j$ , and  $\mathbb{1}$  is the identity operator. The action of  $\hat{\mathcal{P}}_{i,j}$  is to permute the  $i^{\text{th}}$  and  $j^{\text{th}}$  vector spaces. For example,

$$\hat{\Pi}|\uparrow\downarrow\uparrow\downarrow\rangle = |\downarrow\uparrow\downarrow\uparrow\rangle.$$

The physical meaning of reflection symmetry can be visualized by imagining a mirror placed at one edge of the chain. If parity is conserved, the probability of finding the system in a given basis state is equal to that of finding it in its mirror-reflected configuration.

As an example, consider a chain with  $L = 4$  and a single excitation. The eigenstates of  $\hat{H}$ , which are also eigenstates of  $\hat{\Pi}$ , are given by

$$|\psi^{(j)}\rangle = a_1^{(j)}|\uparrow\downarrow\downarrow\downarrow\rangle + a_2^{(j)}|\downarrow\uparrow\downarrow\downarrow\rangle + a_3^{(j)}|\downarrow\downarrow\uparrow\downarrow\rangle + a_4^{(j)}|\downarrow\downarrow\downarrow\uparrow\rangle.$$

If the state has even parity,  $\Pi = +1$ , then the probability amplitudes are either

$$a_1^{(j)} = a_4^{(j)} \quad \text{and} \quad a_2^{(j)} = a_3^{(j)}, \quad (3.16)$$

whereas for odd parity,  $\Pi = -1$ ,

$$a_1^{(j)} = -a_4^{(j)} \quad \text{and} \quad a_2^{(j)} = -a_3^{(j)}. \quad (3.17)$$

Here, the hat in  $\hat{\Pi}$  indicates the operator and its absence indicates the eigenvalue,  

$$\hat{\Pi}|\psi^{(j)}\rangle = \Pi|\psi^{(j)}\rangle.$$

**Note:** By definition the permutation (swap) operator must satisfy

$$\hat{\mathcal{P}}_{i,j}|\alpha\rangle_i|\beta\rangle_j = |\beta\rangle_i|\alpha\rangle_j$$

for **all** basis states. This is what  $\hat{\mathcal{P}}_{ij} = \frac{1}{2}(\hat{\sigma}_i^x\hat{\sigma}_j^x + \hat{\sigma}_i^y\hat{\sigma}_j^y + \hat{\sigma}_i^z\hat{\sigma}_j^z + \mathbb{1})$  does. This operator swaps (exchanges) the states at sites  $i$  and  $j$ , is unitary, is Hermitian, satisfies  $\hat{\mathcal{P}}_{ij}^2 = \mathbb{1}$ , and has eigenvalues  $\pm 1$ . In contrast, the truncated version  $\frac{1}{2}(\hat{\sigma}_i^x\hat{\sigma}_j^x + \hat{\sigma}_i^y\hat{\sigma}_j^y)$  only flips opposite spins, but does **NOT** act as identity on equal spins. That is, while  $\hat{\mathcal{P}}_{ij}|00\rangle = |00\rangle$ , as a swap operator should do,  $\frac{1}{2}(\hat{\sigma}_i^x\hat{\sigma}_j^x + \hat{\sigma}_i^y\hat{\sigma}_j^y)|00\rangle = 0$ . Therefore, the truncated operator is not a swap operator: it is not invertible, is not unitary, and its square is not the identity.

### Taking parity into account

There are two ways to separate the eigenvalues and eigenstates according to parity. As an illustrative example, consider the XXZ model with open boundary conditions and nearest-neighbor couplings in Eq. (3.9), restricted to the zero- $z$ -magnetization sector  $\mathcal{S}_z = 0$  for a chain of length  $L = 4$  and 2 up-spins.

1. One may first diagonalize the full Hamiltonian matrix in the  $\mathcal{S}_z = 0$  sector and subsequently analyze the parity of each eigenstate. This can be done by inspecting the coefficients of the eigenvectors in the computational basis, following the discussion around Eqs. (3.16) and (3.17), and assigning each eigenstate to the even or odd parity sector.
2. Alternatively, one may construct the Hamiltonian already block-diagonalized by parity. This approach requires generating orthonormal bases for the even- and odd-parity subspaces and writing the Hamiltonian directly in each sector.

#### Odd-parity sector.

An orthonormal basis for the odd-parity subspace is given by

$$|e_1\rangle = \frac{1}{\sqrt{2}}(|1100\rangle - |0011\rangle), \quad (3.18)$$

$$|e_2\rangle = \frac{1}{\sqrt{2}}(|1010\rangle - |0101\rangle). \quad (3.19)$$

In this basis, the Hamiltonian matrix reads

$$H_{\text{odd}} = \begin{pmatrix} \frac{J_z}{4} & \frac{J}{2} \\ \frac{J}{2} & -\frac{3J_z}{4} \end{pmatrix}.$$

#### Even-parity sector.

An orthonormal basis for the even-parity subspace is

$$|e_1\rangle = \frac{1}{\sqrt{2}} (|1100\rangle + |0011\rangle), \quad (3.20)$$

$$|e_2\rangle = \frac{1}{\sqrt{2}} (|1010\rangle + |0101\rangle), \quad (3.21)$$

$$|e_3\rangle = |1001\rangle, \quad (3.22)$$

$$|e_4\rangle = |0110\rangle. \quad (3.23)$$

The states  $|1001\rangle$  and  $|0110\rangle$  are invariant under reflection and therefore belong entirely to the even-parity sector. In the ordered basis  $\{|e_1\rangle, |e_2\rangle, |e_3\rangle, |e_4\rangle\}$ , the Hamiltonian matrix takes the form

$$H_{\text{even}} = \begin{pmatrix} \frac{J_z}{4} & \frac{J}{2} & 0 & 0 \\ \frac{J}{2} & -\frac{3J_z}{4} & \frac{J}{\sqrt{2}} & \frac{J}{\sqrt{2}} \\ 0 & \frac{J}{\sqrt{2}} & -\frac{J_z}{4} & 0 \\ 0 & \frac{J}{\sqrt{2}} & 0 & -\frac{J_z}{4} \end{pmatrix}.$$

### EXERCISE 1.2.2.:

**A)** Obtain the eigenstates and eigenvalues of the Hamiltonian matrix in Eq. (3.15). Identify the eigenstates with even parity and their eigenvalues and do the same for odd parity.

**B)** In analogy with the case of conservation of the total  $z$ -component of the spin, where the Hamiltonian was written within a single symmetry sector, write the Hamiltonian matrix in Eq. (3.15) restricted to the odd-parity sector, and determine its eigenvalues.

Hint for (A): The eigenstate with the lowest eigenvalue  $E_1 = -1.62637$  is

$$|\psi_1\rangle = \begin{pmatrix} -0.070439 \\ 0.26434 \\ -0.396572 \\ 0.243838 \\ -0.260649 \\ 0.583484 \\ -0.396572 \\ -0.260649 \\ 0.26434 \\ -0.070439 \end{pmatrix},$$

and it has **even** parity, while the first excited eigenstate with eigenvalue  $E_2 = -1.01814$  is

$$|\psi_2\rangle = \begin{pmatrix} 0.206639 \\ -0.524096 \\ 0.341145 \\ 4.12 \times 10^{-17} = 0 \\ 0.257378 \\ -1.40 \times 10^{-16} = 0 \\ -0.341145 \\ -0.257378 \\ 0.524096 \\ -0.206639 \end{pmatrix},$$

and has **odd** parity.

Hint for (B): The parity pair of state  $|11000\rangle$  is the state  $|00011\rangle$ . Together they form a state with odd parity  $(|11000\rangle - |00011\rangle)/\sqrt{2}$ . This state is directly coupled with another state of odd parity  $(|10100\rangle - |00101\rangle)/\sqrt{2}$ .

### 3.2.3 Global spin-flip symmetry

If  $L$  is even and the system is restricted to the sector with  $n = L/2$  up-spins (zero total  $z$ -magnetization), the Hamiltonian also possesses a discrete symmetry corresponding to a global  $\pi$  rotation of all spins around the  $x$  axis. This transformation flips all spins according to

$$|\uparrow\rangle \longleftrightarrow |\downarrow\rangle$$

and is implemented by the operator

$$\hat{R}_\pi^x = \hat{\sigma}_1^x \hat{\sigma}_2^x \dots \hat{\sigma}_L^x.$$

One can verify that

$$[\hat{H}, \hat{R}_\pi^x] = 0.$$

As an example, consider  $L = 4$  and  $n = 2$ . An eigenstate in this sector can be written as

$$\begin{aligned} |\psi^{(j)}\rangle &= a_1^{(j)} |\uparrow\uparrow\downarrow\downarrow\rangle + a_2^{(j)} |\uparrow\downarrow\uparrow\downarrow\rangle + a_3^{(j)} |\uparrow\downarrow\downarrow\uparrow\rangle \\ &+ a_4^{(j)} |\downarrow\uparrow\uparrow\downarrow\rangle + a_5^{(j)} |\downarrow\uparrow\downarrow\uparrow\rangle + a_6^{(j)} |\downarrow\downarrow\uparrow\uparrow\rangle. \end{aligned}$$

If the state has  $R_\pi^x = +1$ , the coefficients satisfy

$$a_1^{(j)} = a_6^{(j)}, \quad a_2^{(j)} = a_5^{(j)}, \quad a_3^{(j)} = a_4^{(j)}$$

If the state has  $R_\pi^x = -1$ , the coefficients satisfy

$$a_1^{(j)} = -a_6^{(j)}, \quad a_2^{(j)} = -a_5^{(j)}, \quad a_3^{(j)} = -a_4^{(j)}$$

Other symmetries may emerge depending on the choice of parameters and on the geometry of the system. One important example is conservation of the total spin,  $\hat{\mathcal{S}}_T = \sum_n \vec{\mathcal{S}}_n$ , which occurs only in isotropic systems ( $\Delta = 1$ ), where  $[\hat{H}, \hat{\mathcal{S}}_T^2] = 0$ .

### 3.2.4 Spatial translation invariance

Another example is **conservation of momentum**, which arises for a closed (periodic) chain as a consequence of invariance under discrete spatial translations. In a periodic chain, site  $L + 1$  is identified with site 1, so that the system is unchanged when every spin is shifted by one lattice site. The corresponding symmetry operator is the **translation operator**  $\hat{T}$ . We define its action on a basis state as

$$\hat{T}|\sigma_1, \sigma_2, \dots, \sigma_{L-1}, \sigma_L\rangle = |\sigma_L, \sigma_1, \sigma_2, \dots, \sigma_{L-1}\rangle, \quad (3.24)$$

where  $\sigma_i = \uparrow, \downarrow$ . Thus,  $\hat{T}$  translates every spin by one site to the right. One could equivalently define translation to the left; this would only change the sign convention used for the momentum below.

For example,

$$\hat{T}|\uparrow\downarrow\uparrow\downarrow\rangle = |\downarrow\uparrow\downarrow\uparrow\rangle.$$

Because of the periodic boundary conditions, the spin originally at site  $L$  moves to site 1.

The translation operator can also be constructed from permutation (swap) operators. With the convention in Eq. (3.24), it can be written as

$$\hat{T} = \hat{\mathcal{P}}_{1,2}\hat{\mathcal{P}}_{2,3}\cdots\hat{\mathcal{P}}_{L-1,L}, \quad (3.25)$$

where the rightmost operator acts first! If the Hamiltonian is translationally invariant, then

$$[\hat{H}, \hat{T}] = 0. \quad (3.26)$$

Therefore, the eigenstates of the Hamiltonian can be chosen to be simultaneous eigenstates of the translation operator,

$$\hat{T}|\psi_k\rangle = e^{-ik}|\psi_k\rangle. \quad (3.27)$$

The phase convention  $e^{-ik}$  follows from our definition of  $\hat{T}$  as translation to the right. The quantity  $k$  is the **lattice momentum**, or **crystal momentum**, associated with the state.

Since translating a periodic chain by  $L$  sites brings the system back to exactly the same configuration,

$$\hat{T}^L = \mathbb{1}. \quad (3.28)$$

Applying this relation to a momentum eigenstate gives

$$\hat{T}^L|\psi_k\rangle = e^{-ikL}|\psi_k\rangle = |\psi_k\rangle.$$

Hence

$$e^{-ikL} = 1,$$

which implies

$$\boxed{k = \frac{2\pi n}{L}}, \quad n = 0, 1, \dots, L-1. \quad (3.29)$$

Thus, because translations on a lattice form a discrete symmetry, the allowed momenta are also discrete.

The consequences of translation symmetry for the components of an eigenstate can be seen explicitly. Consider, for example, a periodic chain with  $L = 4$  and a single excitation. A general state in this sector is

$$|\psi\rangle = a_1 |\uparrow\downarrow\downarrow\downarrow\rangle + a_2 |\downarrow\uparrow\downarrow\downarrow\rangle + a_3 |\downarrow\downarrow\uparrow\downarrow\rangle + a_4 |\downarrow\downarrow\downarrow\uparrow\rangle. \quad (3.30)$$

For convenience, define

$$\begin{aligned} |1\rangle &= |\uparrow\downarrow\downarrow\downarrow\rangle, & |2\rangle &= |\downarrow\uparrow\downarrow\downarrow\rangle, \\ |3\rangle &= |\downarrow\downarrow\uparrow\downarrow\rangle, & |4\rangle &= |\downarrow\downarrow\downarrow\uparrow\rangle. \end{aligned}$$

With our convention for translation,

$$\hat{T}|1\rangle = |2\rangle, \quad \hat{T}|2\rangle = |3\rangle, \quad \hat{T}|3\rangle = |4\rangle, \quad \hat{T}|4\rangle = |1\rangle.$$

Acting with  $\hat{T}$  on Eq. (3.30) therefore gives

$$\hat{T}|\psi\rangle = a_1|2\rangle + a_2|3\rangle + a_3|4\rangle + a_4|1\rangle,$$

or, after rearranging the terms in the original order,

$$\hat{T}|\psi\rangle = a_4|1\rangle + a_1|2\rangle + a_2|3\rangle + a_3|4\rangle. \quad (3.31)$$

If  $|\psi\rangle$  has a definite momentum  $k$ , then

$$\hat{T}|\psi_k\rangle = e^{-ik}|\psi_k\rangle.$$

Comparing the coefficients on both sides gives

$$a_4 = e^{-ik}a_1, \quad a_1 = e^{-ik}a_2, \quad a_2 = e^{-ik}a_3, \quad a_3 = e^{-ik}a_4. \quad (3.32)$$

Equivalently,

$$a_j = e^{ik(j-1)}a_1, \quad j = 1, \dots, L. \quad (3.33)$$

Thus, translation symmetry fixes the relative phases of the probability amplitudes associated with configurations that are related by spatial translations. For the  $L = 4$  example, the allowed momenta are

$$k = 0, \quad \frac{\pi}{2}, \quad \pi, \quad \frac{3\pi}{2}.$$

The corresponding normalized momentum eigenstates are

$$|\psi_k\rangle = \frac{1}{2} (|1\rangle + e^{ik}|2\rangle + e^{i2k}|3\rangle + e^{i3k}|4\rangle). \quad (3.34)$$

For  $k = 0$ ,

$$|\psi_0\rangle = \frac{1}{2} (|1\rangle + |2\rangle + |3\rangle + |4\rangle),$$

so that

$$a_1 = a_2 = a_3 = a_4.$$

For  $k = \pi$ ,

$$|\psi_\pi\rangle = \frac{1}{2}(|1\rangle - |2\rangle + |3\rangle - |4\rangle),$$

so that

$$a_1 = -a_2 = a_3 = -a_4.$$

For  $k = \pi/2$ ,

$$|\psi_{\pi/2}\rangle = \frac{1}{2}(|1\rangle + i|2\rangle - |3\rangle - i|4\rangle),$$

while for  $k = 3\pi/2$ , equivalently  $k = -\pi/2$ ,

$$|\psi_{-\pi/2}\rangle = \frac{1}{2}(|1\rangle - i|2\rangle - |3\rangle + i|4\rangle).$$

This illustrates a difference between reflection and translation symmetry. For reflection symmetry, the eigenvalues of the symmetry operator are  $\Pi = \pm 1$ , and therefore the coefficients of mirror-related basis states are either equal or opposite,

$$a_i = \pm a_{L+1-i}.$$

For translation symmetry, the eigenvalues of the symmetry operator are phases  $e^{-ik}$ , and therefore the coefficients of translation-related basis states differ by corresponding phase factors,

$$a_{j+1} = e^{ik} a_j.$$

In both cases, however, the basic idea is the same: a symmetry relates different basis states and imposes constraints on their probability amplitudes in an eigenstate with a definite value of the corresponding symmetry quantum number.

More generally, let  $|\phi\rangle$  be an arbitrary spin configuration. Repeated translations generate its **translation orbit**,

$$|\phi\rangle, \quad \hat{T}|\phi\rangle, \quad \hat{T}^2|\phi\rangle, \quad \dots$$

A state with definite momentum can be constructed from this orbit as

$$|\phi; k\rangle = \frac{1}{\sqrt{\mathcal{N}}} \sum_{r=0}^{L-1} e^{ikr} \hat{T}^r |\phi\rangle, \quad (3.35)$$

where  $\mathcal{N}$  is the appropriate normalization factor. Indeed,

$$\hat{T}|\phi; k\rangle = \frac{1}{\sqrt{\mathcal{N}}} \sum_{r=0}^{L-1} e^{ikr} \hat{T}^{r+1} |\phi\rangle = e^{-ik} |\phi; k\rangle.$$

Thus, basis configurations related by translation are combined with momentum-dependent phase factors to form states belonging to a definite momentum sector. The Hamiltonian does not couple states belonging to different momentum sectors. Consequently, in a basis organized according to momentum, the Hamiltonian becomes block diagonal,

$$\hat{H} = \bigoplus_k \hat{H}_k.$$

This reduction of the Hilbert space into independent symmetry sectors is particularly important in exact diagonalization and in studies of spectral statistics, where eigenvalues belonging to different symmetry sectors should not be mixed.

In summary, the larger the number of conserved quantities, the smaller the invariant subspaces into which the Hilbert space decomposes. This reduction in the effective dimensionality can complicate the analysis of quantum chaos, since it reduces the amount of spectral data within each symmetry sector. For this reason, in studies of quantum chaos and thermalization it is often advantageous to choose parameters and geometries that minimize or avoid additional symmetries.

### 3.3 Integrability and Chaos in Spin-1/2 Models

The XX and XXZ chains with nearest-neighbor couplings only are both integrable models, but for different reasons. The XX model can be mapped onto free fermions via a Jordan–Wigner transformation (see Sec. 3.5) and is diagonalized by a simple Fourier transform. The XXZ model is genuinely interacting, yet remains integrable due to the existence of an extensive set of local conserved quantities and is solvable by Bethe ansatz techniques.

In integrable systems, energy levels belonging to the same symmetry sector do not exhibit the strong correlations characteristic of chaotic systems. as if they were drawn independently from a random process. The expected nearest-neighbor level spacing distribution is therefore *Poissonian*,

$$P_P(s) = e^{-s}, \quad (3.36)$$

which reflects the absence of level repulsion.

#### Breaking integrability in the XXZ model

There are many ways to break the integrability of the XXZ chain and drive it into the chaotic regime. Common mechanisms include:

- adding couplings between further neighbors (e.g. next-nearest-neighbor or dipolar interactions),
- introducing a single impurity (local defect),
- randomizing coupling strengths,
- adding on-site disorder.

In assignment 02, you will study the case where couplings between next-nearest neighbors are added. For open boundary conditions, the Hamiltonian becomes

$$\hat{H}_\lambda = \sum_{n=1}^{L-1} \left[ J_{xy} \left( \hat{S}_n^x \hat{S}_{n+1}^x + \hat{S}_n^y \hat{S}_{n+1}^y \right) + J_z \hat{S}_n^z \hat{S}_{n+1}^z \right] + \lambda \sum_{n=1}^{L-2} \left[ J'_{xy} \left( \hat{S}_n^x \hat{S}_{n+2}^x + \hat{S}_n^y \hat{S}_{n+2}^y \right) + J'_z \hat{S}_n^z \hat{S}_{n+2}^z \right], \quad (3.37)$$

where  $\lambda$  controls the relative strength of the interactions between next-nearest neighbors. In the assignment, you will consider  $J_{xy} = J'_{xy} \neq 0$  and  $J_z = J'_z \neq 0$ , with  $J_{xy} \sim J_z$ .

For  $\lambda = 0$  the model is integrable. As  $\lambda$  increases, integrability is progressively destroyed. In finite systems, the level spacing distribution  $P(s)$  typically evolves in three stages:

1. For small  $\lambda$ ,  $P(s)$  remains close to Poisson.
2. For intermediate  $\lambda$ ,  $P(s)$  displays an intermediate form between Poisson and Wigner–Dyson.
3. For sufficiently large  $\lambda$ ,  $P(s)$  approaches the Wigner–Dyson distribution characteristic of quantum chaos. [Attention! Large here means  $\lambda \sim 1$ . If  $\lambda \gg 1$ , we reach another integrable point.]

Several distinct nonintegrable scenarios arise depending on which terms are present in Eq. (3.37). For sufficiently large  $\lambda$ , quantum chaos can develop in all of the following cases:

- absence of Ising interactions:

$$J_z = J'_z = 0;$$

- absence of next-nearest neighbor flip–flop term:

$$J'_{xy} = 0;$$

- absence of next-nearest neighbor Ising interaction:

$$J'_z = 0;$$

- presence of all four terms.

Although these models differ microscopically, they all generically break the integrable structure of the nearest-neighbor XXZ chain and produce level statistics consistent with random matrix theory.

## Symmetry sectors and level statistics

To compute meaningful level spacing distributions, it is essential to first separate the spectrum into its symmetry sectors (e.g. total magnetization, parity, spin inversion, momentum for periodic chains).

If eigenvalues from different symmetry sectors are mixed together, the resulting level spacing distribution may fail to show Wigner–Dyson behavior even when the system is fully chaotic. This happens because eigenvalues from different subspaces are statistically independent and therefore do not repel each other.

Thus, a necessary condition to observe level repulsion and random-matrix statistics is:

Level statistics must be computed within a single irreducible symmetry sector of the Hamiltonian.

### 3.4 Eigenstates and Basis Choices

Consider an eigenstate

$$|\psi_\alpha\rangle = \sum_{k=1}^{\mathcal{D}} C_\alpha^{(k)} |\phi_k\rangle, \quad (3.38)$$

written in terms of the orthonormal basis vectors  $|\phi_k\rangle$ , where  $C_\alpha^{(k)} = \langle\phi_k|\psi_\alpha\rangle$ . As we have already seen, the participation ratio, defined as

$$\text{PR}_\alpha \equiv \frac{1}{\sum_{k=1}^{\mathcal{D}} |C_\alpha^{(k)}|^4}, \quad (3.39)$$

is proportional to the number of basis vectors that contribute to each eigenstate  $|\psi_\alpha\rangle$ . This quantity is small when the state is localized and large when the state is delocalized in the chosen basis. Thus, PR is a measure of the delocalization of the states.

There are other measures of delocalization, such as the Shannon entropy

$$\text{Sh}_\alpha^{(k)} \equiv - \sum_k^{\mathcal{D}} |C_\alpha^{(k)}|^2 \ln |C_\alpha^{(k)}|^2. \quad (3.40)$$

These quantities depend on the basis in which states are represented. A state that looks localized in one basis may appear highly delocalized in another one. For example, in the *site basis* (computational basis), eigenstates of a lattice Hamiltonian may appear extended, while in the *energy basis* of another operator (say, an integrable Hamiltonian), the same states may look localized. Let us review how to change basis.

#### Notation and basic setup

We assume a finite-dimensional Hilbert space of dimension  $\mathcal{D}$ .

- $\{|\phi_k\rangle\}_{k=1}^{\mathcal{D}}$  : **old basis** (e.g. site basis/computational basis).
- $\{|\xi_\nu\rangle\}_{\nu=1}^{\mathcal{D}}$  : **new basis** (e.g. eigenstates of  $\hat{H}_{XX}$ ).
- $\{|\psi_\alpha\rangle\}_{\alpha=1}^{\mathcal{D}}$  : eigenstates of the Hamiltonian being studied (e.g. eigenstates of  $\hat{H}_{XZX}$ ).

All bases are assumed orthonormal and complete:

$$\sum_k |\phi_k\rangle\langle\phi_k| = \sum_\nu |\xi_\nu\rangle\langle\xi_\nu| = \mathbb{I}.$$

We use the following compact notation:

- $\psi^{\text{in } \phi}$  : matrix whose columns are eigenstates written in the  $\phi$  basis.
- $\psi^{\text{in } \xi}$  : same states written in the  $\xi$  basis.
- $\xi^{\text{in } \phi}$  : columns are the  $\xi$  basis vectors written in the  $\phi$  basis.

## Two equivalent strategies to change basis

There are two mathematically equivalent ways to express eigenstates in a new basis.

### Method (i): Project eigenstates onto the new basis

First diagonalize the Hamiltonian in the old basis:

$$|\psi_\alpha\rangle = \sum_{k=1}^{\mathcal{D}} |\phi_k\rangle \langle \phi_k | \psi_\alpha \rangle.$$

Now insert the identity in the new basis:

$$\mathbb{1} = \sum_{\nu=1}^{\mathcal{D}} |\xi_\nu\rangle \langle \xi_\nu|,$$

which gives

$$|\psi_\alpha\rangle = \sum_{\nu=1}^{\mathcal{D}} |\xi_\nu\rangle \underbrace{\left( \sum_{k=1}^{\mathcal{D}} \langle \xi_\nu | \phi_k \rangle \langle \phi_k | \psi_\alpha \rangle \right)}_{\langle \xi_\nu | \psi_\alpha \rangle}.$$

Thus, the coefficients in the new basis are

$$\boxed{\langle \xi_\nu | \psi_\alpha \rangle = \sum_{k=1}^{\mathcal{D}} \langle \xi_\nu | \phi_k \rangle \langle \phi_k | \psi_\alpha \rangle.}$$

**Matrix form.** Assuming that we have three eigenstates, the expression above is written as:

$$\begin{pmatrix} \psi_1^{\text{in } \xi} & \psi_2^{\text{in } \xi} & \psi_3^{\text{in } \xi} \\ \langle \xi_1 | \psi_1 \rangle & \langle \xi_1 | \psi_2 \rangle & \langle \xi_1 | \psi_3 \rangle \\ \langle \xi_2 | \psi_1 \rangle & \langle \xi_2 | \psi_2 \rangle & \langle \xi_2 | \psi_3 \rangle \\ \langle \xi_3 | \psi_1 \rangle & \langle \xi_3 | \psi_2 \rangle & \langle \xi_3 | \psi_3 \rangle \end{pmatrix} = \begin{pmatrix} \langle \xi_1 | \phi_1 \rangle & \langle \xi_1 | \phi_2 \rangle & \langle \xi_1 | \phi_3 \rangle \\ \langle \xi_2 | \phi_1 \rangle & \langle \xi_2 | \phi_2 \rangle & \langle \xi_2 | \phi_3 \rangle \\ \langle \xi_3 | \phi_1 \rangle & \langle \xi_3 | \phi_2 \rangle & \langle \xi_3 | \phi_3 \rangle \end{pmatrix} \begin{pmatrix} \psi_1^{\text{in } \phi} & \psi_2^{\text{in } \phi} & \psi_3^{\text{in } \phi} \\ \langle \phi_1 | \psi_1 \rangle & \langle \phi_1 | \psi_2 \rangle & \langle \phi_1 | \psi_3 \rangle \\ \langle \phi_2 | \psi_1 \rangle & \langle \phi_2 | \psi_2 \rangle & \langle \phi_2 | \psi_3 \rangle \\ \langle \phi_3 | \psi_1 \rangle & \langle \phi_3 | \psi_2 \rangle & \langle \phi_3 | \psi_3 \rangle \end{pmatrix},$$

which is the same as

$$\begin{pmatrix} \psi_1^{\text{in } \xi} & \psi_2^{\text{in } \xi} & \psi_3^{\text{in } \xi} \\ \langle \xi_1 | \psi_1 \rangle & \langle \xi_1 | \psi_2 \rangle & \langle \xi_1 | \psi_3 \rangle \\ \langle \xi_2 | \psi_1 \rangle & \langle \xi_2 | \psi_2 \rangle & \langle \xi_2 | \psi_3 \rangle \\ \langle \xi_3 | \psi_1 \rangle & \langle \xi_3 | \psi_2 \rangle & \langle \xi_3 | \psi_3 \rangle \end{pmatrix} = \begin{pmatrix} \xi_1^{\text{in } \phi} & \xi_2^{\text{in } \phi} & \xi_3^{\text{in } \phi} \\ \langle \phi_1 | \xi_1 \rangle & \langle \phi_1 | \xi_2 \rangle & \langle \phi_1 | \xi_3 \rangle \\ \langle \phi_2 | \xi_1 \rangle & \langle \phi_2 | \xi_2 \rangle & \langle \phi_2 | \xi_3 \rangle \\ \langle \phi_3 | \xi_1 \rangle & \langle \phi_3 | \xi_2 \rangle & \langle \phi_3 | \xi_3 \rangle \end{pmatrix}^\dagger \begin{pmatrix} \psi_1^{\text{in } \phi} & \psi_2^{\text{in } \phi} & \psi_3^{\text{in } \phi} \\ \langle \phi_1 | \psi_1 \rangle & \langle \phi_1 | \psi_2 \rangle & \langle \phi_1 | \psi_3 \rangle \\ \langle \phi_2 | \psi_1 \rangle & \langle \phi_2 | \psi_2 \rangle & \langle \phi_2 | \psi_3 \rangle \\ \langle \phi_3 | \psi_1 \rangle & \langle \phi_3 | \psi_2 \rangle & \langle \phi_3 | \psi_3 \rangle \end{pmatrix}.$$

In general, define the matrices:

$$\Psi_{k\alpha}^{(\phi)} = \langle \phi_k | \psi_\alpha \rangle, \quad \Xi_{k\nu}^{(\phi)} = \langle \phi_k | \xi_\nu \rangle.$$

Then

$$\boxed{\Psi^{(\xi)} = \Xi^{(\phi)\dagger} \Psi^{(\phi)}}.$$

This is the fundamental basis-change formula.

**Interpretation.**

- $\Xi^{(\phi)}$  is a unitary matrix.
- Its dagger rotates vectors from  $\phi$  to  $\xi$ .

**Inverse transformation**

If we already know  $\psi^{\text{in } \xi}$  and want  $\psi^{\text{in } \phi}$ :

$$\boxed{\Psi^{(\phi)} = \Xi^{(\phi)} \Psi^{(\xi)}}.$$

This works because

$$\Xi^{(\phi)} \Xi^{(\phi)\dagger} = \mathbb{I}.$$

**Method (ii): Transform the Hamiltonian first**

Instead of transforming states, we may transform the Hamiltonian itself.

Hamiltonian elements in old basis:

$$\begin{aligned} H_{kl}^{(\phi)} &= \langle \phi_k | H | \phi_l \rangle \\ &= \sum_j \sum_i \langle \phi_k | \xi_j \rangle \langle \xi_j | H | \xi_i \rangle \langle \xi_i | \phi_l \rangle = \sum_j \sum_i \Xi_{kj}^{(\phi)} H_{ji}^{(\xi)} \Xi_{il}^{(\phi)\dagger}. \end{aligned} \quad (3.41)$$

Hamiltonian in new basis:

$$\boxed{H^{(\xi)} = \Xi^{(\phi)\dagger} H^{(\phi)} \Xi^{(\phi)}}.$$

Then diagonalize  $H^{(\xi)}$  directly. This is the standard unitary similarity transformation:

$$H^{(\xi)} \mapsto U^\dagger H^{(\phi)} U,$$

with  $U = \Xi^{(\phi)}$ . The eigenvalues of  $H^{(\xi)}$  and  $H^{(\phi)}$  are the same.

Both strategies for changing basis give exactly the same coefficients for the eigenstates.

**Physical meaning**

- A basis transformation is simply a rotation in Hilbert space.
- States themselves are invariant; only their coordinates change.
- Delocalization measures are **not invariant** under such rotations.

Therefore:

Localization is not an intrinsic property of a state, but a relational property between a state and a chosen basis.

This is why in many-body physics one must always specify:

- which basis is used,
- and whether it has physical meaning (e.g. local operators).

### 3.5 Mappings of the XXZ chain

Spin- $\frac{1}{2}$  operators obey the SU(2) algebra and act on a finite-dimensional Hilbert space. Jordan–Wigner and Holstein–Primakoff transformations provide systematic mappings of spin operators onto canonical fermionic or bosonic degrees of freedom. The Jordan–Wigner transformation maps spins onto fermions in a way that preserves the local two-dimensional Hilbert space and can convert certain spin Hamiltonians into quadratic fermionic models. The Holstein–Primakoff transformation expresses spins in terms of bosons with an occupancy constraint. These mappings often reveal hidden structures (such as free quasiparticle dynamics or interaction terms) and enable the use of many-body techniques developed for fermions and bosons.

Let us describe these transformations for the spin-1/2 XXZ chain with nearest-neighbor couplings,

$$\hat{H}_{\text{XXZ}} = \sum_{j=1}^{L-1} \left[ J \left( \hat{S}_j^x \hat{S}_{j+1}^x + \hat{S}_j^y \hat{S}_{j+1}^y \right) + J\Delta \hat{S}_j^z \hat{S}_{j+1}^z \right] = \sum_{j=1}^{L-1} \left[ \frac{J}{2} \left( \hat{S}_j^+ \hat{S}_{j+1}^- + \hat{S}_{j+1}^+ \hat{S}_j^- \right) + J\Delta \hat{S}_j^z \hat{S}_{j+1}^z \right]. \quad (3.42)$$

#### 3.5.1 Jordan–Wigner mapping to spinless fermions

To introduce the Jordan–Wigner (JW) transformation, we first recall the algebra of spinless fermions.

##### Spinless fermions

In general, spin-1/2 fermions are described by annihilation and creation operators  $c_{i\sigma}$  and  $c_{i\sigma}^\dagger$ , where  $\sigma = \uparrow, \downarrow$  labels the spin degree of freedom. These operators satisfy the canonical anticommutation relations

$$\{c_{i\sigma}, c_{j\sigma'}^\dagger\} = \delta_{ij} \delta_{\sigma\sigma'}, \quad (3.43)$$

together with

$$\{c_{i\sigma}, c_{j\sigma'}\} = 0, \quad \{c_{i\sigma}^\dagger, c_{j\sigma'}^\dagger\} = 0. \quad (3.44)$$

Here, the curly brackets denote the *anticommutator*,

$$\{A, B\} \equiv AB + BA. \quad (3.45)$$

single-particle state.

We can think of scenarios, where the spin degree of freedom is frozen or irrelevant. For example, a strong magnetic field or exchange interaction may fully polarize the system, leaving only one spin component ( $\uparrow$ ) active. In this case,

$$c_{i\uparrow} \rightarrow c_i, \quad c_{i\downarrow} \text{ absent}, \quad (3.46)$$

yielding an effective spinless fermion description. The term “spinless” therefore means that each site hosts only one fermionic degree of freedom (either occupied or empty), not that the original particles lacked spin.

We thus define spinless fermion operators  $\hat{c}_j, \hat{c}_j^\dagger$  and number operators  $\hat{n}_j = \hat{c}_j^\dagger \hat{c}_j$ . The fermion operators satisfy the anticommutation relations

$$\{\hat{c}_i, \hat{c}_j^\dagger\} = \hat{c}_i \hat{c}_j^\dagger + \hat{c}_j^\dagger \hat{c}_i = \delta_{ij}, \quad \{\hat{c}_i, \hat{c}_j\} = 0, \quad \{\hat{c}_i^\dagger, \hat{c}_j^\dagger\} = 0.$$

The anticommutation relation  $\{\hat{c}_i^\dagger, \hat{c}_j^\dagger\} = 0$  implies that  $(\hat{c}_i^\dagger)^2 = 0$ , so we cannot create two fermions on the same site and the occupation number is restricted to  $n_i = \hat{c}_i^\dagger \hat{c}_i \in \{0, 1\}$ . This is the Pauli exclusion principle: no more than one fermion can occupy a given site.

The Jordan–Wigner (JW) transformation is

$$\hat{S}_j^+ = \hat{c}_j^\dagger \exp\left(i\pi \sum_{\ell < j} \hat{n}_\ell\right), \quad \hat{S}_j^- = \exp\left(-i\pi \sum_{\ell < j} \hat{n}_\ell\right) \hat{c}_j, \quad \hat{S}_j^z = \hat{n}_j - \frac{1}{2}. \quad (3.47)$$

For nearest neighbors, the JW strings cancel in the hopping terms, yielding

$$\hat{S}_{j+1}^+ \hat{S}_j^- = \hat{c}_{j+1}^\dagger \hat{c}_j, \quad \hat{S}_j^+ \hat{S}_{j+1}^- = \hat{c}_j^\dagger \hat{c}_{j+1}. \quad (3.48)$$

Let us check this in detail.

$$\hat{S}_{j+1}^+ \hat{S}_j^- = \hat{c}_{j+1}^\dagger e^{i\pi \hat{n}_j} e^{(i\pi \sum_{\ell < j} \hat{n}_\ell)} e^{(-i\pi \sum_{\ell < j} \hat{n}_\ell)} \hat{c}_j = \hat{c}_{j+1}^\dagger e^{i\pi \hat{n}_j} \hat{c}_j \quad (3.49)$$

and

$$e^{i\pi \hat{n}_j} = \sum_{m=0}^{\infty} \frac{(i\pi)^m}{m!} \hat{n}_j^m. \quad (3.50)$$

Using the anticommutator and  $(\hat{c}_i^2) = 0$ ,  $(\hat{c}_i^\dagger)^2 = 0$  in  $\hat{n}_j^2$ ,

$$\hat{n}_j^2 = \hat{c}_j^\dagger \hat{c}_j \hat{c}_j^\dagger \hat{c}_j = \hat{c}_j^\dagger (1 - \hat{c}_j^\dagger \hat{c}_j) \hat{c}_j = \hat{c}_j^\dagger \hat{c}_j = \hat{n}_j, \quad (3.51)$$

we verify that  $\hat{n}_j^2 = \hat{n}_j$  and all higher powers in Eq. (3.50) collapse,

$$\hat{n}_j^m = \begin{cases} 1, & m = 0, \\ \hat{n}_j, & m \geq 1. \end{cases} \quad (3.52)$$

Therefore the exponential becomes

$$e^{i\pi \hat{n}_j} = 1 + \hat{n}_j \sum_{m=1}^{\infty} \frac{(i\pi)^m}{m!} = 1 + \hat{n}_j (e^{i\pi} - 1) = 1 - 2\hat{n}_j. \quad (3.53)$$

Recall again that  $(\hat{c}_i^2) = 0$ , so Eq. (3.49) becomes

$$\hat{S}_{j+1}^+ \hat{S}_j^- = \hat{c}_{j+1}^\dagger (1 - 2\hat{n}_j) \hat{c}_j = \hat{c}_{j+1}^\dagger (1 - 2\hat{c}_j^\dagger \hat{c}_j) \hat{c}_j = \hat{c}_{j+1}^\dagger \hat{c}_j$$

and Eq. (3.48) is obtained.

The Ising part becomes

$$\hat{S}_j^z \hat{S}_{j+1}^z = \left(\hat{n}_j - \frac{1}{2}\right) \left(\hat{n}_{j+1} - \frac{1}{2}\right) = \hat{n}_j \hat{n}_{j+1} - \frac{1}{2}(\hat{n}_j + \hat{n}_{j+1}) + \frac{1}{4}. \quad (3.54)$$

Therefore, up to an additive constant and a boundary-dependent chemical-potential term, the XXZ chain maps to interacting spinless fermions:

$$\hat{H}_{\text{XXZ}} = \sum_{j=1}^{L-1} \left[ \frac{J}{2} \left( \hat{c}_j^\dagger \hat{c}_{j+1} + \hat{c}_{j+1}^\dagger \hat{c}_j \right) + J\Delta \left( \hat{n}_j - \frac{1}{2} \right) \left( \hat{n}_{j+1} - \frac{1}{2} \right) \right]. \quad (3.55)$$

Equivalently, expanding the last factor,

$$\hat{H}_{\text{XXZ}} = \sum_{j=1}^{L-1} \left[ \frac{J}{2} \left( \hat{c}_j^\dagger \hat{c}_{j+1} + \hat{c}_{j+1}^\dagger \hat{c}_j \right) + J\Delta \hat{n}_j \hat{n}_{j+1} \right] - \frac{J\Delta}{2} \sum_{j=1}^L \hat{n}_j + \text{const.} \quad (3.56)$$

(The chemical-potential term  $\propto \sum_j \hat{n}_j$  can be absorbed into a  $z$ -field  $h \sum_j \hat{S}_j^z$  in the spin language.)

### Quadratic models

In second quantization, a many-body Hamiltonian is called noninteracting (or quadratic) if it contains only terms that are bilinear in the creation and annihilation operators,

$$H_{\text{quad}} = \sum_{i,j} t_{ij} a_i^\dagger a_j. \quad (3.57)$$

Such a Hamiltonian describes particles that move independently in an effective single-particle potential. For example, the term

$$a_i^\dagger a_j \quad (3.58)$$

represents hopping of a particle from site  $j$  to site  $i$ . It annihilates one particle at site  $j$  and creates one at site  $i$ . Whether its action is effective or not is determined by the occupation of the initial and final single-particle states, but the hopping amplitude is a fixed single-particle matrix element that does not depend on the occupation of other sites. Likewise,

$$a_i^\dagger a_i = n_i \quad (3.59)$$

is the number operator at site  $i$  and corresponds to a single-particle on-site energy contribution. A quadratic Hamiltonian can always be diagonalized by a linear transformation of the operators.

In contrast, a term of the form

$$a_i^\dagger a_i a_j^\dagger a_j = n_i n_j \quad (3.60)$$

is quartic in the operators. It couples the occupations of sites  $i$  and  $j$ . The energy now depends simultaneously on the presence of particles at both sites. This term cannot be removed by a linear transformation of the operators and therefore cannot be reduced to a sum of independent single-particle modes. Terms such as this one generates genuine **many-body interactions**.

The Jordan–Wigner transformation can reveal an exact quadratic structure in certain one-dimensional spin-1/2 models. Consider, for example, the 1D XX model with nearest-neighbor coupling,

$$H_{XX} = J \sum_j (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y). \quad (3.61)$$

In spin variables, the Hamiltonian contains products of operators acting on neighboring sites, which may suggest two-body interactions. However, applying the Jordan–Wigner transformation, one finds that the Hamiltonian becomes

$$H_{XX} = \frac{J}{2} \sum_j (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j), \quad (3.62)$$

which is quadratic in fermionic operators and therefore describes free fermions hopping on a lattice.

This example illustrates an important point: a Hamiltonian that appears as a two-body interaction in spin language may correspond to a quadratic (noninteracting) theory in fermionic variables. The Jordan–Wigner transformation thus distinguishes between generic interacting spin models and those that, despite their appearance, possess an underlying free-fermion structure and are consequently integrable.

### ATTENTION! A non-quadratic Hamiltonian revealed by the JW transformation

Consider the Hamiltonian

$$H = J_1 \sum_j (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) + J_2 \sum_j (S_j^x S_{j+2}^x + S_j^y S_{j+2}^y). \quad (3.63)$$

Using the Jordan–Wigner mapping for the next-nearest neighbors ( $l = j + 2$ ):  $\hat{S}_{j+2}^+ \hat{S}_j^-$ . Using the Jordan–Wigner transformation,

$$\begin{aligned} \hat{S}_{j+2}^+ \hat{S}_j^- &= \hat{c}_{j+2}^\dagger \exp \left( i\pi \sum_{\ell < j+2} \hat{n}_\ell \right) \exp \left( -i\pi \sum_{\ell < j} \hat{n}_\ell \right) \hat{c}_j \\ &= \hat{c}_{j+2}^\dagger e^{i\pi(\hat{n}_{j+1} + \hat{n}_j)} \hat{c}_j \\ &= \hat{c}_{j+2}^\dagger e^{i\pi\hat{n}_{j+1}} e^{i\pi\hat{n}_j} \hat{c}_j. \end{aligned} \quad (3.64)$$

As shown above,  $e^{i\pi\hat{n}_j} = 1 - 2\hat{n}_j$  and  $(1 - 2\hat{n}_j)\hat{c}_j = \hat{c}_j$ . Therefore,

$$\boxed{\hat{S}_{j+2}^+ \hat{S}_j^- = \hat{c}_{j+2}^\dagger (1 - 2\hat{n}_{j+1}) \hat{c}_j.} \quad (3.65)$$

In contrast with the nearest-neighbor case, the Jordan–Wigner string does not cancel completely; a factor associated with the intermediate site  $j + 1$  remains. We now have we obtain

$$J_2 \sum_j (\hat{S}_j^x \hat{S}_{j+2}^x + \hat{S}_j^y \hat{S}_{j+2}^y) = \frac{J_2}{2} \sum_j \left[ \hat{c}_{j+2}^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_{j+2} - 2 \left( \hat{c}_{j+2}^\dagger \hat{n}_{j+1} \hat{c}_j + \hat{c}_j^\dagger \hat{n}_{j+1} \hat{c}_{j+2} \right) \right]. \quad (3.66)$$

The first two terms describe ordinary next-nearest-neighbor hopping. The remaining terms contain the occupation of the intermediate site. For example,

$$\hat{c}_{j+2}^\dagger \hat{n}_{j+1} \hat{c}_j = \hat{c}_{j+2}^\dagger \hat{c}_{j+1}^\dagger \hat{c}_{j+1} \hat{c}_j, \quad (3.67)$$

which is quartic in the fermionic operators and represents genuine many-body interactions. Thus, a simple next-nearest-neighbor  $XY$  coupling in the spin representation maps onto an *interacting* fermionic model. The hopping between sites  $j$  and  $j+2$  depends on whether the intermediate site  $j+1$  is occupied. This Hamiltonian is **non-integrable**!

### 3.5.2 Holstein–Primakoff mapping to bosons

Bosonic operators  $\hat{a}_j$  and  $\hat{a}_j^\dagger$  satisfy the canonical commutation relations

$$[\hat{a}_j, \hat{a}_k^\dagger] = \delta_{jk}, \quad [\hat{a}_j, \hat{a}_k] = 0, \quad [\hat{a}_j^\dagger, \hat{a}_k^\dagger] = 0. \quad (3.68)$$

The corresponding number operator is

$$\hat{n}_j^{(b)} = \hat{a}_j^\dagger \hat{a}_j. \quad (3.69)$$

The vanishing commutator between creation operators,  $[\hat{a}_j^\dagger, \hat{a}_k^\dagger] = 0$ , implies that bosonic creation operators commute and therefore the order in which bosons are created does not matter. Moreover, there is no algebraic constraint forcing  $(\hat{a}_j^\dagger)^2$  to vanish, so repeated applications of  $\hat{a}_j^\dagger$  generate states with arbitrarily large occupation number.

The Holstein–Primakoff (HP) transformation expresses spin operators in terms of bosonic operators as

$$\hat{S}_j^+ = \hat{a}_j^\dagger \sqrt{2S - \hat{n}_j^{(b)}}, \quad \hat{S}_j^- = \sqrt{2S - \hat{n}_j^{(b)}} \hat{a}_j, \quad \hat{S}_j^z = \hat{n}_j^{(b)} - S. \quad (3.70)$$

This mapping is exact and preserves the spin commutation relations, provided the bosonic Hilbert space is restricted to  $\hat{n}_j^{(b)} \leq 2S$ . The square-root factors enforce this constraint dynamically: once the occupation reaches  $2S$ , further creation is suppressed, ensuring that the bosonic representation reproduces the finite dimension of the spin Hilbert space.

One important advantage of the HP transformation is that it provides a natural route to the semiclassical (large- $S$ ) limit. When the boson number satisfies  $\langle \hat{n}_j^{(b)} \rangle \ll 2S$ , the square root can be expanded as

$$\sqrt{2S - \hat{n}_j^{(b)}} = \sqrt{2S} \left( 1 - \frac{\hat{n}_j^{(b)}}{4S} + \mathcal{O}(S^{-2}) \right), \quad (3.71)$$

so that spin operators become approximately linear in the bosonic fields. In this regime the Hamiltonian often reduces to a quadratic bosonic theory, allowing a systematic expansion in powers of  $1/S$  and making the semiclassical fluctuation structure explicit.

For a spin- $\frac{1}{2}$  chain, this semiclassical advantage is absent, since  $S = \frac{1}{2}$  and no large parameter exists. In that case the HP representation remains exact only if the bosonic occupation is restricted to

$$\hat{n}_j^{(b)} \in \{0, 1\}, \quad (3.72)$$

which corresponds to the hard-core boson constraint. Thus, for  $S = \frac{1}{2}$ , the HP transformation reduces to a mapping between spins and hard-core bosons rather than to a true large- $S$  semiclassical expansion. In this hard-core boson subspace one may write

$$\hat{S}_j^+ \leftrightarrow \hat{b}_j^\dagger, \quad \hat{S}_j^- \leftrightarrow \hat{b}_j, \quad \hat{S}_j^z = \hat{n}_j^{(b)} - \frac{1}{2}, \quad \hat{n}_j^{(b)} = \hat{b}_j^\dagger \hat{b}_j, \quad (3.73)$$

with on-site constraints  $\hat{b}_j^{\dagger 2} = \hat{b}_j^2 = 0$  and  $\hat{n}_j^{(b)} \in \{0, 1\}$ .

Substituting (3.73) into (3.42) yields the hard-core boson form

$$\hat{H}_{\text{XXZ}} = \sum_{j=1}^{L-1} \left[ \frac{J}{2} (\hat{b}_j^\dagger \hat{b}_{j+1} + \hat{b}_{j+1}^\dagger \hat{b}_j) + \Delta \left( \hat{n}_j^{(b)} - \frac{1}{2} \right) \left( \hat{n}_{j+1}^{(b)} - \frac{1}{2} \right) \right], \quad (3.74)$$

i.e., hopping hard-core bosons with nearest-neighbor density–density interactions.

Although the first term in Eq. (3.74) has the form of a quadratic hopping Hamiltonian, its interpretation requires care. For canonical (unconstrained) bosons, a hopping Hamiltonian is strictly quadratic and therefore describes a noninteracting, exactly solvable model in any spatial dimension. However, the operators  $\hat{b}_j$  in Eq. (3.74) are hard-core bosons, which satisfy the on-site constraint  $\hat{b}_j^2 = 0$  and  $\hat{n}_j^{(b)} \in \{0, 1\}$ . This constraint acts as an infinite on-site interaction and renders the theory nontrivial, even when only the hopping term is present.

In one dimension, the hopping-only hard-core boson model ( $\Delta = 0$ ) is nevertheless equivalent to free spinless fermions via the Jordan–Wigner transformation. This mapping removes the local constraint and transforms the Hamiltonian into a quadratic fermionic form, making its noninteracting character explicit. Thus, in 1D, the hopping term alone describes an integrable free theory.

In higher dimensions, however, the Jordan–Wigner transformation becomes nonlocal and does not reduce the model to independent quadratic modes. As a result, in two dimensions the hopping Hamiltonian of hard-core bosons represents a genuinely interacting many-body system, despite its quadratic operator appearance. This contrasts with the case of canonical bosons, for which a pure hopping Hamiltonian remains quadratic and therefore noninteracting in any dimension.

### 3.5.3 Interaction and the role of basis

In the chapter on random matrices, we used a  $2 \times 2$  matrix as an example in which a diagonal matrix represents two uncoupled levels, while an off-diagonal perturbation mixes them, lifts degeneracies, and produces level repulsion. At that stage, however, the role of the basis was not emphasized. The discussion of the Jordan–Wigner transformation now allows us to clarify that the physically meaningful notion of interaction emerges most clearly in the basis that diagonalizes the noninteracting (quadratic) part of the Hamiltonian.

Let us be more specific. Consider the XXZ model. When the Hamiltonian is written in the computational ( $S^z$ ) basis, the Ising term  $S_j^z S_{j+1}^z$  is diagonal, whereas the flip–flop (XX) term produces off-diagonal matrix elements. From this representation alone, one might be tempted to interpret the off-diagonal part as the “interaction.” However, whether a term

is off-diagonal depends on the chosen basis and does not by itself determine whether the system is interacting.

After performing a Jordan-Wigner transformation, the XX term maps to a quadratic fermionic Hamiltonian, which describes free (noninteracting) fermions. In the basis that diagonalizes  $H_{XX}$ , the XXZ Hamiltonian takes a form, where the Ising term becomes quartic in fermionic operators and couples different many-body eigenstates. In this basis, it is the Ising term that generates genuine particle-particle interactions, thereby justifying the terminology “Ising interaction.”

For this reason, it is illuminating to analyze the eigenstates of the XXZ Hamiltonian in the eigenbasis of the XX model. In this basis, the effect of the Ising term is seen explicitly as mixing and reshaping free-fermion states, revealing how interactions deform the structure of the noninteracting eigenstates.

In the case of the 1D spin-1/2 XXZ model with nearest- and next-nearest-neighbor couplings, the nearest-neighbor (XXZ) Hamiltonian is integrable and can be solved exactly by means of the Bethe ansatz. For this reason, it is common to regard the nearest-neighbor part as the unperturbed (integrable) Hamiltonian and to treat the next-nearest-neighbor couplings as the perturbation that breaks integrability, leading to more complex dynamics and signatures of quantum chaos.

In this context, the eigenbasis of the nearest-neighbor Hamiltonian provides a natural reference basis, and the next-nearest-neighbor couplings act as the interaction that mixes its eigenstates and induces nonintegrable behavior. Therefore, when analyzing the structure of the eigenstates in this nonintegrable model, it is insightful to express them in the eigenbasis of the nearest-neighbor Hamiltonian, since this basis makes explicit how integrability-breaking terms spread and hybridize the original integrable states.

## 3.6 Bipartite entanglement: Concepts and measures

Consider a quantum system composed of two subsystems,  $A$  and  $B$ . The total Hilbert space is the tensor product

$$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B.$$

A pure state  $|\Psi\rangle \in \mathcal{H}$  is said to be *separable* (or unentangled) if it can be written as a simple product,

$$|\Psi\rangle = |\psi_A\rangle \otimes |\psi_B\rangle.$$

If this is not possible, the state is called ***entangled***. Physically, entanglement means that the state of subsystem  $A$  cannot be specified independently of subsystem  $B$ . Measurements performed on one subsystem affect the outcomes on the other, even if the two are spatially separated.

### Example: two qubits

Let us consider two qubits, with computational basis

$$\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}.$$

**An entangled state.** The state

$$|\Psi_1\rangle = \frac{|10\rangle + |01\rangle}{\sqrt{2}}$$

is one of the Bell states and is maximally entangled. To see why, suppose it could be factorized:

$$|\Psi_1\rangle = (a|0\rangle + b|1\rangle) \otimes (c|0\rangle + d|1\rangle).$$

Expanding the product gives

$$|\Psi_1\rangle = ac|00\rangle + ad|01\rangle + bc|10\rangle + bd|11\rangle.$$

Matching coefficients with  $|\Psi_1\rangle$  requires

$$ac = 0, \quad bd = 0, \quad ad = \frac{1}{\sqrt{2}}, \quad bc = \frac{1}{\sqrt{2}},$$

which is impossible to satisfy simultaneously. Therefore  $|\Psi_1\rangle$  cannot be written as a product and is entangled. Physically, if qubit  $A$  is measured and found in state  $|1\rangle$ , then qubit  $B$  is guaranteed to be in state  $|0\rangle$ , and vice versa. The outcomes are perfectly correlated.

**A non-entangled state.** Now consider the state

$$|\Psi_2\rangle = \frac{|00\rangle + |10\rangle + |01\rangle + |11\rangle}{2}.$$

This state can be factorized as

$$|\Psi_2\rangle = \left( \frac{|0\rangle + |1\rangle}{\sqrt{2}} \right) \otimes \left( \frac{|0\rangle + |1\rangle}{\sqrt{2}} \right).$$

Hence it is a product state and therefore *not entangled*. Although it is a superposition of all four basis states, there are no quantum correlations between the two qubits.

This illustrates an important point:

Superposition does not imply entanglement. Entanglement is about *non-factorizability*, not about how many terms appear in a sum.

### 3.6.1 Reduced density matrix

To quantify bipartite entanglement, consider a pure state  $|\Psi\rangle$  of the composite system  $A+B$  and the corresponding density matrix

$$\rho = |\Psi\rangle\langle\Psi|.$$

The reduced density matrix of subsystem  $A$  is obtained by tracing over subsystem  $B$ :

$$\rho_A = \text{Tr}_B(\rho).$$

Similarly,

$$\rho_B = \text{Tr}_A(\rho).$$

**Example:**

Consider a spin-1/2 chain with  $L = 4$  sites. We work in the fixed-magnetization sector with  $N_\uparrow = 2$  (equivalently  $S_{\text{tot}}^z = 0$ ) and use the computational basis

$$\{|1100\rangle, |1010\rangle, |1001\rangle, |0110\rangle, |0101\rangle, |0011\rangle\}. \quad (3.75)$$

Any pure state in this sector can be written as

$$|\psi\rangle = c_1|1100\rangle + c_2|1010\rangle + c_3|1001\rangle + c_4|0110\rangle + c_5|0101\rangle + c_6|0011\rangle, \quad \sum_{k=1}^6 |c_k|^2 = 1. \quad (3.76)$$

**Full density matrix.** The density matrix of this pure state is

$$\rho \equiv |\psi\rangle\langle\psi| = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \\ c_6 \end{pmatrix} (c_1^* \ c_2^* \ c_3^* \ c_4^* \ c_5^* \ c_6^*). \quad (3.77)$$

In the ordered basis  $(|1100\rangle, |1010\rangle, |1001\rangle, |0110\rangle, |0101\rangle, |0011\rangle)$ ,  $\rho$  is the  $6 \times 6$  matrix with entries  $\rho_{mn} = c_m c_n^*$ , i.e.

$$\rho = \begin{pmatrix} & \langle 1100| & \langle 1010| & \langle 1001| & \langle 0110| & \langle 0101| & \langle 0011| \\ \begin{matrix} |1100\rangle \\ |1010\rangle \\ |1001\rangle \\ |0110\rangle \\ |0101\rangle \\ |0011\rangle \end{matrix} & \begin{matrix} c_1 c_1^* & c_1 c_2^* & c_1 c_3^* & c_1 c_4^* & c_1 c_5^* & c_1 c_6^* \\ c_2 c_1^* & c_2 c_2^* & c_2 c_3^* & c_2 c_4^* & c_2 c_5^* & c_2 c_6^* \\ c_3 c_1^* & c_3 c_2^* & c_3 c_3^* & c_3 c_4^* & c_3 c_5^* & c_3 c_6^* \\ c_4 c_1^* & c_4 c_2^* & c_4 c_3^* & c_4 c_4^* & c_4 c_5^* & c_4 c_6^* \\ c_5 c_1^* & c_5 c_2^* & c_5 c_3^* & c_5 c_4^* & c_5 c_5^* & c_5 c_6^* \\ c_6 c_1^* & c_6 c_2^* & c_6 c_3^* & c_6 c_4^* & c_6 c_5^* & c_6 c_6^* \end{matrix} \end{pmatrix}. \quad (3.78)$$

**Bipartition and partial trace.** Now partition the chain into sites  $A = \{1, 2\}$  and  $B = \{3, 4\}$ . The reduced density matrix of subsystem  $A$  is obtained by tracing out the last two sites:

$$\rho_A \equiv \text{Tr}_B \rho = \sum_{b \in \{00, 01, 10, 11\}} (\mathbb{1}_A \otimes \langle b|) \rho (\mathbb{1}_A \otimes |b\rangle). \quad (3.79)$$

To compute  $\rho_A$  explicitly, rewrite  $\rho$  grouping the degrees of freedom in  $A$  and  $B$  as

$$\rho = \sum_{i,j=1}^6 c_i c_j^* |\phi_i\rangle\langle\phi_j|$$

Below: terms that exist in  $\rho_A$

$$\begin{aligned} &= |c_1|^2 |11\rangle_A \boxed{|00\rangle_B \langle 00|_B} \langle 11|_A \\ &+ |c_2|^2 |10\rangle_A \boxed{|10\rangle_B \langle 10|_B} \langle 10|_A + c_2 c_4^* |10\rangle_A \boxed{|10\rangle_B \langle 10|_B} \langle 01|_A \\ &+ |c_4|^2 |01\rangle_A \boxed{|10\rangle_B \langle 10|_B} \langle 01|_A + c_4 c_2^* |01\rangle_A \boxed{|10\rangle_B \langle 10|_B} \langle 10|_A \\ &+ |c_3|^2 |10\rangle_A \boxed{|01\rangle_B \langle 01|_B} \langle 10|_A + c_3 c_5^* |10\rangle_A \boxed{|01\rangle_B \langle 01|_B} \langle 01|_A \\ &+ |c_5|^2 |01\rangle_A \boxed{|01\rangle_B \langle 01|_B} \langle 01|_A + c_5 c_3^* |01\rangle_A \boxed{|01\rangle_B \langle 01|_B} \langle 10|_A \\ &+ |c_6|^2 |00\rangle_A \boxed{|11\rangle_B \langle 11|_B} \langle 00|_A \end{aligned}$$

Below: terms that do not survive in  $\rho_A$

$$\begin{aligned} &+ c_1 c_2^* |11\rangle_A \boxed{|00\rangle_B \langle 10|_B} \langle 10|_A + \dots \\ &+ \dots \\ &+ c_6 c_1^* |00\rangle_A \boxed{|11\rangle_B \langle 00|_B} \langle 11|_A + \dots \end{aligned} \tag{3.80}$$

This makes evident which terms survive in  $\rho_A$ , such as

$${}_B\langle 00|\rho_{11}|00\rangle_B = |c_1|^2 (|11\rangle_{AA}\langle 11|) \otimes ({}_B\langle 00|00\rangle_B {}_B\langle 00|00\rangle_B),$$

from those that do not exist, such as

$$c_1 c_2^* (|11\rangle_{AA}\langle 10|) \otimes ({}_B\langle 00|00\rangle_B {}_B\langle 00|10\rangle_B).$$

In the two-site basis for  $A$  ordered as

$$\{|11\rangle_A, |10\rangle_A, |01\rangle_A, |00\rangle_A\}, \tag{3.81}$$

the reduced density matrix  $\rho_A$  becomes

$$\rho_A = \begin{pmatrix} |c_1|^2 & 0 & 0 & 0 \\ 0 & |c_2|^2 + |c_3|^2 & c_2 c_4^* + c_3 c_5^* & 0 \\ 0 & c_4 c_2^* + c_5 c_3^* & |c_4|^2 + |c_5|^2 & 0 \\ 0 & 0 & 0 & |c_6|^2 \end{pmatrix}. \tag{3.82}$$

### 3.6.2 Entanglement entropy

The entanglement entropy is defined as the von Neumann entropy of either reduced density matrix,

$$S_A = -\text{Tr}(\rho_A \log \rho_A), \quad S_B = -\text{Tr}(\rho_B \log \rho_B). \quad (3.83)$$

For a pure global state,  $S_A = S_B$ .

**Attention!** Different conventions are used for the logarithm in Eq. (3.83), including base 10 ( $\log_{10}$ ), base 2 ( $\log_2$ ), and the natural logarithm ( $\ln$ ).

#### Interpretation.

- If  $|\Psi\rangle$  is a product state, then  $\rho_A$  is pure and  $S_A = 0$ . Nothing about  $A$  depends on  $B$ . In this case, we have full information about  $A$ . There is no entanglement between  $A$  and  $B$ .
- If  $|\Psi\rangle$  is entangled, then  $\rho_A$  is mixed and  $S_A > 0$ .
- For two qubits, the maximum entanglement entropy is  $S_A = \log 2$ , achieved by Bell states.

#### Matrix logarithm

It is important to emphasize that  $\log \rho$  is the *matrix logarithm* of  $\rho$ , **not** the element-by-element logarithm of the entries of  $\rho$ . In general, a matrix represents a linear operator, and functions of an operator are defined in a basis-independent way.

#### Spectral definition of $\log \rho$

To compute  $\log \rho$ , we need to diagonalize the density matrix and only then compute the logarithm of its eigenvalues. A density matrix is Hermitian and positive semidefinite (that is, its eigenvalues are not negative). It can be diagonalized as

$$\rho = \sum_n \lambda_n |n\rangle\langle n|, \quad \lambda_n \geq 0, \quad \sum_n \lambda_n = 1, \quad (3.84)$$

where  $\{|n\rangle\}$  are orthonormal eigenvectors and  $\{\lambda_n\}$  are eigenvalues.

Functions of  $\rho$  are then defined spectrally:

$$f(\rho) = \sum_n f(\lambda_n) |n\rangle\langle n|. \quad (3.85)$$

In particular,

$$\log \rho = \sum_n \log(\lambda_n) |n\rangle\langle n|. \quad (3.86)$$

Therefore, the von Neumann entropy reduces to a Shannon-like expression in terms of the eigenvalues:

$$S(\rho) = - \sum_n \lambda_n \log \lambda_n, \quad (3.87)$$

with the convention  $0 \log 0 \equiv 0$  (understood as a limit).

**How a computer computes  $\log(\rho)$** 

There are two common numerical strategies:

- \*) Diagonalize and apply log to the eigenvalues (best for Hermitian  $\rho$ ).
- \*) Use a dedicated matrix-log function when needed (for non-Hermitian or general matrices).

**Practical computation in Python**

In Python, one should **NOT** use `np.log(rho)` because that applies log element-by-element and does *not* produce the matrix logarithm.

I) If  $\rho$  is Hermitian, the most pedagogical approach is:

1. Compute eigenvalues  $\{\lambda_n\}$  (using a Hermitian eigensolver).
2. Compute  $S(\rho) = -\sum_n \lambda_n \log \lambda_n$ .

This avoids forming  $\log \rho$  explicitly.

II) If one truly needs the operator  $\log \rho$ , one can use a matrix-logarithm routine (from `scipy`):

$$\log \rho \leftrightarrow \text{scipy.linalg.logm}(\rho).$$

This computes the matrix logarithm of a general matrix.

**Example: Entanglement in a Two-Qubit System**

1) Consider a two-qubit system prepared in the Bell state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|10\rangle + |01\rangle). \quad (3.88)$$

The density matrix of the full system is

$$\rho = |\psi\rangle\langle\psi| = \frac{1}{2}(|10\rangle\langle 10| + |10\rangle\langle 01| + |01\rangle\langle 10| + |01\rangle\langle 01|). \quad (3.89)$$

In matrix form, this reads

$$\rho = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (3.90)$$

where the computational basis ordering is  $|00\rangle, |01\rangle, |10\rangle, |11\rangle$ .

The reduced density matrix of qubit 1 is obtained by tracing out qubit 2,

$$\rho_1 = \text{Tr}_2(\rho) = \sum_{k=0}^1 {}_2\langle k|\rho|k\rangle_2. \quad (3.91)$$

Evaluating the partial trace yields

$$\rho_1 = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}. \quad (3.92)$$

The **entanglement entropy** of the reduced density matrix is

$$S = -\text{Tr}(\rho_1 \log \rho_1). \quad (3.93)$$

The eigenvalues of  $\rho_1$  are  $\lambda_1 = \lambda_2 = 1/2$ , so the entropy is

$$S = -\sum_{i=1}^2 \lambda_i \log \lambda_i = \log 2. \quad (3.94)$$

Using logarithms base 2, this corresponds to  $S = 1$ , indicating maximal entanglement between the two qubits.

Matrix Eq. (3.92) tells us that if we only look at  $A$ , we have 50% probability to get  $|0\rangle$  and 50% to get  $|1\rangle$ . This uncertainty in  $A$  comes from the fact that its state is correlated with  $B$ . Only if we could measure  $B$ , we would immediately know  $A$ .

2) Now consider the same two-qubit system prepared in a product state

$$|\psi\rangle = |11\rangle.$$

If you go through the same procedure, you find that the entanglement entropy is  $S = 0$ .

Entanglement entropy measures how much information about the full system is inaccessible when only one part is observed.

### Entanglement entropy vs basis

Entanglement entropy is not an intrinsic property of the state alone; it is a property of (state + bipartition). Entanglement entropy depends on how you split the system into  $A$  and  $B$ , but does not depend on the choice of basis within each subsystem. In this sense, it differs from measures of delocalization as the participation ratio, which depend on the basis choice.

One can define entanglement in different “spaces” (real space, momentum space, energy space, mode space). This means that entanglement is not an absolute property of the state alone – it depends on how one chooses to decompose the Hilbert space. The statement: “A state is entangled” is meaningless unless we also specify: “With respect to which partition?” A state can obey area laws in real space, but show volume-law entanglement in momentum space. Free fermions, for example, are weakly entangled in energy modes, but strongly entangled in real space.

## 3.7 Assignment 02: Spectrum and Level Statistics of Spin-1/2 Chains

*Consider a spin-1/2 chain with  $L = 15$  sites and 5 up-spins, so the total  $z$ -magnetization  $S^z$  is fixed (total number of up-spins is fixed). The system is described by the following Hamiltonian:*

$$\begin{aligned} \hat{H}_{NNN} = & \sum_{j=1}^{L-1} \left[ J \left( \hat{S}_j^x \hat{S}_{j+1}^x + \hat{S}_j^y \hat{S}_{j+1}^y \right) + \Delta \hat{S}_j^z \hat{S}_{j+1}^z \right] \\ & + \lambda \sum_{j=1}^{L-2} \left[ \left( \hat{S}_j^x \hat{S}_{j+2}^x + \hat{S}_j^y \hat{S}_{j+2}^y \right) + \Delta \hat{S}_j^z \hat{S}_{j+2}^z \right]. \end{aligned} \quad (3.95)$$

### 3.7. ASSIGNMENT 02: SPECTRUM AND LEVEL STATISTICS OF SPIN-1/2 CHAINS85

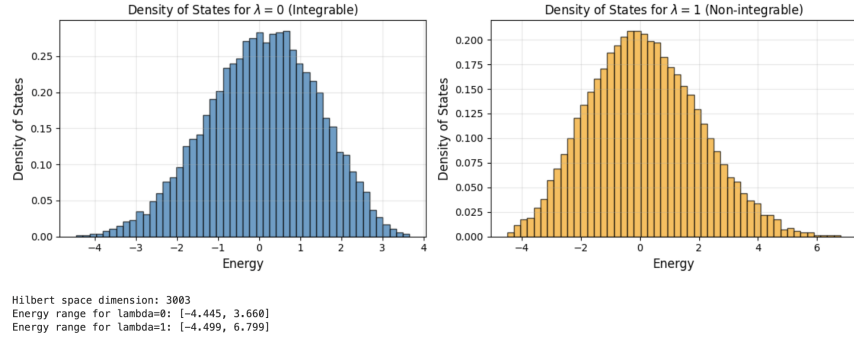


Figure 3.2: Question 1: Density of states.

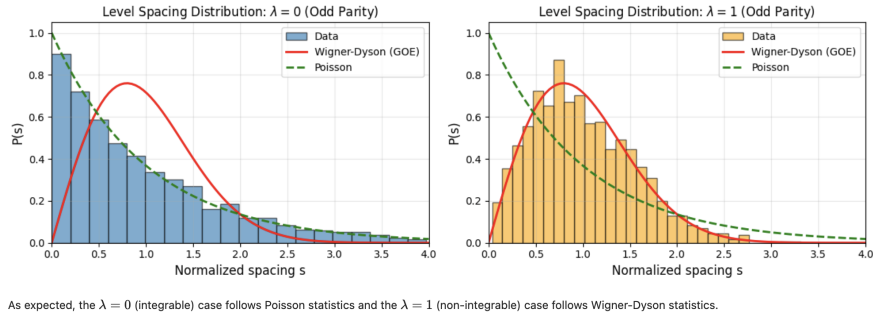


Figure 3.3: Question 2: Level spacing distribution.

Consider  $J = 1$  and  $\Delta = 0.48$ . The value of  $\lambda$  is varied according to the problem.

- 1) Obtain the density of states for  $\lambda = 0$  and  $\lambda = 1$ .
- 2) Obtain the level spacing distribution,  $P(s)$ , for  $\lambda = 0$  and  $\lambda = 1$ . Attention! You need to separate the eigenvalues by symmetry sector. Show your results for the odd parity sector. [You can also do an average over the results for the odd and for the even sectors, if you want].
- 3) Plot  $\langle \tilde{r} \rangle$  vs  $\lambda$  for  $0 \leq \lambda \leq 1$ . Attention! You need to separate the eigenvalues by symmetry sector. Show your results for the odd parity sector. [You can also do an average over the results for the odd and even sectors, if you want].
- 4) Plot the participation ratio (PR) vs energy (E) for  $\hat{H}_{NNN}$  with  $\lambda = 0$  and  $\lambda = 1$ , using the computational basis, so no need to separate by parity sector. [You can also plot the Shannon entropy vs energy, if you want].
- 5) Repeat (4) using as basis the eigenstates of the Hamiltonian with  $\lambda = 0$ . [Alternative/Additional: Use instead the basis of the XX-Hamiltonian].
- 6) **OPTIONAL!** Plot the entanglement entropy vs energy in two cases: the integrable case  $\lambda = 0$  and the nonintegrable case  $\lambda = 1$ . Consider a real-space partition of the chain, where subsystem  $A$  consists of the first 7 spins and subsystem  $B$  consists of the last 8 spins.
- 7) Compute and display the level spacing distribution  $P(s)$  for the Hamiltonian  $\hat{H}_{NNN}$  in Eq. (3.95) with  $L = 14$ , 7 up-spins,  $J = 1$ , and  $\Delta = 1$ . The spectrum should be restricted only by the conservation of total magnetization,  $\mathcal{S}_z$ , without further separation into additional symmetry sectors. How do you explain the resulting level-spacing distribution?

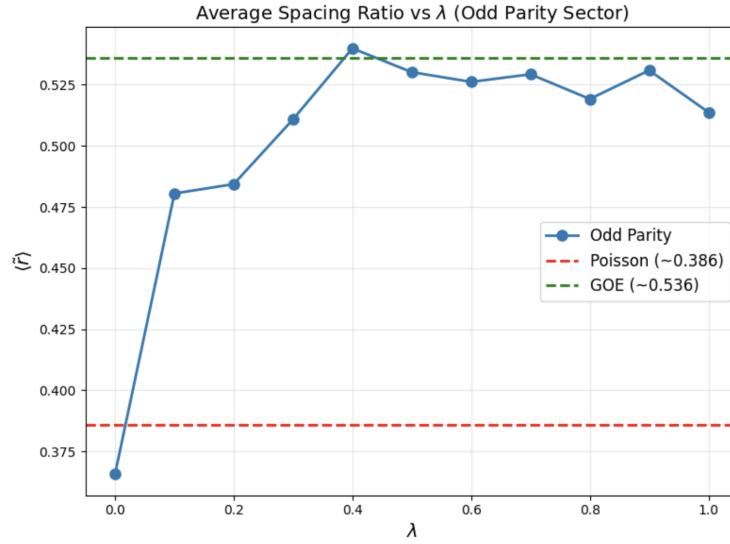


Figure 3.4: Question 3: Ratio of consecuting spacings.

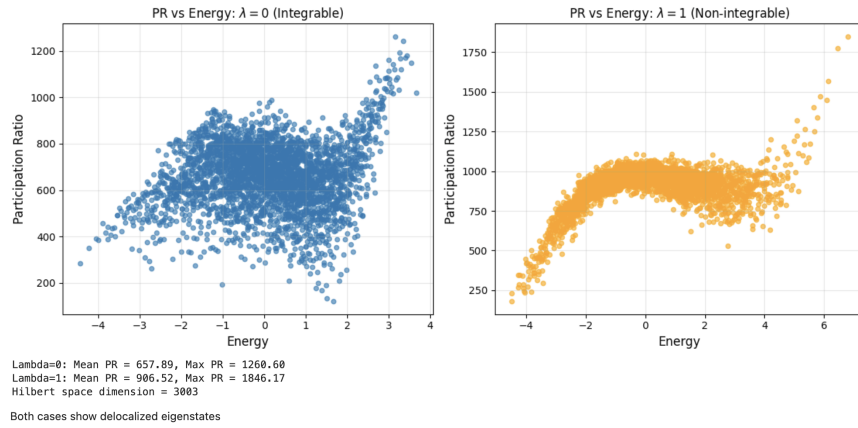
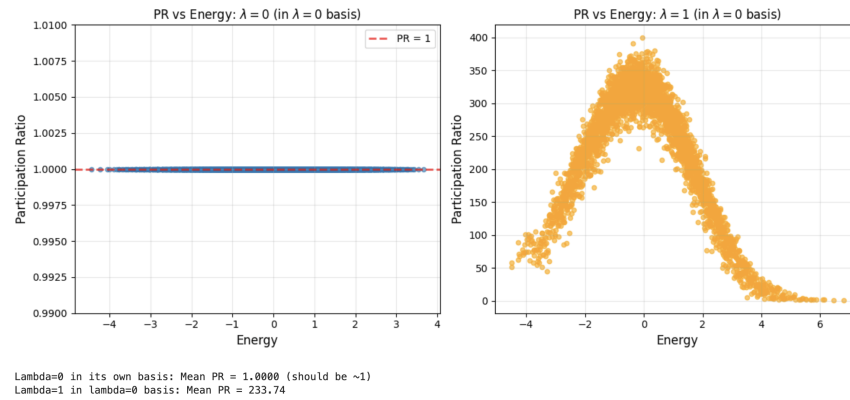
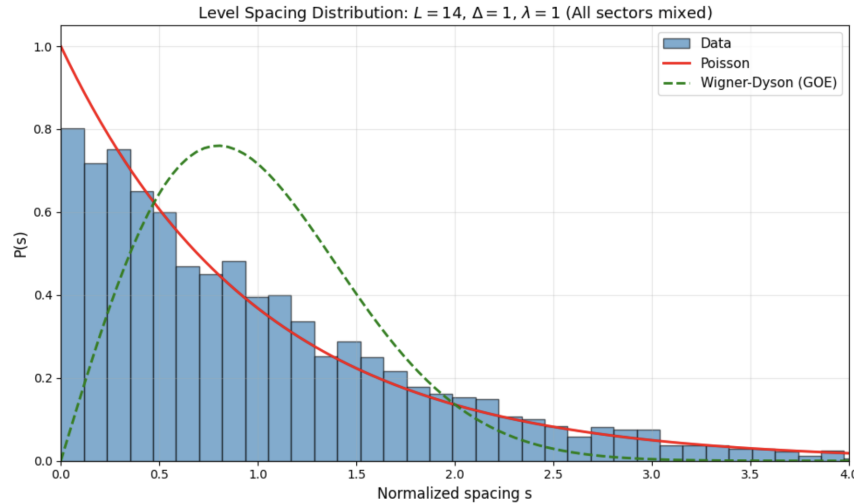
Figure 3.5: Question 4: Participation ratio in the computational basis ( $z$ -direction).

Figure 3.6: Question 5: Participation ratio in the XXZ-basis.

Figure 3.7: Question 7: Level spacing distribution;  $L = 14$ .

## 3.8 Tools for Spin Hamiltonians

In the previous sections, we constructed the Hamiltonian matrix in Eq. (3.12) by explicitly analyzing how each term of the Hamiltonian acts on the many-body basis vectors, focusing on the action of pairs of spin operators. This approach makes the physical content of the model transparent and is particularly well suited for understanding how local operators generate transitions between basis states.

There exists, however, an alternative strategy to build spin Hamiltonians, which is based on tensor products of Pauli matrices. In this operator-level construction, local spin operators are embedded into the full many-body Hilbert space by taking tensor products with identity operators on all other sites. The Python library **QuTiP** (Quantum Toolbox in Python) follows precisely this tensor-product approach, explicitly constructing operators as matrices acting on the full Hilbert space.

By contrast, another efficient library, **QuSpin**, avoids the explicit construction of tensor-product operators altogether. Instead, it works directly in a chosen basis—such as a fixed magnetization sector—and builds the Hamiltonian by encoding how local operators act on basis states, closely mirroring the method we employed earlier.

Before discussing these two libraries in more detail, we first review the tensor-product construction of spin-1/2 Hamiltonians.

### Building spin-1/2 Hamiltonians from tensor products

A spin-1/2 chain with  $L$  sites lives in a Hilbert space of dimension  $2^L$ . As explained above, a convenient basis is the computational (Ising) basis

$$|s_1 s_2 \cdots s_L\rangle \equiv |s_1\rangle \otimes |s_2\rangle \otimes \cdots \otimes |s_L\rangle, \quad s_n \in \{0, 1\},$$

where  $\otimes$  denotes the tensor (Kronecker) product, indicating that the full many-body Hilbert space is constructed as the product of the local Hilbert spaces associated with each spin.

To represent a single-site operator acting on site  $n$  inside an  $L$ -site chain, one uses Kronecker (tensor) products:

$$\sigma_n^{x,y,z} = \mathbb{1}_1 \otimes \mathbb{1}_2 \otimes \dots \otimes \sigma_n^{x,y,z} \otimes \dots \otimes \mathbb{1}_{L-1} \otimes \mathbb{1}_L = \mathbb{1}^{\otimes(n-1)} \otimes \sigma_n^{x,y,z} \otimes \mathbb{1}^{\otimes(L-n)}. \quad (3.96)$$

Similarly, a two-site operator acting on sites  $n$  and  $m$  is

$$\sigma_n^{x,y,z} \sigma_m^{x,y,z} = \mathbb{1}^{\otimes(n-1)} \otimes \sigma_n^{x,y,z} \otimes \mathbb{1}^{\otimes(m-n-1)} \otimes \sigma_m^{x,y,z} \otimes \mathbb{1}^{\otimes(L-m)}. \quad (3.97)$$

This is what is implicitly meant by expressions like  $\sigma_n^x \sigma_{n+1}^x$  in the Hamiltonian. Each term is a  $2^L \times 2^L$  matrix built from tensor products, and the full Hamiltonian is obtained by summing all such terms.

**Example: For  $L=2$ , build the  $4 \times 4$  matrix for  $\sigma_1^x \sigma_2^x$**

For this case,

$$\sigma_1^x \sigma_2^x = \sigma^x \otimes \sigma^x = \begin{pmatrix} 0(\sigma^x) & 1(\sigma^x) \\ 1(\sigma^x) & 0(\sigma^x) \end{pmatrix} = \left( \begin{array}{cc|cc} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{array} \right).$$

**Example: For  $L=4$ , build the  $16 \times 16$  matrix for  $\sigma_2^x \sigma_3^x$**

The operator acting as identity on sites 1 and 4 and as  $\sigma^x$  on sites 2 and 3 is

$$\mathbb{1}_1 \otimes \sigma_2^x \otimes \sigma_3^x \otimes \mathbb{1}_4 = \mathbb{1} \otimes \sigma^x \otimes \sigma^x \otimes \mathbb{1},$$

which leads to the matrix

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (3.98)$$

Once each term (e.g.,  $\sigma_n^x \sigma_{n+1}^x$ ,  $\sigma_n^y \sigma_{n+1}^y$ ,  $\sigma_n^z \sigma_{n+1}^z$ , local fields, etc.) is written as a  $2^L \times 2^L$  matrix, the full Hamiltonian matrix is obtained simply by summing all contributions.

## BASIS

**Attention!** The order of the basis states follows binary numbers, from smallest to largest, using  $L$  bits.

For example, when  $L = 2$

For  $L = 4$ , we have

| Basis state  | Binary index |
|--------------|--------------|
| $ 00\rangle$ | 0            |
| $ 01\rangle$ | 1            |
| $ 10\rangle$ | 2            |
| $ 11\rangle$ | 3            |

| Basis state    | Binary index |
|----------------|--------------|
| $ 0000\rangle$ | 0            |
| $ 0001\rangle$ | 1            |
| $ 0010\rangle$ | 2            |
| $ 0011\rangle$ | 3            |
| $ 0100\rangle$ | 4            |
| $ 0101\rangle$ | 5            |
| $ 0110\rangle$ | 6            |
| $ 0111\rangle$ | 7            |
| $ 1000\rangle$ | 8            |
| $ 1001\rangle$ | 9            |
| $ 1010\rangle$ | 10           |
| $ 1011\rangle$ | 11           |
| $ 1100\rangle$ | 12           |
| $ 1101\rangle$ | 13           |
| $ 1110\rangle$ | 14           |
| $ 1111\rangle$ | 15           |

### 3.8.1 QuTiP

QuTiP (Quantum Toolbox in Python) is a library for quantum dynamics, especially used for:

- \*) Open quantum systems (Lindblad master equations).
- \*) Time-dependent Hamiltonians.
- \*) State vectors, density matrices, expectation values.

You can learn more about it here:

<https://qutip.org/>

A simple example of how it works:

Listing 3.1: Construction of the  $L = 2$  XXZ Hamiltonian using QuTiP

```
import numpy as np
import qutip as qt

# --- Pauli matrices ---
sigx = qt.sigmax()
sigy = qt.sigmay()
sigz = qt.sigmaz()

# --- Identity ---
```

```

I = qt.qeye(2)

# --- For two sites ---
sigx1, sigy1, sigz1 = qt.tensor(sigx, I), qt.tensor(sigy, I), qt.
    tensor(sigz, I)
sigx2, sigy2, sigz2 = qt.tensor(I, sigx), qt.tensor(I, sigy), qt.
    tensor(I, sigz)
# [Note: For three sites, sigx1 = qt.tensor(sigx, I, I), etc.]

# --- XXZ Hamiltonian: H = Jxy (SxSx + SySy) + Jz SzSz ---
Jxy = 1.0
Jz = 0.5

# Remember the factor 1/4, since S = sigma/2
H_xxz = (Jxy / 4.0) * (sigx1 * sigx2 + sigy1 * sigy2) + (Jz / 4.0) *
    (sigz1 * sigz2)

print("XXZ Hamiltonian matrix for L=2:")
print(H_xxz.full())

# Eigenvalues
evals = np.linalg.eigvalsh(H_xxz.full())
print("\nEigenvalues:", evals)

```

**Attention!**

QuTiP supports spins larger than 1/2. For general spin  $S$  you should use:

$$S = 1, 3/2, 2, \dots$$

qt.jmat( $S$ , 'x')

qt.jmat( $S$ , 'y')

qt.jmat( $S$ , 'z')

**3.8.2 QuSpin**

QuSpin (Quantum Spin Dynamics) is a library specifically designed for lattice many-body systems, especially:

- \*) Spin chains
- \*) Fermionic and bosonic lattice models
- \*) Symmetry resolution (magnetization, momentum, parity, etc.)
- \*) Floquet

More information can be found here:

<https://quspin.github.io/QuSpin/>

Example:

Listing 3.2: Construction of the XXZ Hamiltonian for  $L = 4$  with fixed  $N_{\uparrow} = 2$  using QuSpin

```

import numpy as np
from quspin.basis import spin_basis_1d
from quspin.operators import hamiltonian

# -----
# Parameters
# -----
L = 4
Jxy = 1.0
Jz = 0.5

# -----
# Basis: fix number of up-spins
# -----
# Full Hilbert space dimension would be  $2^L = 16$ .
# In the  $N_{\text{up}}=2$  sector the dimension is  $C(4,2) = 6$ .
N_up = 2
basis = spin_basis_1d(L, Nup=N_up, pauli=False)
# pauli=False means that QuSpin uses spin-1/2 operators  $S^\alpha = \sigma^\alpha/2$ .
# In this way, usual factors of 1/2 and 1/4 are automatically
# included in the Hamiltonian.

# Show which basis states are kept (as bitstrings)
# NOTE: QuSpin stores states as integers; here they are
# printed as L-bit binary strings for readability.
print("Basis states in this sector:")
for s_int in basis.states:
    print(format(s_int, f"0{L}b"))
print()

# -----
# Build the open-boundary XXZ Hamiltonian
# -----
# Bonds for open boundaries: (0,1), (1,2), (2,3)
bonds = [(i, i + 1) for i in range(L - 1)]

# Coupling lists: [coupling strength, site i, site j]
Jxy_list = [[Jxy, i, j] for (i, j) in bonds]
Jz_list = [[Jz, i, j] for (i, j) in bonds]

# Static = time-independent terms of the Hamiltonian
static = [
    ["xx", Jxy_list],
    ["yy", Jxy_list],
    ["zz", Jz_list],
]

```

```

# Dynamic = time-dependent terms (none in this model)
dynamic = []

H = hamiltonian(static, dynamic, basis=basis, dtype=np.float64)

# -----
# Inspect matrix and spectrum
# -----
H_mat = H.toarray()
print("Hamiltonian matrix in the N_up=2 sector (shape):", H_mat.
      shape)
print(H_mat)

evals = np.linalg.eigvalsh(H_mat)
print("\nEigenvalues in the N_up=2 sector:")
print(evals)

```

More details on how to use QuSpin (provided by Sriram C. Lakshmanan):

### Importing the Required Libraries

We begin by importing the libraries required to build the Hamiltonian and analyze the system.

```

import numpy as np
import matplotlib.pyplot as plt
from quspin.basis import spin_basis_1d
from quspin.operators import hamiltonian

```

### Defining the System

We consider a spin-1/2 chain of length  $N$  described by the XXZ Hamiltonian. The main parameters are

- $N$  : number of spins
- $J$  : interaction strength
- $\Delta$  : anisotropy parameter

```

N = 4
J = 1
Delta = 0.5

```

## Constructing the Basis

The Hilbert space basis for the spin chain is generated with QuSpin.

```
basis = spin_basis_1d(N, S='1/2', pauli=0)
print(basis)
```

This lists all computational basis states of the  $2^N$ -dimensional Hilbert space.

Note: The way we wrote “basis” above is equivalent to using:

```
basis = spin_basis_1d(N, pauli=False)
```

## Initializing a Product State

A particular basis state can be chosen as the initial state. Note that below “Ns” is a QuSpin object corresponding to the dimension of the full Hilbert space.

```
State = "1010"
i_0 = basis.index(State)

Psi = np.zeros(basis.Ns)
Psi[i_0] = 1
```

This creates a vector representing the product state

$$|\psi\rangle = |1\,0\,1\,0\rangle.$$

## Incorporating Symmetries

One of the advantages of QuSpin is the ability to restrict calculations to symmetry sectors. QuSpin allows us to restrict the Hilbert space to different symmetry sectors. Some commonly used options are

- **Nup**: fixes the number of up spins (equivalently, the total magnetization  $S^z$ );
- **pblock**: selects a spatial-parity (reflection) sector;
- **zblock**: selects a spin-inversion sector;
- **kblock**: selects a translation (momentum) sector.

### • Conservation of $z$ -Magnetization

We can restrict the basis to the sector with fixed total magnetization

$$S^z = \sum_i S_i^z.$$

```
basis = spin_basis_1d(N, S='1/2', pauli=0, Nup=N//2)
print(basis)
```

This selects the sector with  $N/2$  spins up.

- **Conservation of  $z$ -total magnetization and parity symmetry**

For an open spin chain with reflection symmetry, one may restrict the system to a fixed-magnetization and parity sector. Below, we restrict the system to the  $p = 1$  parity block

```
basis = spin_basis_1d(N,
                      S='1/2',
                      pauli=0,
                      Nup=N//2,
                      pblock=1)
```

- **Total  $z$ -magnetization, parity, and spin-inversion symmetry**

At zero magnetization,  $N_{\text{up}} = N/2$ , spin inversion also preserves the fixed-magnetization sector. If the Hamiltonian has spin-inversion symmetry, we can therefore additionally impose

```
basis = spin_basis_1d(N,
                      S='1/2',
                      pauli=0,
                      Nup=N//2,
                      pblock=1,
                      zblock=1)
```

The basis states printed in a symmetry-reduced basis should be understood as representative states of symmetry orbits, rather than simply as the original computational-basis states.

- **Momentum Conservation**

Translational symmetry can also be imposed, restricting the system to a momentum sector. Below, the system is restricted to the  $k = 0$  momentum sector. Here,  $a=1$  specifies that the unit cell contains one lattice site, so the elementary translation is by one site. Notice that  $a$  is determined by the spatial periodicity of the Hamiltonian, not by the range of the interactions.

```
basis = spin_basis_1d(N,
                      S='1/2',
                      pauli=0,
                      a=1,
                      kblock=0)
```

## Open Boundary Conditions

For open boundaries the couplings are defined as

```
Coupling_xy = [[J, i, (i+1)] for i in range(basis.N-1)]
Coupling_z = [[J*Delta, i, (i+1)] for i in range(basis.N-1)]

static = [['xx', Coupling_xy],
          ['yy', Coupling_xy],
          ['zz', Coupling_z]]
```

```
H = hamiltonian(static, [],
                basis=basis,
                dtype=np.float64,
                check_symm=False,
                check_herm=False,
                check_pcon=False)
```

## Periodic Boundary Conditions

Periodic boundaries connect the last site to the first.

```
Coupling_xy = [[J, i, (i+1)%basis.N] for i in range(basis.N)]
Coupling_z = [[J*Delta, i, (i+1)%basis.N] for i in range(basis.N)]
```

## Hamiltonian Matrix

The Hamiltonian matrix can be converted to a dense array.

```
Ham = H.toarray()
Diag = np.diagonal(Ham)
```

The diagonal elements correspond to the classical Ising energies of the computational basis states.

## Diagonalization

To obtain the spectrum we diagonalize the Hamiltonian.

```
E1, V1 = H.eigh()
```

Here

- $E_1$  are the eigenvalues
- $V_1$  are the eigenvectors

## Histogram of Diagonal Elements

```
fig, ax = plt.subplots(figsize=(14,10))

ax.hist(Diag.real,
        bins=np.sort(np.append(np.unique(Diag),
                                max(Diag)+0.2)),
        rwidth=0.05)

ax.set_ylabel("Number of elements")
ax.set_xlabel(r"$H_{ii}/J$")
```

### Histogram of Energy Eigenvalues

The density of states can be visualized through a histogram.

```
binwidth = 0.2

ax.hist(E1/J,
        bins=np.arange(min(E1/J),
                        max(E1/J)+binwidth,
                        binwidth),
        histtype="step")
```

## 3.9 Beyond Spin-1/2 Models

Now you have the tools to investigate other physical models. Below, we briefly discuss the one-dimensional spin-1 Heisenberg model and the Bose-Hubbard model.

### Spin matrices – General

In the Zeeman basis  $\{|S, m\rangle\}$ ,  $m = -S, \dots, S$ , the spin operators have matrix elements

$$\langle S, m' | \hat{S}_x | S, m \rangle = \frac{1}{2} (\delta_{m', m+1} + \delta_{m', m-1}) \sqrt{S(S+1) - m'm}, \quad (3.99)$$

$$\langle S, m' | \hat{S}_y | S, m \rangle = \frac{1}{2i} (\delta_{m', m+1} - \delta_{m', m-1}) \sqrt{S(S+1) - m'm}, \quad (3.100)$$

$$\langle S, m' | \hat{S}_z | S, m \rangle = \delta_{m', m} m, \quad (3.101)$$

$$\langle S, m' | \hat{S}_+ | S, m \rangle = \delta_{m', m+1} \sqrt{S(S+1) - m'm}, \quad (3.102)$$

$$\langle S, m' | \hat{S}_- | S, m \rangle = \delta_{m', m-1} \sqrt{S(S+1) - m'm}, \quad (3.103)$$

$$\langle S, m' | \hat{S}^2 | S, m \rangle = \delta_{m', m} S(S+1). \quad (3.104)$$

### 3.9.1 Spin-1 Heisenberg XXZ chain

For a length- $L$  chain with open boundaries, the spin-1 XXZ Hamiltonian is

$$\hat{H} = J \sum_{i=1}^{L-1} \left( \hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y + \Delta \hat{S}_i^z \hat{S}_{i+1}^z \right) \quad (3.105)$$

$$= \frac{J}{2} \sum_{i=1}^{L-1} \left( \hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+ \right) + J\Delta \sum_{i=1}^{L-1} \hat{S}_i^z \hat{S}_{i+1}^z. \quad (3.106)$$

**Block diagonal form for  $L = 3$  (spin-1)**

Work in the product Zeeman basis  $|m_1, m_2, m_3\rangle$  with  $m_j \in \{+1, 0, -1\}$ . The total magnetization

$$M = m_1 + m_2 + m_3$$

is conserved, so  $\hat{H}$  is block diagonal in  $M$  sectors.

**Sector  $M = 3$  (dim 1).** Basis:  $\{|1, 1, 1\rangle\}$ .

$$H^{(3)} = (2J\Delta).$$

**Sector  $M = 2$  (dim 3).** Basis:  $\{|1, 1, 0\rangle, |1, 0, 1\rangle, |0, 1, 1\rangle\}$ .

$$H^{(2)} = \begin{pmatrix} J\Delta & J & 0 \\ J & 0 & J \\ 0 & J & J\Delta \end{pmatrix}.$$

**Sector  $M = 1$  (dim 6).** Basis:  $\{|1, 1, -1\rangle, |1, 0, 0\rangle, |1, -1, 1\rangle, |0, 1, 0\rangle, |0, 0, 1\rangle, |-1, 1, 1\rangle\}$ .

$$H^{(1)} = \begin{pmatrix} 0 & J & 0 & 0 & 0 & 0 \\ J & 0 & J & J & 0 & 0 \\ 0 & J & -2J\Delta & 0 & J & 0 \\ 0 & J & 0 & 0 & J & 0 \\ 0 & 0 & J & J & 0 & J \\ 0 & 0 & 0 & 0 & J & 0 \end{pmatrix}.$$

**Sector  $M = 0$  (dim 7).** Basis:  $\{|1, 0, -1\rangle, |1, -1, 0\rangle, |0, 1, -1\rangle, |0, 0, 0\rangle, |0, -1, 1\rangle, |-1, 1, 0\rangle, |-1, 0, 1\rangle\}$ .

$$H^{(0)} = \begin{pmatrix} 0 & J & J & 0 & 0 & 0 & 0 \\ J & -J\Delta & 0 & J & 0 & 0 & 0 \\ J & 0 & -J\Delta & J & 0 & 0 & 0 \\ 0 & J & J & 0 & J & J & 0 \\ 0 & 0 & 0 & J & -J\Delta & 0 & J \\ 0 & 0 & 0 & J & 0 & -J\Delta & J \\ 0 & 0 & 0 & 0 & J & J & 0 \end{pmatrix}.$$

**Sector  $M = -1$  (dim 6).** Basis:  $\{|1, -1, -1\rangle, |0, 0, -1\rangle, |0, -1, 0\rangle, |-1, 1, -1\rangle, |-1, 0, 0\rangle, |-1, -1, 1\rangle\}$ .

$$H^{(-1)} = \begin{pmatrix} 0 & J & 0 & 0 & 0 & 0 \\ J & 0 & J & J & 0 & 0 \\ 0 & J & 0 & 0 & J & 0 \\ 0 & J & 0 & -2J\Delta & J & 0 \\ 0 & 0 & J & J & 0 & J \\ 0 & 0 & 0 & 0 & J & 0 \end{pmatrix}.$$

**Sector  $M = -2$  (dim 3).** Basis:  $\{|0, -1, -1\rangle, |-1, 0, -1\rangle, |-1, -1, 0\rangle\}$ .

$$H^{(-2)} = \begin{pmatrix} J\Delta & J & 0 \\ J & 0 & J \\ 0 & J & J\Delta \end{pmatrix}.$$

**Sector  $M = -3$  (dim 1).** Basis:  $\{|-1, -1, -1\rangle\}$ .

$$H^{(-3)} = (2J\Delta).$$

### 3.9.2 Bose–Hubbard model

The Bose–Hubbard Hamiltonian is

$$H_{\text{BH}} = -J \sum_{\langle i,j \rangle} (b_i^\dagger b_j + b_j^\dagger b_i) + \frac{U}{2} \sum_i n_i(n_i - 1), \quad (3.107)$$

where  $b_i$  are bosonic operators and  $n_i = b_i^\dagger b_i$ . Let us choose  $L = 2$  sites and a total boson number  $N = 2$ . For the Fock-basis in this order

$$|1\rangle = |2, 0\rangle, \quad (3.108)$$

$$|2\rangle = |1, 1\rangle, \quad (3.109)$$

$$|3\rangle = |0, 2\rangle, \quad (3.110)$$

the Hamiltonian matrix is

$$H_{\text{BH}} = \begin{pmatrix} U & -\sqrt{2}J & 0 \\ -\sqrt{2}J & 0 & -\sqrt{2}J \\ 0 & -\sqrt{2}J & U \end{pmatrix}. \quad (3.111)$$

When writing the off-diagonal elements, recall that

$$b|n\rangle = \sqrt{n}|n-1\rangle \quad \text{and} \quad b^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle.$$

# Chapter 4

## Thermalization

When we first learn thermodynamics, we describe systems at equilibrium in terms of macroscopic variables such as temperature, pressure, volume, number of particles. These variables characterize the state of the system without reference to its microscopic constituents. Statistical mechanics takes a deeper step by recognizing that macroscopic objects are composed of an enormous number of microscopic particles governed by laws of classical mechanical. Temperature, for instance, acquires a microscopic interpretation. In a classical ideal gas it is proportional to the average kinetic energy of the particles, while more generally it is related to how the number of accessible microstates changes with energy. In this way, statistical mechanics connects thermodynamic variables to the collective behavior of microscopic degrees of freedom.

To make this connection precise, statistical mechanics introduces the concept of ensembles. An ensemble is a probability distribution over the possible microscopic states of a system consistent with given macroscopic constraints, such as fixed energy (microcanonical ensemble), fixed temperature (canonical ensemble), or fixed temperature and chemical potential (grand canonical ensemble). The central idea is that macroscopic observables can be computed as averages over these ensembles. This probabilistic description reflects our lack of knowledge of the exact microscopic configuration and, more fundamentally, captures the typical behavior of large systems in the thermodynamic limit.

---

**Microcanonical ensemble (fixed  $E, V, N$ ).** In the microcanonical ensemble, the system has fixed energy  $E$ , volume  $V$ , and particle number  $N$ . All microstates consistent with this energy are assumed to be equally probable. In classical mechanics, a microstate is specified by a point in phase space  $(\mathbf{q}, \mathbf{p})$ , and the ensemble average (expectation value) of a dynamical variable (observable)  $O(\mathbf{q}, \mathbf{p})$  is given by

$$\langle O \rangle_{\text{micro}} = \frac{1}{\Omega(E)} \int \delta(H(\mathbf{q}, \mathbf{p}) - E) O(\mathbf{q}, \mathbf{p}) d\mathbf{q} d\mathbf{p}, \quad (4.1)$$

where  $\Omega(E)$  is the volume of phase space accessible at energy  $E$ ,

$$\Omega(E) = \int \delta(H(\mathbf{q}, \mathbf{p}) - E) d\mathbf{q} d\mathbf{p}. \quad (4.2)$$

**Canonical ensemble (fixed  $T, V, N$ ).** In the canonical ensemble, the system is in contact with a heat bath at temperature  $T$ . The probability density in phase space is given

by the Boltzmann distribution,

$$\rho_{\text{can}}(\mathbf{q}, \mathbf{p}) = \frac{e^{-\beta H(\mathbf{q}, \mathbf{p})}}{Z}, \quad Z = \int e^{-\beta H(\mathbf{q}, \mathbf{p})} d\mathbf{q} d\mathbf{p}, \quad (4.3)$$

where  $\beta = 1/(k_B T)$  and  $Z$  is the partition function. The ensemble average of an observable is

$$\langle O \rangle_{\text{can}} = \int O(\mathbf{q}, \mathbf{p}) \rho_{\text{can}}(\mathbf{q}, \mathbf{p}) d\mathbf{q} d\mathbf{p}. \quad (4.4)$$

For example, the average energy is

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \ln Z. \quad (4.5)$$

**Grand canonical ensemble (fixed  $T, V, \mu$ ).** In the grand canonical ensemble, both energy and particle number may fluctuate, while temperature  $T$  and chemical potential  $\mu$  are fixed. The phase-space probability density becomes

$$\rho_{\text{gc}}(\mathbf{q}, \mathbf{p}) = \frac{e^{-\beta(H(\mathbf{q}, \mathbf{p}) - \mu N)}}{\Xi}, \quad \Xi = \sum_N \int e^{-\beta(H(\mathbf{q}, \mathbf{p}) - \mu N)} d\mathbf{q} d\mathbf{p}, \quad (4.6)$$

and ensemble averages are computed accordingly. For instance,

$$\langle N \rangle = \frac{1}{\beta} \frac{\partial}{\partial \mu} \ln \Xi. \quad (4.7)$$

---

Importantly, equilibrium does not imply that the system is static. Even at equilibrium, microscopic particles continue to move and evolve in time according to deterministic dynamical laws. The conceptual bridge between this microscopic motion and ensemble averages is provided by the notion of ergodicity. In classical many-body systems, the equations of motion are typically nonlinear due to interactions between particles. This nonlinearity can give rise to complex, and often chaotic, dynamics characterized by sensitive dependence on initial conditions. In systems with sufficiently chaotic behavior, trajectories explore the constant-energy surface in phase space in a way that effectively samples all accessible microstates. As a consequence, macroscopic observables become progressively insensitive to the precise details of the initial condition, effectively losing memory of how the system was prepared. In this case, long-time averages of observables along a single trajectory coincide with ensemble averages over phase space. This is ergodicity caused by chaos. This emergence of ergodicity (equivalence between time averages and ensemble averages) provides a dynamical justification for statistical mechanics, linking microscopic motion to macroscopic equilibrium behavior.

**Attention!** Chaos is the dynamical mechanism that generates mixing and ergodicity. However, ergodicity does not necessarily imply chaos – e.g. a particle moving on a rectangular billiard with irrational velocity components explores the energy shell ergodically despite exhibiting completely regular dynamics.

The discussion so far has remained within the framework of classical mechanics. However, the true microscopic description of matter is quantum mechanical. Therefore, a deeper and more fundamental question is whether thermodynamics can be derived directly from quantum mechanics itself. In other words, can the macroscopic laws of equilibrium arise from the unitary evolution of many-body quantum systems, without relying on classical notions such as trajectories or phase-space mixing? Addressing this question amounts to seeking a first-principles derivation of thermodynamics from the laws of quantum mechanics.

Quantum mechanics, however, poses a conceptual challenge to this picture. The Schrödinger equation is linear, the dynamics is unitary, and the full many-body wave function preserves complete information about the initial state at all times. How, then, can such reversible and information-preserving dynamics give rise to the effective irreversibility and ensemble-based descriptions of thermodynamics? How to address the microscopic origin of statistical mechanics within quantum mechanics caught von Neumann’s attention in 1932. The subject was an active topic of research within the quantum chaos and nuclear physics communities in the 1990s, where it was studied in terms of chaotic eigenstates and random-matrix-like structures by researchers such as Zelevinsky, Izrailev and Flambaum. The question also motivated studies that led to what became known as the eigenstate thermalization hypothesis (ETH), a term coined by Srednicki. Many core ETH ideas were already present in the quantum-chaos studies, although ETH evolved in parallel, using a different language and communities, which explains why works by the quantum chaos and nuclear physics communities are often not cited by the newer studies in condensed matter physics, AMO, and high energy physics.

## 4.1 Eigenstate Thermalization Hypothesis

ETH (and similar developments) addresses the microscopic origin of statistical mechanics by shifting the focus from classical trajectories to the properties of energy eigenstates. Rather than invoking ergodicity in phase space, can we talk about some notion of ergodicity in Hilbert space? The emphasis is now placed on signatures of quantum chaos and, specially, the structure of the eigenstates. The quantum chaos community introduced the notion of chaotic many-body eigenstates. Similarly, ETH proposes that in generic interacting quantum systems, individual many-body eigenstates already encode thermal properties: expectation values of few-body observables evaluated in a single eigenstate depend smoothly on energy and coincide with microcanonical predictions. As a result, thermal behavior emerges not from information loss or coupling to an external environment, but from the intrinsic structure of the Hamiltonian eigenstates themselves. The many-body eigenstates act as an effective “bath” for local degrees of freedom. In this sense, ETH provides a microscopic, fully quantum-mechanical foundation for statistical mechanics in isolated systems.

The importance of thermalization in isolated quantum systems extends well beyond conceptual foundations. The framework makes concrete, experimentally testable predictions, including the equivalence between long-time averages and ensemble averages for local observables, as well as the systematic suppression of temporal fluctuations as the system size increases.

### Equilibration

Consider an initial state  $|\Psi(0)\rangle$  that evolves under a Hamiltonian  $\hat{H}$  with eigenstates  $\{|\alpha\rangle\}$  and eigenvalues  $\{E_\alpha\}$ ,

$$|\Psi(0)\rangle = \sum_{\alpha} C_{\alpha} |\alpha\rangle, \quad |\Psi(t)\rangle = \sum_{\alpha} C_{\alpha} e^{-iE_{\alpha}t} |\alpha\rangle, \quad C_{\alpha} = \langle\alpha|\Psi(0)\rangle. \quad (4.8)$$

For an observable  $\hat{O}$ ,

$$\langle O(t) \rangle = \langle \Psi(t) | \hat{O} | \Psi(t) \rangle \quad (4.9)$$

$$\begin{aligned} &= \sum_{\alpha, \beta} C_{\beta}^* C_{\alpha} e^{i(E_{\beta} - E_{\alpha})t} O_{\beta\alpha}, \quad \text{where } O_{\beta\alpha} = \langle \beta | \hat{O} | \alpha \rangle \\ &= \underbrace{\sum_{\alpha \neq \beta} C_{\beta}^* C_{\alpha} e^{i(E_{\beta} - E_{\alpha})t} O_{\beta\alpha}}_{O_{\text{off}}(t)} + \underbrace{\sum_{\alpha} |C_{\alpha}|^2 O_{\alpha\alpha}}_{O_{\text{diag}}}. \end{aligned} \quad (4.10)$$

### When the off-diagonal term averages out at long times.

If the spectrum is nondegenerate, as in chaotic systems, or the degeneracies are rare, and the gaps  $E_{\beta} - E_{\alpha}$  are incommensurate enough, the phases  $e^{i(E_{\beta} - E_{\alpha})t}$  dephase. Then the long-time average kills the oscillatory term:

$$\overline{O(t)} \equiv \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \langle O(t) \rangle = \sum_{\alpha} |C_{\alpha}|^2 O_{\alpha\alpha} \equiv O_{\text{diag}}. \quad (4.11)$$

Thus the infinite-time average is determined by the diagonal matrix elements  $O_{\alpha\alpha}$  weighted by the overlaps  $|C_{\alpha}|^2$ . This saturation value is often denoted by “diagonal ensemble” prediction.

### Thermalization.

Thermalization in the microcanonical sense means:

$$O_{\text{diag}} \approx O_{\text{mic}}, \quad (4.12)$$

where

$$O_{\text{mic}} = \frac{1}{\mathcal{N}} \sum_{\substack{\alpha \\ |E_0 - E_{\alpha}| < \Delta E}} \langle \alpha | O | \alpha \rangle \quad (4.13)$$

is the microcanonical average around the energy of the initial state,  $E_0 = \langle \Psi(0) | \hat{H} | \Psi(0) \rangle$ . In the equation above,  $\mathcal{N}$  is the number of states in the energy window  $\Delta E$ .

## 4.2 Diagonal ETH

The infinite-time average of an observable,

$$\overline{O} = \sum_{\alpha} |C_{\alpha}|^2 O_{\alpha\alpha}, \quad (4.14)$$

depends explicitly on the initial state through the weights  $|C_{\alpha}|^2$ , whereas the microcanonical average does not. A central question is therefore how these two quantities can coincide in thermalizing systems.

For a few-body (local) observable  $\hat{O}$ , the diagonal eigenstate thermalization hypothesis (diagonal ETH) states that the eigenstate expectation values (EEVs)

$$O_{\alpha\alpha} \equiv \langle \alpha | \hat{O} | \alpha \rangle \quad (4.15)$$

are smooth functions of the eigenenergy. Consequently, eigenstates with nearby energies yield nearly identical expectation values, with fluctuations that decrease as the system size increases. This is naturally what we expect for chaotic eigenstates (see Sec. 4.2.2). As a result, if the initial state has significant support only within a narrow energy window, all eigenstates contributing appreciably to  $\overline{O}$  give essentially the same value. In this case,

$$\overline{O} \approx O_{\alpha\alpha} \approx O_{\text{mic}}.$$

In this sense, a single many-body eigenstate already reproduces the thermodynamic value of local observables, which is the essence of the term *eigenstate thermalization*. Individual eigenstates already look thermal to few-body probes.

A convenient finite-size diagnostic is to compare the eigenstate expectation values against the microcanonical average in a small energy window. This can be done with the relative deviation, defined as

$$\Delta_O^{\text{mic}} \equiv \frac{\sum_{\alpha \in \text{window}} |O_{\alpha\alpha} - O_{\text{mic}}|}{\sum_{\alpha \in \text{window}} |O_{\alpha\alpha}|}. \quad (4.16)$$

The decay of  $\Delta_O^{\text{mic}}$  with the system size is a good indication of the validity of ETH.

One may also test the worst-case fluctuations via the normalized extremal deviation

$$\Delta_O^{e,\text{mic}} \equiv \left| \frac{\max_{\alpha \in \text{window}} O_{\alpha\alpha} - \min_{\alpha \in \text{window}} O_{\alpha\alpha}}{O_{\text{mic}}} \right|, \quad (4.17)$$

which also needs to decrease as the system size increases for satisfying the diagonal ETH.

### 4.2.1 Diagonal ETH is automatic in full random matrix models

The eigenvalues of full random matrices, such as GOE matrices, are strongly correlated (spectral rigidity). Level repulsion ensures dephasing and relaxation to the infinite-time average. Furthermore, the eigenvectors behave as random vectors constrained only by normalization. Therefore, in any fixed basis, the components  $C_{\alpha}^k$  of an eigenstate  $|\alpha\rangle = \sum_{k=1}^D C_{\alpha}^k |k\rangle$  are (approximately) Gaussian (real or complex) random numbers. The fact that all eigenstates are statistically equivalent ensures diagonal ETH.

### 4.2.2 Diagonal ETH is subtler in physical Hamiltonians than GOE

Realistic many-body Hamiltonians with few-body interactions are sparse and banded. Even when level statistics are Wigner–Dyson-like, eigenstates are not perfectly random vectors. Nevertheless, in the chaotic regime and away from spectral edges, eigenstates become highly delocalized in the relevant energy shell, eigenstate expectation values become smooth functions of energy, and ETH becomes an excellent approximation. This is precisely why, in practice, *local observables* tend to thermalize in nonintegrable spin chains, while deviations may persist: (i) near integrable points, (ii) near localization regimes, (iii) near spectral edges, or (iv) for carefully chosen nonlocal observables that can resolve fine structure.

#### What are chaotic eigenstates in physical systems?

Consider a many-body Hamiltonian written as

$$H = H_0 + V,$$

and expand an exact energy eigenstate in a physically motivated mean-field basis  $\{|n\rangle\}$  that diagonalizes  $H_0$ ,

$$|\alpha\rangle = \sum_n C_n^\alpha |n\rangle.$$

Because realistic few-body interactions couple only a subset of mean-field basis states, the eigenstate can spread only within an *energy shell*: the maximal set (and envelope) of basis states that are accessible due to the structure and strength of the couplings induced by  $V$ .

One distinguishes:

- **Localized eigenstates**: only a small fraction of the shell is populated (e.g., very few significant  $C_n^\alpha$ ).
- **Sparse delocalized eigenstates**: many basis states participate, but the components fluctuate strongly and do not fill the shell uniformly.
- **Ergodic filling of the energy shell**: the eigenstate fills the shell uniformly in a statistical sense.

A **chaotic eigenstate** fills the energy shell ergodically. Within the shell, the coefficients behave as random variables with (approximately) Gaussian statistics, so that  $|C_n^\alpha|^2$  fluctuates around a smooth envelope set by the energy shell. In this regime, a statistical description of the isolated system becomes possible. These states can only emerge **away from the edges** of the spectrum.

#### Why do chaotic eigenstates imply diagonal ETH?

Let  $O$  be a few-body (local) observable. In the energy eigenbasis,

$$O_{\alpha\alpha} = \langle\alpha|O|\alpha\rangle = \sum_{m,n} (C_m^\alpha)^* C_n^\alpha O_{mn}.$$

In the chaotic (ergodic) regime, the coefficients  $C_n^\alpha$  within the energy shell behave as random variables with Gaussian statistics, subject only to normalization and global constraints. As a result:  $O_{\alpha\alpha}$  becomes a sum of many almost uncorrelated contributions and the fluctuations are suppressed as the system size grows.

Away from the edges of the spectrum, the typical value of  $O_{\alpha\alpha}$  depends smoothly on the eigenenergy  $E_\alpha$  and

$$\langle \alpha | O | \alpha \rangle \approx O_{\text{mc}}(E_\alpha).$$

This is precisely the content of *diagonal ETH*: individual eigenstates already encode thermal (microcanonical) values of few-body observables, and eigenstates close in energy are statistically similar.

### 4.3 Off-diagonal ETH

The first term in Eq. (4.10),

$$\sum_{\alpha \neq \beta} C_\alpha^* C_\beta O_{\alpha\beta} e^{i(E_\alpha - E_\beta)t},$$

controls the relaxation toward equilibrium and the temporal fluctuations around equilibrium. Thus, the magnitude and statistics of  $O_{\alpha\beta}$  determine how efficiently dephasing and equilibration occur.

In chaotic many-body systems, we expect  $\langle |O_{\alpha\beta}|^2 \rangle$  to decrease exponentially with system size and their distribution to be approximately Gaussian. Gaussianity arises because few-body operators acting on chaotic eigenstates produce matrix elements that are sums of many very weakly correlated (almost uncorrelated) random contributions,

$$O_{\alpha\beta} = \langle \alpha | O | \beta \rangle = \sum_{m,n} (C_m^\alpha)^* C_n^\beta O_{mn}.$$

leading (via the central limit theorem) to a normal distribution.

In integrable interacting systems, the distributions can differ strongly from Gaussian form and may exhibit skewed or log-normal-like features.

**Attention!** In few-body or single-particle quantum-chaotic systems, the distribution of off-diagonal elements need not be Gaussian. The reason is that for simple one-body observables, the matrix elements are built from only a small number of random components. The central limit theorem does not apply, and therefore non-Gaussian distributions are typical. Gaussian distributions emerge only when the observable effectively sums over many independent contributions (e.g., operators involving extensive mode sums).

### 4.4 Assignment 03: Thermalization

Consider the following three spin-1/2 models with an odd number  $L$  of sites:

- XXZ model,

$$\hat{H} = \epsilon J \hat{S}_1^z + \sum_{n=1}^{L-1} \left[ J_{xy} \left( \hat{S}_n^x \hat{S}_{n+1}^x + \hat{S}_n^y \hat{S}_{n+1}^y \right) + J_z \hat{S}_n^z \hat{S}_{n+1}^z \right] \quad (4.18)$$

- defect-XXZ model with a single defect on site  $(L+1)/2$  when  $L$  is odd and  $(L+2)/2$  when  $L$  is even,

$$\hat{H} = \epsilon J \hat{S}_1^z + d_{(L+1)/2} J \hat{S}_{(L+1)/2}^z + \sum_{n=1}^{L-1} \left[ J_{xy} \left( \hat{S}_n^x \hat{S}_{n+1}^x + \hat{S}_n^y \hat{S}_{n+1}^y \right) + J_z \hat{S}_n^z \hat{S}_{n+1}^z \right] \quad (4.19)$$

- NNN-XXZ model with second neighboring couplings.

$$\begin{aligned} \hat{H} = & \epsilon J \hat{S}_1^z + \sum_{n=1}^{L-1} \left[ J_{xy} \left( \hat{S}_n^x \hat{S}_{n+1}^x + \hat{S}_n^y \hat{S}_{n+1}^y \right) + J_z \hat{S}_n^z \hat{S}_{n+1}^z \right] \\ & + \lambda \sum_{n=1}^{L-2} \left[ J'_{xy} \left( \hat{S}_n^x \hat{S}_{n+2}^x + \hat{S}_n^y \hat{S}_{n+2}^y \right) + J'_z \hat{S}_n^z \hat{S}_{n+2}^z \right]. \end{aligned} \quad (4.20)$$

Consider open boundary conditions,  $J, J' = 1$ ;  $J_z, J'_z = 0.48$ ; and  $L/3$  up-spins. Include also a small defect on the first site of the chain  $\epsilon_1 J = 0.1$ , so you do not need to worry about parity. For all questions below, except (1) and (4), use defect size  $d_{(L+1)/2} J = 0.9$  and strength of second neighboring couplings  $\lambda = 0.44$ .

1) Make a plot of  $\langle \tilde{r} \rangle$  vs  $d_{(L+1)/2}$  and of  $\langle \tilde{r} \rangle$  vs  $\lambda$  that includes the values selected above. Use  $L = 15$

2) Plot participation ratio (PR) vs energy (E) for the three models. Use the eigenstates of the XX model as basis for the XXZ model and the eigenstates of the XXZ model as basis for the other two models;  $L = 15$ . What do you observe and how do you interpret your results?

3) For the three models, plot the eigenstate expectation values of  $S_{L/2}^z$ , of  $S_{L/2}^z S_{(L+1)/2}^z$ , and of the Ising interaction energy  $I = \sum_{j=1}^{L-1} J_z \hat{S}_j^z \hat{S}_{j+1}^z + \lambda \sum_{j=1}^{L-2} J'_z \hat{S}_j^z \hat{S}_{j+2}^z$  vs energy. Compare on the same plot the results for  $L = 9, 12, 15$ . How do your results compare with those for the participation ratio in question 2?

4) Using the Ising interaction energy as your observable, plot Eq. (4.16) and/or Eq. (4.17) vs  $d_{(L+1)/2}$  and vs  $\lambda$ . Show on each plot the results for  $L = 9, 12, 15$ . What do you observe?

5) Using  $S_{L/2}^z$  as your observable, make a plot of the distribution of its off-diagonal elements for the three models with  $L = 15$ . Consider only few eigenstates with energy closest to zero. It could be around 150 eigenstates. What do your distributions look like?

# Chapter 5

## Quench Dynamics

A quantum quench is a nonequilibrium protocol in which a system is prepared at  $t = 0$  in a state that is stationary with respect to an *initial* (unperturbed) Hamiltonian  $H_I$  (often denoted also by  $H_0$ ), and then the Hamiltonian is changed abruptly (in a time much shorter than any intrinsic timescale of the system), so that for  $t > 0$  the evolution is governed by a *final* (perturbed) Hamiltonian  $H_F$  (often denoted also just by  $H$ ). One can write

$$H_F = H_I + g V, \quad (5.1)$$

where  $V$  is the perturbation and  $g$  controls its strength.

In this setting, the initial state  $|\Psi(0)\rangle$  is an eigenstate of  $H_I$ ,

$$H_I |\phi_n\rangle = \varepsilon_n |\phi_n\rangle, \quad (5.2)$$

so  $|\Psi(0)\rangle = |\phi_{\text{ini}}\rangle$ .

### Expansion in the eigenbasis of the post-quench Hamiltonian

Let  $\{|\psi_\alpha\rangle\}$  be the eigenstates of  $H_F$  with eigenvalues  $\{E_\alpha\}$ :

$$H_F |\psi_\alpha\rangle = E_\alpha |\psi_\alpha\rangle. \quad (5.3)$$

Expand the initial state in this basis,

$$|\Psi(0)\rangle = \sum_{\alpha} C_{\alpha}^{\text{ini}} |\psi_{\alpha}\rangle, \quad C_{\alpha}^{\text{ini}} \equiv \langle \psi_{\alpha} | \Psi(0) \rangle. \quad (5.4)$$

The unitary time evolution for  $t > 0$  is then

$$|\Psi(t)\rangle = e^{-iH_F t} |\Psi(0)\rangle = \sum_{\alpha} C_{\alpha}^{\text{ini}} e^{-iE_{\alpha} t} |\psi_{\alpha}\rangle. \quad (5.5)$$

### 5.1 Survival probability

The survival amplitude is the overlap of the evolved state with the initial state:

$$A(t) \equiv \langle \Psi(0) | \Psi(t) \rangle = \langle \Psi(0) | e^{-iH_F t} | \Psi(0) \rangle. \quad (5.6)$$

The survival probability (often also called return probability or, simply, fidelity) is

$$S_p(t) \equiv |A(t)|^2 = \left| \langle \Psi(0) | e^{-iH_F t} | \Psi(0) \rangle \right|^2. \quad (5.7)$$

Using (5.5),

$$S_p(t) = \left| \sum_{\alpha} |C_{\alpha}^{\text{ini}}|^2 e^{-iE_{\alpha} t} \right|^2. \quad (5.8)$$

### 5.1.1 Local density of states (LDOS)

Define the local density of states (LDOS), also known as the strength function, as the energy distribution of the initial state, or equivalently, the weighted distribution of energies of  $H_F$  populated by the initial state:

$$\rho_{\text{ini}}(E) \equiv \sum_{\alpha} |C_{\alpha}^{\text{ini}}|^2 \delta(E - E_{\alpha}). \quad (5.9)$$

Then the survival amplitude is the absolute square of the Fourier transform of the LDOS,

$$S_p(t) = \left| \int_{E_{\min}}^{E_{\max}} dE \rho_{\text{ini}}(E) e^{-iEt} \right|^2, \quad (5.10)$$

where  $E_{\min}$  and  $E_{\max}$  are the energy bounds of the LDOS.

#### Very short-time universal behavior: quadratic decay and $\sigma_{\text{ini}}^2$

The post-quench energy of the initial state is the LDOS mean,

$$E_{\text{ini}} \equiv \langle E \rangle_{\text{ini}} = \langle (0) | H_F | (0) \rangle = \sum_{\alpha} |C_{\alpha}^{\text{ini}}|^2 E_{\alpha} = \int dE E \rho_{\text{ini}}(E), \quad (5.11)$$

and the LDOS variance (energy dispersion) is

$$\begin{aligned} \sigma_{\text{ini}}^2 &\equiv \sum_{\alpha} |C_{\alpha}^{\text{ini}}|^2 (E_{\alpha} - E_{\text{ini}})^2 = \int dE (E - E_{\text{ini}})^2 \rho_{\text{ini}}(E). \\ &= \sum_{\alpha} |C_{\alpha}^{\text{ini}}|^2 E_{\alpha}^2 - 2E_{\text{ini}} \sum_{\alpha} |C_{\alpha}^{\text{ini}}|^2 E_{\alpha} + E_{\text{ini}}^2 \sum_{\alpha} |C_{\alpha}^{\text{ini}}|^2 \\ &= \left( \sum_{\alpha} |C_{\alpha}^{\text{ini}}|^2 E_{\alpha}^2 \right) - E_{\text{ini}}^2 = \langle E^2 \rangle_{\text{ini}} - \langle E \rangle_{\text{ini}}^2 \end{aligned} \quad (5.12)$$

Expand  $S_p(t)$  for short times,

$$\begin{aligned} S_p(t) &= \left| e^{-iE_{\text{ini}} t} \sum_{\alpha} |C_{\alpha}^{\text{ini}}|^2 e^{-i(E_{\alpha} - E_{\text{ini}})t} \right|^2 \\ &= \left| e^{-iE_{\text{ini}} t} \sum_{\alpha} |C_{\alpha}^{\text{ini}}|^2 \left[ 1 - it(E_{\alpha} - E_{\text{ini}}) + \frac{t^2}{2}(E_{\alpha} - E_{\text{ini}})^2 + \mathcal{O}(t^3) \right] \right|^2. \end{aligned}$$

Since

$$\sum_{\alpha} |C_{\alpha}^{\text{ini}}|^2 (E_{\alpha} - E_{\text{ini}}) = 0,$$

we have

$$S_p(t) \approx \left[ 1 + \frac{t^2}{2} \sum_{\alpha} |C_{\alpha}^{\text{ini}}|^2 (E_{\alpha} - E_{\text{ini}})^2 \right]^2 \approx 1 + t^2 \sum_{\alpha} |C_{\alpha}^{\text{ini}}|^2 (E_{\alpha} - E_{\text{ini}})^2 \quad (5.13)$$

Therefore,

$$S_p(t) \approx 1 - \sigma_{\text{ini}}^2 t^2. \quad (5.14)$$

This quadratic decay is universal for the unitary evolution of a pure state. Another way to show this result is directly from

$$S_p(t) = \langle \Psi(0) | e^{-iH_F t} | \Psi(0) \rangle^2 \approx \left| \langle \Psi(0) | 1 - iH_F t - \frac{1}{2} H_F^2 t^2 | \Psi(0) \rangle \right|^2,$$

which gives

$$\begin{aligned} S_p(t) &\approx \left( 1 - \frac{t^2}{2} \langle \Psi(0) | H_F^2 | \Psi(0) \rangle \right)^2 + t^2 \langle \Psi(0) | H_F | \Psi(0) \rangle^2 \\ &\approx 1 - t^2 [\langle \Psi(0) | H_F^2 | \Psi(0) \rangle - \langle \Psi(0) | H_F | \Psi(0) \rangle^2] = 1 - \sigma_{\text{ini}}^2 t^2. \end{aligned}$$

**Why does  $\sigma_{\text{ini}}^2$  depend only on off-diagonal couplings?**

A very useful identity expresses  $\sigma_{\text{ini}}^2$  directly in terms of matrix elements of  $H_F$  in the basis that contains  $|\Psi(0)\rangle = |\phi_{\text{ini}}\rangle$  as a basis vector.

$$\sigma_{\text{ini}}^2 = \langle \Psi(0) | H_F^2 | \Psi(0) \rangle - \langle \Psi(0) | H_F | \Psi(0) \rangle^2 \quad (5.15)$$

$$= \sum_n \langle \phi_{\text{ini}} | H_F | \phi_n \rangle \langle \phi_n | H_F | \phi_{\text{ini}} \rangle - (\langle \phi_{\text{ini}} | H_F | \phi_{\text{ini}} \rangle)^2 \quad (5.16)$$

$$= \sum_n |\langle \phi_n | H_F | \phi_{\text{ini}} \rangle|^2 - |\langle \phi_{\text{ini}} | H_F | \phi_{\text{ini}} \rangle|^2 \quad (5.17)$$

$$= \sum_{\phi_n \neq \text{ini}} |\langle \phi_n | H_F | \phi_{\text{ini}} \rangle|^2. \quad (5.18)$$

So the initial decay of  $S_p(t)$  is controlled by the total strength of couplings from the initial state to all other basis states under  $H_F$ .

## 5.2 Short-Time Behavior and Saturation

Beyond the universal quadratic decay of the survival probability, valid for  $\sigma_{\text{ini}} t < 1$ , different behaviors emerge at different timescales. In this section, we will discuss only the behavior at short times, for  $\sigma_{\text{ini}} t \gtrsim 1$ , and the saturation of the dynamics. The behavior at intermediate timescales will be discussed in the next section.

### 5.2.1 Survival Probability: Bessel decay

Because  $S_p(t)$  is the squared modulus of the Fourier transform of the LDOS, different functional forms of  $\rho_{\text{ini}}(E)$  lead to characteristic decays.

#### Semicircular LDOS and its Fourier transform

For full random matrices from the GOE, the density of states approaches Wigner's semicircle. In this case, the LDOS for an arbitrary initial state is itself semicircular,

$$\rho_{\text{ini}}^{SC}(E) = \frac{1}{\pi\sigma_{\text{ini}}} \sqrt{1 - \left(\frac{E}{2\sigma_{\text{ini}}}\right)^2}, \quad |E| \leq 2\sigma_{\text{ini}}. \quad (5.19)$$

We then need to compute the Fourier transform,

$$A(t) = \int_{-2\sigma_{\text{ini}}}^{2\sigma_{\text{ini}}} dE \frac{1}{\pi\sigma_{\text{ini}}} \sqrt{1 - \left(\frac{E}{2\sigma_{\text{ini}}}\right)^2} e^{-iEt}. \quad (5.20)$$

Introduce the dimensionless variable

$$x = \frac{E}{2\sigma_{\text{ini}}}, \quad E = 2\sigma_{\text{ini}}x, \quad dE = 2\sigma_{\text{ini}}dx.$$

The integration limits become  $x \in [-1, 1]$ , and

$$A(t) = \frac{2}{\pi} \int_{-1}^1 dx \sqrt{1 - x^2} e^{-i(2\sigma_{\text{ini}}t)x} = \frac{2}{\pi} \left( \pi \frac{J_1(2\sigma_{\text{ini}}t)}{2\sigma_{\text{ini}}t} \right) = \frac{2J_1(2\sigma_{\text{ini}}t)}{2\sigma_{\text{ini}}t}, \quad (5.21)$$

where  $J_1(a)$  is the Bessel function of the first kind. Therefore, the survival probability is

$$S_p^{SC}(t) = \left[ \frac{J_1(2\sigma_{\text{ini}}t)}{\sigma_{\text{ini}}t} \right]^2. \quad (5.22)$$

Expanding this function for very short times gives the quadratic decay that we derived above. Using  $J_1(x) = x/2 - x^3/16 + \mathcal{O}(x^5)$ , we find

$$S_p^{SC}(t) \approx \left[ \frac{1}{2} \frac{(2\sigma_{\text{ini}}t)}{\sigma_{\text{ini}}t} - \frac{1}{16} \left( \frac{(2\sigma_{\text{ini}}t)}{\sigma_{\text{ini}}t} \right)^3 \right]^2 \Rightarrow S_p^{SC}(t) \approx 1 - \sigma_{\text{ini}}^2 t^2 \quad (5.23)$$

consistent with (5.14).

### 5.2.2 Survival Probability: Gaussian Decay

The density of states of generic many-body quantum systems with few-body couplings, such as chaotic models with short-range two-body interactions, is Gaussian. As a result, when the initial state is very far from any eigenstate of  $H_F$  (that is, when the perturbation  $g$  is very strong) and when the energy of the initial state  $E_{\text{ini}}$  is away from the edges of the spectrum, the LDOS itself has a Gaussian shape.

**Gaussian LDOS  $\Rightarrow$  Gaussian decay**

Consider a Gaussian LDOS centered at  $E_{\text{ini}}$  with variance  $\sigma_{\text{ini}}^2$ ,

$$\rho_{\text{ini}}^G(E) = \frac{1}{\sqrt{2\pi}\sigma_{\text{ini}}} \exp\left[-\frac{(E - E_{\text{ini}})^2}{2\sigma_{\text{ini}}^2}\right]. \quad (5.24)$$

Let us examine two scenarios for Eq. (5.10).

**1. Infinite limits:**  $E_{\text{min}} = -\infty$ ,  $E_{\text{max}} = \infty$ 

The integral becomes

$$A(t) = \int_{-\infty}^{\infty} dE \frac{1}{\sqrt{2\pi}\sigma_{\text{ini}}} \exp\left[-\frac{(E - E_{\text{ini}})^2}{2\sigma_{\text{ini}}^2} - iEt\right]. \quad (5.25)$$

Shift the integration variable

$$x = E - E_{\text{ini}}, \quad E = x + E_{\text{ini}}.$$

Then

$$A(t) = e^{-iE_{\text{ini}}t} \int_{-\infty}^{\infty} dx \frac{1}{\sqrt{2\pi}\sigma_{\text{ini}}} \exp\left[-\frac{x^2}{2\sigma_{\text{ini}}^2} - ixt\right]. \quad (5.26)$$

This is the Fourier transform of a Gaussian. Completing the square,

$$-\frac{x^2}{2\sigma_{\text{ini}}^2} - ixt = -\frac{1}{2\sigma_{\text{ini}}^2} (x + i\sigma_{\text{ini}}^2 t)^2 - \frac{\sigma_{\text{ini}}^2 t^2}{2},$$

gives

$$A(t) = e^{-iE_{\text{ini}}t} e^{-\frac{\sigma_{\text{ini}}^2 t^2}{2}} \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}\sigma_{\text{ini}}} \exp\left[-\frac{(x + i\sigma_{\text{ini}}^2 t)^2}{2\sigma_{\text{ini}}^2}\right]. \quad (5.27)$$

The remaining integral is unity, because it is a normalized Gaussian. Thus

$$A(t) = e^{-iE_{\text{ini}}t} e^{-\frac{\sigma_{\text{ini}}^2 t^2}{2}}, \quad (5.28)$$

and

$$S_p(t) = |A(t)|^2 = e^{-\sigma_{\text{ini}}^2 t^2}. \quad (5.29)$$

We conclude that when the Gaussian energy distribution extends over the whole energy axis, the decay is Gaussian.

**Attention!** This is, however, an over simplification. The LDOS (and even the density of states itself) is bounded in energy. This means that  $E_{\text{min}}$  and  $E_{\text{max}}$  have finite values.

## 2. Finite limits: $E_{\min}$ and $E_{\max}$ finite

Let us examine the realistic case,

$$A(t) = \int_{E_{\min}}^{E_{\max}} dE \frac{1}{\sqrt{2\pi}\sigma_{\text{ini}}} \exp\left[-\frac{(E - E_{\text{ini}})^2}{2\sigma_{\text{ini}}^2} - iEt\right]. \quad (5.30)$$

Following the same steps as above, we arrive at

$$A(t) = e^{-iE_{\text{ini}}t} e^{-\frac{\sigma_{\text{ini}}^2 t^2}{2}} \int_{E_{\min} - E_{\text{ini}}}^{E_{\max} - E_{\text{ini}}} \frac{dx}{\sqrt{2\pi}\sigma_{\text{ini}}} \exp\left[-\frac{(x + i\sigma_{\text{ini}}^2 t)^2}{2\sigma_{\text{ini}}^2}\right]. \quad (5.31)$$

Introducing

$$u = \frac{x + i\sigma_{\text{ini}}^2 t}{\sqrt{2}\sigma_{\text{ini}}},$$

the integral becomes expressible in terms of the error function:

$$A(t) = \frac{e^{-iE_{\text{ini}}t} e^{-\frac{\sigma_{\text{ini}}^2 t^2}{2}}}{2} [\text{erf}(u_{\max}) - \text{erf}(u_{\min})], \quad (5.32)$$

where

$$u_{\max} = \frac{E_{\max} - E_{\text{ini}} + i\sigma_{\text{ini}}^2 t}{\sqrt{2}\sigma_{\text{ini}}}, \quad (5.33)$$

$$u_{\min} = \frac{E_{\min} - E_{\text{ini}} + i\sigma_{\text{ini}}^2 t}{\sqrt{2}\sigma_{\text{ini}}}. \quad (5.34)$$

The final result is

$$S_p(t) = |A(t)|^2 = \frac{e^{-\sigma_{\text{ini}}^2 t^2}}{4} |\text{erf}(u_{\max}) - \text{erf}(u_{\min})|^2. \quad (5.35)$$

For sufficiently large bandwidth  $(E_{\max} - E_{\min}) \gg \sigma_{\text{ini}}$ , where  $E_{\max} - E_{\text{ini}} \gg \sigma_{\text{ini}}$  and  $E_{\text{ini}} - E_{\min} \gg \sigma_{\text{ini}}$ , and provided the initial energy  $E_{\text{ini}}$  is well inside the band, far from the edges, then the error functions approach  $\pm 1$  and the Gaussian decay  $S_p(t) = e^{-\sigma_{\text{ini}}^2 t^2}$  is recovered.

### 5.2.3 Survival Probability: Exponential Decay

when we increase the perturbation  $g$  in Eq. (5.1) from zero, we observe that before reaching the point where the LDOS achieves a Gaussian shape, we obtain a Lorentzian shape.

#### Lorentzian (Breit-Wigner or Cauchy) LDOS $\Rightarrow$ exponential decay

Assume a Lorentzian LDOS centered at  $E_{\text{ini}}$  with full width at half maximum  $\Gamma$ ,

$$\rho_{\text{ini}}^L(E) = \frac{1}{\pi} \frac{\Gamma/2}{(E - E_{\text{ini}})^2 + (\Gamma/2)^2}. \quad (5.36)$$

This distribution reaches its maximum at  $E = E_{\text{ini}}$ , where

$$\rho_{\text{ini}}^L(E_{\text{ini}}) = \frac{2}{\pi\Gamma}.$$

To determine the full width at half maximum, we evaluate the energy values for which the distribution equals half of this maximum,

$$\rho_{\text{ini}}^L(E) = \frac{1}{2}\rho_{\text{ini}}^L(E_{\text{ini}}).$$

Substituting Eq. (5.36) gives  $(E - E_{\text{ini}})^2 = (\Gamma/2)^2$ , so the two half-maximum points occur at

$$E = E_{\text{ini}} \pm \frac{\Gamma}{2}.$$

The distance between these two points defines the full width at half maximum (FWHM),  $\Gamma$ .

To obtain the survival probability, we need to compute the Fourier transform,

$$A(t) = \int_{-\infty}^{\infty} dE \frac{1}{2\pi} \frac{\Gamma}{(E - E_{\text{ini}})^2 + (\Gamma/2)^2} e^{-iEt}. \quad (5.37)$$

Shifting the integration variable

$$x = E - E_{\text{ini}}, \quad E = x + E_{\text{ini}}, \quad dE = dx,$$

gives

$$A(t) = e^{-iE_{\text{ini}}t} \int_{-\infty}^{\infty} dx \frac{1}{2\pi} \frac{\Gamma}{x^2 + (\Gamma/2)^2} e^{-ixt} = e^{-iE_{\text{ini}}t} \frac{1}{2\pi} (2\pi e^{-\Gamma t/2}). \quad (5.38)$$

Therefore,

$$S_p^L(t) = |A_L(t)|^2 = e^{-\Gamma t}. \quad (5.39)$$

**Attention!** Notice that at very short times, we still have the quadratic decay controlled by the variance  $\sigma_{\text{ini}}^2$  of the energy distribution of the initial state.

**Attention!** Notice also that we avoided equating  $\Gamma$  with  $\sigma_{\text{ini}}$ . The reason is that the mean and the variance of Lorentzians are not well defined. This is because the Lorentzian has very heavy tails, so the natural width parameter is the full width at half maximum.

### 5.2.4 Survival Probability: Cosine-squared behavior

The fastest decay of the survival probability is given by

$$S_p(t) \geq \cos^2(\sigma_{\text{ini}}t), \quad 0 \leq t \leq \frac{\pi}{2\sigma_{\text{ini}}}. \quad (5.40)$$

This limit is achieved with the idealized two-delta LDOS

$$\rho_{\text{ini}}^C(E) = \frac{1}{2} [\delta(E - E_1) + \delta(E - E_2)], \quad (5.41)$$

which yields

$$A_C(t) = \frac{1}{2} (e^{-iE_1 t} + e^{-iE_2 t}) = e^{-i(E_1+E_2)t/2} \cos\left(\frac{(E_2 - E_1)t}{2}\right), \quad (5.42)$$

and therefore

$$S_p^C(t) = \cos^2\left(\frac{(E_2 - E_1)t}{2}\right). \quad (5.43)$$

This exactly saturates the speed-limit structure with  $\sigma_{\text{ini}} = |E_2 - E_1|/2$ .

A comparison between the decay of the survival probability for three cases is shown in Fig. 5.1.

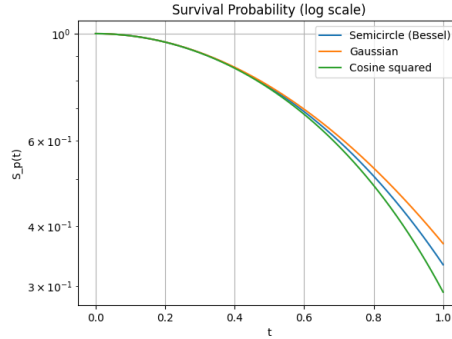


Figure 5.1: The fastest survival probability decay is that for  $\cos^2(\sigma_{\text{ini}} t)$ , followed by the GOE random matrix result, and then the Gaussian behavior achieved for a very strong perturbation of a realistic system with few-body couplings.

### Connection to local quench in space

An example of a realistic scenario that approaches the speed-limit decay in Eq. (5.40) is obtained by preparing an initial state of the 1D XXZ model with energy near the middle of the spectrum and evolving it under a defect Hamiltonian with a strong local defect,  $d_{L/2} \gg J$ . In this regime, both the density of states and the LDOS split into a bimodal distribution, with two peaks separated by an energy difference approximately equal to  $d_{L/2}$ .

The LDOS has the form

$$\rho_{\text{ini}}(E) \approx w_1 \rho_{\text{ini}}^{(1)}(E) + w_2 \rho_{\text{ini}}^{(2)}(E), \quad (5.44)$$

where  $w_1 + w_2 = 1$  and the centers of  $\rho_{\text{ini}}^{(1,2)}$  are separated by an energy gap  $\Delta E$  much larger than their individual widths. The survival amplitude is then approximately

$$A(t) \approx w_1 e^{-iE_1 t} \phi_1(t) + w_2 e^{-iE_2 t} \phi_2(t), \quad (5.45)$$

where  $\phi_{1,2}(t)$  are slowly decaying envelopes (Fourier transforms of the individual peaks). In the regime where  $\phi_1(t) \approx \phi_2(t) \approx e^{-\sigma^2 t^2}$  for the early times of interest, the interference between the two phases produces

$$S_p(t) \approx \cos^2\left(\frac{\Delta E}{2} t\right) \exp(-\sigma^2 t^2), \quad \Delta E = E_2 - E_1, \quad (5.46)$$

so the *initial* decay can approach the cosine-squared quantum limit. As time increases, the finite widths of the peaks cause dephasing and the oscillations become damped, eventually leading to saturation in finite systems.

### 5.2.5 Saturation of the survival probability

Expanding the modulus squared of Eq. (5.8),

$$S_p(t) = \sum_{\alpha} |C_{\alpha}^{\text{ini}}|^4 + \sum_{\alpha \neq \beta} |C_{\alpha}^{\text{ini}}|^2 |C_{\beta}^{\text{ini}}|^2 e^{-i(E_{\alpha} - E_{\beta})t}. \quad (5.47)$$

Defining the infinite-time average as

$$\overline{S_p} = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T S_p(t) dt, \quad (5.48)$$

we get

$$\overline{S_p} = \sum_{\alpha} |C_{\alpha}^{\text{ini}}|^4 + \sum_{\alpha \neq \beta} |C_{\alpha}^{\text{ini}}|^2 |C_{\beta}^{\text{ini}}|^2 \left[ \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T e^{-i(E_{\alpha} - E_{\beta})t} dt \right]. \quad (5.49)$$

For non-degenerate spectra,

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T e^{-i(E_{\alpha} - E_{\beta})t} dt = 0 \quad \text{if } E_{\alpha} \neq E_{\beta}. \quad (5.50)$$

Therefore, all off-diagonal terms vanish in the infinite-time average and we obtain

$$\boxed{\overline{S_p} = \sum_{\alpha} |C_{\alpha}^{\text{ini}}|^4} \quad (5.51)$$

The quantity

$$\sum_{\alpha} |C_{\alpha}^{\text{ini}}|^4 \quad (5.52)$$

is the inverse participation ratio (IPR) of the initial state in the eigenbasis of  $H_F$ . Thus, the infinite-time saturation value of the survival probability is  $\overline{S_p} = \text{IPR}_{\text{ini}}$

Physical meaning:

- If the initial state is highly delocalized in the eigenbasis of  $H_F$ , then  $|C_{\alpha}^{\text{ini}}|^2 \sim 1/\mathcal{D}$ , where  $\mathcal{D}$  is the Hilbert space dimension. In this case,

$$\overline{S_p} \sim \frac{1}{\mathcal{D}}.$$

- If the initial state is localized in few eigenstates then  $\overline{S_p}$  is much larger.

### 5.3 Assignment 04: Survival Probability

#### GOE and survival probability

Question 1) Consider a GOE matrix ( $N=3000$ ). Let the initial state be the basis vector corresponding to the middle index  $m \sim N/2$ .

a) Show the LDOS for a single realization.

b) For a single realization, compute  $\sigma_{\text{ini}}^2$ . Make a log-log plot of your numerical result for  $S_p(t)$  together with the analytical result in Eq. (5.22). Comment on the time window for the agreement. Mark with a horizontal line the saturation value of  $S_p(t)$  according to Eq. (5.51).

#### Spin-1/2 model and Gaussian decay of the survival probability

Consider the nearest-neighbor (NN) XXZ Hamiltonian

$$H_{\text{NN}} = J \sum_{i=1}^{L-1} \left( S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z \right) = \frac{J}{2} \sum_{i=1}^{L-1} \left( S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ \right) + J\Delta \sum_{i=1}^{L-1} S_i^z S_{i+1}^z \quad (5.53)$$

and the next-nearest-neighbor (NNN) extension

$$H_{\text{NNN}}(\lambda) = H_{\text{NN}} + \lambda J \sum_{i=1}^{L-2} \left( S_i^x S_{i+2}^x + S_i^y S_{i+2}^y + \Delta S_i^z S_{i+2}^z \right) \quad (5.54)$$

Use  $J = 1$ ,  $\Delta = 0.48$  and  $\lambda = 1$  throughout.

Use the following three initial product states in the  $S^z$  basis:

1. **Néel:**

$$|\text{Néel}\rangle = |\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\rangle.$$

2. **Domain wall:**

$$|\text{DW}\rangle = |\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\rangle.$$

3. **Pattern state:**

$$|\text{P}\rangle = |\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\uparrow\rangle.$$

Question 2-a) Write down general equations providing the energy of the three initial states above and the variance of their LDOS for any system size  $L$ , where  $L$  is even and  $L/2$  is odd, as in  $L = 10, 14, 18, 22, \dots$

For chain size  $L = 14$  and  $N_{\uparrow} = 7$ :

Question 2-b) Make plots of the density of states (DOS) for the XXZ model and the NNN model. Obtain the mean and variance of the distributions and fit your histograms with a Gaussian distribution.

Question 2-c) Make a plot of the local density of states (LDOS) for the domain wall state in the nearest-neighbor Hamiltonian. What is the mean energy and variance of the distribution? Where are the mean energy of this initial state with respect to the DOS?

Question 2-d) Make a plot of the LDOS for the Néel state in the next-nearest-neighbor Hamiltonian. What are the mean energy and variance of the distribution? Where is the mean energy of this initial state with respect to the DOS?

Question 2-e) Make a log-log plot showing the numerical result for  $S_p(t)$  together with the Gaussian-decay prediction using your analytic  $\sigma_{\text{ini}}$  for the Néel state and the domain wall state. Compare and explain your results. Which initial state leads to faster decay of  $S_p(t)$  and why? Comment on the time window where the Gaussian prediction works. Mark with a horizontal line the saturation value of  $S_p(t)$ .

Question 2-f) **OPTIONAL!** Analyze the LDOS and  $S_p(t)$  for the “pattern state” and compare with your results for the other two states.

### Spin-1/2 model: Exponential vs Gaussian decay of the survival probability

To solve these problems, it might be useful to review how we change the basis when writing the Hamiltonian matrix. Go back to the chapter on spin-1/2 models and read

*“Method (ii): Transform the Hamiltonian first”*

For chain size  $L = 14$  and  $N_{\uparrow} = 7$ :

Question 3-a) Show the LDOS and the survival probability for the XXZ model, when the initial state is an eigenstate of the XX model with energy closest to  $E_{\text{ini}} = 0$ . Consider three cases for the XXZ model:  $\Delta = 0.1, 0.48, 0.9$ .

(i) What is the best fit for the LDOS of  $\Delta = 0.48$ , a Lorentzian or a Gaussian function? Show your plot in linear scale and in log-scale.

(ii) What is the best fit for the LDOS of  $\Delta = 0.9$ , a Lorentzian or a Gaussian function? Show your plot in linear scale and in log-scale.

Question 3-b) Show the LDOS and the survival probability for the NNN model, when the initial state is an eigenstate of the XXZ model with  $\Delta = 0.48$  and energy closest to  $E_{\text{ini}} = 0$ . Consider three cases for the NNN model:  $\lambda = 0.1, 0.48, 0.9$ .

(i) What is the best fit for the LDOS of  $\lambda = 0.48$ , a Lorentzian or a Gaussian function? Show your plot in linear scale and in log-scale.

(ii) What is the best fit for the LDOS of  $\lambda = 0.9$ , a Lorentzian or a Gaussian function? Show your plot in linear scale and in log-scale.

### Spin-1/2 model: Fastest decay

Consider a quench from the XXZ model to the defect (impurity) model with defect strength  $d = 8.0$ . The initial state is chosen from the middle of the energy spectrum of the XXZ Hamiltonian. Work in the sector with  $L = 14$  sites and  $N_{\uparrow} = 7$  spins up.

Question 4-(i) Compute and plot the local density of states (LDOS) of the initial state with respect to the eigenbasis of the defect Hamiltonian. Do you observe two well-separated peaks in the LDOS? If so, attempt to fit each peak with a Gaussian distribution. Determine the mean energy and variance of each Gaussian and report the corresponding fitting parameters.

Question 4-(ii) Compute and plot the time evolution of the survival probability. Using the parameters obtained in part (i), fit the decay of the survival probability according to

Eq. (5.46). Discuss how well the analytical expression reproduces the numerical results.

## 5.4 Other Observables

In addition to the survival probability, there are several other commonly investigated physically meaningful observables. They provide information about relaxation, thermalization, correlations, information spreading, and the development of many-body quantum chaos. Below we summarize the quantities most frequently studied in systems such as spin chains and bosonic lattice models like the Bose–Hubbard model.

### 5.4.1 Loschmidt echo

Closely related to the survival probability is the Loschmidt echo,

$$\mathcal{L}(t) = |\langle \psi_0 | e^{i\hat{H}_2 t} e^{-i\hat{H}_1 t} | \psi_0 \rangle|^2, \quad (5.55)$$

which quantifies the sensitivity of the dynamics to perturbations in the Hamiltonian. The central idea is simple. One evolves an initial state forward in time with some Hamiltonian  $\hat{H}_1$ , and then attempts to reverse the dynamics. If the reversal were perfect, the system would return exactly to its initial state. In practice, however, the backward evolution is never exact, there is always some imperfection. The Loschmidt echo quantifies how well the system returns.

NMR is among the earliest and most influential experimental settings for studying Loschmidt echo, because it provides control over many-spin dynamics and makes it possible to implement, to a very good approximation, forward and backward time evolution. But this quantity has also been investigated in cold atoms, trapped ions, and superconducting circuits. It plays an important role in studies of quantum chaos, dynamical phase transitions, nonequilibrium quantum dynamics, and quantum information science.

Loschmidt echo gives access to questions such as: How reversible is quantum dynamics? How sensitive is the evolution to small perturbations? How do interactions, disorder, chaos, or decoherence affect the possibility of recovering the initial state?

The name “Loschmidt echo” has historical and conceptual roots in the Loschmidt paradox. In the XIXth century, Loschmidt raised an objection to Boltzmann’s explanation of irreversibility. The paradox can be phrased as follows: if the microscopic laws of motion are reversible in time, then why do macroscopic systems display irreversible behavior, such as entropy increase? In classical language, Loschmidt argued that if one could reverse all particle velocities at some instant, then the system should retrace its trajectory and return to its earlier state, apparently undoing entropy growth. The Loschmidt echo is related to this idea because it asks, in a quantum setting, how well one can reverse the dynamics and recover the initial state. It is called an “echo” by analogy with the spin echo procedure realized in NMR.

### 5.4.2 Expectation values of local observables

The most direct observable is the expectation value of an operator  $\hat{O}$  evolving under a Hamiltonian  $\hat{H}$ . The expectation value of  $\hat{O}$  is

$$O(t) = \langle \Psi(t) | \hat{O} | \Psi(t) \rangle. \quad (5.56)$$

These quantities are particularly relevant when  $\hat{O}$  is a *local observable*, meaning that it acts on a small subset of degrees of freedom. Local observables are the quantities that correspond most directly to experimental measurements.

In spin chains, common examples include

$$\hat{S}_i^z, \quad \hat{S}_i^x, \quad \hat{S}_i^z \hat{S}_{i+1}^z, \quad (5.57)$$

while in the Bose–Hubbard model typical observables are

$$\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i, \quad (5.58)$$

which measures the number of bosons on lattice site  $i$ .

The relaxation of local observables toward stationary values is one of the main signatures of thermalization in isolated quantum systems.

### 5.4.3 Correlations in space

Two-point correlation functions reveal the development of spatial correlations during the dynamics. They are defined as

$$C_{ij}(t) = \langle \Psi(t) | \hat{O}_i \hat{O}_j | \Psi(t) \rangle - \langle \Psi(t) | \hat{O}_i | \Psi(t) \rangle \langle \Psi(t) | \hat{O}_j | \Psi(t) \rangle. \quad (5.59)$$

This quantity measures how fluctuations of the observable  $\hat{O}_i$  at site  $i$  are correlated with fluctuations of  $\hat{O}_j$  at site  $j$  at time  $t$ . The subtraction of the product of expectation values removes the trivial part of the signal, leaving only the genuine correlations between the two observables.

If  $C_{ij}(t) = 0$ , the fluctuations at sites  $i$  and  $j$  are independent. Knowing the outcome of a measurement at site  $i$  gives no information about the outcome at site  $j$ . If  $C_{ij}(t) \neq 0$ , the fluctuations are correlated.

For spin chains one frequently studies

$$C_{ij}^{(zz,xx,yy)}(t) = \langle \hat{S}_i^{z,x,y} \hat{S}_j^{z,x,y} \rangle - \langle \hat{S}_i^{z,x,y} \rangle \langle \hat{S}_j^{z,x,y} \rangle, \quad (5.60)$$

while in the Bose–Hubbard model one often examines

$$C_{ij}^{(n)}(t) = \langle \hat{n}_i \hat{n}_j \rangle - \langle \hat{n}_i \rangle \langle \hat{n}_j \rangle. \quad (5.61)$$

Correlation functions provide information about how correlations build up and propagate through the system and they are useful in studies of transport behavior. Their spreading is often characterized by a light-cone structure associated with Lieb–Robinson bounds.

### 5.4.4 Correlations in time

Above, we discussed correlations in space, that is, how observables associated with different sites or degrees of freedom are related at a given time. One may also ask a different question: How strongly is an observable at a later time related to the same observable, or to another observable, at an earlier time? This leads to the notion of correlations in time.

A general two-time correlation function has the form

$$C_{AB}(t, t') = \langle \Psi_0 | \hat{A}(t) \hat{B}(t') | \Psi_0 \rangle, \quad (5.62)$$

where, in the Heisenberg picture,

$$\hat{A}(t) = e^{i\hat{H}t} \hat{A} e^{-i\hat{H}t}, \quad \hat{B}(t') = e^{i\hat{H}t'} \hat{B} e^{-i\hat{H}t'}. \quad (5.63)$$

This quantity measures how the value of observable  $\hat{B}$  at time  $t'$  is related to the value of observable  $\hat{A}$  at time  $t$ .

When the reference state is time independent, one often sets  $t' = 0$  and writes

$$C_{AB}(t) = \langle \Psi_0 | \hat{A}(t) \hat{B}(0) | \Psi_0 \rangle. \quad (5.64)$$

If  $\hat{A} = \hat{B}$ , this is called an *autocorrelation function*,

$$C_A(t) = \langle \Psi_0 | \hat{A}(t) \hat{A}(0) | \Psi_0 \rangle. \quad (5.65)$$

It tells us how much **memory** of the initial value of  $\hat{A}$  remains at time  $t$ .

Temporal correlations are important because they quantify memory, relaxation, equilibration, and transport. If an autocorrelation function decays rapidly, the system quickly loses memory of its initial condition as far as that observable is concerned. If it decays slowly, the system retains memory for a long time. Persistent oscillations may indicate coherent dynamics, conserved quantities, or the proximity to integrability. Exponential, Gaussian, power-law, or stretched-exponential decays can reveal different dynamical regimes.

**Spin autocorrelation functions.** A standard example of a temporal autocorrelation for observables is the spin autocorrelation function. For a local spin operator  $\hat{S}_k^z$ , one writes

$$C_k(t) = \langle \Psi_0 | \hat{S}_k^z(t) \hat{S}_k^z(0) | \Psi_0 \rangle = \langle \Psi_0 | e^{i\hat{H}t} \hat{S}_k^z e^{-i\hat{H}t} \hat{S}_k^z | \Psi_0 \rangle. \quad (5.66)$$

This measures how the value of the  $z$ -component of the spin at site  $k$  at time  $t$  is correlated with its value at time 0.

A site-averaged version is

$$C_s(t) = \frac{1}{L} \sum_{k=1}^L \langle \Psi_0 | \hat{S}_k^z(t) \hat{S}_k^z(0) | \Psi_0 \rangle. \quad (5.67)$$

This is one of the most common temporal autocorrelation functions in spin systems. It tells us how much local spin memory remains on average throughout the chain.

- If  $C_s(t)$  remains large, the system retains memory of its initial local spin configuration.

- If  $C_s(t)$  decays to a small value, the initial spin information has been lost locally.
- If  $C_s(t)$  decays slowly, this may indicate slow relaxation, localization, glassiness, or conservation laws.
- If  $C_s(t)$  oscillates, this may signal coherent dynamics or finite-size effects.

For transport problems, spin autocorrelations are especially important. Slow decay of local spin memory is often associated with inhibited transport, whereas rapid decay is associated with efficient spreading of spin information.

**Survival probability: An autocorrelation function.** The survival probability is a temporal autocorrelation function. It measures correlation in time, but now the object being correlated is the *full quantum state* with itself at different times. It quantifies how much the state at time  $t$  still resembles the initial state.

The survival probability is not the same as the autocorrelation of a specific observable. It is more global. A local observable may have already relaxed even when the full state still retains some structure.

**Connected temporal correlations.** Just as for equal-time spatial correlations, one may remove the trivial product of averages and define the connected two-time correlator,

$$C_{AB}^{\text{conn}}(t) = \langle \Psi_0 | \hat{A}(t) \hat{B}(0) | \Psi_0 \rangle - \langle \Psi_0 | \hat{A}(t) | \Psi_0 \rangle \langle \Psi_0 | \hat{B}(0) | \Psi_0 \rangle. \quad (5.68)$$

This isolates the genuine temporal correlation between the fluctuations of  $\hat{A}$  and  $\hat{B}$ .

**Connected spin autocorrelation.** If one wants to remove the trivial contribution from the average magnetization, one may define

$$C_s^{\text{conn}}(t) = \frac{1}{L} \sum_{k=1}^L \left[ \langle \Psi_0 | \hat{S}_k^z(t) \hat{S}_k^z(0) | \Psi_0 \rangle - \langle \Psi_0 | \hat{S}_k^z(t) | \Psi_0 \rangle \langle \Psi_0 | \hat{S}_k^z(0) | \Psi_0 \rangle \right]. \quad (5.69)$$

This isolates the genuine temporal correlation of spin fluctuations.

### 5.4.5 Entanglement entropy

Entanglement measures the quantum correlations between subsystems. If the system is divided into two parts  $A$  and  $B$ , the reduced density matrix of subsystem  $A$  is

$$\rho_A(t) = \text{Tr}_B [|\psi(t)\rangle\langle\psi(t)|]. \quad (5.70)$$

The von Neumann entanglement entropy is

$$S_A(t) = -\text{Tr} [\rho_A(t) \ln \rho_A(t)]. \quad (5.71)$$

In nonequilibrium dynamics, entanglement entropy typically grows in time and eventually saturates. Its growth rate and saturation value provide information about thermalization, integrability, and many-body localization.

### 5.4.6 Participation ratio and Shannon/Participation entropy

Another important quantity to characterize nonequilibrium dynamics is the spreading of the quantum state over the Hilbert space. This spreading can be quantified through the participation ratio (PR), which measures how many basis states significantly contribute to the wave function.

Consider the expansion of the time-evolved state in some chosen basis  $\{|\phi_n\rangle\}$ ,

$$|\Psi(t)\rangle = \sum_n C_n(t) |\phi_n\rangle, \quad (5.72)$$

where

$$C_n(t) = \langle \phi_n | \Psi(t) \rangle. \quad (5.73)$$

The probabilities

$$P_n(t) = |C_n(t)|^2 \quad (5.74)$$

represent the weight of the state  $|\Psi(t)\rangle$  on the basis vector  $|\phi_n\rangle$ . The participation ratio is defined as

$$\text{PR}(t) = \frac{1}{\sum_n P_n(t)^2}. \quad (5.75)$$

This quantity estimates the effective number of basis states occupied by the wavefunction.

If the initial state is one of the states of the chosen basis,  $\text{PR}(0)=1$ , and it grows as the wavefunction spreads over the Hilbert space during the dynamics. The participation ratio provides a direct measure of the degree of delocalization of the wavefunction in the chosen basis.

Closely related to the participation ratio is the Shannon entropy (also called information entropy),

$$S_{\text{Sh}}(t) = - \sum_n P_n(t) \ln P_n(t) \quad (5.76)$$

or the participation entropy

$$S_2(t) = - \ln \left[ \sum_n P_n(t)^2 \right]. \quad (5.77)$$

In studies of nonequilibrium quantum dynamics, the participation ratio and the Shannon/participation entropy are often computed in the basis where the initial state is localized. For example, in spin-1/2 chains one may use the computational basis (eigenstates of  $\hat{S}_i^z$ ),

$$|\phi_n\rangle = |s_1, s_2, \dots, s_L\rangle, \quad (5.78)$$

with  $s_i = \uparrow, \downarrow$ . The growth of  $\text{PR}(t)$  and related quantities reveal how the initially localized configuration spreads through the many-body Hilbert space.

The growth in time of the participation ratio and related entropies signals the spreading of the quantum state in Hilbert space, the buildup of complexity, and the approach toward equilibrium. These quantities provide complementary information to observables such as entanglement entropy, correlation functions, and out-of-time-ordered correlators.

⇒ **Spread in the many-body Hilbert space and timescales**

Let us consider the XXZ model with nearest neighbor couplings and open boundary conditions,

$$\hat{H} = J \sum_{i=1}^{L-1} \left( \hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y + \Delta \hat{S}_i^z \hat{S}_{i+1}^z \right), \quad (5.79)$$

where  $J$  sets the overall energy scale and  $\Delta$  is the anisotropy. Suppose  $L = 4$  and our initial state is the Néel state

$$|\Psi(0)\rangle = |1010\rangle.$$

This state is directly coupled with the states

$$|m\rangle = |0110\rangle, \quad |1100\rangle, \quad |1001\rangle,$$

while it couples with its mirror state

$$|0101\rangle$$

in second order of perturbation theory.

**Question:**

**How long does it take for the mirror state  $|0101\rangle$  to show up in the dynamics?**

There are two very different scenarios:

(a)  $\Delta \sim 1$ . Here, there is a hierarchy in the timescales for the participation of states coupled in first  $[|m\rangle]$  and second  $[|0101\rangle]$  order only at very short times. Once time  $\sim 1/J$ , both classes of states show similar contributions.

(b)  $\Delta \gg 1$ . Here, the states  $|m\rangle$  coupled in first order are virtual states, and the timescale of the participation of the state coupled in second order  $[|0101\rangle]$  is long and can be obtained by perturbation theory.

Let us examine each case more carefully.

**(a)  $\Delta \sim 1$ .** The evolution operator is

$$e^{-iHt} = 1 - iHt - \frac{1}{2}H^2t^2 \dots$$

For states directly coupled, the expansion above implies

$$A_{1010 \rightarrow m}(t) \approx -it \langle m | H | 1010 \rangle, \quad P_{1010 \rightarrow m}(t) \sim \frac{J^2}{4} t^2,$$

while for the second-order transition, we first go through  $|0110\rangle$  and  $|1001\rangle$ , leading to

$$A_{1010 \rightarrow 0101}(t) \approx -\frac{t^2}{2} \langle 0101 | H^2 | 1010 \rangle = -\frac{t^2}{2} 2 \frac{J^2}{4}, \quad P_{1010 \rightarrow 0101}(t) \sim \frac{J^4}{16} t^4,$$

Thus, at very short times

$$P_{1010 \rightarrow 0101} \ll P_{1010 \rightarrow m}.$$

because  $t^4 \ll t^2$ . Initially there is a hierarchy, but at relevant dynamical times,

$$t \sim \frac{2}{J}$$

both contributions are similar

$$P_{1010 \rightarrow m}(t = \frac{2}{J}) \sim 1 \quad \text{and} \quad P_{1010 \rightarrow 0101}(t = \frac{2}{J}) \sim 1.$$

After times of order  $1/J$ , the second-order process has had enough time to accumulate amplitude comparable to the first-order processes.

**(b)  $\Delta \gg 1$ .** The two Néel states that we are studying are degenerate

$$E_{1010}^{(0)} = J\Delta \left( -\frac{1}{4} - \frac{1}{4} - \frac{1}{4} \right) = -\frac{3J\Delta}{4}, \quad E_{0101}^{(0)} = -\frac{3J\Delta}{4}, \quad (5.80)$$

while the energies of the virtual states are

$$E_{0110}^{(0)} = -\frac{J\Delta}{4}, \quad E_{1001}^{(0)} = -\frac{J\Delta}{4}. \quad (5.81)$$

Therefore, the energy cost of the intermediate virtual states is

$$E_{1010}^{(0)} - E_{0110}^{(0)} = E_{1010}^{(0)} - E_{1001}^{(0)} = -\frac{J\Delta}{2}. \quad (5.82)$$

In this case, we can treat the flip-flop term perturbatively, writing the XXZ Hamiltonian as

$$\hat{H} = \hat{H}_0 + \hat{V}, \quad (5.83)$$

with the unperturbed part being

$$\hat{H}_0 = J\Delta \sum_{i=1}^{L-1} \hat{S}_i^z \hat{S}_{i+1}^z, \quad (5.84)$$

and the perturbation

$$\hat{V} = \frac{J}{2} \sum_{i=1}^{L-1} \left( \hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+ \right). \quad (5.85)$$

In degenerate perturbation theory, the second-order effective Hamiltonian in the degenerate subspace is

$$\begin{aligned} \langle 0101 | \hat{H}_{\text{eff}}^{(2)} | 1010 \rangle &= \sum_m \frac{\langle 0101 | \hat{V} | m \rangle \langle m | \hat{V} | 1010 \rangle}{E_0^{(0)} - E_m^{(0)}} \\ &= \frac{\langle 1010 | \hat{V} | 0110 \rangle \langle 0110 | \hat{V} | 0101 \rangle}{E_0^{(0)} - E_{0110}^{(0)}} + \frac{\langle 1010 | \hat{V} | 1001 \rangle \langle 1001 | \hat{V} | 0101 \rangle}{E_0^{(0)} - E_{1001}^{(0)}} \\ &= \frac{\left(\frac{J}{2}\right) \left(\frac{J}{2}\right)}{-\frac{J\Delta}{2}} + \frac{\left(\frac{J}{2}\right) \left(\frac{J}{2}\right)}{-\frac{J\Delta}{2}} = -\frac{J}{\Delta}. \end{aligned}$$

So, if we start in  $|1010\rangle$ , the coupling to  $|0101\rangle$  occurs on a timescale of order

$$\boxed{t_2 \sim \frac{\Delta}{J}}.$$

To be more precise, let us examine the effective Hamiltonian in the  $\{|1010\rangle, |0101\rangle\}$  subspace. Collecting zeroth- and second-order contributions, the effective Hamiltonian is

$$\hat{H}_{\text{eff}} = \begin{pmatrix} -\frac{3J\Delta}{4} - \frac{5J}{4\Delta} & -\frac{J}{\Delta} \\ -\frac{J}{\Delta} & -\frac{3J\Delta}{4} - \frac{5J}{4\Delta} \end{pmatrix}. \quad (5.86)$$

The shift in the diagonal elements come from

$$\langle 1010 | \hat{H}_{\text{eff}}^{(2)} | 1010 \rangle = \frac{|\langle 0110 | \hat{V} | 1010 \rangle|^2}{E_0^{(0)} - E_{0110}^{(0)}} + \frac{|\langle 1001 | \hat{V} | 1010 \rangle|^2}{E_0^{(0)} - E_{1001}^{(0)}} + \frac{|\langle 1100 | \hat{V} | 1010 \rangle|^2}{E_0^{(0)} - E_{1100}^{(0)}} \quad (5.87)$$

$$= -\frac{5J}{4\Delta}. \quad (5.88)$$

The eigenstates of  $\hat{H}_{\text{eff}}$  are the symmetric and antisymmetric combinations

$$|\pm\rangle = \frac{1}{\sqrt{2}} (|1010\rangle \pm |0101\rangle), \quad (5.89)$$

with energies

$$E_+ = -\frac{3J\Delta}{4} - \frac{9J}{4\Delta}, \quad E_- = -\frac{3J\Delta}{4} - \frac{J}{4\Delta}. \quad (5.90)$$

This means that in the effective two-state Hamiltonian the oscillation frequency is set by the energy splitting

$$E_- - E_+ = \frac{2J}{\Delta},$$

so the probability oscillates as

$$P_{1010 \rightarrow 0101}(t) = \sin^2\left(\frac{J}{\Delta}t\right), \quad (5.91)$$

and the first full maximum occurs at

$$t_{\text{max}} = \frac{\pi}{2} \frac{\Delta}{J}. \quad (5.92)$$

The same analysis can be done in terms of the Schrieffer–Wolff transformation.

I also suggest that you analyze the density of states when  $\Delta \gg 1$ . It splits into several energy bands, depending on the number of parallel and antiparallel spins.

- The two Néel states belong to their own energy band, creating their own quasi-subspace.
- In a chain with open boundary conditions, the same is true for the two domain wall states,  $|111\dots 000\dots\rangle$  and  $|000\dots 111\dots\rangle$ . When the chain has periodic boundary conditions, there are  $L$  states forming a quasi-subspace.
- The case with separated pairs of parallel spins is more subtle. Even though a state such as  $|0011011000\rangle$  has the same energy as the state  $|0011101000\rangle$ , and therefore belong to the same energy band, they do not couple!

### 5.4.7 Out-of-time-ordered correlators (OTOCs)

OTOCs quantify the growth of operator complexity and the sensitivity of observables to perturbations. They are defined as

$$C(t) = -\langle [\hat{W}(t), \hat{V}(0)]^2 \rangle, \quad (5.93)$$

where

$$\hat{W}(t) = e^{i\hat{H}t} \hat{W} e^{-i\hat{H}t}. \quad (5.94)$$

In spin chains one often chooses local spin operators such as

$$\hat{W} = \hat{S}_i^z, \quad \hat{V} = \hat{S}_j^z. \quad (5.95)$$

OTOCs characterize the spreading of local perturbations and are widely used as diagnostics of information scrambling and instability.

**The motivation for measuring OTOCs** comes from classical mechanics. There is a close connection between quantum commutators and classical Poisson brackets, which in turn quantify sensitivity to initial conditions in classical chaotic systems.

A defining feature of classical chaos is the exponential sensitivity of trajectories to small perturbations of the initial conditions. Consider a dynamical variable  $x(t)$  that evolves according to Hamilton's equations. A small perturbation of the initial coordinate  $x(0)$  produces a deviation

$$\delta x(t) = \frac{\partial x(t)}{\partial x(0)} \delta x(0). \quad (5.96)$$

This is because for the initial condition  $x(0), p(0)$  we have trajectory

$$x_1(t) = x(x(0), p(0), t)$$

and for the initial condition  $x(0) + \delta x(0), p(0)$  we have trajectory

$$x_2(t) = x(x(0) + \delta x(0), p(0), t) \approx x(x(0), p(0), t) + \frac{\partial x(t)}{\partial x(0)} \delta x(0) + \mathcal{O}(\delta x(0)^2),$$

so

$$\delta x(t) = x_2(t) - x_1(t) \approx \frac{\partial x(t)}{\partial x(0)} \delta x(0)$$

In chaotic systems the derivative grows exponentially,

$$\boxed{\frac{\partial x(t)}{\partial x(0)} \sim e^{\lambda t}}, \quad (5.97)$$

where  $\lambda$  is the classical Lyapunov exponent.

Therefore, the quantity  $\frac{\partial x(t)}{\partial x(0)}$  measures the amplification of small perturbations and it can be written in terms of the Poisson bracket

$$\boxed{\frac{\partial x(t)}{\partial x(0)} = \{x(t), p(0)\}}. \quad (5.98)$$

This comes from the definition of Poisson brackets. Recall that the Poisson bracket of two phase-space functions  $A(q, p)$  and  $B(q, p)$  is

$$\{A, B\} = \sum_i \left( \frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial q_i} \right). \quad (5.99)$$

Write  $x(0) = x_0$  and  $p(0) = p_0$ , where  $x_0$  and  $p_0$  are two independent variables labeling a point in phase space. We then have

$$\{x(t), p_0\} = \frac{\partial x(t)}{\partial x_0} \frac{\partial p_0}{\partial p_0} - \frac{\partial x(t)}{\partial p_0} \frac{\partial p_0}{\partial x_0} = \frac{\partial x(t)}{\partial x_0}$$

since

$$\frac{\partial p_0}{\partial p_0} = 1 \quad \text{and} \quad \frac{\partial p_0}{\partial x_0} = 0$$

In the semiclassical correspondence between classical and quantum mechanics, Poisson brackets are replaced by commutators according to

$$\{A, B\} \longrightarrow \frac{1}{i\hbar} [\hat{A}, \hat{B}]. \quad (5.100)$$

Applying this rule to Eq. (5.98) suggests that the quantum analogue of the classical sensitivity is

$$[\hat{x}(t), \hat{p}(0)]. \quad (5.101)$$

More generally, one considers two Hermitian operators  $\hat{W}$  and  $\hat{V}$ , leading to the commutator

$$[\hat{W}(t), \hat{V}(0)]. \quad (5.102)$$

If the system exhibits chaotic dynamics, the magnitude of this commutator is expected to grow rapidly with time.

The quantity used in practice is not the commutator itself but the square of the commutator,

$$C(t) = -\langle [\hat{W}(t), \hat{V}(0)]^2 \rangle. \quad (5.103)$$

The square makes the quantity positive for Hermitian operators. Squaring also removes cancellations that could occur if the commutator were averaged over states or ensembles. The expectation value of  $[\hat{W}(t), \hat{V}(0)]$  often vanishes due to symmetries.

Expanding the square reveals a four-point correlation function with a characteristic time ordering:

$$[\hat{W}(t), \hat{V}(0)]^2 = \hat{W}(t)\hat{V}(0)\hat{W}(t)\hat{V}(0) + \hat{V}(0)\hat{W}(t)\hat{V}(0)\hat{W}(t) - \hat{W}(t)\hat{V}(0)^2\hat{W}(t) - \hat{V}(0)\hat{W}(t)^2\hat{V}(0).$$

The first two terms contain operator sequences such as

$$\langle \hat{W}(t)\hat{V}(0)\hat{W}(t)\hat{V}(0) \rangle, \quad (5.104)$$

in which the operators are not ordered chronologically. These are the “out-of-time-ordered” correlators that give the OTOC its name.

### 5.4.8 Fidelity out-of-time-ordered correlators (FOTOCs)

A quantity closely related to OTOCs is the fidelity out-of-time-ordered correlator (FOTOC), which quantifies the sensitivity of the quantum state to small perturbations applied during the evolution. FOTOCs are particularly useful because they can often be measured experimentally through echo protocols.

Consider a unitary evolution generated by a Hamiltonian  $\hat{H}$ ,

$$\hat{U}(t) = e^{-i\hat{H}t}. \quad (5.105)$$

Let the system start from an initial state  $|\Psi(0)\rangle$ . At time  $t$  a small unitary perturbation is applied,

$$\hat{W}(\theta) = e^{-i\theta\hat{G}}, \quad (5.106)$$

where  $\hat{G}$  is a Hermitian operator and  $\theta$  is a small parameter that controls the perturbation strength. The system is then evolved backward in time. The resulting echo state is

$$|\Psi_{\text{echo}}(t, \theta)\rangle = \hat{U}^\dagger(t) \hat{W}(\theta) \hat{U}(t) |\Psi(0)\rangle. \quad (5.107)$$

The fidelity between the echo state and the initial state defines the FOTOC,

$$F(t, \theta) = |\langle\Psi(0)|\Psi_{\text{echo}}(t, \theta)\rangle|^2 = |\langle\Psi(0)|e^{i\hat{H}t}e^{-i\theta\hat{G}}e^{-i\hat{H}t}|\Psi(0)\rangle|^2. \quad (5.108)$$

To simplify this expression we use the identity  $\hat{U}^\dagger e^{\hat{A}} \hat{U} = e^{\hat{U}^\dagger \hat{A} \hat{U}}$ , which follows from the power-series definition of the exponential,  $e^{\hat{A}} = \sum_{n=0}^{\infty} \frac{\hat{A}^n}{n!}$ , so the unitary transformation gives

$$\hat{U}^\dagger e^{\hat{A}} \hat{U} = \hat{U}^\dagger \left( \sum_{n=0}^{\infty} \frac{\hat{A}^n}{n!} \right) \hat{U} = \sum_{n=0}^{\infty} \frac{\hat{U}^\dagger \hat{A}^n \hat{U}}{n!} = \sum_{n=0}^{\infty} \frac{(\hat{U}^\dagger \hat{A} \hat{U})^n}{n!} = e^{\hat{U}^\dagger \hat{A} \hat{U}}. \quad (5.109)$$

Applying this identity to the operator  $\hat{A} = -i\theta\hat{G}$  gives

$$\hat{U}^\dagger(t) e^{-i\theta\hat{G}} \hat{U}(t) = e^{-i\theta\hat{U}^\dagger(t)\hat{G}\hat{U}(t)}. \quad (5.110)$$

Using the Heisenberg-picture operator

$$\hat{G}(t) = \hat{U}^\dagger(t) \hat{G} \hat{U}(t), \quad (5.111)$$

the fidelity becomes

$$F(t, \theta) = \left| \langle\Psi(0)|e^{-i\theta\hat{G}(t)}|\Psi(0)\rangle \right|^2. \quad (5.112)$$

We now expand the exponential for small  $\theta$ ,

$$e^{-i\theta\hat{G}(t)} = 1 - i\theta\hat{G}(t) - \frac{\theta^2}{2}\hat{G}(t)^2 + \mathcal{O}(\theta^3). \quad (5.113)$$

Taking the expectation value gives

$$\langle e^{-i\theta\hat{G}(t)} \rangle = 1 - i\theta\langle\hat{G}(t)\rangle - \frac{\theta^2}{2}\langle\hat{G}(t)^2\rangle + \mathcal{O}(\theta^3), \quad (5.114)$$

where  $\langle \cdots \rangle \equiv \langle \Psi(0) | \cdots | \Psi(0) \rangle$ . The fidelity is the modulus squared of this quantity,

$$F(t, \theta) = \left| 1 - i\theta \langle \hat{G}(t) \rangle - \frac{\theta^2}{2} \langle \hat{G}(t)^2 \rangle \right|^2. \quad (5.115)$$

Keeping terms up to order  $\theta^2$ , we obtain

$$F(t, \theta) = 1 - \theta^2 \left( \langle \hat{G}(t)^2 \rangle - \langle \hat{G}(t) \rangle^2 \right) + \mathcal{O}(\theta^4). \quad (5.116)$$

where

$$\text{Var}[\hat{G}(t)] = \langle \hat{G}(t)^2 \rangle - \langle \hat{G}(t) \rangle^2. \quad (5.117)$$

Thus the decay of the FOTOC is governed by the growth of the variance of the operator  $\hat{G}$  in the Heisenberg picture. This connects FOTOCs directly to operator spreading and quantum chaos.

**Collective Models:** For collective spin systems it is natural to choose  $\hat{G}$  as a collective spin operator, for example

$$\hat{G} = \hat{S}_z. \quad (5.118)$$

In this case the short-time expansion becomes

$$F(t, \theta) \approx 1 - \theta^2 \left( \langle \hat{S}_z^2(t) \rangle - \langle \hat{S}_z(t) \rangle^2 \right). \quad (5.119)$$

Therefore, the decay of the FOTOC is directly controlled by the growth of collective spin fluctuations. In chaotic collective spin systems or systems with local dynamical instabilities, such as those with hyperbolic fixed points, these fluctuations can grow exponentially in time,

$$\text{Var}[\hat{S}_z(t)] \sim e^{2\lambda t}, \quad (5.120)$$

where  $\lambda$  is the Lyapunov exponent associated with the underlying classical instability.

FOTOCs are diagnostics of instability, quantum chaos, operator growth, and information scrambling. They are also closely connected to quantities such as the quantum Fisher information and the anti-squeezing of collective spin fluctuations.

#### 5.4.9 Momentum distribution in bosonic systems

In lattice boson systems the momentum distribution is a key observable,

$$n(k, t) = \frac{1}{L} \sum_{i,j} e^{ik(i-j)} \langle \hat{a}_i^\dagger(t) \hat{a}_j(t) \rangle. \quad (5.121)$$

This quantity reveals coherence properties of the bosonic gas and is routinely measured in cold-atom experiments through time-of-flight imaging.

## 5.5 Transport in 1D spin models

Transport describes how a spatial imbalance in a conserved quantity spreads through a system. In spin chains, the conserved quantity is often the local magnetization along the  $z$  direction, so transport corresponds to the spreading of

$$\hat{n}_i \equiv \hat{S}_i^z. \quad (5.122)$$

The central idea is that if magnetization is conserved globally, then any decrease of magnetization at site  $i$  must be caused by a flow of magnetization to neighboring sites. This flow is quantified by the *current operator*.

### 5.5.1 Why the current operator appears: continuity equation

For any operator  $\hat{O}$ , the Heisenberg equation of motion is

$$\frac{d\hat{O}}{dt} = i[\hat{H}, \hat{O}], \quad (5.123)$$

where we set  $\hbar = 1$ .

If  $\hat{n}_i = \hat{S}_i^z$  is the local density of a conserved quantity, then its time evolution can often be written in the form

$$\frac{d\hat{S}_i^z}{dt} = \hat{J}_{i-1} - \hat{J}_i, \quad (5.124)$$

which is the lattice version of the continuity equation. Here,  $\hat{J}_i$  is the current from site  $i$  to site  $i + 1$ .

Equation (5.124) says the following: the magnetization at site  $i$  increases if more current enters from the left than leaves to the right, and decreases if more leaves than enters. This is why the current operator is the natural quantity to study transport.

### 5.5.2 A useful commutator identity

To derive the current operator, we use the spin commutation relations

$$[\hat{S}_i^\alpha, \hat{S}_j^\beta] = i\delta_{ij} \epsilon_{\alpha\beta\gamma} \hat{S}_i^\gamma, \quad (5.125)$$

so that, in particular,

$$[\hat{S}_i^x, \hat{S}_i^z] = -i\hat{S}_i^y, \quad [\hat{S}_i^y, \hat{S}_i^z] = i\hat{S}_i^x. \quad (5.126)$$

Operators acting on different sites commute.

### 5.5.3 Current operator for the nearest-neighbor XX model

The one-dimensional XX model with nearest-neighbor couplings is

$$\hat{H}_{\text{XX}} = J \sum_{i=1}^{L-1} \left( \hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y \right) \quad (5.127)$$

for open boundary conditions.

For periodic (closed) boundary conditions, one adds the bond connecting site  $L$  back to site 1,

$$\hat{H}_{\text{XX}}^{(\text{pbc})} = J \sum_{i=1}^L \left( \hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y \right), \quad \hat{S}_{L+1}^\alpha \equiv \hat{S}_1^\alpha. \quad (5.128)$$

To derive the local current, we compute  $i[\hat{H}, \hat{S}_i^z]$ . Only the terms involving sites  $i-1, i$  and  $i, i+1$  contribute, because all other terms commute with  $\hat{S}_i^z$ . After a straightforward calculation, one finds

$$\frac{d\hat{S}_i^z}{dt} = J \left( \hat{S}_{i-1}^x \hat{S}_i^y - \hat{S}_{i-1}^y \hat{S}_i^x \right) - J \left( \hat{S}_i^x \hat{S}_{i+1}^y - \hat{S}_i^y \hat{S}_{i+1}^x \right). \quad (5.129)$$

Comparing with Eq. (5.124), the local spin current is

$$\hat{J}_i = J \left( \hat{S}_i^x \hat{S}_{i+1}^y - \hat{S}_i^y \hat{S}_{i+1}^x \right). \quad (5.130)$$

Therefore, the XX model current operator has exactly the form in Eq. (5.130).

**Open boundary conditions.** For open chains, the local current is still given by Eq. (5.130) for bonds  $i = 1, \dots, L-1$ . There is no bond between  $L$  and 1, so there is no current across that boundary.

**Periodic boundary conditions.** For periodic chains, Eq. (5.130) still holds, but now  $i = 1, \dots, L$ , with the identification  $L+1 \equiv 1$ . Thus there is also a current on the bond  $(L, 1)$ .

### 5.5.4 Current operator for the nearest-neighbor XXZ model

The XXZ Hamiltonian is

$$\hat{H}_{\text{XXZ}} = J \sum_{i=1}^{L-1} \left( \hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y + \Delta \hat{S}_i^z \hat{S}_{i+1}^z \right) \quad (5.131)$$

for open boundary conditions, and

$$\hat{H}_{\text{XXZ}}^{(\text{pbc})} = J \sum_{i=1}^L \left( \hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y + \Delta \hat{S}_i^z \hat{S}_{i+1}^z \right), \quad \hat{S}_{L+1}^\alpha \equiv \hat{S}_1^\alpha \quad (5.132)$$

for periodic boundary conditions.

The  $\hat{S}_i^z \hat{S}_{i+1}^z$  term does *not* contribute to  $i[\hat{H}, \hat{S}_i^z]$ , because it commutes with  $\hat{S}_i^z$ . Therefore, the local spin current is the same as for the XX model:

$$\hat{J}_i = J \left( \hat{S}_i^x \hat{S}_{i+1}^y - \hat{S}_i^y \hat{S}_{i+1}^x \right). \quad (5.133)$$

This is an important lesson: two Hamiltonians may have different interactions, but the current associated with a given conserved quantity may still have the same form.

### 5.5.5 Current operator for the XXZ model with second-neighbor couplings

Now consider a model with both nearest-neighbor and second-neighbor couplings:

$$\begin{aligned}\hat{H} = & J_1 \sum_i \left( \hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y + \Delta_1 \hat{S}_i^z \hat{S}_{i+1}^z \right) \\ & + J_2 \sum_i \left( \hat{S}_i^x \hat{S}_{i+2}^x + \hat{S}_i^y \hat{S}_{i+2}^y + \Delta_2 \hat{S}_i^z \hat{S}_{i+2}^z \right).\end{aligned}\quad (5.134)$$

For open chains, the sums run only over bonds that exist:

$$i = 1, \dots, L-1 \quad \text{for nearest neighbors}, \quad i = 1, \dots, L-2 \quad \text{for second neighbors.} \quad (5.135)$$

For periodic chains, the indices are taken modulo  $L$ .

In this case, magnetization can flow not only between  $i$  and  $i+1$ , but also between  $i$  and  $i+2$ . Therefore, the continuity equation is more naturally written as

$$\frac{d\hat{S}_i^z}{dt} = \left( \hat{J}_{i-1 \rightarrow i}^{(1)} - \hat{J}_{i \rightarrow i+1}^{(1)} \right) + \left( \hat{J}_{i-2 \rightarrow i}^{(2)} - \hat{J}_{i \rightarrow i+2}^{(2)} \right), \quad (5.136)$$

where

$$\hat{J}_{i \rightarrow i+1}^{(1)} = J_1 \left( \hat{S}_i^x \hat{S}_{i+1}^y - \hat{S}_i^y \hat{S}_{i+1}^x \right) \quad (5.137)$$

is the nearest-neighbor current and

$$\hat{J}_{i \rightarrow i+2}^{(2)} = J_2 \left( \hat{S}_i^x \hat{S}_{i+2}^y - \hat{S}_i^y \hat{S}_{i+2}^x \right) \quad (5.138)$$

is the second-neighbor current.

So in the presence of second-neighbor hopping or exchange, there is not a single simple nearest-neighbor current only; the current has several contributions, one for each allowed transport channel.

**Important remark.** The current operator must always be derived from the Hamiltonian through the continuity equation. Therefore, it *depends on the model*. For nearest-neighbor XX and XXZ chains, the current has the simple form in Eq. (5.133). For models with longer-range couplings, additional current terms appear.

### 5.5.6 Total current

The total current is obtained by summing the local currents over all bonds:

$$\hat{J} = \sum_i \hat{J}_i \quad (5.139)$$

for nearest-neighbor models, or

$$\hat{J} = \sum_i \hat{J}_{i \rightarrow i+1}^{(1)} + \sum_i \hat{J}_{i \rightarrow i+2}^{(2)} \quad (5.140)$$

when second-neighbor currents are also present.

The total current is especially useful in linear-response theory and in the Green–Kubo approach discussed below.

### 5.5.7 How transport is characterized

The current operator by itself does not tell us whether transport is ballistic or diffusive. Instead, it is used inside dynamical quantities whose time dependence reveals the transport regime.

The most common possibilities are:

- **Ballistic transport:** the disturbance travels with a well-defined velocity, so its width grows linearly in time and the mean-square displacement grows as  $t^2$ .
- **Diffusive transport:** the disturbance spreads like ordinary diffusion, so its mean-square displacement grows as  $t$ .
- **Subdiffusive transport:** spreading is slower than diffusion, with mean-square displacement growing as  $t^\alpha$  with  $0 < \alpha < 1$ .
- **Superdiffusive transport:** spreading is faster than diffusion but slower than ballistic, with  $1 < \alpha < 2$ .

Below we explain in detail two standard methods.

### 5.5.8 Method 1: spreading of a local excitation

This method is very intuitive and is often the best choice for beginners because it directly visualizes transport in real space.

#### Step 1: create a local excess of magnetization

Suppose the system is in some reference state or ensemble that we call “equilibrium.” This may mean, for example:

- the infinite-temperature state,
- a thermal state,
- or simply a state with no special local inhomogeneity.

Then one creates a local perturbation near the center of the chain.

When people write something like

$$\hat{S}_{L/2}^z |\text{equilibrium}\rangle, \quad (5.141)$$

they mean: act with the local magnetization operator at the middle site on the chosen reference state in order to create a state with a local magnetization imbalance.

**Why this notation can be confusing.** Strictly speaking, if  $|\text{equilibrium}\rangle$  is a pure state, then  $\hat{S}_{L/2}^z |\text{equilibrium}\rangle$  is generally *not normalized*. So, in careful notation, one should write something like

$$|\psi(0)\rangle = \frac{\hat{S}_{L/2}^z |\phi\rangle}{\sqrt{\langle \phi | (\hat{S}_{L/2}^z)^2 | \phi \rangle}}, \quad (5.142)$$

where  $|\phi\rangle$  is the reference state.

**Physical meaning.** The operator  $\hat{S}_{L/2}^z$  picks out or creates extra weight associated with magnetization at the middle site. Then one lets the system evolve and asks: how does this initially local magnetization spread?

### Example 1: simple product state

For a spin-1/2 chain with  $L = 7$ , consider

$$|\psi(0)\rangle = |\downarrow\downarrow\downarrow\uparrow\downarrow\downarrow\downarrow\rangle, \quad (5.143)$$

where the only up-spin is at the middle site. This is already a localized magnetization excitation. Its time evolution directly shows how magnetization spreads.

### Example 2: infinite-temperature correlation function

In many numerical studies, instead of preparing one special pure state, one studies the correlation function

$$C_{i,j}(t) = \frac{1}{\mathcal{D}} \text{Tr} \left[ \hat{S}_i^z(t) \hat{S}_j^z(0) \right], \quad (5.144)$$

where  $\mathcal{D}$  is the Hilbert-space dimension. This corresponds to infinite temperature. If we choose  $j = L/2$ , then  $C_{i,L/2}(t)$  tells us how magnetization that was initially localized at the middle site spreads to site  $i$  at time  $t$ .

This is often cleaner numerically than working with a single special state.

### Step 2: define the width of the packet

From the magnetization profile, define the mean-square displacement

$$x^2(t) = \sum_i (i - i_0)^2 p_i(t), \quad (5.145)$$

where  $i_0$  is the site where the excitation started, and  $p_i(t)$  is a normalized profile. For example, one may use

$$p_i(t) = \frac{C_{i,i_0}(t)}{\sum_j C_{j,i_0}(t)} \quad (5.146)$$

when the denominator is nonzero and the profile is positive, or use a suitably normalized excess density.

### Step 3: determine the transport exponent

One then fits the growth of the mean-square displacement to

$$x^2(t) \sim t^\alpha. \quad (5.147)$$

The exponent  $\alpha$  determines the transport regime:

$$\alpha = 2 \quad \text{ballistic}, \quad \alpha = 1 \quad \text{diffusive}, \quad 0 < \alpha < 1 \quad \text{subdiffusive}, \quad 1 < \alpha < 2 \quad \text{superdiffusive}. \quad (5.148)$$

**Why this works.** If particles or magnetization move almost freely, the packet expands linearly in space, so its squared width grows as  $t^2$ . If the motion is random and resembles a random walk, then the squared width grows as  $t$ . Slower growth indicates inhibited transport.

### Advantages and disadvantages of Method 1

#### Advantages.

- Very intuitive.
- Gives direct real-space pictures of spreading.
- Works naturally for open boundary conditions.
- Especially useful in numerical time evolution methods.

#### Disadvantages.

- Finite-size effects appear when the excitation reaches the boundaries.
- Extracting a clean exponent  $\alpha$  may require long times and large systems.
- One must define the initial perturbation carefully.

### 5.5.9 Method 2: current autocorrelation and the Green–Kubo approach

This method uses the total current operator and is the standard route in linear-response theory.

#### Step 1: define the total current

For nearest-neighbor XX or XXZ chains,

$$\hat{J} = \sum_i J \left( \hat{S}_i^x \hat{S}_{i+1}^y - \hat{S}_i^y \hat{S}_{i+1}^x \right). \quad (5.149)$$

For open chains, the sum runs over existing bonds only. For periodic chains, it includes the bond  $(L, 1)$  as well.

#### Step 2: compute the current autocorrelation function

Define

$$C_J(t) = \langle \hat{J}(t) \hat{J}(0) \rangle, \quad (5.150)$$

where the average may be taken in thermal equilibrium or at infinite temperature.

This quantity tells us how much memory the current keeps of its initial value. If the current remains correlated with itself for very long times, transport tends to be ballistic. If the correlation decays sufficiently fast, transport tends to be diffusive.

**Step 3: diffusion constant and Drude weight**

In linear-response theory, the conductivity can be decomposed as

$$\sigma(\omega) = 2\pi D \delta(\omega) + \sigma_{\text{reg}}(\omega), \quad (5.151)$$

where  $D$  is the *Drude weight*.

- If  $D > 0$ , there is a persistent dissipationless part of the transport, which signals *ballistic* transport.
- If  $D = 0$  and the current correlation decays normally, transport is typically *diffusive*.

The diffusion constant is related to the time integral of the current autocorrelation,

$$D_{\text{diff}} \propto \int_0^\infty dt C_J(t), \quad (5.152)$$

up to model-dependent constants such as temperature and susceptibility.

**Physical interpretation**

This method measures the memory of the current:

- **Ballistic transport:** the current does not fully decay; it keeps memory for arbitrarily long times.
- **Diffusive transport:** the current loses memory sufficiently fast, but the integral in Eq. (5.152) remains finite.
- **Anomalous transport:** the decay is neither fully persistent nor normal enough to give simple diffusion.

**Advantages and disadvantages of Method 2****Advantages.**

- Closely connected to conductivity measurements and linear-response theory.
- Very powerful for translationally invariant systems.
- Particularly natural for periodic boundary conditions.

**Disadvantages.**

- Conceptually more abstract than Method 1.
- More difficult for beginners.
- In finite systems, long-time behavior may be hard to interpret.
- For nonintegrable systems, extracting asymptotic behavior from exact diagonalization can be challenging.

### 5.5.10 Which method is best for numerical analysis of spin models?

There is no single best method for all purposes, but for most undergraduate-level numerical studies the most practical choice is usually **Method 1**, the spreading of a local excitation.

**Why Method 1 is often best numerically.**

- It is easy to visualize.
- It works naturally with time evolution of pure states.
- It is well suited for exact diagonalization and tensor-network methods.
- One immediately sees whether the packet spreads quickly, slowly, or barely at all.

**When Method 2 is preferable.** Method 2 is especially valuable when one wants:

- a direct connection to conductivity,
- a comparison with linear-response theory,
- or a careful study of ballistic transport through the Drude weight.

### 5.5.11 Typical expectations for common models

For the one-dimensional nearest-neighbor XX model, transport of  $S^z$  is typically ballistic. This is because the model maps to free fermions, and the excitations propagate without scattering.

For the nearest-neighbor XXZ model, the situation depends on parameters and on the sector studied. Different regimes can show ballistic, diffusive, or anomalous behavior.

For XXZ chains with second-neighbor couplings, integrability is broken, and transport often becomes more diffusive, although the details depend on energy, filling, anisotropy, and system size.

## 5.6 Temporal Fluctuations



# Chapter 6

## Many-body localization and multifractality

### 6.1 Many-Body Localization

### 6.2 Multifractality



# Chapter 7

## Floquet systems

Many physical systems are subject to external driving that varies in time. Examples include atoms in oscillating electromagnetic fields, electrons in solids under laser illumination, and spins manipulated by time-dependent magnetic fields.

We will focus first on **periodically driven quantum systems**, also known as **Floquet systems**. These are systems whose Hamiltonian satisfies

$$H(t + T) = H(t), \quad (7.1)$$

where  $T$  is the period of the drive.

### Why are Floquet systems important?

- They allow us to engineer new phases of matter (“Floquet engineering”).
- They can generate effective interactions that do not exist in static systems.
- They are widely used in quantum control and quantum computing.
- They provide a natural setting to study thermalization, chaos, and heating in isolated quantum systems.

The central idea is that even though the Hamiltonian depends on time, its periodicity allows us to describe the dynamics in a simple way.

## 7.1 Floquet theorem and Floquet states

Floquet’s theorem applies to linear differential equations with periodic coefficients. It states that if the dynamics of a system is periodic in time, then its solutions can be written as the product of a periodic function and an exponential evolution. It is analog of Bloch’s theorem for periodic crystals, but for time instead of space.

The mathematical statement is as follows. If the system is described by

$$\frac{d}{dt}x(t) = A(t)x(t)$$

where the matrix  $A(t)$  is periodic with period  $T$ ,

$$A(t + T) = A(t),$$

then the solutions can be written as

$$x(t) = P(t)e^{Rt},$$

where

- $P(t)$  is a periodic matrix,  $P(t + T) = P(t)$ ,
- $R$  is a constant (time-independent) matrix.

This is precisely the situation encountered for periodically driven quantum systems, where the Hamiltonian satisfies  $H(t + T) = H(t)$  [Eq. (7.1)] and the corresponding Schrödinger equation is

$$\frac{d}{dt}|\Psi(t)\rangle = -iH(t)|\Psi(t)\rangle. \quad (7.2)$$

According to Floquet's theorem, the solutions can be written as

$$\boxed{|\psi_\alpha(t)\rangle = e^{-i\varepsilon_\alpha t} |\phi_\alpha(t)\rangle}, \quad (7.3)$$

where

- $|\psi_\alpha(t)\rangle$  are called **Floquet states**,
- $|\phi_\alpha(t)\rangle$  are called **Floquet modes** and they are periodic functions,

$$\boxed{|\phi_\alpha(t + T)\rangle = |\phi_\alpha(t)\rangle}$$

- $\varepsilon_\alpha$  are called **quasienergies**.

In what follows, we will learn how to obtain  $|\phi_\alpha(0)\rangle$  and  $\varepsilon_\alpha$ .

The states  $|\psi_\alpha(t)\rangle$  form a particular set of solutions of the Schrödinger equation, obtained by choosing the initial condition

$$|\psi_\alpha(0)\rangle = |\phi_\alpha(0)\rangle.$$

They provide a natural basis for describing the dynamics of periodically driven systems.

In particular, any arbitrary initial state  $|\Psi(0)\rangle$  can be expanded in this basis as

$$|\Psi(0)\rangle = \sum_{\alpha} c_{\alpha} |\phi_{\alpha}(0)\rangle,$$

so that its time evolution follows as

$$|\Psi(t)\rangle = \sum_{\alpha} c_{\alpha} e^{-i\varepsilon_{\alpha} t} |\phi_{\alpha}(t)\rangle.$$

This decomposition separates the dynamics into a simple phase evolution governed by the quasienergies and a periodic motion encoded in the Floquet modes.

The Floquet states in Eq. (7.3) play a role analogous to the stationary states in time-independent systems. In the latter case, if  $H|\psi_n\rangle = E_n|\psi_n\rangle$ , the stationary states are  $|\psi_n(t)\rangle = e^{-iE_n t}|\psi_n(0)\rangle$ , with  $|\psi_n(0)\rangle = |\psi_n\rangle$ . Similarly, Floquet states evolve with a simple phase factor, but with an **additional periodic modulation** encoded in  $|\phi_\alpha(t)\rangle$ . If, however, we observe the system stroboscopically at multiples of the period,  $t = nT$ , the picture simplifies even further, as we shall see in the next subsections.

## 7.2 Floquet operator

Since the Schrödinger equation now involves a time-dependent Hamiltonian,

$$i \frac{d}{dt} |\Psi(t)\rangle = H(t) |\Psi(t)\rangle. \quad (7.4)$$

we **CANNOT** write  $|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$ . Instead, we have

$$|\Psi(t)\rangle = U(t, 0) |\Psi(0)\rangle. \quad (7.5)$$

The time evolution operator from time 0 to time  $t$  is given by

$$U(t, 0) = \mathcal{T} \exp \left( -i \int_0^t H(t') dt' \right), \quad (7.6)$$

where  $\mathcal{T}$  denotes time ordering.

Because the Hamiltonian is periodic, a special role is played by the evolution over one full period  $T$ . This defines the **Floquet operator**

$$U_F \equiv U(T, 0) = \mathcal{T} \exp \left( -i \int_0^T H(t) dt \right). \quad (7.7)$$

**Key idea:** Once we know  $U_F$ , we can determine the evolution at all times that are integer multiples of  $T$ .

### 7.2.1 Stroboscopic evolution

If we observe the system only at times  $t = nT$  (with  $n$  integer), we obtain the so-called **stroboscopic evolution**:

$$|\Psi(nT)\rangle = U_F^n |\Psi(0)\rangle. \quad (7.8)$$

Instead of solving a continuous-time Schrödinger equation, we repeatedly apply the same operator  $U_F$ . As it will become evident in the next subsection, this reduces a time-dependent problem to an effective time-independent one.

### 7.2.2 Floquet modes and quasienergies

The eigenstates of the Floquet operator are

$$\boxed{U_F |\phi_\alpha\rangle = \eta_\alpha |\phi_\alpha\rangle}. \quad (7.9)$$

These **Floquet eigenstates** correspond to the **Floquet modes** in Eq. (7.3) at time  $t = 0$ , that is,  $|\phi_\alpha\rangle = |\phi_\alpha(0)\rangle$ .

Since  $U_F$  is unitary, the eigenvalues  $\eta_\alpha$  lie on the unit circle, that is, they are pure phases,

$$\eta_\alpha = e^{-i\theta_\alpha} = e^{-i\varepsilon_\alpha T}.$$

The **quasienergies** are defined from the phases  $\theta_\alpha$  as

$$\varepsilon_\alpha = \frac{\theta_\alpha}{T}. \quad (7.10)$$

Thus, the Floquet eigenstates diagonalize the evolution operator over one period,

$$U(T, 0) |\phi_\alpha\rangle = e^{-i\varepsilon_\alpha T} |\phi_\alpha\rangle,$$

just as energy eigenstates diagonalize the Hamiltonian in time-independent systems,

$$H |E_n\rangle = E_n |E_n\rangle.$$

#### IMPORTANT!!

We now see that if we observe the system only at times  $t = nT$  (integer multiples of the period), the explicitly time-dependent problem simplifies dramatically. For  $|\psi_\alpha(0)\rangle = |\phi_\alpha\rangle$ , the evolution after one period is

$$|\psi_\alpha(T)\rangle = U(T, 0) |\psi_\alpha(0)\rangle = U_F |\phi_\alpha(0)\rangle, \quad (7.11)$$

which implies that

$$\boxed{|\psi_\alpha(T)\rangle = e^{-i\varepsilon_\alpha T} |\psi_\alpha(0)\rangle}. \quad (7.12)$$

More generally, at stroboscopic times  $t = nT$ , we obtain

$$\boxed{|\psi_\alpha(nT)\rangle = e^{-in\varepsilon_\alpha T} |\psi_\alpha(0)\rangle}. \quad (7.13)$$

Therefore, when viewed stroboscopically, the dynamics reduces to that of an effective time-independent problem governed by the unitary operator  $U_F$ . The quasienergies  $\varepsilon_\alpha$  play a role analogous to energies in static systems, and the Floquet states behave like stationary states under discrete-time evolution.

---

**Review of unitary matrices.** A matrix  $U$  is called *unitary* if

$$U^\dagger U = U U^\dagger = I, \quad (7.14)$$

where  $U^\dagger$  denotes the Hermitian conjugate of  $U$ .

**Orthonormal columns.** Let the columns of  $U$  be denoted by  $\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_N$ . Then the matrix element of  $U^\dagger U$  in row  $i$ , column  $j$  is

$$(U^\dagger U)_{ij} = \mathbf{u}_i^\dagger \mathbf{u}_j. \quad (7.15)$$

Since  $U^\dagger U = I$ , we obtain

$$\mathbf{u}_i^\dagger \mathbf{u}_j = \delta_{ij}. \quad (7.16)$$

Thus, the columns of a unitary matrix form an orthonormal set of vectors.

**Eigenvalues have modulus one.** Let  $\lambda$  be an eigenvalue of  $U$  with eigenvector  $\mathbf{v} \neq 0$ , so that

$$U\mathbf{v} = \lambda\mathbf{v}. \quad (7.17)$$

Consider the inner product:

$$\langle U\mathbf{v}, U\mathbf{v} \rangle = \langle U\mathbf{v}, U\mathbf{v} \rangle = \langle \mathbf{v} | U^\dagger U | \mathbf{v} \rangle. \quad (7.18)$$

Using the unitarity of  $U$ , we have

$$\langle U\mathbf{v} | U\mathbf{v} \rangle = \langle \mathbf{v} | \mathbf{v} \rangle. \quad (7.19)$$

Using the eigenvalue equation,

$$\langle U\mathbf{v} | U\mathbf{v} \rangle = \langle \lambda\mathbf{v} | \lambda\mathbf{v} \rangle = |\lambda|^2 \langle \mathbf{v} | \mathbf{v} \rangle. \quad (7.20)$$

Since  $\mathbf{v} \neq 0$

$$|\lambda|^2 \langle \mathbf{v} | \mathbf{v} \rangle = \langle \mathbf{v} | \mathbf{v} \rangle \Rightarrow |\lambda| = 1. \quad (7.21)$$

Hence, all eigenvalues of a unitary matrix lie on the unit circle in the complex plane.

---

— END of review —

### 7.2.3 Floquet Hamiltonian

It is often useful to define an effective Hamiltonian  $H_F$  such that

$$U_F \equiv U(T, 0) = e^{-iH_F T}. \quad (7.22)$$

The operator  $H_F$  is called the **Floquet Hamiltonian**. It governs the dynamics at stroboscopic times  $t = nT$  and plays a role analogous to the Hamiltonian in time-independent systems.

The eigenstates of  $H_F$  coincide with those of the Floquet operator. Indeed, if

$$U_F |\phi_\alpha\rangle = e^{-i\varepsilon_\alpha T} |\phi_\alpha\rangle,$$

then

$$H_F|\phi_\alpha\rangle = \varepsilon_\alpha|\phi_\alpha\rangle,$$

where  $\varepsilon_\alpha$  are the quasienergies, defined modulo  $2\pi/T$ .

Thus, the Floquet Hamiltonian provides an effective time-independent description of the system when observed at stroboscopic times. In particular,

$$U(nT, 0) = (U_F)^n = e^{-iH_F nT}.$$

However, it is important to note that  $H_F$  is not unique, since the logarithm of  $U_F$  is defined only up to multiples of  $2\pi/T$ . Moreover, obtaining  $H_F$  exactly can be challenging in practice.

In many relevant situations, particularly in the high-frequency regime (when the driving period  $T$  is short), one can approximate  $H_F$  using systematic expansions. The leading-order approximation is given by the **average Hamiltonian**,

$$H_F \approx \frac{1}{T} \int_0^T H(t) dt,$$

which captures the dominant effect of the drive.

Higher-order corrections can be obtained through methods such as the Magnus expansion.

**Magnus expansion.** Consider the time-evolution operator

$$U(t) = \mathcal{T} \exp \left( -i \int_0^t H(t_1) dt_1 \right), \quad (7.23)$$

where  $H(t)$  is the Hamiltonian.

The Magnus expansion writes

$$U(t) = \exp(\Omega(t)), \quad (7.24)$$

with

$$\Omega(t) = \Omega_0(t) + \Omega_1(t) + \Omega_2(t) + \cdots. \quad (7.25)$$

**Zeroth order:**

$$\Omega_0(t) = -i \int_0^t dt_1 H(t_1). \quad (7.26)$$

**First order:**

$$\Omega_1(t) = -\frac{1}{2} \int_0^t dt_1 \int_0^{t_1} dt_2 [H(t_1), H(t_2)]. \quad (7.27)$$

**Second order:**

$$\begin{aligned} \Omega_2(t) = \frac{i}{6} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 & \left( [H(t_1), [H(t_2), H(t_3)]] \right. \\ & \left. + [H(t_3), [H(t_2), H(t_1)]] \right). \end{aligned} \quad (7.28)$$

These approximations form the basis of **Floquet engineering**, where periodic driving is used to design effective Hamiltonians with desired properties that may not be accessible in static systems.

Despite the subtleties, the Floquet Hamiltonian is an important tool, as it allows one to interpret periodically driven systems in terms of an effective static Hamiltonian.

### 7.2.4 Practical recipe to compute quasienergies

The eigenphase  $\theta_\alpha$  is not unique. Since

$$e^{-i\theta_\alpha} = e^{-i(\theta_\alpha + 2\pi)},$$

the eigenphases are defined modulo  $2\pi$ . We then choose a interval of length  $2\pi$  (a branch cut), typically  $\theta_\alpha \in [-\pi, \pi)$ , although  $\theta_\alpha \in [0, 2\pi)$  is also correct.

We now explain step by step how to extract quasienergies in practice.

#### 1. Diagonalize the Floquet operator

Compute  $U(T)$  and diagonalize it:

$$U(T) |\phi_\alpha\rangle = \eta_\alpha |\phi_\alpha\rangle.$$

#### 2. Extract the phase $\theta_\alpha$

In practice, numerical diagonalization gives  $\eta_\alpha$  as a complex number,

$$\eta_\alpha = x + iy,$$

but we want  $\theta_\alpha$  from

$$\eta_\alpha = e^{-i\theta_\alpha} = \cos \theta_\alpha - i \sin \theta_\alpha.$$

This means that

$$\begin{aligned} x &= \cos \theta_\alpha = \cos(-\theta_\alpha) = \cos \chi, \\ y &= -\sin \theta_\alpha = \sin(-\theta_\alpha) = \sin \chi, \end{aligned} \tag{7.29}$$

where we defined

$$\boxed{\chi = -\theta_\alpha}.$$

Therefore

$$\tan \chi = \frac{y}{x}.$$

To extract  $\chi$ , and thus  $\theta_\alpha$ , we need to use the complex argument,

$$\chi = \arg(\eta_\alpha) = \text{atan2}(y, x)$$

$$\theta_\alpha = -\chi = -\arg(\eta_\alpha).$$

Notice that we use `atan2` not `arctan(y/x)`. This is because `arctan(y/x)` uses the ratio  $y/x$ , so it cannot distinguish between opposite directions and gives  $\theta_\alpha \in (-\pi/2, \pi/2)$ . For example,

$$\arctan\left(\frac{1/\sqrt{2}}{1/\sqrt{2}}\right) = \arctan\left(\frac{-1/\sqrt{2}}{-1/\sqrt{2}}\right)$$

both give  $\pi/4$ , but the correct angles are

$$\arctan2\left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right) = \pi/4$$

and

$$\arctan2\left(-\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}\right) = -3\pi/4.$$

The complex argument `atan2` determines the correct quadrant and gives

$$\theta_\alpha \in (-\pi, \pi].$$

Most programming languages provide a function for this:

- Python: `theta = -np.angle(eta)`,  
or equivalently,  
`np.arctan2(eta.imag, eta.real)`
- MATLAB: `theta = -angle(eta)`
- Mathematica: `theta = -Arg[eta]`
- Fortran: `theta = -atan2(aimag(eta), real(eta))`

### 3. Compute the quasienergies

Once  $\theta_\alpha$  is obtained, compute

$$\varepsilon_\alpha = \frac{\theta_\alpha}{T}.$$

Since  $\theta_\alpha$  is already in  $(-\pi, \pi]$ , then the quasienergies automatically lie in

$$[-\pi/T, \pi/T],$$

which is the standard choice.

### 4. (Optional) Changing the branch

Sometimes one may want quasienergies in  $[0, 2\pi/T]$ . This can be done by shifting negative values:

$$\theta_\alpha \rightarrow \begin{cases} \theta_\alpha, & \theta_\alpha \geq 0, \\ \theta_\alpha + 2\pi, & \theta_\alpha < 0. \end{cases}$$

Then compute  $\varepsilon_\alpha = \theta_\alpha/T$ .

### 5. Sort the quasienergies

Finally, sort  $\varepsilon_\alpha$  in increasing order for visualization and analysis.

## Physical interpretation

The quasienergies  $\varepsilon_\alpha$  play a role analogous to energies in time-independent systems, but are defined modulo  $2\pi/T$  due to the periodic driving. This periodicity is a feature of Floquet systems and underlies many of their unique properties.

### 7.2.5 Using quasienergies to diagnose chaos

To determine whether the system is chaotic or not, one studies the statistical properties of the quasienergy spectrum. The most common diagnostic is the distribution of nearest-neighbor spacings. Before describing the procedure, we first discuss the random-matrix ensembles used to benchmark quasienergy statistics in physical models.

#### Circular random-matrix ensembles

In Floquet systems, the time-evolution operator  $U_F$  is unitary. Chaotic Floquet systems are therefore described by random matrices drawn from the **circular ensembles**.

**Circular Unitary Ensemble (CUE).** The CUE consists of unitary matrices distributed uniformly (with respect to the Haar measure) over the unitary group. It describes systems without time-reversal symmetry.

**Circular Orthogonal Ensemble (COE).** The COE consists of unitary matrices that are also symmetric,

$$U = U^T,$$

and describes systems with time-reversal symmetry.

#### How to generate these matrices in practice

**CUE matrices.** A random matrix from the CUE can be generated in a practical way starting from a completely random complex matrix. The idea is to turn a set of random vectors into an orthonormal basis, which then forms a unitary matrix.

1. Generate an  $N \times N$  complex matrix  $Z$  whose entries are independent Gaussian random variables,

$$Z_{jk} = x_{jk} + iy_{jk},$$

where  $x_{jk}$  and  $y_{jk}$  are independent real Gaussian variables.

The columns of  $Z$  are therefore random complex vectors. However, they are not orthogonal to one another and are not normalized, so  $Z$  is not unitary.

2. Perform a QR decomposition,

$$Z = QR.$$

Here:

- $Q$  is a matrix whose columns are orthonormal,
- $R$  is an upper-triangular matrix.

The important point is that the columns of  $Q$  are obtained by orthonormalizing the columns of  $Z$  (this is closely related to the Gram–Schmidt procedure).

Since the columns of  $Q$  are orthonormal,  $Q$  satisfies

$$Q^\dagger Q = I,$$

so  $Q$  is unitary.

3. At this stage,  $Q$  is unitary, but there is still an ambiguity: each column of  $Q$  can be multiplied by a complex phase factor without changing orthonormality. For example, if one column is multiplied by  $e^{i\varphi}$ , it is still normalized and still orthogonal to the others.

This ambiguity is compensated by the matrix  $R$ . Therefore, the QR decomposition is not unique unless we impose an additional convention.

4. To remove this ambiguity, we adjust the phases so that the diagonal entries of  $R$  are real and positive.

To do this, write each diagonal entry of  $R$  as

$$R_{jj} = |R_{jj}|e^{i\varphi_j}.$$

Then define a diagonal matrix

$$D = \text{diag}(e^{i\varphi_1}, e^{i\varphi_2}, \dots, e^{i\varphi_N}).$$

Now redefine

$$Q' = QD, \quad R' = D^{-1}R.$$

This does not change the product:

$$Q'R' = (QD)(D^{-1}R) = QR = Z,$$

but now the diagonal entries of  $R'$  are real and positive.

5. The matrix

$$U = Q'$$

is then a random unitary matrix drawn from the CUE.

**COE matrices.** A random matrix from the COE can be constructed from a CUE matrix  $U$  via

$$U_{\text{COE}} = U_{\text{CUE}} U_{\text{CUE}}^T.$$

The resulting matrix  $U_{\text{COE}}$  is unitary and symmetric, as required for the COE.

*Unitarity.* Since  $U_{\text{CUE}}$  is unitary, we have

$$\begin{aligned} U_{\text{COE}}^\dagger U_{\text{COE}} &= (U_{\text{CUE}} U_{\text{CUE}}^T)^\dagger (U_{\text{CUE}} U_{\text{CUE}}^T) \\ &= U_{\text{CUE}}^* U_{\text{CUE}}^\dagger U_{\text{CUE}} U_{\text{CUE}}^T \\ &= U_{\text{CUE}}^* U_{\text{CUE}}^T \\ &= I, \end{aligned}$$

where we used  $U^\dagger U = I$  and  $U^* U^T = I$ .

*Symmetry.* The matrix  $U_{\text{COE}}$  is symmetric because

$$U_{\text{COE}}^T = (U_{\text{CUE}} U_{\text{CUE}}^T)^T = U_{\text{CUE}} U_{\text{CUE}}^T = U_{\text{COE}}.$$

## PROCEDURE TO ANALYZE QUASIENERGY LEVEL STATISTICS

### Step 1: Order the quasienergies

Choose a branch for the quasienergies, for example

$$\varepsilon_\alpha \in [-\pi/T, \pi/T),$$

and sort them in increasing order,

$$\varepsilon_1 < \varepsilon_2 < \cdots < \varepsilon_{\mathcal{N}}.$$

Equivalently, one may work directly with the eigenphases

$$\theta_\alpha \in [-\pi, \pi),$$

sorted in increasing order.

### Step 2: Compute the spacings

The nearest-neighbor spacings are

$$s_\alpha = \varepsilon_{\alpha+1} - \varepsilon_\alpha.$$

If one works with eigenphases instead, then

$$s_\alpha = \theta_{\alpha+1} - \theta_\alpha.$$

Because quasienergies live on a circle, one must also include the spacing across the boundary,

$$s_{\mathcal{N}} = \theta_1 + 2\pi - \theta_{\mathcal{N}}.$$

### Step 3: Normalize the spacings

The spacing distribution should be computed using normalized spacings,

$$\tilde{s}_\alpha = \frac{s_\alpha}{\langle s \rangle},$$

where  $\langle s \rangle$  is the average spacing.

If the calculation is done with eigenphases on the interval  $[-\pi, \pi)$ , then the mean spacing is simply

$$\langle s \rangle = \frac{2\pi}{\mathcal{N}},$$

since

$$\langle s \rangle = \frac{s_1 + s_2 + \dots + s_{\mathcal{N}-1} + s_{\mathcal{N}}}{\mathcal{N}} = \frac{(\theta_2 - \theta_1) + (\theta_3 - \theta_2) + \dots + (\theta_{\mathcal{N}} - \theta_{\mathcal{N}-1}) + (\theta_1 + 2\pi - \theta_{\mathcal{N}})}{\mathcal{N}}$$

### Why normalize the spacings?

The raw spacings

$$s_\alpha = \theta_{\alpha+1} - \theta_\alpha$$

depend on the total number of levels and therefore on the system size. The average spacing scales as

$$\langle s \rangle = \frac{2\pi}{\mathcal{N}}.$$

To compare spectra of different systems and to test universal predictions from random matrix theory, it is necessary to remove this trivial scale. This is achieved by defining the normalized spacings

$$\tilde{s}_\alpha = \frac{s_\alpha}{\langle s \rangle},$$

which satisfy

$$\langle \tilde{s} \rangle = 1.$$

The statistical properties of  $\tilde{s}_\alpha$  reflect genuine correlations between levels, such as level repulsion, and can be directly compared with universal distributions (Poisson, COE, CUE). Without this normalization, the spacing distribution would depend on system size and would not reveal universal behavior.

### Do we need unfolding?

For Floquet systems, one usually works with the eigenphases of the unitary Floquet operator, which lie on the unit circle. In this case, the average density of phases is constant along the circle, so for nearest-neighbor spacing statistics one typically **does not need unfolding**. It is enough to sort the phases and divide the spacings by the mean spacing.

This is one advantage of Floquet spectra over energy spectra of time-independent Hamiltonians, where unfolding is often necessary because the density of states varies with energy.

**Step 4: Compare with the expected distributions**

The behavior of the spacing distribution reveals whether the system is regular or chaotic.

**Integrable or regular systems.** If the system is regular, the quasienergies are essentially uncorrelated, and the spacing distribution is approximately Poissonian,

$$P(s) = e^{-s}.$$

In this case, level crossings are common and there is no level repulsion.

**Chaotic systems.** If the system is chaotic, the quasienergies repel each other and the spacing distribution follows random-matrix theory. The precise form depends on the symmetries of the Floquet operator.

For example:

- if the Floquet operator has time-reversal symmetry and belongs to the circular orthogonal ensemble (COE), then the spacing distribution is well approximated by the Wigner-Dyson form

$$P_{\text{COE}}(s) \approx \frac{\pi}{2} s e^{-\pi s^2/4};$$

- if time-reversal symmetry is absent and the Floquet operator belongs to the circular unitary ensemble (CUE), then the spacing distribution is approximately

$$P_{\text{CUE}}(s) \approx \frac{32}{\pi^2} s^2 e^{-4s^2/\pi}.$$

**Very important: resolve symmetries first**

Before computing level-spacing statistics, one must diagonalize the Floquet operator separately in each symmetry sector. If different symmetry sectors are mixed together, the spacing distribution can look artificially Poissonian even when the dynamics is chaotic.

**Alternative diagnostic: spacing ratios**

A useful alternative, which avoids even the normalization by the mean spacing, is the ratio of consecutive spacings,

$$\tilde{r}_\alpha = \frac{\min(s_\alpha, s_{\alpha-1})}{\max(s_\alpha, s_{\alpha-1})}.$$

Its average value distinguishes regular and chaotic spectra:

- Poisson:  $\langle \tilde{r} \rangle \approx 0.386$ ,
- COE:  $\langle \tilde{r} \rangle \approx 0.536$ ,
- CUE:  $\langle \tilde{r} \rangle \approx 0.603$ .

This ratio method is often convenient in numerical work.

### 7.3 Example 1: Piecewise constant drive (spin chain)

We will focus on two examples that will allow us to get a general picture of Floquet systems and the techniques used to study them.

For the first example, consider a spin- $\frac{1}{2}$  chain with a two-step periodic drive:

$$H(t) = \begin{cases} H_1, & 0 \leq t < T/2, \\ H_2, & T/2 \leq t < T, \end{cases} \quad (7.30)$$

with

$$H_1 = J \sum_{i=1}^{L-1} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y), \quad (7.31)$$

$$H_2 = J\Delta \sum_{i=1}^{L-1} S_i^z S_{i+1}^z + \epsilon_1 S_1^z. \quad (7.32)$$

Notice that  $H_2$  includes a defect on site 1 to break symmetries, such as parity and spin reversal. We also assume that  $\Delta \neq 1$  and open boundaries.

#### Step 1: Evolution within each interval

In each half-period, the Hamiltonian is **time independent**. Therefore, the evolution operator is simply:

$$U_1 = e^{-iH_1 T/2}, \quad U_2 = e^{-iH_2 T/2}. \quad (7.33)$$

#### Step 2: One-period evolution

The total evolution over one period is obtained by composing the two steps:

$$U_F = e^{-iH_2 T/2} e^{-iH_1 T/2}. \quad (7.34)$$

**ATTENTION!** The order matters because, in general,

$$[H_1, H_2] \neq 0.$$

$\Rightarrow$  **Numerical remark:** Since  $H_1$  and  $H_2$  are time independent within each interval, the exponentials  $e^{-iH_2 T/2}$  and  $e^{-iH_1 T/2}$  can be computed using exact diagonalization or standard matrix exponential routines.

**ATTENTION!** If exact diagonalization is used, care must be taken to express both exponentials in the same basis before multiplying them, since  $H_1$  and  $H_2$  generally have different eigenbases. Each exponential must therefore be transformed back to a common basis (e.g., the computational basis) before constructing the Floquet operator.

### 7.3.1 Symmetry considerations

Both  $H_1$  and  $H_2$  conserve the total magnetization in the  $z$ -direction:

$$S_{\text{tot}}^z = \sum_i S_i^z. \quad (7.35)$$

Therefore,

$$[U_F, S_{\text{tot}}^z] = 0.$$

#### Consequences:

- The Hilbert space splits into sectors of fixed magnetization.
- The dynamics remains confined to the sector where the initial state lives.
- Numerical calculations can be performed in each sector independently, greatly reducing computational cost.
- Chaos must be analyzed within each symmetry sector.

### 7.3.2 Average Hamiltonian and Magnus Expansion

As mentioned above, computing the Floquet Hamiltonian  $H_F$  exactly is, in general, difficult. However, for short driving periods  $T$  (high-frequency driving), one can approximate  $H_F$  using systematic expansions.

**Average Hamiltonian.** To leading order, the Floquet Hamiltonian is given by the time average of the Hamiltonian over one period:

$$H_F^{(0)} = \frac{1}{T} \int_0^T H(t) dt. \quad (7.36)$$

For the two-step drive considered here, this becomes

$$H_F^{(0)} = \frac{H_1 + H_2}{2}, \quad (7.37)$$

which gives the integrable 1D XXZ model with nearest-neighbor couplings. This approximation captures the dominant effect of the drive when  $T$  is small.

**Magnus expansion.** Higher-order corrections to  $H_F$  can be obtained using the Magnus expansion. The first correction is

$$H_F \approx H_F^{(0)} + \frac{1}{2iT} \int_0^T dt_1 \int_0^{t_1} dt_2 [H(t_1), H(t_2)] + \dots \quad (7.38)$$

For the piecewise drive, the Magnus expansion is equivalent to the Baker–Campbell–Hausdorff (BCH) expansion. In this case, since

$$U_F = e^{-iH_2 T/2} e^{-iH_1 T/2} = \exp \left[ -i \frac{T}{2} (H_2 + H_1) + \frac{1}{2} \left[ -iH_2 \frac{T}{2}, -iH_1 \frac{T}{2} \right] + \mathcal{O}(T^3) \right],$$

we find that

$$H_F \approx \frac{H_1 + H_2}{2} - \frac{iT}{8}[H_2, H_1] + \mathcal{O}(T^2). \quad (7.39)$$

These higher-order terms generate new effective interactions that are not present in  $H_1$  or  $H_2$  individually. This mechanism underlies **Floquet engineering**, where periodic driving is used to design effective Hamiltonians with tailored properties.

### 7.3.3 Level statistics

The level statistics of the quasienergies  $\{\varepsilon_\alpha\}$  provide a diagnostic of integrability and chaos.

**Small driving period** ( $T \ll 1$ ). In the high-frequency regime, the Floquet Hamiltonian is well approximated by the average Hamiltonian,

$$H_F \approx \frac{H_1 + H_2}{2}.$$

In this limit, the system behaves approximately as a time-independent XXZ-type Hamiltonian, which is integrable. The quasienergy level statistics are therefore expected to follow a **Poisson distribution**,

$$P(s) = e^{-s}.$$

**Intermediate and large  $T$ .** As the driving period increases, higher-order terms in the Magnus expansion become important. These involve commutators such as  $[H_1, H_2]$  and generically break integrability by generating more complex interactions. As a result, the system becomes chaotic, and the quasienergy statistics are expected to follow **Wigner-Dyson statistics**. Since the Floquet operator is time-reversal symmetric in this case, the appropriate ensemble is the **circular orthogonal ensemble (COE)**.

Thus, by tuning the driving period  $T$ , one can induce a transition from integrable to chaotic dynamics.

### 7.3.4 Prethermalization

In periodically driven systems, the dynamics can exhibit a long-lived intermediate regime known as **prethermalization**. This occurs most prominently in the high-frequency regime (small driving period  $T$ ).

For  $T \ll 1$ , the Floquet Hamiltonian is well approximated by the average Hamiltonian,

$$H_F \approx \frac{H_1 + H_2}{2},$$

and higher-order corrections are small. As a result, the system initially evolves as if it were governed by an effective time-independent Hamiltonian.

During this regime, observables relax to values consistent with thermal equilibrium under  $H_F$ , rather than the fully driven system. This defines the **prethermal state**.

**Time scales.** The prethermal regime persists up to a time scale that grows rapidly as the driving frequency increases (i.e., as  $T \rightarrow 0$ ). Beyond this time, heating effects become important.

**In our spin-chain example.** For small  $T$ , the dynamics of the spin- $\frac{1}{2}$  chain is approximately governed by the effective XXZ-type Hamiltonian  $(H_1 + H_2)/2$ . Observables such as spin correlations or local magnetization relax toward values consistent with this effective model before eventual heating sets in.

### 7.3.5 Heating and the infinite-temperature state

At long times, generic periodically driven interacting systems absorb energy from the drive and approach a featureless state known as the **infinite-temperature state**.

Unlike time-independent systems, energy is not conserved in driven systems. As a result, the system can continuously absorb energy from the periodic drive. In generic (non-integrable) systems, this leads to heating toward a state where all accessible configurations are equally likely.

At infinite temperature, expectation values of observables correspond to those of a completely mixed state within each symmetry sector. For example,

$$\langle S_i^z \rangle \approx 0,$$

and correlations become trivial.

**How to measure heating.** Heating can be quantified in several ways:

- **Energy absorption:** Track the expectation value of the average Hamiltonian,

$$H_{\text{avg}} = \frac{1}{T} \int_0^T H(t) dt = \frac{H_1 + H_2}{2},$$

$$E(t) = \langle \psi(t) | H_{\text{avg}} | \psi(t) \rangle. \quad (7.40)$$

In the prethermal regime,  $E(t)$  remains approximately constant, while at longer times it increases and approaches its infinite-temperature value.

- **Local observables:** Monitor quantities such as  $\langle S_i^z(t) \rangle$  or spin correlations. Their relaxation toward zero (or trivial values) signals heating.
- **Entanglement entropy:** The growth and eventual saturation of entanglement entropy to a maximal value is a hallmark of the infinite-temperature state.
- **Level statistics:** Wigner-Dyson statistics of quasienergies indicate chaotic dynamics, which is typically associated with thermalization toward infinite temperature.

**In our spin-chain example.** For larger driving periods  $T$ , the commutator terms in the effective Hamiltonian break integrability and lead to chaotic dynamics. As a result, the system absorbs energy and evolves toward the infinite-temperature state, where observables become featureless and lose memory of the initial state.

**Infinite-temperature value of the energy for a general spin model.** Consider a quantum spin system with Hamiltonian  $\hat{H}$  acting on a Hilbert space  $\mathcal{H}$  of dimension  $D$ .

At infinite temperature, all states in the accessible Hilbert space are equally likely. The corresponding density matrix is therefore the completely mixed state,

$$\hat{\rho}_\infty = \frac{\mathbb{I}}{D}, \quad (7.41)$$

where  $\mathbb{I}$  is the identity operator on  $\mathcal{H}$ . This density matrix is obtained from the density matrix of the canonical ensemble,

$$\hat{\rho}(\beta) = \frac{e^{-\beta\hat{H}}}{Z}, \quad Z = \text{Tr} \left( e^{-\beta\hat{H}} \right), \quad (7.42)$$

where  $\beta = 1/(k_B T)$ , using  $\beta \rightarrow 0$ .

The infinite-temperature expectation value of the energy is then

$$E_\infty = \text{Tr}(\hat{\rho}_\infty \hat{H}) = \frac{1}{D} \text{Tr}(\hat{H}). \quad (7.43)$$

Thus, the infinite-temperature energy is the trace of the Hamiltonian divided by the dimension of the accessible Hilbert space. When comparing heating dynamics to the infinite-temperature state, it is important to compute the trace in the *same sector* where the dynamics takes place.

**Practical computation.** In the assignment, we are going to consider the average Hamiltonian as our observable, so when we write above  $\hat{H}$ , we mean  $\hat{H}_{\text{avg}}$ .

There are two ways to compute  $E_\infty$ :

1. *Directly from the matrix representation of  $\hat{H}$ :*

$$E_\infty = \frac{1}{D} \sum_{\alpha=1}^D H_{\alpha\alpha}, \quad (7.44)$$

where  $H_{\alpha\alpha}$  is written in any orthonormal basis.

2. *From the eigenvalues  $E_n$  of  $\hat{H}$ :*

$$E_\infty = \frac{1}{D} \sum_{n=1}^D E_n. \quad (7.45)$$

The reason why both expressions are equal is because the trace is independent of the basis used to represent the operator.

## 7.4 Trotter decomposition and Trotter–Suzuki approximation

In quantum mechanics, the time-evolution operator is determined by the Hamiltonian. For a time-independent Hamiltonian  $H$ , the evolution over a time  $t$  is given by

$$U(t) = e^{-iHt}. \quad (7.46)$$

In many physically relevant situations, the Hamiltonian can be written as a sum of simpler terms,

$$H = \sum_{\alpha} H_{\alpha}, \quad (7.47)$$

which do not commute with one another,

$$[H_{\alpha}, H_{\beta}] \neq 0 \quad \text{for some } \alpha \neq \beta. \quad (7.48)$$

In this case, the exponential of the sum cannot be factorized into a product of exponentials,

$$e^{-i(H_1+H_2)t} \neq e^{-iH_1t} e^{-iH_2t}. \quad (7.49)$$

While direct evaluation of the exponential may be feasible for small systems, it becomes computationally prohibitive for many-body systems, where the Hilbert space dimension grows exponentially with system size. This motivates the use of the *Trotter decomposition*, which approximates the exponential of a sum of noncommuting operators in terms of products of exponentials of simpler operators.

### Example: spin chain

Consider the Hamiltonian

$$H = J \sum_{i=1}^{L-1} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y). \quad (7.50)$$

The evolution operator is

$$U(t) = e^{-iHt} = e^{-iH\Delta t} \dots e^{-iH\Delta t} e^{-iH\Delta t} = (e^{-iH\Delta t})^N,$$

where  $t = N\Delta$ . The equation above is exact.

We can also split the Hamiltonian into two parts,

$$H = H^{\text{even}} + H^{\text{odd}}, \quad (7.51)$$

where

$$H_1 = H^{\text{even}} = J \sum_{\substack{i=1 \\ i \text{ even}}}^{L-1} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) = J \sum_{\substack{i=1 \\ i \text{ even}}}^{L-1} h_{i,i+1}, \quad (7.52)$$

$$H_2 = H^{\text{odd}} = J \sum_{\substack{i=1 \\ i \text{ odd}}}^{L-1} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) = J \sum_{\substack{i=1 \\ i \text{ odd}}}^{L-1} h_{i,i+1}. \quad (7.53)$$

Within each set (even or odd bonds), all terms commute, but in general

$$[H^{\text{even}}, H^{\text{odd}}] \neq 0. \quad (7.54)$$

**Basic idea**

We divide the total evolution time into small steps,

$$t = N\Delta t, \quad \Delta t = \frac{t}{N}. \quad (7.55)$$

For sufficiently small  $\Delta t$ , we approximate the short-time evolution as

$$e^{-i(H_1+H_2)\Delta t} \approx e^{-iH_1\Delta t} e^{-iH_2\Delta t} + \mathcal{O}(\Delta t^2). \quad (7.56)$$

Repeating this  $N$  times gives

$$U(t) = e^{-i(H_1+H_2)t} \approx \left( e^{-iH_1\Delta t} e^{-iH_2\Delta t} \right)^N. \quad (7.57)$$

This approximation is known as the **first-order Trotter decomposition**. Its error scales linearly with the total time and as  $\mathcal{O}(\Delta t)$  globally.

**Conclusion:** The smaller  $\Delta t$ , the more accurate the approximation.

**Computational advantage.** Since within each block, all terms commute,

$$e^{-iH_{\text{odd}}\Delta t} = \prod_{i \text{ odd}} e^{-ih_{i,i+1}\Delta t}, \quad (7.58)$$

with  $h_{i,i+1}$  acting only on two spins. Each local term  $h_{i,i+1}$  acts on a two-spin Hilbert space of dimension  $2^2 = 4$ , so its exponential can be computed as a  $4 \times 4$  matrix. This avoids constructing the full  $2^L \times 2^L$  matrix exponential, whose cost scales exponentially with system size. Instead, the dynamics is implemented as a sequence of local operations, leading to a computational cost that scales polynomially with system size for local Hamiltonians.

**Physical and practical relevance.** Trotterization is not only a numerical tool, but also reflects the physical structure of local quantum systems. It underlies:

- quantum circuit decompositions, where time evolution is implemented as a sequence of local gates,
- digital quantum simulation, where Hamiltonian dynamics is approximated by gate sequences,
- tensor network methods (e.g., TEBD), where local updates are applied sequentially,
- Floquet engineering, where piecewise time evolution naturally leads to product forms of unitary operators.

### 7.4.1 Second-order (symmetric) Trotter-Suzuki decomposition

A better approximation is obtained by symmetrizing the product:

$$e^{-i(H_1+H_2)\Delta t} \approx e^{-iH_1\Delta t/2} e^{-iH_2\Delta t} e^{-iH_1\Delta t/2}. \quad (7.59)$$

This is called the **second-order Trotter-Suzuki decomposition**. In this case,

- The leading error is now of order  $(\Delta t)^3$ .
- This is significantly more accurate than the first-order scheme.

The full evolution becomes:

$$U(t) \approx \left( e^{-iH_1\Delta t/2} e^{-iH_2\Delta t} e^{-iH_1\Delta t/2} \right)^N. \quad (7.60)$$

#### Error:

Let us verify that the symmetrization implies a leading error of order  $(\Delta t)^3$ .

The Baker-Campbell-Hausdorff (BCH) formula states that for two operators  $X$  and  $Y$ ,

$$e^X e^Y = e^Z, \quad (7.61)$$

where

$$Z = X + Y + \frac{1}{2}[X, Y] + \frac{1}{12}[X, [X, Y]] + \frac{1}{12}[Y, [Y, X]] + \dots. \quad (7.62)$$

We want to understand the accuracy of the symmetric decomposition

$$e^{A+B} \approx e^{A/2} e^B e^{A/2}, \quad (7.63)$$

where

$$A = -iH_1\Delta t, \quad B = -iH_2\Delta t. \quad (7.64)$$

#### Step 1: Combine the first two exponentials

First consider

$$e^{A/2} e^B = e^C, \quad (7.65)$$

with

$$C = \frac{A}{2} + B + \frac{1}{2} \left[ \frac{A}{2}, B \right] + \frac{1}{12} \left[ \frac{A}{2}, \left[ \frac{A}{2}, B \right] \right] + \frac{1}{12} \left[ B, \left[ B, \frac{A}{2} \right] \right] + \dots. \quad (7.66)$$

Simplifying the commutators,

$$C = \frac{A}{2} + B + \frac{1}{4}[A, B] + \frac{1}{48}[A, [A, B]] + \frac{1}{24}[B, [B, A]] + \dots. \quad (7.67)$$

**Step 2: Multiply by the last exponential**

Now consider

$$e^C e^{A/2} = e^Z. \quad (7.68)$$

Using BCH again,

$$Z = C + \frac{A}{2} + \frac{1}{2} \left[ C, \frac{A}{2} \right] + \frac{1}{12} \left[ C, \left[ C, \frac{A}{2} \right] \right] + \frac{1}{12} \left[ \frac{A}{2}, \left[ \frac{A}{2}, C \right] \right] + \dots \quad (7.69)$$

Substituting  $C$  and keeping terms up to second order in  $A$  and  $B$ ,

$$Z = A + B + \frac{1}{4}[A, B] + \frac{1}{2} \left[ \frac{A}{2} + B, \frac{A}{2} \right] + \mathcal{O}((\Delta t)^3). \quad (7.70)$$

But the term,

$$\frac{1}{2} \left[ \frac{A}{2} + B, \frac{A}{2} \right] = \frac{1}{8}[A, A] + \frac{1}{4}[B, A] = -\frac{1}{4}[A, B], \quad (7.71)$$

so

$$Z = A + B + \mathcal{O}((\Delta t)^3) \quad (7.72)$$

and we have then shown that

$$e^{A/2} e^B e^{A/2} = e^{A+B+\mathcal{O}((\Delta t)^3)}. \quad (7.73)$$

**7.4.2 Higher-order decompositions**

Suzuki showed that it is possible to construct higher-order approximations recursively. Using the second-order (symmetric) Trotter-Suzuki decomposition is given by

$$S_2(\Delta t) = e^{-iH_1\Delta t/2} e^{-iH_2\Delta t} e^{-iH_1\Delta t/2}, \quad (7.74)$$

Suzuki realized that we can improve the accuracy by combining several second-order steps in such a way that the leading error cancels.

**General fourth-order formula**

A fourth-order approximation can be constructed as

$$S_4(\Delta t) = S_2(p_1\Delta t) S_2(p_2\Delta t) S_2(p_1\Delta t), \quad (7.75)$$

where the coefficients are

$$p_1 = \frac{1}{2 - 2^{1/3}}, \quad p_2 = -\frac{2^{1/3}}{2 - 2^{1/3}}. \quad (7.76)$$

These coefficients are universal constants; they do not depend on the specific Hamiltonian.

The resulting approximation satisfies

$$S_4(\Delta t) = e^{-i(H_1+H_2)\Delta t + \mathcal{O}((\Delta t)^5)}. \quad (7.77)$$

Thus, the leading error is now of order  $(\Delta t)^5$ , which is why this method is called **fourth order**.

**Why do these coefficients appear?**

To understand the origin of the coefficients  $p_1$  and  $p_2$ , let us examine the structure of the second-order approximation.

The symmetric step can be written schematically as

$$S_2(\Delta t) = \exp \left[ X\Delta t + E_3(\Delta t)^3 + E_5(\Delta t)^5 + \cdots \right], \quad (7.78)$$

where

$$X = -i(H_1 + H_2), \quad (7.79)$$

and  $E_3, E_5, \dots$  are operator-valued error terms involving commutators such as  $[H_1, H_2]$ .

Now consider the composition

$$S_4(\Delta t) = S_2(p_1\Delta t) S_2(p_2\Delta t) S_2(p_1\Delta t). \quad (7.80)$$

Each factor contributes:

- a first-order term proportional to  $p_i\Delta t$ ,
- a third-order error proportional to  $p_i^3(\Delta t)^3$ .

**Step 1: Correct total time step**

To reproduce the correct evolution time  $\Delta t$ , the coefficients must satisfy

$$2p_1 + p_2 = 1. \quad (7.81)$$

**Step 2: Cancellation of cubic error**

To eliminate the leading error term, we require that the total cubic contribution vanishes:

$$2p_1^3 + p_2^3 = 0. \quad (7.82)$$

Solving these two equations yields

$$p_1 = \frac{1}{2 - 2^{1/3}}, \quad p_2 = -\frac{2^{1/3}}{2 - 2^{1/3}}. \quad (7.83)$$

**Key insight:** The coefficients are chosen so that the third-order errors cancel exactly, leaving the fifth-order term as the leading correction.

For example, a fourth-order decomposition has the general structure:

$$U(\Delta t) \approx S_2(p_1\Delta t) S_2(p_2\Delta t) S_2(p_1\Delta t), \quad (7.84)$$

where  $S_2$  is the second-order propagator and  $p_1, p_2$  are specific coefficients.

**General rule:**

- First order: error  $\sim (\Delta t)^2$
- Second order: error  $\sim (\Delta t)^3$
- Fourth order: error  $\sim (\Delta t)^5$

**Note:** Fourth-order methods are more accurate but require more exponentials per time step, so there is a trade-off between accuracy and computational cost.

### 7.4.3 Practical remarks

- Smaller  $\Delta t$  increases accuracy but also computational cost.
- Second-order schemes are often the best compromise between accuracy and efficiency.
- In many-body systems,  $H_1$  and  $H_2$  are often chosen as sums of commuting local terms, making exponentials easy to compute.

## 7.5 Example 2: Continuously driven two-level system

Consider a single spin- $\frac{1}{2}$  with Hamiltonian

$$H(t) = [A + B \sin(\omega t)] \sigma_z + C \sigma_x. \quad (7.85)$$

This is an example solved in the QuTiP webpage (an open-source Python library designed for simulating quantum systems, especially in quantum optics, many-body physics, and quantum information). You can find it here:

<https://qutip.org/docs/4.1/guide/dynamics/dynamics-floquet.html>

### Why is this problem harder?

Unlike the previous example, the Hamiltonian is now explicitly time dependent within each interval. Therefore, we cannot, in general, write it as a simple exponential of the time-integrated Hamiltonian due to the noncommutativity of  $H(t)$  at different times

### 7.5.1 Time discretization

For a time-dependent Hamiltonian, the evolution over one period is

$$U(T) = \mathcal{T} \exp \left[ -i \int_0^T H(t') dt' \right], \quad (7.86)$$

where  $\mathcal{T}$  denotes time ordering. To approximate this operator numerically, we divide the period into  $N$  small intervals of size  $\Delta t = T/N$ , with

$$t_k = k \Delta t, \quad k = 0, 1, \dots, N. \quad (7.87)$$

Then,

$$U(T) = \prod_{k=1}^N U(t_k, t_{k-1}), \quad (7.88)$$

where the exact short-time propagator on each interval is

$$U(t_k, t_{k-1}) = \mathcal{T} \exp \left[ -i \int_{t_{k-1}}^{t_k} H(t') dt' \right]. \quad (7.89)$$

If  $\Delta t$  is sufficiently small, one may approximate

$$U(t_k, t_{k-1}) \approx e^{-iH(t_k^*)\Delta t}, \quad (7.90)$$

where  $t_k^* \in [t_{k-1}, t_k]$  is, for example, the left endpoint, right endpoint, or midpoint. Thus,

$$U(T) \approx \prod_{k=1}^N e^{-iH(t_k^*)\Delta t}. \quad (7.91)$$

### 7.5.2 Left endpoint: First-order accurate

For the left endpoint,  $t_k^* = t_k$ ,

$$U(T) \approx \prod_{k=1}^N e^{-iH(t_k)\Delta t}, \quad (7.92)$$

The approximation in Eq. (7.92) is first-order accurate. The approximation error in each time step is of order  $\Delta t^2$ . Since the total number of steps scales as  $N = T/\Delta t$ , the accumulated global error over a fixed total time  $T$  scales as

$$N \times \mathcal{O}(\Delta t^2) = \mathcal{O}(T \Delta t),$$

which is therefore linear in  $\Delta t$ . Over a fixed total time the accumulated global error scales as  $\mathcal{O}(\Delta t)$ .

---

To understand the accuracy of the approximation

$$U(t_k, t_{k-1}) \approx e^{-iH(t_k)\Delta t}, \quad (7.93)$$

we compare it with the exact short-time propagator,

$$U(t_k, t_{k-1}) = \mathcal{T} \exp \left[ -i \int_{t_{k-1}}^{t_k} H(t') dt' \right]. \quad (7.94)$$

For a sufficiently small time step  $\Delta t$ , the exact propagator can be expanded as

$$U(t_k, t_{k-1}) = \mathbb{I} - i \int_{t_{k-1}}^{t_k} H(t') dt' + \mathcal{O}(\Delta t^2). \quad (7.95)$$

The neglected terms are of order  $\Delta t^2$ , because the next term in the Dyson expansion involves two time integrals over an interval of size  $\Delta t$ .

We now expand the integral of the Hamiltonian around the endpoint  $t_k$ . Using the Taylor expansion,

$$H(t') = H(t_k) + (t' - t_k) \dot{H}(t_k) + \mathcal{O}(\Delta t^2), \quad (7.96)$$

and integrating from  $t_{k-1}$  to  $t_k$ , we obtain

$$\begin{aligned} \int_{t_{k-1}}^{t_k} H(t') dt' &= \int_{t_{k-1}}^{t_k} \left[ H(t_k) + (t' - t_k) \dot{H}(t_k) + \mathcal{O}(\Delta t^2) \right] dt' \\ &= H(t_k)\Delta t + \dot{H}(t_k) \int_{t_{k-1}}^{t_k} (t' - t_k) dt' + \mathcal{O}(\Delta t^3) \\ &= H(t_k)\Delta t - \frac{\Delta t^2}{2} \dot{H}(t_k) + \mathcal{O}(\Delta t^3). \end{aligned} \quad (7.97)$$

Above, we used

$$\int_{t_{k-1}}^{t_k} (t' - t_k) dt' = \int_{t_{k-1}-t_k}^0 x dx = \int_{-\Delta t}^0 x dx \quad (7.98)$$

Substituting Eq. (7.97) into Eq. (7.95) gives

$$U(t_k, t_{k-1}) = \mathbb{I} - iH(t_k)\Delta t + \mathcal{O}(\Delta t^2). \quad (7.99)$$

On the other hand, expanding the approximate propagator yields

$$e^{-iH(t_k)\Delta t} = \mathbb{I} - iH(t_k)\Delta t + \mathcal{O}(\Delta t^2). \quad (7.100)$$

Therefore, the exact and approximate propagators agree up to first order in  $\Delta t$ , and their difference begins at order  $\Delta t^2$ :

$$U(t_k, t_{k-1}) - e^{-iH(t_k)\Delta t} = \mathcal{O}(\Delta t^2). \quad (7.101)$$

This shows that the approximation

$$U(t_k, t_{k-1}) \approx e^{-iH(t_k)\Delta t} \quad (7.102)$$

has a *local error* of order  $\Delta t^2$  per time step, which is why the method is said to be first-order accurate overall.

### 7.5.3 Midpoint: Second-order accurate

Using the endpoint  $t_k$  gives only a first-order approximation. A better choice is to evaluate the Hamiltonian at the midpoint of each interval,

$$t_{k-\frac{1}{2}} = \frac{t_k + t_{k-1}}{2}, \quad (7.103)$$

and write

$$U(T) \approx \prod_{k=1}^N e^{-iH(t_{k-\frac{1}{2}})\Delta t}. \quad (7.104)$$

This is called the *midpoint rule*. It is more accurate because the term  $\propto \Delta t^2$  in Eq. (7.97) vanishes when the midpoint is used. This is because Eq. (7.98) now becomes

$$\int_{t_{k-1}}^{t_k} (t' - t_{k-\frac{1}{2}}) dt' = \int_{t_{k-1}-t_{k-\frac{1}{2}}}^{t_k-t_{k-\frac{1}{2}}} x dx = \int_{\frac{t_{k-1}-t_k}{2}}^{\frac{t_k-t_{k-1}}{2}} x dx = 0. \quad (7.105)$$

Therefore,

$$\int_{t_{k-1}}^{t_k} H(t') dt' = H(t_{k-\frac{1}{2}}) \Delta t + \frac{\ddot{H}(t_{k-\frac{1}{2}})}{24} \Delta t^3 + \mathcal{O}(\Delta t^5). \quad (7.106)$$

This shows that the midpoint approximation differs from the exact integral by a term of order  $\Delta t^3$ :

$$\int_{t_{k-1}}^{t_k} H(t') dt' = H(t_{k-\frac{1}{2}}) \Delta t + \mathcal{O}(\Delta t^3). \quad (7.107)$$

Thus, over a fixed total time  $T$ , the errors from all intervals accumulate, giving

$$n \times \mathcal{O}(\Delta t^3) = \frac{T}{\Delta t} \mathcal{O}(\Delta t^3) = \mathcal{O}(T \Delta t^2). \quad (7.108)$$

For fixed final time  $t$ , this is usually written simply as

$$\mathcal{O}(\Delta t^2), \quad (7.109)$$

which is why the midpoint method is called *second-order accurate*.

#### 7.5.4 Symmetrized Trotter-Suzuki decomposition

As written above, we have the Hamiltonian in Eq. (7.85)

$$H(t) = [A + B \sin(\omega t)] \sigma_z + C \sigma_x, \quad (7.110)$$

and the exact propagator over a period is

$$U(T) = \mathcal{T} \exp \left[ -i \int_0^T H(t') dt' \right] = \prod_{k=1}^N U(t_k, t_{k-1}), \quad (7.111)$$

where the exact short-time propagator on each interval is

$$U(t_k, t_{k-1}) = \mathcal{T} \exp \left[ -i \int_{t_{k-1}}^{t_k} H(t') dt' \right]. \quad (7.112)$$

We can separate the Hamiltonian into

$$H(t) = H_1 + H_2(t), \quad (7.113)$$

with

$$H_1 = A \sigma_z + C \sigma_x, \quad (7.114)$$

$$H_2(t) = B \sin(\omega t) \sigma_z. \quad (7.115)$$

The time integral can then be performed explicitly,

$$\int_{t_{k-1}}^{t_k} H(t') dt' = H_1 \Delta t + B \left( \int_{t_{k-1}}^{t_k} \sin(\omega t') dt' \right) \sigma_z, \quad (7.116)$$

and since

$$\int_{t_{k-1}}^{t_k} \sin(\omega t') dt' = \frac{\cos(\omega t_{k-1}) - \cos(\omega t_k)}{\omega}, \quad (7.117)$$

we obtain

$$U(t_k, t_{k-1}) = \mathcal{T} \exp \left\{ -i H_1 \Delta t - i \frac{B}{\omega} [\cos(\omega t_{k-1}) - \cos(\omega t_k)] \sigma_z \right\}. \quad (7.118)$$

**Short-time approximation (removing time ordering).**

**ATTENTION!** Notice that the time ordering  $\mathcal{T}$  is still in the equation above and **cannot** be ignored! What we can do, when  $\Delta t = t_k - t_{k-1} \rightarrow 0$ , is to **approximate** the propagator as

$$U(t_k, t_{k-1}) \approx \exp \left\{ -i H_1 \Delta t - i \frac{B}{\omega} [\cos(\omega t_{k-1}) - \cos(\omega t_k)] \sigma_z \right\}. \quad (7.119)$$

This is an **APPROXIMATION** that works when  $\Delta t$  is small. For sufficiently small  $\Delta t$ , the effect of time ordering enters only at higher order through commutators of the Hamiltonian at different times.

NOTE: If one would do the same for the whole period, for example, we would entirely eliminate the effect of the sinusoidal function,  $[\cos(\omega T) - \cos(\omega 0)] = 0$  which would be clearly **wrong!**

**Symmetric Trotter–Suzuki approximation.**

In Eq. (7.119), the exponent is a sum of two noncommuting operators, so one may apply the second-order symmetric Trotter-Suzuki formula,

$$e^{X+Y} \approx e^{X/2} e^Y e^{X/2}, \quad (7.120)$$

with

$$X = -i H_1 \Delta t, \quad (7.121)$$

$$Y = -i \frac{B}{\omega} [\cos(\omega t_{k-1}) - \cos(\omega t_k)] \sigma_z. \quad (7.122)$$

This yields

$$U(t_k, t_{k-1}) \approx \exp \left( -i H_1 \frac{\Delta t}{2} \right) \exp \left[ -i \frac{B}{\omega} (\cos(\omega t_{k-1}) - \cos(\omega t_k)) \sigma_z \right] \exp \left( -i H_1 \frac{\Delta t}{2} \right), \quad (7.123)$$

where  $H_1 = A \sigma_z + C \sigma_x$ .

For the Floquet operator, we finally have approximately

$$\begin{aligned} U(T, 0) \approx & \exp \left( -i H_1 \frac{\Delta t}{2} \right) \exp \left( i \frac{B}{\omega} [\cos(n\omega\Delta t) - \cos((n-1)\omega\Delta t)] \sigma_z \right) \exp \left( -i H_1 \frac{\Delta t}{2} \right) \\ & \dots \\ & \exp \left( -i H_1 \frac{\Delta t}{2} \right) \exp \left( i \frac{B}{\omega} [\cos(2\omega\Delta t) - \cos(\omega\Delta t)] \sigma_z \right) \exp \left( -i H_1 \frac{\Delta t}{2} \right) \\ & \exp \left( -i H_1 \frac{\Delta t}{2} \right) \exp \left( i \frac{B}{\omega} [\cos(\omega\Delta t) - \cos(0)] \sigma_z \right) \exp \left( -i H_1 \frac{\Delta t}{2} \right). \end{aligned} \quad (7.124)$$

**7.5.5 Exact evaluation of each time step**

At each time step  $t_k^*$ , the Hamiltonian takes the form

$$H(t_k^*) = h_z(t_k^*) \sigma_z + C \sigma_x, \quad h_z(t_k^*) = A + B \sin(\omega t_k^*), \quad (7.125)$$

which can be written as

$$H(t_k^*) = \vec{h}(t_k^*) \cdot \vec{\sigma}, \quad (7.126)$$

with  $\vec{h}(t_k^*) = (C, 0, h_z(t_k^*))$  and  $|\vec{h}(t_k^*)| = h(t_k^*) = \sqrt{C^2 + h_z(t_k^*)^2}$ .

The exponential of such a  $2 \times 2$  Hamiltonian can be computed exactly using the identity (the derivation is below)

$$e^{-i(\vec{h} \cdot \vec{\sigma}) \Delta t} = \cos(h \Delta t) \mathbb{I} - i \sin(h \Delta t) \frac{\vec{h}}{h} \cdot \vec{\sigma}. \quad (7.127)$$

Applying this to  $H(t_k^*)$ , we obtain

$$e^{-iH(t_k^*) \Delta t} = \cos(h(t_k^*) \Delta t) \mathbb{I} - i \sin(h(t_k^*) \Delta t) \left( \frac{C}{h(t_k^*)} \sigma_x + \frac{h_z(t_k^*)}{h(t_k^*)} \sigma_z \right). \quad (7.128)$$

Therefore, although the full time evolution requires time ordering, each short-time propagator can be evaluated exactly in closed form using trigonometric functions and  $2 \times 2$  matrices.

### Derivation of the exponential of a Pauli-vector operator.

Let

$$H = \vec{h} \cdot \vec{\sigma} = h_x \sigma_x + h_y \sigma_y + h_z \sigma_z, \quad (7.129)$$

and define

$$h = |\vec{h}| = \sqrt{h_x^2 + h_y^2 + h_z^2}. \quad (7.130)$$

We want to compute

$$e^{-i(\vec{h} \cdot \vec{\sigma}) \delta t}. \quad (7.131)$$

We begin from the Taylor expansion of the exponential:

$$e^{-i(\vec{h} \cdot \vec{\sigma}) \delta t} = \sum_{n=0}^{\infty} \frac{1}{n!} \left[ -i(\vec{h} \cdot \vec{\sigma}) \delta t \right]^n. \quad (7.132)$$

The key step is to compute the square of  $\vec{h} \cdot \vec{\sigma}$ . Using

$$\sigma_i \sigma_j = \delta_{ij} \mathbb{I} + i \sum_k \epsilon_{ijk} \sigma_k, \quad (7.133)$$

we have

$$(\vec{h} \cdot \vec{\sigma})^2 = \sum_{i,j} h_i h_j \sigma_i \sigma_j \quad (7.134)$$

$$= \sum_{i,j} h_i h_j \left( \delta_{ij} \mathbb{I} + i \sum_k \epsilon_{ijk} \sigma_k \right). \quad (7.135)$$

The first term gives

$$\sum_{i,j} h_i h_j \delta_{ij} \mathbb{I} = \sum_i h_i^2 \mathbb{I} = h^2 \mathbb{I}. \quad (7.136)$$

The second term vanishes because  $h_i h_j$  is symmetric under  $i \leftrightarrow j$ , while  $\epsilon_{ijk}$  is antisymmetric:

$$\sum_{i,j,k} h_i h_j \epsilon_{ijk} \sigma_k = 0. \quad (7.137)$$

Therefore,

$$(\vec{h} \cdot \vec{\sigma})^2 = h^2 \mathbb{I}. \quad (7.138)$$

This immediately implies the pattern

$$(\vec{h} \cdot \vec{\sigma})^{2m} = h^{2m} \mathbb{I}, \quad (7.139)$$

$$(\vec{h} \cdot \vec{\sigma})^{2m+1} = h^{2m} (\vec{h} \cdot \vec{\sigma}), \quad (7.140)$$

for any integer  $m \geq 0$ .

We now separate the exponential series into even and odd powers:

$$e^{-i(\vec{h} \cdot \vec{\sigma})\delta t} = \sum_{m=0}^{\infty} \frac{1}{(2m)!} \left[ -i(\vec{h} \cdot \vec{\sigma})\delta t \right]^{2m} + \sum_{m=0}^{\infty} \frac{1}{(2m+1)!} \left[ -i(\vec{h} \cdot \vec{\sigma})\delta t \right]^{2m+1}. \quad (7.141)$$

Using the power relations above,

$$e^{-i(\vec{h} \cdot \vec{\sigma})\delta t} = \sum_{m=0}^{\infty} \frac{(-i)^{2m} (h\delta t)^{2m}}{(2m)!} \mathbb{I} + \sum_{m=0}^{\infty} \frac{(-i)^{2m+1} (h\delta t)^{2m}}{(2m+1)!} (\vec{h} \cdot \vec{\sigma}) \delta t \quad (7.142)$$

$$= \sum_{m=0}^{\infty} \frac{(-1)^m (h\delta t)^{2m}}{(2m)!} \mathbb{I} - i \sum_{m=0}^{\infty} \frac{(-1)^m (h\delta t)^{2m+1}}{(2m+1)!} \frac{\vec{h} \cdot \vec{\sigma}}{h}. \quad (7.143)$$

Recognizing the cosine and sine series,

$$\cos(h\delta t) = \sum_{m=0}^{\infty} \frac{(-1)^m (h\delta t)^{2m}}{(2m)!}, \quad (7.144)$$

$$\sin(h\delta t) = \sum_{m=0}^{\infty} \frac{(-1)^m (h\delta t)^{2m+1}}{(2m+1)!}, \quad (7.145)$$

we obtain

$$e^{-i(\vec{h} \cdot \vec{\sigma})\delta t} = \cos(h\delta t) \mathbb{I} - i \sin(h\delta t) \frac{\vec{h}}{h} \cdot \vec{\sigma}. \quad (7.146)$$

## 7.6 Assignment: Floquet Systems

Work in units where  $\hbar = 1$  and set  $J = 1$ .

## Part I: Piecewise constant drive in a spin chain

Consider the periodically driven spin- $\frac{1}{2}$  chain

$$H(t) = \begin{cases} H_1, & 0 \leq t < T/2, \\ H_2, & T/2 \leq t < T, \end{cases}$$

with

$$H_1 = \sum_{i=1}^{L-1} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y), \quad (7.147)$$

$$H_2 = \Delta \sum_{i=1}^{L-1} S_i^z S_{i+1}^z + \epsilon_1 S_1^z. \quad (7.148)$$

Assume open boundary conditions,  $\Delta = 0.48$ ,  $\epsilon_1 = 0.1$ , and choose  $L = 12$  with 6 up-spins, so that the dynamics is restricted to the zero-magnetization sector.

Construct the Floquet operator

$$U_F = e^{-iH_2 T/2} e^{-iH_1 T/2}.$$

**ATTENTION!** Check your code first for a small chain. When you are sure everything is correct, you can run for  $L = 12$  with 6 up-spins. If your code gets too slow, you can use  $L = 10$  and 5 up-spins.

### 1. Quasienergies and spacing-ratio statistics.

For a range of periods  $T \in [0.1, 8]$ , diagonalize  $U_F$  in the sector with 6 up-spins and compute the quasienergies  $\varepsilon_\alpha$ . Then compute the ratio of consecutive spacings,

$$\tilde{r}_\alpha = \frac{\min(s_\alpha, s_{\alpha-1})}{\max(s_\alpha, s_{\alpha-1})}, \quad s_\alpha = \theta_{\alpha+1} - \theta_\alpha,$$

where  $\theta_\alpha$  are the ordered eigenphases of  $U_F$ .

Plot the average

$$\langle \tilde{r} \rangle = \frac{1}{N-2} \sum_{\alpha=2}^{N-1} \tilde{r}_\alpha$$

as a function of  $T$ .

- Compare your results with the expected values

$$\langle \tilde{r} \rangle_{\text{Poisson}} \approx 0.386, \quad \langle \tilde{r} \rangle_{\text{COE}} \approx 0.536.$$

- Identify the range of  $T$  where the dynamics is close to integrable and the range where it becomes chaotic.
- Briefly explain why varying  $T$  changes the quasienergy statistics.

## 2. Spacing distribution.

- For one relatively small value of  $T = 2$  and one larger value of  $T = 7$ , compute the normalized quasienergy spacing distribution  $P(s)$  and compare it with:

$$P_{\text{Poisson}}(s) = e^{-s}, \quad P_{\text{COE}}(s) \approx \frac{\pi}{2} s e^{-\pi s^2/4}.$$

Discuss whether your results are consistent with the behavior of  $\langle r \rangle$ .

- Choose a value of  $T$  and make a normalized histogram with the eigenphases (DOS). Does it look flat?

## 3. Participation ratio in the Floquet basis.

Choose two computational-basis initial states:

- Néel state,  $|1010 \cdots 10\rangle$ ,
- Domain-wall type state  $|111111000000\rangle$ .

Expand each state in the eigenbasis of the Floquet operator,

$$|\psi(0)\rangle = \sum_{\alpha} c_{\alpha} |\phi_{\alpha}\rangle, \quad U_F |\phi_{\alpha}\rangle = e^{-i\theta_{\alpha}} |\phi_{\alpha}\rangle,$$

and compute the participation ratio. Evaluate the PR for  $T = 0.2, 1, 7$ .

- Which initial state is more delocalized in the Floquet basis?
- How does the PR change as  $T$  increases?
- Relate your findings to the change from Poisson-like to COE-like level statistics.

## 4. Heating and the approach to infinite temperature.

Take the Néel state from the previous question and evolve it stroboscopically,

$$|\psi(nT)\rangle = U_F^n |\psi(0)\rangle.$$

Compute the expectation value of the average Hamiltonian

$$H_{\text{avg}} = \frac{H_1 + H_2}{2}, \quad E(nT) = \langle \psi(nT) | H_{\text{avg}} | \psi(nT) \rangle,$$

as a function of  $nT$ .

- Show that

$$E(0) = -0.635.$$

- Show that the infinite-temperature value of the energy is

$$E_{\infty} = -0.06.$$

- Compare the time dependence of  $E(nT)$  for different values of the period,  $T = 1, 2.5, 7$ . Show in your plot (or plots, if you prefer) the values  $E(0)$  and  $E_\infty$  with a horizontal line.
- Discuss whether the system absorbs energy more efficiently for large  $T$ .

### 5. Average Hamiltonian.

Consider the Néel state  $|\psi(0)\rangle = |1010\cdots\rangle$  and compute the stroboscopic survival probability

$$S_P(nT) = |\langle\psi(0)|\psi(nT)\rangle|^2, \quad |\psi(nT)\rangle = U_F^n |\psi(0)\rangle,$$

using the exact Floquet operator.

Compare this result with the approximate dynamics generated by the average Hamiltonian

$$H_{\text{avg}} = \frac{H_1 + H_2}{2},$$

Compute the approximate evolution as

$$|\psi(nT)\rangle \approx e^{-iH_{\text{avg}}nT} |\psi(0)\rangle.$$

- Plot the survival probability  $S_P(nT)$  as a function of  $n$  on a semi-logarithmic scale (logarithmic scale on the vertical axis) for both the exact and approximate dynamics at  $T = 0.5$ .
- Repeat the comparison for  $T = 4$ .
- For which value of  $T$  does the average Hamiltonian provide a good approximation? Why?

### 6. Exact evolution vs. second-order Trotter-Suzuki.

Instead of constructing the exact Floquet operator

$$U_F = e^{-iH_2T/2} e^{-iH_1T/2},$$

approximate the evolution over one period using a second-order Trotter-Suzuki decomposition with a time step  $\Delta t$ .

Divide each half-period into small intervals, as in Eqs. (7.52)-(7.53), and approximate the propagator over one period numerically. [NOTE: This is an approximation only for the Hamiltonian with noncommuting terms.]

- Plot the error  $\mathcal{E}_{\tilde{r}}(\Delta t)$  in  $\langle\tilde{r}\rangle$  as a function of  $\Delta t$ .

$$\mathcal{E}_{\tilde{r}}(\Delta t) = |\langle\tilde{r}\rangle_{\Delta t} - \langle\tilde{r}\rangle_{\text{exact}}|.$$

Consider  $T = 2.0$  and some values of  $\Delta t \in [0.02, 0.50]$ .

- In one plot, show the stroboscopic dynamics of the local magnetization at the center of the chain,

$$\langle S_6^z(nT) \rangle,$$

computed using the exact Floquet operator and using the second-order Trotter-Suzuki approximation for at least three different values of  $\Delta t$ . Verify that the approximate results converge to the exact one as  $\Delta t$  decreases. Consider  $T = 2.0$  and some values of  $\Delta t \in [0.1, 1.0]$ .

## Part II: Continuously driven two-level system

Consider the Hamiltonian

$$H(t) = [A + B \sin(\omega t)]\sigma^z + C\sigma^x,$$

with period

$$T = \frac{2\pi}{\omega},$$

and

$$A = -\pi \quad B = 2.5\pi \quad C = -0.2\pi \quad \omega = 2\pi.$$

This is an example considered in

<https://qutip.org/docs/4.1/guide/dynamics/dynamics-floquet.html>

### 7. Convergence of quasienergies.

Compute the quasienergies of the Floquet operator using the left endpoint in Eq. (7.92), the midpoint in Eq. (7.104), and the Trotter-Suzuki approximation in Eq. (7.124) for several values of  $\Delta t$ .

- Show that the quasienergies converge as  $\Delta t$  decreases.
- Discuss why the midpoint choice is more accurate than the endpoint choice.
- How do the midpoint choice and Trotter-Suzuki approximation compare?

### 7.6.1 Illustrations of the solutions

These plots give you an idea of what to expect for the assignment.

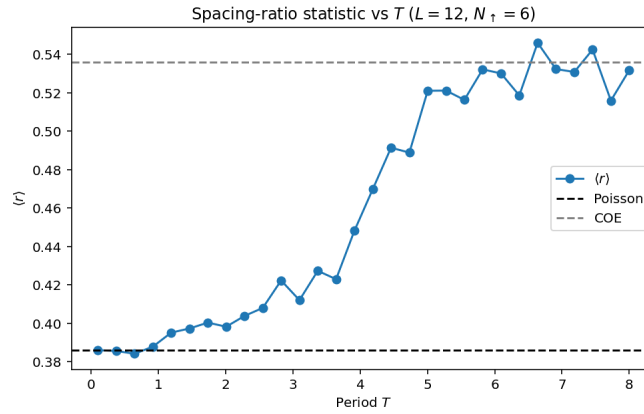


Figure 7.1: 1. Plot of the average  $\langle r \rangle$  vs  $T$ .

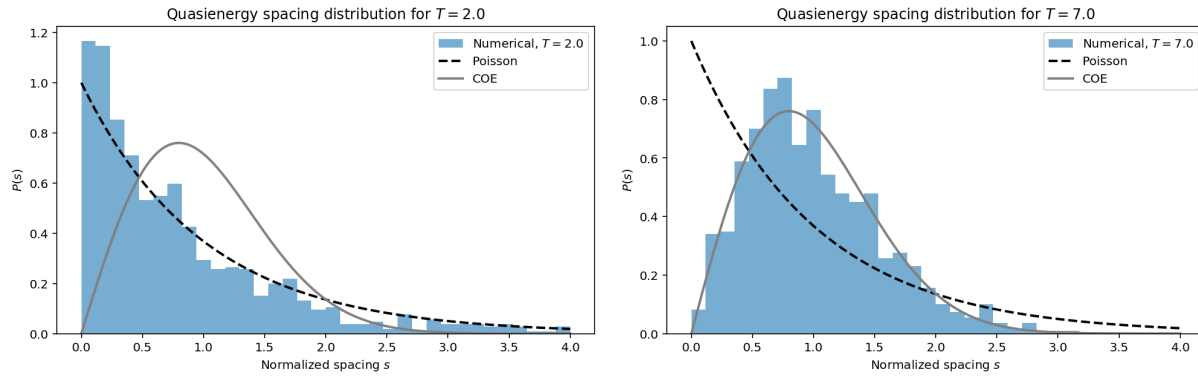


Figure 7.2: 2. Level statistics: Poisson for  $T = 2$ ; COE for  $T = 7$

Question 3:

| $T$ | PR (Néel state) | PR (Domain wall) |
|-----|-----------------|------------------|
| 0.2 | 39.1420         | 60.8342          |
| 1.0 | 40.3828         | 60.8899          |
| 7.0 | 230.2250        | 253.1880         |

Table 7.1: 3. Participation ratios in the Floquet eigenbasis for different driving periods  $T$ .

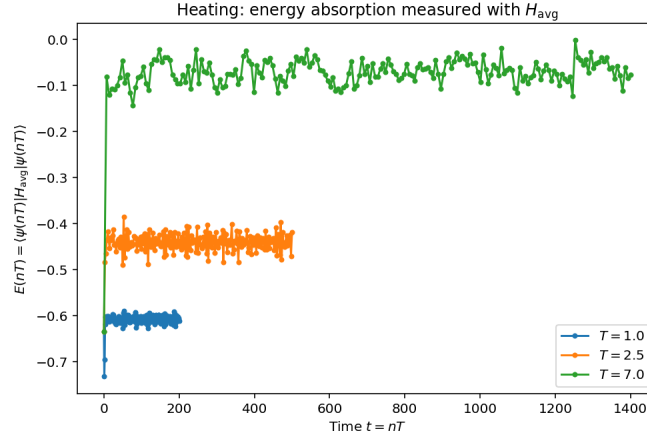
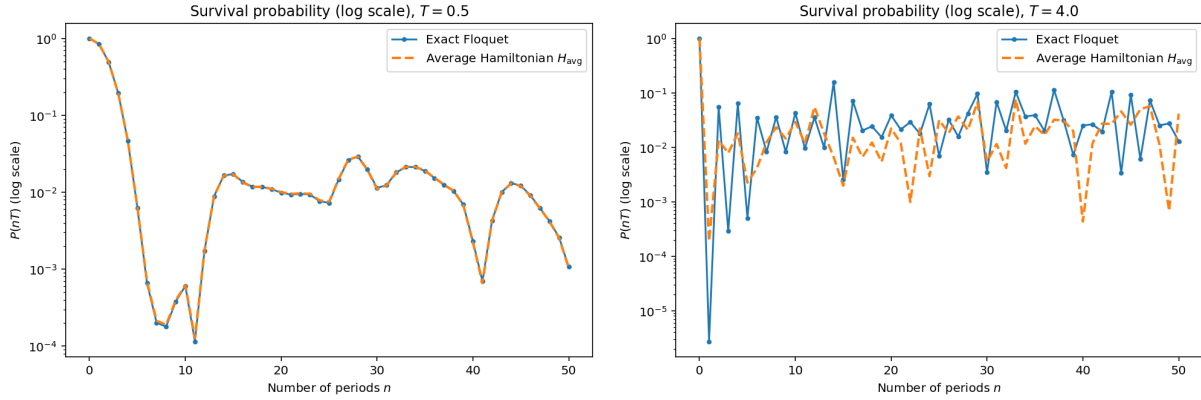
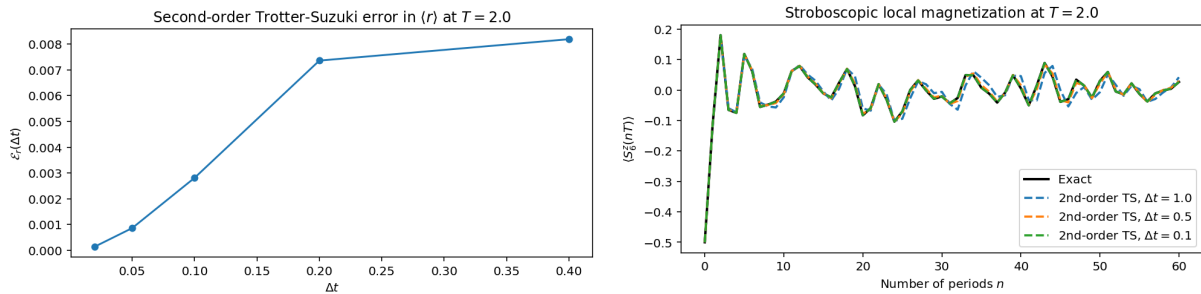


Figure 7.3: 4. Heating.

Figure 7.4: 5. Average Hamiltonian vs Exact Result :  $S_P(nT)$  for  $T = 0.5$  and  $S_P(nT)$  for  $T = 4$ .Figure 7.5: 6. Trotter-Suzuki vs Exact Result: Error for  $\langle r \rangle$  and  $\langle S_6(nT) \rangle$ .

## 7. Convergence of quasienergies with Trotter-Suzuki approximations.

**Reference quasienergies** ( $\omega = 2\pi$ ).

$$\varepsilon_\alpha = \{-2.83131209, 2.83131209\}. \quad (7.149)$$



# Chapter 8

## Open Quantum Systems

In this chapter we discuss how open-system dynamics differs from ordinary Schrödinger evolution, and how the Lindblad equation arises as a common description of dissipation in quantum systems. Before introducing the Lindblad equation, it is useful to briefly review the concepts of density matrices and purity.

### 8.1 Density matrices for pure and mixed states

**Pure state:** For simplicity, we focus on a two-level system with basis states  $|\psi_0\rangle$  and  $|\psi_1\rangle$ . The density matrix of a pure state  $|\Psi(t)\rangle = c_0(t)|\psi_0\rangle + c_1(t)|\psi_1\rangle$  is given by the outer product of the state vector,

$$\rho(t) = |\Psi(t)\rangle\langle\Psi(t)| = \begin{pmatrix} c_0(t) \\ c_1(t) \end{pmatrix} \begin{pmatrix} c_0^*(t) & c_1^*(t) \end{pmatrix} = \begin{pmatrix} |c_0(t)|^2 & c_0(t)c_1^*(t) \\ c_0^*(t)c_1(t) & |c_1(t)|^2 \end{pmatrix}. \quad (8.1)$$

The diagonal elements are known as *populations*, while the off-diagonal elements are called *coherences*. The populations quantify the probability of finding the system in each basis state upon measurement. The coherences encode phase relations between the states and are responsible for quantum interference effects.

**Mixed state:** In contrast, a mixed state describes a statistical ensemble of pure states. In general, it can be written as

$$\rho(t) = \sum_{\alpha} p_{\alpha}(t) |\Psi_{\alpha}\rangle\langle\Psi_{\alpha}|, \quad (8.2)$$

where  $p_{\alpha} \geq 0$  and  $\sum_{\alpha} p_{\alpha} = 1$ . A simple example is a mixture of the basis states,

$$\rho(t) = p_0(t) |\psi_0\rangle\langle\psi_0| + p_1(t) |\psi_1\rangle\langle\psi_1| = \begin{pmatrix} p_0(t) & 0 \\ 0 & p_1(t) \end{pmatrix}. \quad (8.3)$$

In this case, the density matrix is diagonal in the chosen basis, and there are no coherences. This reflects classical uncertainty about the state: the system is in  $|\psi_0\rangle$  with probability  $p_0$  and in  $|\psi_1\rangle$  with probability  $p_1$ , but there is no quantum superposition between them.

**Superposition vs classical mixture:** A pure superposition and a classical mixture are not the same thing. Compare

$$|+\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \implies \rho_+ = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

with

$$\rho_{\text{mix}} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Both have populations  $1/2$  and  $1/2$ , but the pure state has off-diagonal coherence while the mixed state does not. That coherence is what allows interference.

## 8.2 Purity

A very useful quantity is the *purity*,

$$\text{Tr}(\rho^2),$$

which quantifies how mixed a quantum state is. It provides a measure of the degree of coherence of the system and is often used to track decoherence and the loss of quantum information.

For a pure state,

$$\rho = |\psi\rangle \langle\psi| \implies \rho^2 = \rho \implies \text{Tr}(\rho^2) = \text{Tr}(\rho) = 1.$$

For a mixed state, however,

$$\text{Tr}(\rho^2) < 1.$$

In a  $D$ -dimensional Hilbert space,

$$\frac{1}{D} \leq \text{Tr}(\rho^2) \leq 1.$$

The lower bound corresponds to the maximally mixed state,

$$\rho = \frac{\mathbb{1}}{D},$$

which represents maximal classical uncertainty about the system.

### Example of a pure state

Consider

$$|\psi\rangle = a|0\rangle + b|1\rangle, \quad |a|^2 + |b|^2 = 1.$$

Its density matrix is

$$\rho_{\text{pure}} = |\psi\rangle \langle\psi| = \begin{pmatrix} |a|^2 & ab^* \\ a^*b & |b|^2 \end{pmatrix}. \quad (8.4)$$

Now compute the purity:

$$\text{Tr}(\rho_{\text{pure}}^2) = 1.$$

This must happen because  $\rho_{\text{pure}}^2 = \rho_{\text{pure}}$ .

**Example of a mixed state**

Now suppose the system is in  $|0\rangle$  with probability  $p$  and in  $|1\rangle$  with probability  $1 - p$ . Then

$$\rho_{\text{mix}} = p |0\rangle \langle 0| + (1 - p) |1\rangle \langle 1| = \begin{pmatrix} p & 0 \\ 0 & 1 - p \end{pmatrix}. \quad (8.5)$$

Then

$$\text{Tr}(\rho_{\text{mix}}^2) = p^2 + (1 - p)^2 = 1 - 2p(1 - p).$$

Unless  $p = 0$  or  $p = 1$ , this is strictly less than 1. For the maximally mixed qubit,  $p = 1/2$ , so

$$\rho_{\text{max mix}} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \text{Tr}(\rho_{\text{max mix}}^2) = \frac{1}{2}.$$

### 8.3 Lindblad master equation

In the idealized case of *closed* (*isolated*) systems, including periodically driven (Floquet) systems, the dynamics is *unitary* and governed by the Schrödinger equation. Unitary dynamics means that the time evolution is described by a unitary operator, which ensures that the evolution is reversible [ $U^\dagger(t)$  undoes the evolution], total probability is conserved [ $\text{Tr}[\rho(t)] = 1$ ], coherence is (globally) preserved, and pure states remain pure [ $\text{Tr}[\rho^2(t)] = 1$ ].

Real systems, however, are inevitably coupled to their environment, and this coupling is detrimental to quantum behavior. An atom interacts with the electromagnetic vacuum, a spin with fluctuating magnetic fields, a superconducting circuit leaks photons into its surroundings, and a quantum computer/processor is constantly exposed to uncontrolled degrees of freedom. These interactions introduce different physical mechanisms that degrade quantum states.

- *Dissipation* (relaxation) refers to the irreversible exchange of energy or particles with the environment, driving the system toward lower-energy or thermal states. Once populations change, off-diagonal elements typically decay as well, leading to *decoherence*, that is, loss of quantum coherences, or equivalently, decay of the off-diagonal elements of the density matrix (in some basis).
- *Dephasing* corresponds to the randomization of the relative phases between components of a quantum superposition, typically without energy exchange, leading to the suppression of interference effects. Dephasing directly suppresses coherences (off-diagonal elements of the density matrix), being a particular type of decoherence.
- *Decoherence* is the general process by which a quantum system loses its “quantumness” due to entanglement with the environment. Operationally, it corresponds to the decay of off-diagonal elements of the density matrix (in some basis), turning pure states into mixed states. While relaxation and dephasing are distinct environment-induced processes, both contribute to decoherence.

As a result of these processes, quantum states degrade: superpositions lose their phase relations, pure states evolve into mixed states, and entanglement is diminished or destroyed.

The very resources that enable quantum technologies – coherence, interference, and entanglement – are therefore fragile and rapidly eroded. The environment is not merely a perturbation, but a central obstacle that limits the stability, controllability, and scalability of quantum devices.

When investigating *open quantum systems*, instead of following the full state of the system plus its environment, we focus only on the subsystem of interest. As a consequence, the reduced dynamics of the subsystem is, in general, *non-unitary*.

An important equation for describing Markovian open-system dynamics is the *Lindblad* or Gorini–Kossakowski–Sudarshan–Lindblad (GKSL) master equation,

$$\frac{d\rho}{dt} = -i[H, \rho] + \sum_k \left( L_k \rho L_k^\dagger - \frac{1}{2} \{L_k^\dagger L_k, \rho\} \right), \quad (8.6)$$

which gives the most general continuous-time, trace-preserving, completely positive, Markovian evolution of a density matrix. In this equation,  $H$  is the system Hamiltonian and generates the usual unitary evolution through the commutator  $[H, \rho]$ . The operators  $L_k$ , called ***Lindblad operators*** (or ***jump operators***), determine the different dissipative processes affecting the system, such as decay, dephasing, or particle loss. The term  $L_k \rho L_k^\dagger$  represents the action of these processes on the state, while the anticommutator term  $-\frac{1}{2} \{L_k^\dagger L_k, \rho\}$  ensures that the evolution preserves the trace of  $\rho$ .

It is often convenient to separate the evolution into a unitary and a dissipative contribution. Defining the ***dissipator***

$$\mathcal{D}[\rho] = \sum_k \left( L_k \rho L_k^\dagger - \frac{1}{2} \{L_k^\dagger L_k, \rho\} \right), \quad (8.7)$$

the master equation can be written compactly as

$$\frac{d\rho}{dt} = -i[H, \rho] + \mathcal{D}[\rho]. \quad (8.8)$$

The dissipator  $\mathcal{D}$  is a *superoperator* that encodes the effects of the environment.

The Lindblad master equation is an operator equation for the density matrix that can also be written as

$$\boxed{\frac{d\rho}{dt} = \mathcal{L}[\rho]},$$

where  $\mathcal{L}$  is the generator of the dynamics. The map  $\mathcal{L}$  is a *superoperator*.

**Superoperator** is a linear operator that acts on operators rather than on state vectors. In particular, while an ordinary operator acts on a vector in Hilbert space,

$$A : |\psi\rangle \mapsto A|\psi\rangle,$$

a superoperator acts on a matrix (such as the density operator),

$$\mathcal{L} : \rho \mapsto \mathcal{L}[\rho].$$

Just as matrices represent linear maps acting on vectors, superoperators can be represented as matrices acting on vectorized operators. This observation will allow us to rewrite the

Lindblad master equation as an ordinary matrix differential equation in a larger space, as discussed in Sec. 8.7.

Next, we recall the concepts of continuous-time, trace-preserving, completely positive, and Markovian dynamics, as well as the notion of purity. Before doing so, we briefly review the definitions of pure and mixed states.

## 8.4 Properties of the Lindblad equation

We review the concepts of continuous-time, trace-preserving, completely positive, and Markovian dynamics, which are associated with the Lindblad master equation.

### 8.4.1 Continuous-time

The state  $\rho(t)$  evolves smoothly in time according to a differential equation (no discrete jumps in time).

### 8.4.2 Markovian

The evolution has no memory; the future state depends only on the present state  $\rho(t)$  and not on its past history.

### 8.4.3 Trace preserving: Normalization

In both cases, pure or mixed states, the trace of the density matrix is equal to one. The trace is defined as the sum of the diagonal elements in any orthonormal basis  $\{|n\rangle\}$ ,

$$\text{Tr}(\rho) = \sum_n \langle n | \rho | n \rangle = \sum_n \rho_{nn} = 1,$$

which ensures normalization of the state. This result is *independent of the choice of basis*. This follows from the cyclic property of the trace, and guarantees that normalization is a physical property of the state, not an artifact of a particular representation.

For a pure state,  $\rho = |\Psi\rangle\langle\Psi|$ , one finds

$$\text{Tr}(\rho) = \langle\Psi|\Psi\rangle = 1,$$

while for a mixed state,  $\rho = \sum_\alpha p_\alpha |\Psi_\alpha\rangle\langle\Psi_\alpha|$ , the normalization condition becomes

$$\text{Tr}(\rho) = \sum_\alpha p_\alpha = 1.$$

### 8.4.4 Completely positive

To understand complete positivity, we first recall the notion of positivity for a density matrix.

### Positivity

A physical density matrix must satisfy

$$\langle \phi | \rho | \phi \rangle \geq 0 \quad \text{for every state } |\phi\rangle.$$

This condition ensures that all measurable probabilities are nonnegative. Here, “for every state” means for all normalized vectors in the Hilbert space, not only for the vectors of a particular basis. This definition is therefore basis independent.

In practice, however, it is not feasible to check this condition for all possible states. There is an equivalent and much more useful criterion: a density matrix is positive if and only if all its eigenvalues are nonnegative. Therefore, positivity is typically verified by diagonalizing  $\rho$ . This means that a density matrix is a *positive semidefinite* operator, that is, all its eigenvalues are nonnegative (but may be zero), ensuring that probabilities are never negative.

### Dynamical maps

The time evolution of a quantum system is described by a map

$$\mathcal{E} : \rho \longmapsto \mathcal{E}(\rho),$$

which takes an initial density matrix to a final one. For this evolution to be physically meaningful, it must map any valid density matrix to another valid density matrix.

### Complete positivity

A map  $\mathcal{E}$  is called *positive* if it maps positive operators to positive operators. However, this condition is not sufficient in quantum mechanics. The issue is that the system of interest may be entangled with another system (for example, its environment). To ensure physical consistency in this more general situation, we require a stronger condition known as *complete positivity*.

Complete positivity means that for any auxiliary system (of arbitrary dimension), the extended map

$$\mathcal{E} \otimes \mathbb{1}$$

also preserves positivity, where  $\mathbb{1}$  denotes the identity map acting on the auxiliary system. In other words, for any joint state  $\rho_{SA}$  of the system  $S$  and an auxiliary system  $A$  (including entangled states),

$$(\mathcal{E} \otimes \mathbb{1})(\rho_{SA})$$

must be a valid density matrix, i.e., it must remain positive (all eigenvalues are  $\geq 0$ ).

### Physical meaning

This requirement is essential because the system may be entangled with its environment. If a map were only positive but not completely positive, applying it locally to part of an entangled state could produce a matrix with negative eigenvalues. This would lead to negative probabilities, which are unphysical. Thus, complete positivity guarantees that the evolution remains physically consistent even when the system is part of a larger quantum system.

These ideas are central across quantum optics, atomic physics, condensed matter, quantum thermodynamics, and quantum information science. In particular, the Lindblad framework is used to describe spontaneous emission, dephasing, cavity loss, driven-dissipative phase transitions, dissipative state preparation, noise in quantum processors, and engineered dissipation for control and sensing.

## 8.5 Unitary evolution: Closed system

For a closed quantum system, the state vector evolves according to the Schrödinger equation,

$$\frac{d}{dt} |\psi(t)\rangle = -iH |\psi(t)\rangle,$$

where we set  $\hbar = 1$ . If the Hamiltonian is time independent, the solution is

$$|\psi(t)\rangle = e^{-iHt} |\psi(0)\rangle. \quad (8.9)$$

The operator  $U(t) = e^{-iHt}$  is unitary because  $H$  is Hermitian, i.e.,  $U^\dagger U = \mathbb{1}$ . As a result, it preserves the norm of the state and therefore all probabilities.

### 8.5.1 Von Neumann equation for density matrices

The density-matrix formalism provides a unified description of both pure and mixed states. Unlike the Schrödinger equation, which applies to state vectors, the von Neumann equation governs the evolution of density matrices and is valid in both cases.

For a mixed state written as

$$\rho(t) = \sum_i p_i |\psi_i(t)\rangle \langle \psi_i(t)|,$$

we can evolve each pure component according to the Schrödinger equation and then reconstruct  $\rho(t)$ . Differentiating with respect to time and using the Schrödinger equation for each component, one obtains

$$\dot{\rho} = -i[H, \rho], \quad (8.10)$$

which is the density-matrix analog of Schrödinger evolution.

The commutator indicates that the Hamiltonian acts on  $\rho$  both from the left and from the right,

$$[H, \rho] = H\rho - \rho H.$$

### Conservation of purity

A key property of unitary evolution is that the purity,  $\text{Tr}(\rho^2)$ , is conserved in time. Using Eq. (8.10), we compute

$$\frac{d}{dt} \text{Tr}(\rho^2) = \text{Tr}(\dot{\rho}\rho + \rho\dot{\rho}) = 2 \text{Tr}(\rho\dot{\rho}),$$

where we used the cyclic property of the trace. Substituting  $\dot{\rho} = -i[H, \rho]$ , we obtain

$$\frac{d}{dt} \text{Tr}(\rho^2) = -2i \text{Tr}(\rho(H\rho - \rho H)).$$

Using again the cyclic property of the trace,  $\text{Tr}(ABC) = \text{Tr}(BCA) = \text{Tr}(CAB)$ , we find

$$\text{Tr}(\rho H \rho) = \text{Tr}(H \rho^2) = \text{Tr}(\rho^2 H),$$

so the two terms cancel. Therefore,

$$\frac{d}{dt} \text{Tr}(\rho^2) = 0. \quad (8.11)$$

Under *closed* (unitary) evolution, a pure state remains pure, and a mixed state retains exactly the same degree of mixedness. In particular, no loss of coherence or increase in entropy can occur in an isolated system.

## 8.6 Open systems and reduced density matrices

We begin with a total (closed) system consisting of the system  $S$  and the environment  $E$ , with Hamiltonian

$$H_T = H_S + H_E + \alpha H_I, \quad H_I = \sum_i S_i \otimes E_i,$$

where  $S_i$  are the operators acting on the system Hilbert space and  $E_i$  are operators acting on the environment Hilbert space. The total density matrix evolves according to the von Neumann equation,

$$\frac{d\rho_T(t)}{dt} = -i[H_T, \rho_T(t)].$$

Our goal is to obtain an effective equation for the reduced density matrix

$$\rho_S(t) = \text{Tr}_E(\rho_T(t)).$$

**Interaction picture.** To separate the effect of the interaction from the free evolution, we move to the interaction picture, where operators evolve as

$$\hat{O}(t) = e^{i(H_S+H_E)t} O e^{-i(H_S+H_E)t}.$$

The time derivative of  $\hat{\rho}_T(t)$  is

$$\begin{aligned} \frac{d\hat{\rho}_T(t)}{dt} &= \frac{d}{dt} (e^{iH_0t} \rho_T(t) e^{-iH_0t}) \\ &= iH_0 e^{iH_0t} \rho_T(t) e^{-iH_0t} + e^{iH_0t} \frac{d\rho_T(t)}{dt} e^{-iH_0t} - e^{iH_0t} \rho_T(t) e^{-iH_0t} iH_0 \\ &= i[H_0, \hat{\rho}_T(t)] + e^{iH_0t} \frac{d\rho_T(t)}{dt} e^{-iH_0t}. \end{aligned} \quad (8.12)$$

Substituting the von Neumann equation,  $\frac{d\rho_T(t)}{dt} = -i[H_0 + \alpha H_I, \rho_T(t)]$ , we get

$$\frac{d\hat{\rho}_T(t)}{dt} = i[H_0, \hat{\rho}_T(t)] - i e^{iH_0 t} [H_0, \rho_T(t)] e^{-iH_0 t} - i\alpha e^{iH_0 t} [H_I, \rho_T(t)] e^{-iH_0 t}. \quad (8.13)$$

Therefore, in this picture, the evolution of the density matrix is governed only by the interaction Hamiltonian,

$$\frac{d\hat{\rho}_T(t)}{dt} = -i\alpha [\hat{H}_I(t), \hat{\rho}_T(t)]. \quad (8.14)$$

This equation is exact.

We can formally integrate Eq. (8.14),

$$\hat{\rho}_T(t) = \hat{\rho}_T(0) - i\alpha \int_0^t ds [\hat{H}_I(s), \hat{\rho}_T(s)]. \quad (8.15)$$

**Iterating once (Born expansion).** Substituting Eq. (8.15) back into Eq. (8.14), we obtain

$$\frac{d\hat{\rho}_T(t)}{dt} = -i\alpha [\hat{H}_I(t), \hat{\rho}_T(0)] - \alpha^2 \int_0^t ds [\hat{H}_I(t), [\hat{H}_I(s), \hat{\rho}_T(s)]]. \quad (8.16)$$

This equation is still exact, but it explicitly shows that the evolution depends on the past history through the integral.

To obtain a closed equation for the reduced system density matrix, several standard approximations are introduced, as listed below. The derivation of the final Lindblad equation is shown at the end of this chapter in Sec. 8.12.

- **Born approximation.** We assume weak coupling between system and environment, so that the total density matrix factorizes at all times,

$$\hat{\rho}_T(t) \approx \hat{\rho}(t) \otimes \hat{\rho}_E,$$

where  $\hat{\rho}_E$  is a stationary state of the environment. This allows us to trace out the environment degrees of freedom.

- **Tracing over the environment.** Taking the partial trace over the environment eliminates the first-order term (under the usual assumption  $\text{Tr}_E[\hat{H}_I(t)\hat{\rho}_E] = 0$ ) and produces an equation for the reduced density matrix  $\hat{\rho}(t)$  involving environment correlation functions.
- **Markov approximation.** We assume that the environment correlation time is much shorter than the system evolution time. As a result, we replace

$$\hat{\rho}(s) \approx \hat{\rho}(t),$$

and extend the upper limit of the integral to infinity, obtaining a time-local (memoryless) equation.

- **Secular (rotating-wave) approximation.** We decompose system operators into eigenoperators of the system Hamiltonian and neglect rapidly oscillating terms. This step ensures that the generator is of Gorini–Kossakowski–Sudarshan–Lindblad form and preserves complete positivity.
- **Return to the Schrödinger picture.** Finally, transforming back to the Schrödinger picture restores the unitary part of the dynamics, yielding a Hamiltonian contribution together with dissipative terms.

### The Lindblad master equation

After these steps, the master equation takes the standard Lindblad form, as written in Eq. (8.6),

$$\dot{\rho} = -i[H, \rho] + \sum_k \left( L_k \rho L_k^\dagger - \frac{1}{2} \{L_k^\dagger L_k, \rho\} \right), \quad (8.17)$$

where  $H$  includes possible environment-induced shifts (Lamb shift), and the operators  $L_k$  encode the dissipative processes determined by the system–environment coupling and bath correlations.

### When should one be cautious?

The Lindblad equation is excellent when the bath is memoryless enough and the coupling is weak enough. One should be cautious when:

- the system and environment are strongly coupled,
- bath correlations decay slowly,
- different Bohr frequencies are not well separated,
- the initial system–environment correlations are important.

In those cases, non-Markovian or more microscopic treatments may be needed.

## 8.7 Vectorization of the density matrix

The Lindblad master equation in Eq. (8.6) [or above in Eq. (8.17)] is an operator equation for the density matrix that can be written as

$$\boxed{\frac{d\rho}{dt} = \mathcal{L}[\rho]},$$

where  $\mathcal{L}$  is the generator of the dynamics. In analytical and numerical work, it is often convenient to convert this operator equation into an ordinary matrix differential equation. Instead of viewing  $\rho$  as a matrix, we view it as a vector in a larger linear space of dimension  $D^2$ , where  $D$  is the Hilbert-space dimension.

This larger space is often called *Liouville space*, *Fock–Liouville space*, or *operator space*. In this representation, the generator  $\mathcal{L}$  becomes an ordinary matrix, called the *Liouvillian* or *Lindbladian*.

**Basis convention.** Throughout this chapter, we use the convention

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \sigma^z|1\rangle = +|1\rangle, \quad \sigma^z|0\rangle = -|0\rangle.$$

Thus, the first basis index corresponds to the state  $|1\rangle$ .

As an example, consider the  $2 \times 2$  density matrix written in this basis:

$$\rho = \begin{pmatrix} \rho_{11} & \rho_{10} \\ \rho_{01} & \rho_{00} \end{pmatrix}.$$

Here,

$$\rho_{11} = \langle 1|\rho|1\rangle, \quad \rho_{00} = \langle 0|\rho|0\rangle,$$

are the populations of the excited and ground states, respectively, while

$$\rho_{10} = \langle 1|\rho|0\rangle, \quad \rho_{01} = \langle 0|\rho|1\rangle,$$

are the coherences.

We define the vectorized form of  $\rho$  by stacking its entries row by row:

$$|\rho\rangle\rangle \equiv \text{vec}(\rho) = \begin{pmatrix} \rho_{11} \\ \rho_{10} \\ \rho_{01} \\ \rho_{00} \end{pmatrix}. \quad (8.18)$$

More generally, for a  $D \times D$  matrix  $\rho$  with entries  $\rho_{ij}$ , we define

$$\text{vec}(\rho) = \begin{pmatrix} \rho_{11} \\ \rho_{12} \\ \dots \\ \rho_{1D} \\ \rho_{21} \\ \rho_{22} \\ \dots \\ \vdots \\ \rho_{DD} \end{pmatrix}.$$

**Remark on conventions.** There are two common vectorization conventions in the literature: row stacking and column stacking. The formulas below are written for the row-stacking convention in Eq. (8.18). If one instead stacks columns, some tensor-product factors are interchanged. It is important to choose one convention and use it consistently.

### 8.7.1 Vectorization identity

A central identity used in the studies of the Lindbladian is

$$\text{vec}(A\rho B) = (A \otimes B^T) \text{vec}(\rho), \quad (8.19)$$

where  $A$  and  $B$  are ordinary matrices and  $B^T$  denotes the transpose of  $B$ .

### Derivation

Let us derive Eq. (8.19) through the components of the matrices involved. The  $(i, j)$  matrix element of  $A\rho B$  is

$$(A\rho B)_{ij} = \sum_{m,n} A_{im} \rho_{mn} B_{nj}.$$

In our row-stacking convention, the component of  $\text{vec}(A\rho B)$  associated with the pair  $(i, j)$  is exactly  $(A\rho B)_{ij}$ .

Now consider the vector  $(A \otimes B^T)\text{vec}(\rho)$ . Its  $(i, j)$  component is

$$\sum_{m,n} A_{im} (B^T)_{jn} \rho_{mn} = \sum_{m,n} A_{im} B_{nj} \rho_{mn},$$

which is precisely  $(A\rho B)_{ij}$ . Therefore,

$$\text{vec}(A\rho B) = (A \otimes B^T) \text{vec}(\rho).$$

### 8.7.2 Vectorization identity for the Lindblad equation

Consider first a Lindblad master equation with a single jump operator  $L$ ,

$$\frac{d\rho}{dt} = -i[H, \rho] + L\rho L^\dagger - \frac{1}{2}\{L^\dagger L, \rho\}. \quad (8.20)$$

Using Eq. (8.19), we can rewrite each term separately.

#### Non-dissipative part

Since

$$\text{vec}(H\rho) = (H \otimes \mathbb{1})\text{vec}(\rho), \quad \text{vec}(\rho H) = (\mathbb{1} \otimes H^T)\text{vec}(\rho),$$

we obtain

$$\text{vec}(-i[H, \rho]) = -i(H \otimes \mathbb{1} - \mathbb{1} \otimes H^T)\text{vec}(\rho). \quad (8.21)$$

#### Dissipative part

For the recycling term,

$$\text{vec}(L\rho L^\dagger) = (L \otimes (L^\dagger)^T)\text{vec}(\rho) = (L \otimes L^*)\text{vec}(\rho),$$

where  $L^*$  is the complex conjugate of  $L$ .

For the anticommutator terms,

$$\text{vec}(L^\dagger L \rho) = (L^\dagger L \otimes \mathbb{1})\text{vec}(\rho),$$

and

$$\text{vec}(\rho L^\dagger L) = (\mathbb{1} \otimes (L^\dagger L)^T)\text{vec}(\rho).$$

Putting everything together, Eq. (8.20) becomes

$$\frac{d}{dt} \|\rho\rangle\rangle = \tilde{\mathcal{L}} \|\rho\rangle\rangle, \quad (8.22)$$

with

$$\tilde{\mathcal{L}} = -i(H \otimes \mathbb{1} - \mathbb{1} \otimes H^T) + L \otimes L^* - \frac{1}{2} \left( L^\dagger L \otimes \mathbb{1} + \mathbb{1} \otimes (L^\dagger L)^T \right). \quad (8.23)$$

For several jump operators  $L_k$ , we simply sum over  $k$ :

$$\tilde{\mathcal{L}} = -i(H \otimes \mathbb{1} - \mathbb{1} \otimes H^T) + \sum_k \left[ L_k \otimes L_k^* - \frac{1}{2} \left( L_k^\dagger L_k \otimes \mathbb{1} + \mathbb{1} \otimes (L_k^\dagger L_k)^T \right) \right]. \quad (8.24)$$

The vectorized form converts the master equation into a standard linear differential equation. The solution can be formally written as

$$\|\rho(t)\rangle\rangle = e^{\tilde{\mathcal{L}}t} \|\rho(0)\rangle\rangle.$$

**The vectorized formulation provides a convenient representation of the Lindblad equation in an enlarged linear space. Its main advantage is that, once the density matrix is expressed as a vector, standard tools of linear algebra can be applied directly.**

### 8.7.3 Spectral properties of the Lindbladian

The Lindbladian  $\tilde{\mathcal{L}}$  is a linear superoperator acting on the space of density matrices. In general, it is *non-Hermitian*, and therefore its eigenvalues are typically complex:

$$\lambda_\alpha \in \mathbb{C}.$$

This is physically natural. The Hamiltonian part of the evolution generates coherent oscillations (purely imaginary contributions), while the dissipative part produces decay (negative real parts). One therefore often writes

$$\lambda_\alpha = -\Gamma_\alpha + i\omega_\alpha,$$

where:

- $\Gamma_\alpha \geq 0$  is a decay rate,
- $\omega_\alpha$  is an oscillation frequency.

A mode proportional to  $e^{\lambda_\alpha t}$  then behaves as

$$e^{\lambda_\alpha t} = e^{-\Gamma_\alpha t} e^{i\omega_\alpha t}.$$

Thus, the real part controls relaxation, while the imaginary part controls oscillations.

*Important constraint:* For physical (completely positive and trace-preserving) Lindblad dynamics, all eigenvalues satisfy

$$\text{Re}(\lambda_\alpha) \leq 0,$$

which ensures that no mode grows exponentially in time.

### Left and right eigenvectors (dynamical modes)

For a Hermitian operator, eigenvectors can be chosen orthonormal,  $\langle n|m \rangle = \delta_{nm}$ . For a non-Hermitian operator such as the Lindbladian  $\tilde{\mathcal{L}}$ , this is no longer true in general. In particular, the right eigenvectors of  $\tilde{\mathcal{L}}$  are not orthogonal to each other under the usual inner product.

We define

$$\tilde{\mathcal{L}} \|\Lambda_\alpha^R\rangle\rangle = \lambda_\alpha \|\Lambda_\alpha^R\rangle\rangle, \quad \langle\langle \Lambda_\alpha^L | \tilde{\mathcal{L}} = \lambda_\alpha \langle\langle \Lambda_\alpha^L |. \quad (8.25)$$

where

- $\|\Lambda_\alpha^R\rangle\rangle$  is a *right eigenvector* (a column vector in Liouville space),
- $\langle\langle \Lambda_\alpha^L |$  is a *left eigenvector* (a row vector),
- $\lambda_\alpha$  is the corresponding eigenvalue.

The right eigenvectors are often referred to as *dynamical modes* of the evolution. As for the left eigenvectors, we can also write them in a column form as

$$\tilde{\mathcal{L}}^\dagger \|\Lambda_\alpha^L\rangle\rangle = \lambda_\alpha^* \|\Lambda_\alpha^L\rangle\rangle. \quad (8.26)$$

**Why do we need left eigenvectors?** The right eigenvectors alone are not enough to expand an arbitrary state. Because  $\tilde{\mathcal{L}}$  is non-Hermitian, the right eigenvectors do not form an orthonormal basis, so we cannot simply project onto them using their Hermitian conjugates. The left eigenvectors provide the correct dual objects that allow us to extract expansion coefficients.

In the double-ket notation,  $\|X\rangle\rangle \equiv \text{vec}(X)$  is the vectorized form of an operator  $X$ , and

$$\langle\langle A|B\rangle\rangle \equiv \text{Tr}(A^\dagger B)$$

is the natural inner product in operator (Liouville) space.

**Biorthonormality.** The left and right eigenvectors of a non-Hermitian operator satisfy the biorthogonality relation

$$\langle\langle \Lambda_\alpha^L | \Lambda_\beta^R \rangle\rangle = 0, \quad \alpha \neq \beta, \quad (8.27)$$

provided the eigenvalues are nondegenerate. The normalization of each pair can be chosen arbitrarily; in particular, one can rescale the eigenvectors so that

$$\langle\langle \Lambda_\alpha^L | \Lambda_\beta^R \rangle\rangle = \delta_{\alpha\beta}. \quad (8.28)$$

The left eigenvectors form a dual basis to the right eigenvectors: each left eigenvector “selects” one right eigenvector and is orthogonal to all others.

When one diagonalizes  $\tilde{\mathcal{L}}$  numerically, one typically obtains:

- right eigenvectors from  $\tilde{\mathcal{L}}$ ,
- left eigenvectors from  $\tilde{\mathcal{L}}^\dagger$  (or equivalently from solving the left eigenvalue problem).

These eigenvectors are defined only up to normalization. In general, they do *not* automatically satisfy Eq. (8.28). However, since eigenvectors can be freely rescaled, one can always enforce biorthonormality by choosing appropriate normalization factors.

Concretely, if

$$\langle\langle \Lambda_\alpha^L | \Lambda_\alpha^R \rangle\rangle = c_\alpha \neq 0,$$

one may rescale the eigenvectors so that their overlap becomes unity. For example, keeping the left eigenvector unchanged and rescaling only the right one,

$$\|\Lambda_\alpha^R\rangle\rangle \rightarrow \frac{1}{c_\alpha} \|\Lambda_\alpha^R\rangle\rangle, \quad \langle\langle \Lambda_\alpha^L | \rightarrow \langle\langle \Lambda_\alpha^L |,$$

gives

$$\langle\langle \Lambda_\alpha^L | \Lambda_\alpha^R \rangle\rangle = 1.$$

More generally, one may rescale both vectors as

$$\|\Lambda_\alpha^R\rangle\rangle \rightarrow a_\alpha \|\Lambda_\alpha^R\rangle\rangle, \quad \langle\langle \Lambda_\alpha^L | \rightarrow b_\alpha \langle\langle \Lambda_\alpha^L |,$$

provided that

$$a_\alpha b_\alpha = \frac{1}{c_\alpha}.$$

For many purposes (e.g., computing eigenvalues or relaxation rates), this normalization is not necessary. However, if one wants to:

- expand the density matrix in terms of eigenmodes,
- write a resolution of the identity,
- or interpret coefficients as amplitudes,

then imposing biorthonormality is extremely convenient and often essential.

**Resolution of the identity.** When Eq. (8.28) holds, we can write

$$\mathbb{1} = \sum_\alpha \|\Lambda_\alpha^R\rangle\rangle \langle\langle \Lambda_\alpha^L |, \quad (8.29)$$

which allows us to expand any density matrix in terms of the dynamical modes of the Lindbladian.

### Mode decomposition of the dynamics

Using Eq. (8.29), the initial state can be expanded as

$$\|\rho(0)\rangle\rangle = \sum_\alpha \|\Lambda_\alpha^R\rangle\rangle \langle\langle \Lambda_\alpha^L | \rho(0)\rangle\rangle. \quad (8.30)$$

The solution at time  $t$  then follows directly:

$$\|\rho(t)\rangle\rangle = \sum_\alpha e^{\lambda_\alpha t} \|\Lambda_\alpha^R\rangle\rangle \langle\langle \Lambda_\alpha^L | \rho(0)\rangle\rangle. \quad (8.31)$$

This expression shows that the dynamics decomposes into independent *dynamical modes* of the Lindbladian. Each mode evolves exponentially as  $e^{\lambda_\alpha t}$ . Each right eigenvector corresponds to a distinct *mode of evolution*, characterized by its own decay rate and oscillation frequency. The left eigenvectors are not usually called modes, because they do not describe independent time evolution.

- Modes with  $\text{Re}(\lambda_\alpha) < 0$  decay in time.
- Modes with  $\text{Re}(\lambda_\alpha) = 0$  persist indefinitely.
- The eigenvalue  $\lambda_\alpha = 0$  corresponds to steady-state contributions (see more details below).

The decomposition in Eq. (8.31) shows that the Lindbladian spectrum fully determines the dynamics:

- eigenvalues with the largest real part (closest to zero) control the long-time behavior,
- the spectral gap (difference between the zero eigenvalue and the eigenvalue whose real part is closest to 0), defined as

$$\Delta = -\max_{\alpha \neq 0} \text{Re}(\lambda_\alpha),$$

sets the relaxation time  $\tau \sim 1/\Delta$ ,

- the imaginary parts  $\text{Im}(\lambda_\alpha)$  determine oscillatory behavior.

#### 8.7.4 Steady states and long-time behavior

An important use of the vectorized form is the determination of the long-time state of the system. Starting from

$$\frac{d}{dt} \|\rho(t)\rangle\rangle = \tilde{\mathcal{L}} \|\rho(t)\rangle\rangle,$$

a *steady state* is, by definition, a density matrix that no longer changes in time. If

$$\rho_{\text{ss}}(t) = \rho_{\text{ss}} = \text{constant},$$

then

$$\frac{d}{dt} \|\rho_{\text{ss}}\rangle\rangle = 0,$$

which implies

$$\tilde{\mathcal{L}} \|\rho_{\text{ss}}\rangle\rangle = 0. \tag{8.32}$$

Thus, steady states correspond to the *right eigenvectors of the Lindbladian with eigenvalue zero*.

Equivalently, we can say that the steady-state density matrices span the kernel of  $\tilde{\mathcal{L}}$ . In linear algebra, the *kernel* (or *null space*) of an operator is the set of all vectors that are mapped to zero:

$$\ker(\tilde{\mathcal{L}}) = \left\{ \|X\rangle\rangle : \tilde{\mathcal{L}} \|X\rangle\rangle = 0 \right\}.$$

Therefore, any steady state must belong to the kernel of  $\tilde{\mathcal{L}}$ . Conversely, any vector in the kernel corresponds to a stationary (time-independent) density matrix.

The statement that *steady-state density matrices span the kernel* means that:

- All steady states are contained in the kernel of  $\tilde{\mathcal{L}}$ ,
- If there is more than one steady state, they form a vector space (the kernel),
- Any linear combination of these steady states (with appropriate normalization and positivity) is also a steady state.

If the kernel is one-dimensional, there is a unique steady state. If the kernel has higher dimension, there are multiple steady states, and the long-time state can depend on the initial condition.

**More than one zero eigenvalue.** It is possible for the Lindbladian to have more than one linearly independent eigenvector with eigenvalue zero. In that case, there is not a unique steady state. Instead, the long-time state depends on the initial condition and is given by the projection of the initial density matrix onto the zero-eigenspace of  $\tilde{\mathcal{L}}$ . Symbolically,

$$\|\rho(t)\rangle\rangle \xrightarrow[t \rightarrow \infty]{} \mathcal{P}_0 \|\rho(0)\rangle\rangle ,$$

where  $\mathcal{P}_0$  is the projector onto the kernel of  $\tilde{\mathcal{L}}$ . This situation may occur, for example, when the dynamics has conserved sectors, strong symmetries, or decoherence-free subspaces. In such cases, different initial states can relax to different stationary density matrices.

**Saturation:** When the zero eigenvalue is unique, saturation means relaxation to a single stationary state. When the zero eigenvalue is degenerate, saturation means relaxation to a stationary state that still depends on the initial condition through its overlap with the steady-state subspace.

**A further possibility: persistent oscillations.** Although the generic situation is relaxation to a time-independent state, one should note that a Lindbladian may also have eigenvalues on the imaginary axis,

$$\lambda_\alpha = i\omega_\alpha, \quad \omega_\alpha \neq 0,$$

with zero real part. In that case, some modes do not decay and the system may display persistent oscillations rather than convergence to a time-independent steady state. Thus, strictly speaking, saturation to a stationary density matrix occurs when the only eigenvalues with zero real part are the zero eigenvalues themselves.

**Practical procedure.** In practice, to determine the long-time behavior one proceeds as follows:

1. Build the Lindbladian matrix  $\tilde{\mathcal{L}}$ .
2. Diagonalize it (or compute its relevant spectral subspace).

3. Identify the eigenvectors with  $\lambda = 0$ .
4. If there is a unique such eigenvector, normalize it to obtain  $\rho_{ss}$ .
5. If there are several, project the initial state onto the zero-eigenspace to determine the asymptotic state.

## 8.8 Example 1: One qubit with one jump operator

We adopt the convention

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (8.33)$$

With this choice,  $|1\rangle$  has eigenvalue  $+1$  of  $\sigma_z$  and will be interpreted as the higher-energy state, while  $|0\rangle$  has eigenvalue  $-1$  and is the lower-energy state.

Let us consider a two-level system (qubit) with basis  $\{|1\rangle, |0\rangle\}$ , Hamiltonian

$$H = \frac{\omega}{2}\sigma_z = \frac{\omega}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} \omega/2 & 0 \\ 0 & -\omega/2 \end{pmatrix}, \quad (8.34)$$

and jump operator

$$L = \sqrt{\gamma}\sigma_- = \sqrt{\gamma} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \sqrt{\gamma}|0\rangle\langle 1|, \quad (8.35)$$

which describes spontaneous decay from  $|1\rangle$  to  $|0\rangle$ .

To obtain the Lindbladian in Eq. (8.23),

$$\tilde{\mathcal{L}} = -i(H \otimes \mathbb{1} - \mathbb{1} \otimes H^T) + L \otimes L^* - \frac{1}{2}(L^\dagger L \otimes \mathbb{1} + \mathbb{1} \otimes (L^\dagger L)^T),$$

we first compute

$$L^\dagger L = \gamma|1\rangle\langle 1| = \begin{pmatrix} \gamma & 0 \\ 0 & 0 \end{pmatrix}. \quad (8.36)$$

We will vectorize the density matrix using the row-stacking convention adapted to the basis ordering  $\{|1\rangle, |0\rangle\}$ :

$$\|\rho\rangle\rangle = \text{vec}(\rho) = \begin{pmatrix} \rho_{11} \\ \rho_{10} \\ \rho_{01} \\ \rho_{00} \end{pmatrix}. \quad (8.37)$$

We now compute the  $4 \times 4$  matrices entering the Lindbladian.

**1. The term  $H \otimes \mathbb{1}$ :**

$$H \otimes \mathbb{1} = \begin{pmatrix} \omega/2 & 0 \\ 0 & -\omega/2 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} \omega/2 & 0 & 0 & 0 \\ 0 & \omega/2 & 0 & 0 \\ 0 & 0 & -\omega/2 & 0 \\ 0 & 0 & 0 & -\omega/2 \end{pmatrix}. \quad (8.38)$$

**2. The term  $\mathbb{1} \otimes H^T$ :** since  $H$  is diagonal,  $H^T = H$ , so

$$\mathbb{1} \otimes H^T = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} \omega/2 & 0 \\ 0 & -\omega/2 \end{pmatrix} = \begin{pmatrix} \omega/2 & 0 & 0 & 0 \\ 0 & -\omega/2 & 0 & 0 \\ 0 & 0 & \omega/2 & 0 \\ 0 & 0 & 0 & -\omega/2 \end{pmatrix}. \quad (8.39)$$

**3. The term  $L \otimes L^*$ :**

$$L = \sqrt{\gamma} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad L^* = \sqrt{\gamma} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},$$

so

$$L \otimes L^* = \sqrt{\gamma} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \otimes \sqrt{\gamma} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \gamma \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \quad (8.40)$$

**4. The term  $L^\dagger L \otimes \mathbb{1}$ :**

$$L^\dagger L \otimes \mathbb{1} = \begin{pmatrix} \gamma & 0 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} \gamma & 0 & 0 & 0 \\ 0 & \gamma & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (8.41)$$

**5. The term  $\mathbb{1} \otimes (L^\dagger L)^T$ :** since  $L^\dagger L$  is diagonal,  $(L^\dagger L)^T = L^\dagger L$ , so

$$\mathbb{1} \otimes (L^\dagger L)^T = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} \gamma & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} \gamma & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \gamma & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (8.42)$$

Putting everything together, the Liouvillian (Lindbladian) matrix becomes

$$\tilde{\mathcal{L}} = \begin{pmatrix} -\gamma & 0 & 0 & 0 \\ 0 & -i\omega - \gamma/2 & 0 & 0 \\ 0 & 0 & i\omega - \gamma/2 & 0 \\ \gamma & 0 & 0 & 0 \end{pmatrix}. \quad (8.43)$$

Therefore, the master equation becomes the system of ordinary differential equations

$$\dot{\rho}_{11} = -\gamma \rho_{11}, \quad (8.44)$$

$$\dot{\rho}_{10} = \left(-i\omega - \frac{\gamma}{2}\right) \rho_{10}, \quad (8.45)$$

$$\dot{\rho}_{01} = \left(i\omega - \frac{\gamma}{2}\right) \rho_{01}, \quad (8.46)$$

$$\dot{\rho}_{00} = \gamma \rho_{11}. \quad (8.47)$$

The solutions are

$$\rho_{11}(t) = \rho_{11}(0) e^{-\gamma t}, \quad (8.48)$$

$$\rho_{10}(t) = \rho_{10}(0) e^{-i\omega t} e^{-\frac{\gamma}{2}t}, \quad (8.49)$$

$$\rho_{01}(t) = \rho_{01}(0) e^{i\omega t} e^{-\frac{\gamma}{2}t}, \quad (8.50)$$

$$\rho_{00}(t) = \rho_{00}(0) + \rho_{11}(0) (1 - e^{-\gamma t}). \quad (8.51)$$

The last equation above is obtained by substituting the solution for  $\rho_{11}(t)$  in  $\dot{\rho}_{00}$

$$\dot{\rho}_{00} = \gamma \rho_{11}(0) e^{-\gamma t} \quad (8.52)$$

and integrating from 0 to  $t$ .

This example is instructive:

- the excited-state population  $\rho_{11}$  decays exponentially;
- the ground-state population  $\rho_{00}$  increases accordingly;
- the coherences  $\rho_{10}$  and  $\rho_{01}$  oscillate with frequency  $\omega$  while decaying with rate  $\gamma/2$ .

## Eigenvalues and eigenvectors of the Lindbladian

The analysis presented above can be recast entirely in terms of the eigenvalues and eigenvectors of the Lindbladian, providing a direct spectral interpretation of the dynamics.

### Eigenvalues of the Lindbladian

To find the eigenvalues, we solve

$$\det(\tilde{\mathcal{L}} - \lambda I) = 0. \quad (8.53)$$

We have

$$\tilde{\mathcal{L}} - \lambda I = \begin{pmatrix} -\gamma - \lambda & 0 & 0 & 0 \\ 0 & -i\omega - \frac{\gamma}{2} - \lambda & 0 & 0 \\ 0 & 0 & i\omega - \frac{\gamma}{2} - \lambda & 0 \\ \gamma & 0 & 0 & -\lambda \end{pmatrix}. \quad (8.54)$$

Expanding along the first row,

$$\det(\tilde{\mathcal{L}} - \lambda I) = (-\gamma - \lambda) \det \begin{pmatrix} -i\omega - \frac{\gamma}{2} - \lambda & 0 & 0 \\ 0 & i\omega - \frac{\gamma}{2} - \lambda & 0 \\ 0 & 0 & -\lambda \end{pmatrix} \quad (8.55)$$

$$= (-\gamma - \lambda) \left( -i\omega - \frac{\gamma}{2} - \lambda \right) \left( i\omega - \frac{\gamma}{2} - \lambda \right) (-\lambda). \quad (8.56)$$

Setting this equal to zero, we obtain the eigenvalues of the Lindbladian

$$\lambda_1 = -\gamma, \quad \lambda_2 = -i\omega - \frac{\gamma}{2}, \quad \lambda_3 = i\omega - \frac{\gamma}{2}, \quad \lambda_4 = 0. \quad (8.57)$$

**Right eigenvectors**

To find the corresponding right eigenstates, let

$$|R\rangle = \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}, \quad (8.58)$$

and solve

$$\tilde{\mathcal{L}}|R\rangle = \lambda|R\rangle. \quad (8.59)$$

This gives

$$-\gamma a = \lambda a, \quad (8.60)$$

$$\left(-i\omega - \frac{\gamma}{2}\right) b = \lambda b, \quad (8.61)$$

$$\left(i\omega - \frac{\gamma}{2}\right) c = \lambda c, \quad (8.62)$$

$$\gamma a = \lambda d. \quad (8.63)$$

Thus, the eigenvalues and corresponding right eigenstates are

$$\lambda_1 = -\gamma, \quad |R_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix}, \quad (8.64)$$

$$\lambda_2 = -i\omega - \frac{\gamma}{2}, \quad |R_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad (8.65)$$

$$\lambda_3 = i\omega - \frac{\gamma}{2}, \quad |R_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad (8.66)$$

$$\lambda_4 = 0, \quad |R_4\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \quad (8.67)$$

**Important remarks:**

- As discussed before, the right eigenvectors are not necessarily orthogonal, which contrasts with the eigenstates of Hermitian Hamiltonians. Indeed,  $|R_1\rangle$  and  $|R_4\rangle$  are not orthogonal.
- Notice also that we did not impose normalization to these eigenvectors;  $|R_1\rangle$  is a clear example. Instead, we choose the elements to ensure that  $\langle L_\alpha | R_\alpha \rangle = 1$ , as shown below.

### Stationary state

The stationary state is obtained from

$$\tilde{\mathcal{L}} \|\rho_{ss}\rangle\rangle = 0,$$

which gives

$$\rho_{ss} = |0\rangle\langle 0|.$$

### Left eigenvectors

Let

$$\langle\langle L_\alpha| = (a_\alpha \ b_\alpha \ c_\alpha \ d_\alpha). \quad (8.68)$$

Then the left-eigenvalue equation  $\langle\langle L_\alpha| \tilde{\mathcal{L}} = \lambda_\alpha \langle\langle L_\alpha|$  determines the coefficients.

1)  $\lambda_1 = -\gamma$ .

We solve

$$(a \ b \ c \ d) \begin{pmatrix} -\gamma & 0 & 0 & 0 \\ 0 & -i\omega - \gamma/2 & 0 & 0 \\ 0 & 0 & i\omega - \gamma/2 & 0 \\ \gamma & 0 & 0 & 0 \end{pmatrix} = -\gamma (a \ b \ c \ d). \quad (8.69)$$

This gives

$$(-\gamma a + \gamma d, (-i\omega - \gamma/2)b, (i\omega - \gamma/2)c, 0) = (-\gamma a, -\gamma b, -\gamma c, -\gamma d). \quad (8.70)$$

Hence  $d = 0$ ,  $b = 0$ , and  $c = 0$ , so we may choose

$$\langle\langle L_1| = (1 \ 0 \ 0 \ 0). \quad (8.71)$$

Indeed,

$$\langle\langle L_1|R_1\rangle\rangle = 1. \quad (8.72)$$

2)  $\lambda_2 = -i\omega - \gamma/2$ .

Similarly, one finds

$$\langle\langle L_2| = (0 \ 1 \ 0 \ 0), \quad (8.73)$$

which satisfies

$$\langle\langle L_2|R_2\rangle\rangle = 1. \quad (8.74)$$

3)  $\lambda_3 = i\omega - \gamma/2$ .

Likewise,

$$\langle\langle L_3| = (0 \ 0 \ 1 \ 0), \quad (8.75)$$

with

$$\langle\langle L_3|R_3\rangle\rangle = 1. \quad (8.76)$$

4)  $\lambda_4 = 0$ .

Now solve

$$\langle\langle L_4 | \tilde{\mathcal{L}} = 0. \quad (8.77)$$

This gives

$$-\gamma a + \gamma d = 0, \quad b = 0, \quad c = 0, \quad (8.78)$$

so  $d = a$ . Choosing the normalization such that  $\langle\langle L_4 | R_4 \rangle\rangle = 1$ , we obtain

$$\langle\langle L_4 | = (1 \quad 0 \quad 0 \quad 1). \quad (8.79)$$

### Biorthonormality

Therefore, a convenient biorthonormal set of left eigenvectors is

$$\langle\langle L_1 | = (1 \quad 0 \quad 0 \quad 0), \quad (8.80)$$

$$\langle\langle L_2 | = (0 \quad 1 \quad 0 \quad 0), \quad (8.81)$$

$$\langle\langle L_3 | = (0 \quad 0 \quad 1 \quad 0), \quad (8.82)$$

$$\langle\langle L_4 | = (1 \quad 0 \quad 0 \quad 1). \quad (8.83)$$

One may verify that

$$\langle\langle L_\alpha | R_\beta \rangle\rangle = \delta_{\alpha\beta}. \quad (8.84)$$

### Time evolution

The time evolution for a generic initial state  $|\psi(0)\rangle = c_1 |1\rangle + c_2 |0\rangle$  is obtained by performing the mode decomposition.

The initial density matrix is

$$\rho(0) = |\psi(0)\rangle\langle\psi(0)| = \begin{pmatrix} |c_1|^2 & c_1 c_2^* \\ c_2 c_1^* & |c_2|^2 \end{pmatrix}, \quad |c_1|^2 + |c_2|^2 = 1. \quad (8.85)$$

Using row stacking,

$$|\rho(0)\rangle\rangle = \begin{pmatrix} |c_1|^2 \\ c_1 c_2^* \\ c_2 c_1^* \\ |c_2|^2 \end{pmatrix}. \quad (8.86)$$

Because the Liouvillian is diagonalizable, the general solution is

$$|\rho(t)\rangle\rangle = \sum_{\alpha=1}^4 e^{\lambda_\alpha t} |R_\alpha\rangle\rangle \langle\langle L_\alpha | \rho(0)\rangle\rangle. \quad (8.87)$$

Let us compute the overlaps one by one:

$$\langle\langle L_1 | \rho(0) \rangle\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} |c_1|^2 \\ c_1 c_2^* \\ c_2 c_1^* \\ |c_2|^2 \end{pmatrix} = |c_1|^2, \quad (8.88)$$

$$\langle\langle L_2 | \rho(0) \rangle\rangle = c_1 c_2^*, \quad (8.89)$$

$$\langle\langle L_3 | \rho(0) \rangle\rangle = c_2 c_1^*, \quad (8.90)$$

$$\langle\langle L_4 | \rho(0) \rangle\rangle = |c_1|^2 + |c_2|^2 = 1. \quad (8.91)$$

Substituting into Eq. (8.87),

$$\begin{aligned} |\rho(t)\rangle\rangle &= e^{-\gamma t} |R_1\rangle\rangle |c_1|^2 + e^{(-i\omega - \gamma/2)t} |R_2\rangle\rangle c_1 c_2^* + e^{(i\omega - \gamma/2)t} |R_3\rangle\rangle c_2 c_1^* + |R_4\rangle\rangle \\ &= e^{-\gamma t} |c_1|^2 \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix} + e^{(-i\omega - \gamma/2)t} c_1 c_2^* \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} + e^{(i\omega - \gamma/2)t} c_2 c_1^* \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \end{aligned} \quad (8.92)$$

Therefore,

$$|\rho(t)\rangle\rangle = \begin{pmatrix} |c_1|^2 e^{-\gamma t} \\ c_1 c_2^* e^{-i\omega t} e^{-\gamma t/2} \\ c_2 c_1^* e^{+i\omega t} e^{-\gamma t/2} \\ 1 - |c_1|^2 e^{-\gamma t} \end{pmatrix}. \quad (8.93)$$

Equivalently, in matrix form,

$$\rho(t) = \begin{pmatrix} |c_1|^2 e^{-\gamma t} & c_1 c_2^* e^{-i\omega t} e^{-\gamma t/2} \\ c_2 c_1^* e^{+i\omega t} e^{-\gamma t/2} & 1 - |c_1|^2 e^{-\gamma t} \end{pmatrix}. \quad (8.94)$$

The result above is equivalent to what we have in Eqs. (8.44)-(8.47). As already discussed above, Equation (8.94) shows that

- the excited-state population  $\rho_{11}(t) = |c_1|^2 e^{-\gamma t}$  decays exponentially,
- the ground-state population increases as  $\rho_{00}(t) = 1 - |c_1|^2 e^{-\gamma t}$ ,
- the coherences decay with rate  $\gamma/2$  and oscillate with frequency  $\omega$ .

At long times,

$$\rho(t \rightarrow \infty) = |0\rangle\langle 0|, \quad (8.95)$$

which is precisely the steady state associated with the zero eigenvalue  $\lambda_4 = 0$ .

## 8.9 Example 2: Two-level atom with decay

We keep the convention

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (8.96)$$

so that  $|1\rangle$  is the higher-energy state and  $|0\rangle$  is the lower-energy state.

Consider a two-level atom in an external field described by the Hamiltonian

$$H = \frac{E}{2}\sigma_z + \Omega\sigma_x = \begin{pmatrix} E/2 & \Omega \\ \Omega & -E/2 \end{pmatrix}. \quad (8.97)$$

The term  $\Omega\sigma_x$  represents coherent driving of the two-level system by an external field. Although the Hamiltonian is time independent, this form is typically obtained after moving to a rotating frame and applying the rotating-wave approximation to an originally time-dependent drive.

The system is subject to spontaneous decay, meaning that when it is in the excited state, it can emit energy into the environment and relax to a lower-energy state even in the absence of external driving. This process arises from the coupling of the system to its environment (for example, the electromagnetic vacuum).

In this convention, spontaneous emission from  $|1\rangle$  to  $|0\rangle$  is described by the lowering operator

$$\sigma_- = \frac{\sigma_x - i\sigma_y}{2} = |0\rangle\langle 1| = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \quad (8.98)$$

The corresponding raising operator

$$\sigma_+ = \frac{\sigma_x + i\sigma_y}{2} = |1\rangle\langle 0| = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad (8.99)$$

describes excitation from the ground state to the excited state.

In this problem, we assume just spontaneous emission, so  $L = \sqrt{\Gamma}\sigma_-$ . The master equation is

$$\frac{d}{dt}\rho(t) = -i[H, \rho] + \Gamma \left( \sigma_- \rho \sigma_+ - \frac{1}{2} \{ \sigma_+ \sigma_-, \rho \} \right). \quad (8.100)$$

The Hamiltonian part drives coherent Rabi oscillations between the ground and excited states. The dissipative term models spontaneous emission from  $|1\rangle$  to  $|0\rangle$  at rate  $\Gamma$ .

Using the row-stacking convention adapted to the basis ordering  $\{|1\rangle, |0\rangle\}$ ,

$$\|\rho\rangle\rangle = \begin{pmatrix} \rho_{11} \\ \rho_{10} \\ \rho_{01} \\ \rho_{00} \end{pmatrix}, \quad (8.101)$$

we can write

$$\frac{d}{dt} \|\rho\rangle\rangle = \tilde{\mathcal{L}} \|\rho\rangle\rangle, \quad (8.102)$$

with

$$\tilde{\mathcal{L}} = \begin{pmatrix} -\Gamma & i\Omega & -i\Omega & 0 \\ i\Omega & -iE - \frac{\Gamma}{2} & 0 & -i\Omega \\ -i\Omega & 0 & iE - \frac{\Gamma}{2} & i\Omega \\ \Gamma & -i\Omega & i\Omega & 0 \end{pmatrix}. \quad (8.103)$$

Each row tells us the time derivative of one component of  $\|\rho\rangle\rangle$ , giving the coupled equations

$$\dot{\rho}_{11} = -i\Omega\rho_{01} + i\Omega\rho_{10} - \Gamma\rho_{11}, \quad (8.104)$$

$$\dot{\rho}_{10} = i\Omega\rho_{11} - \left(iE + \frac{\Gamma}{2}\right)\rho_{10} - i\Omega\rho_{00}, \quad (8.105)$$

$$\dot{\rho}_{01} = -i\Omega\rho_{11} + \left(iE - \frac{\Gamma}{2}\right)\rho_{01} + i\Omega\rho_{00}, \quad (8.106)$$

$$\dot{\rho}_{00} = \Gamma\rho_{11} + i\Omega\rho_{01} - i\Omega\rho_{10}. \quad (8.107)$$

These equations show the competition between coherent oscillation ( $\Omega$  terms) and irreversible decay ( $\Gamma$  terms).

There are four Liouvillian eigenvalues,

$$\Lambda_1, \Lambda_2, \Lambda_3, \Lambda_4,$$

with corresponding left and right eigenvectors. The vectorized density matrix evolves as

$$\|\rho(t)\rangle\rangle = \sum_{i=1}^4 e^{\Lambda_i t} \|\Lambda_i^R\rangle\rangle \langle\langle \Lambda_i^L | \|\rho(0)\rangle\rangle. \quad (8.108)$$

If the initial state is the excited state,

$$\rho(0) = |1\rangle\langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \|\rho(0)\rangle\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad (8.109)$$

then Eq. (8.108) becomes

$$\|\rho(t)\rangle\rangle = \sum_{i=1}^4 e^{\Lambda_i t} \|\Lambda_i^R\rangle\rangle \langle\langle \Lambda_i^L | \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \quad (8.110)$$

The dynamics is a sum of four modes. One mode corresponds to the steady state ( $\Lambda = 0$ ), while the other three decay because their real parts are negative.

**Case 1: no coherent drive**

If  $\Omega = 0$ , the equations decouple and one finds

$$\dot{\rho}_{11} = -\Gamma\rho_{11}, \quad \dot{\rho}_{00} = \Gamma\rho_{11},$$

so

$$\rho_{11}(t) = \rho_{11}(0)e^{-\Gamma t}, \quad \rho_{00}(t) = 1 - \rho_{11}(0)e^{-\Gamma t}.$$

The atom relaxes exponentially to the ground state, which is the steady state. This is exactly the Example 1 above.

**Case 2: drive and decay**

When both  $\Omega \neq 0$  and  $\Gamma \neq 0$ , the atom exhibits damped Rabi oscillations. The coherent part tries to exchange population between  $|0\rangle$  and  $|1\rangle$ , while the dissipative part steadily removes excitation from  $|1\rangle$ . Eventually the system settles into a nonequilibrium stationary state determined by the balance between drive and decay.

## 8.10 Spectrum of the Lindbladian

The spectral analysis of the Lindbladian is useful not only for determining relaxation rates and steady states, but also for characterizing integrability, chaos, and universal spectral correlations in open quantum systems. ***However, recent studies have questioned whether spectral analysis of the Lindbladian can really distinguish chaos from integrability!*** We will proceed with the spectral analysis, which can always be done, but keep in mind that the potential connection with chaos is still under debate.

In closed systems, level statistics of the Hamiltonian spectrum are widely used to distinguish integrable from chaotic dynamics. In open systems, the analogous idea is to study the complex spectrum of the Lindbladian. Because the eigenvalues lie in the complex plane, one must use tools adapted to complex spectra.

A major development in this direction is the analysis of *complex spacing ratios*, introduced to avoid the ambiguities of unfolding in two dimensions and to capture both radial and angular correlations in the complex plane.

**Complex spacing ratios**

Suppose we have computed the complex eigenvalues of a Lindbladian,

$$\{\lambda_1, \lambda_2, \dots, \lambda_N\}, \quad \lambda_k \in \mathbb{C}.$$

Each eigenvalue can be viewed as a point in the complex plane,

$$\lambda_k = x_k + iy_k.$$

To find the nearest neighbor of a given eigenvalue  $\lambda_k$ , we compute its distance to every other eigenvalue  $\lambda_j$  with  $j \neq k$ . The distance is the ordinary Euclidean distance in the complex plane,

$$d_{kj} = |\lambda_j - \lambda_k| = \sqrt{(x_j - x_k)^2 + (y_j - y_k)^2}. \quad (8.111)$$

Then

- The *nearest neighbor*  $\lambda_k^{\text{NN}}$  is the eigenvalue  $\lambda_j$  for which  $d_{kj}$  is smallest.
- The *next-to-nearest neighbor*  $\lambda_k^{\text{NNN}}$  is the eigenvalue  $\lambda_j$  for which  $d_{kj}$  is the second smallest.

One then defines the complex spacing ratio

$$z_k = \frac{\lambda_k^{\text{NN}} - \lambda_k}{\lambda_k^{\text{NNN}} - \lambda_k}. \quad (8.112)$$

We can express  $z_k$  in polar form as

$$z_k = r_k e^{i\theta_k}, \quad 0 \leq r_k \leq 1. \quad (8.113)$$

To obtain  $r_k$  and  $\theta_k$  in practice, we first write  $z_k$  in terms of its real and imaginary parts,

$$z_k = x_k + iy_k, \quad x_k = \text{Re}(z_k), \quad y_k = \text{Im}(z_k). \quad (8.114)$$

The modulus  $r_k$  is then given by

$$r_k = |z_k| = \sqrt{x_k^2 + y_k^2}, \quad (8.115)$$

and the phase  $\theta_k$  is

$$\theta_k = \arg(z_k). \quad (8.116)$$

For numerical implementations, the phase should be computed using the two-argument arc-tangent function,

$$\theta_k = \text{atan2}(y_k, x_k), \quad (8.117)$$

which correctly determines the angle in the appropriate quadrant.

The modulus  $r_k$  measures the relative distances to the two nearest neighbors, while the angle  $\theta_k$  measures the relative orientation of those neighbors in the complex plane.

If the eigenvalues are uncorrelated, the ratios fill the unit disk essentially uniformly. If the eigenvalues are strongly correlated, as in random-matrix ensembles, the distribution becomes nontrivial – there is level repulsion near the origin and a characteristic angular structure. This is illustrated in Fig. 8.1.

The complex-spacing-ratio analysis in Fig. 8.1 compares: (a) a spectrum of uncorrelated complex levels, for which the ratio density is essentially flat in the unit disk; and (b) a spectrum drawn from the GinUE, for which the ratio density is suppressed near the origin and develops a strong angular structure.

The suppression near  $z = 0$  reflects level repulsion. The nearest and next-to-nearest neighbors are typically not both extremely close to the reference eigenvalue. The angular dependence reflects a second effect absent in the uncorrelated case: the neighbors tend to spread around the reference eigenvalue in a correlated way, rather than appearing at random directions.

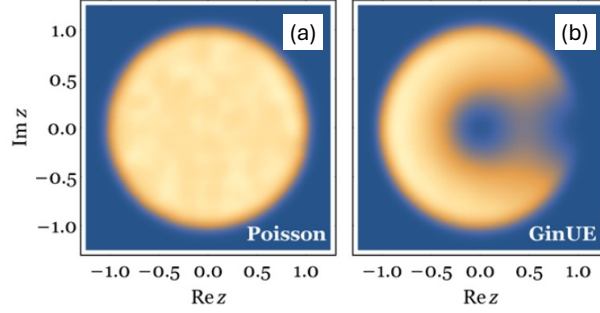


Figure 8.1: Density plot of  $z$  in complex plane for uncorrelated levels and an ensemble of random matrices drawn from the Ginibre unitary ensemble.

### Random-matrix benchmark

For generic non-Hermitian spectra, the relevant random-matrix benchmark is often the *Ginibre unitary ensemble* (GinUE), consisting of complex matrices with independent Gaussian entries. These random matrices are now non-Hermitian. In contrast with Hermitian random matrices, whose eigenvalues lie on the real axis, GinUE eigenvalues fill a two-dimensional region of the complex plane.

For GinUE, the nearest-neighbor spacing distribution in the complex plane after unfolding (see below for details on the unfolding procedure in the complex plane) can be written as

$$P_{\text{GinUE}}(s) = \frac{d^2}{ds^2} \prod_{n=1}^{\infty} \left[ e^{-s^2} \sum_{k=0}^{n-1} \frac{s^{2k}}{k!} \right]. \quad (8.118)$$

It exhibits cubic level repulsion,  $P(s) \propto s^3$ , as  $s \rightarrow 0$ .

Contrary to the nearest-neighbor spacing distribution  $P_{\text{GinUE}}(s)$ , no simple closed-form expression is known for the full distribution of the complex spacing ratio  $\varrho_{\text{GinUE}}(r)$  for GinUE. Nevertheless, its asymptotic behavior near the origin is inherited from the spacing statistics,

$$\varrho_{\text{GinUE}}(r) \propto r^3 \quad \text{for } r \rightarrow 0, \quad (8.119)$$

and the full distribution is typically obtained numerically, displaying universal features characteristic of Ginibre ensembles, as illustrated in Fig. 8.2.

Numerically, one finds the useful single-number signatures

$$\langle r \rangle_{\text{GinUE}} \approx 0.74, \quad -\langle \cos \theta \rangle_{\text{GinUE}} \approx 0.24. \quad (8.120)$$

### Poisson statistics in the complex plane

For the case of completely independent complex levels, after unfolding and ensuring  $\langle s \rangle = 1$ , the nearest-neighbor spacing distribution in the complex plane is given by

$$P_{\text{2DP}}(s) = \frac{\pi}{2} s e^{-\pi s^2/4}. \quad (8.121)$$

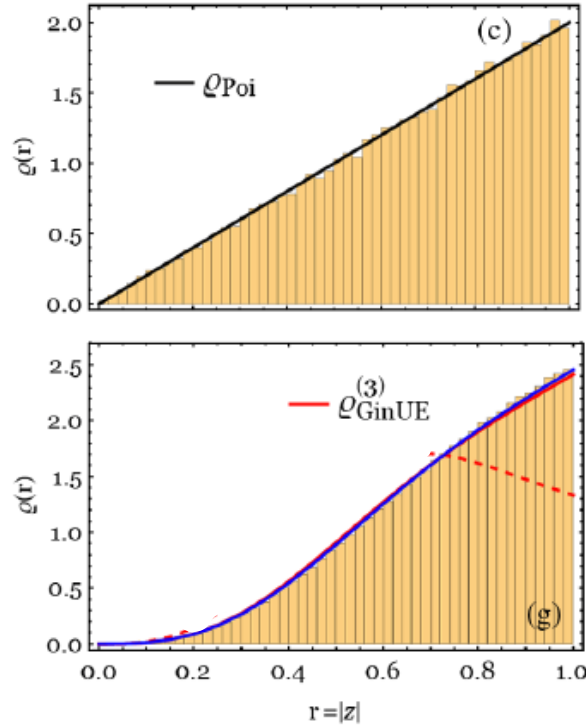


Figure 8.2: Distribution of the real part of the complex spacing ratio  $r = d_{NN}/d_{NNN}$ , where  $d_{NN}$  and  $d_{NNN}$  are the nearest- and next-to-nearest-neighbor distances in the complex plane. For chaotic non-Hermitian systems described by the GinUE, the distribution exhibits cubic level repulsion,  $\varrho(r) \sim r^3$  as  $r \rightarrow 0$ . In contrast, integrable (Poisson-like) shows linear level repulsion.

This distribution exhibits *linear level repulsion*,  $P(s) \propto s$  for small  $s$ . This is a key difference from Hermitian systems. While in one dimension one contrasts level repulsion with its absence, in the complex plane all spectra exhibit repulsion due to geometric constraints. The relevant distinction is therefore between *linear repulsion* (Poisson case) and *cubic repulsion* (Ginibre ensemble).

For the ratio of consecutive spacings in the complex plane, the distribution is uniform inside the unit disk,

$$\varrho_{\text{Poi}}(z) = \frac{1}{\pi} \Theta(1 - |z|), \quad (8.122)$$

where  $\Theta$  is the Heaviside step function. Consequently,

$$\boxed{\varrho_{\text{Poi}}(r) = 2r}, \quad \boxed{\varrho_{\text{Poi}}(\theta) = \frac{1}{2\pi}}, \quad (8.123)$$

and the mean values are

$$\boxed{\langle r \rangle_{\text{Poi}} = \frac{2}{3}}, \quad \boxed{-\langle \cos \theta \rangle_{\text{Poi}} = 0}. \quad (8.124)$$

## Unfolding

For Hermitian matrices, the spectrum lies on the real axis and unfolding can be performed by rescaling the spacings so that the local mean level spacing is equal to one. In practice, this can be achieved by dividing the spectrum into small sets of neighboring levels, computing the average spacing within each set, and rescaling the spacings accordingly. We did this, for example, by splitting the spectrum into sets of 11 consecutive levels, averaging the 10 spacings to obtain  $\langle s \rangle$ , and then rescaling each spacing as

$$\tilde{s}_\mu = \frac{s_\mu}{\langle s \rangle} = s_\mu \rho_\mu,$$

where  $\rho_\mu = 1/\langle s \rangle$  is the local density.

For non-Hermitian matrices, the eigenvalues lie in the complex plane and the notion of unfolding must be generalized. In this case, the relevant quantity is the *local spectral density* in two dimensions, rather than a one-dimensional mean spacing.

To estimate the local density around a given eigenvalue  $\lambda_\mu$ , we consider a disk centered at  $\lambda_\mu$  that contains its  $k$  nearest neighbors. Let  $d_{\mu,k}$  be the distance from  $\lambda_\mu$  to its  $k$ -th nearest neighbor. The area of this disk is

$$A = \pi d_{\mu,k}^2.$$

Since this region contains approximately  $k$  eigenvalues, the local density is estimated as

$$\bar{R}_1(\lambda_\mu) = \frac{k}{\pi d_{\mu,k}^2}.$$

This provides a smooth estimate of the density, provided that  $k$  satisfies  $1 \ll k \ll N$ , so that the averaging is local but reduces statistical fluctuations.

The nearest-neighbor spacing in the complex plane is defined as the Euclidean distance

$$s_\mu = |\lambda_\mu^{\text{NN}} - \lambda_\mu|.$$

To remove the effect of a nonuniform density, the spacings are rescaled using the local density. Since the density has units of inverse area, the appropriate unfolding is given by

$$\tilde{s}_\mu = s_\mu \sqrt{\bar{R}_1(\lambda_\mu)} = \frac{s_\mu}{\sqrt{\pi d_{\mu,k}^2/k}}.$$

This transformation ensures that the unfolded spacings are dimensionless and that their mean value is of order unity across the spectrum. After unfolding, the resulting spacing distribution reflects only universal spectral correlations, independent of the global structure of the spectrum.

The last step is to ensure normalization. The unfolded spacing distribution  $p(\tilde{s})$  needs to be normalized according to

$$\int_0^\infty p(\tilde{s}) d\tilde{s} = 1, \quad \int_0^\infty \tilde{s} p(\tilde{s}) d\tilde{s} = 1. \quad (8.125)$$

The first condition ensures proper normalization of the probability distribution, while the second fixes the mean spacing to unity. This second constraint plays the same role as in the Hermitian case; it sets the natural scale of the unfolded spectrum, allowing for meaningful comparisons between different systems.

For a finite system, the normalization conditions are implemented from the discrete set of unfolded spacings  $\{\tilde{s}_\mu\}_{\mu=1}^M$ . The second condition, which fixes the mean spacing, is enforced directly at the level of the data by computing the empirical average

$$\langle \tilde{s} \rangle = \frac{1}{M} \sum_{\mu=1}^M \tilde{s}_\mu,$$

so that  $\langle \tilde{s} \rangle = 1$ . The first condition is then ensured when estimating the distribution  $p(\tilde{s})$  from the data, for instance by constructing a histogram with bin width  $\Delta s$  and normalizing it as

$$p(s_i) = \frac{n_i}{M \Delta s},$$

where  $n_i$  is the number of spacings in the  $i$ -th bin. By construction, this procedure guarantees  $\sum_i p(s_i) \Delta s = 1$ , providing a discrete approximation to the continuum normalization. In this way, the two normalization conditions are satisfied up to statistical fluctuations inherent to finite data.

### Dissipative quantum chaos

The complex spacing ratios are useful in the study of dissipative quantum chaos, where one wishes to distinguish:

- integrable or regular open systems, whose Lindbladian eigenvalues behave more like uncorrelated points;
- generic or chaotic open systems, whose Lindbladian eigenvalues display Ginibre-like correlations.

In practical studies, one often computes the empirical distribution of  $z_k$ , or simply the averaged quantities

$$\langle r \rangle, \quad -\langle \cos \theta \rangle,$$

and compares them with the Poisson and GinUE benchmarks above.

### A cautionary remarks

- Although GinUE is a natural and widely used benchmark for generic non-Hermitian spectra, not every Lindbladian belongs to the GinUE universality class. Symmetries can change the appropriate random-matrix class. In particular, some non-Hermitian many-body models were shown to approach other symmetry classes, such as  $\text{AI}^\dagger$ , rather than GinUE. Therefore, the comparison with GinUE should be viewed as a first and very useful diagnostic, but not as the only possible universality class.
- The proposed link between Ginibre spectral correlations and dissipative quantum chaos is still under active investigation. Recent findings suggest that such correlations may emerge even when the associated classical system does not exhibit chaos.

## 8.11 Assignment: Open Quantum Systems

### Reference material.

Daniel Manzano, *A short introduction to the Lindblad master equation*,  
AIP Advances **10**, 025106 (2020),  
<https://doi.org/10.1063/1.5115323>.

**Attention!** The paper above uses a notation opposite to ours with respect to  $|0\rangle$  and  $|1\rangle$ .

### Problem 1: Two-level atom with decay

In this problem, use the same convention as in Example 2 in this chapter:

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (8.126)$$

so that  $|1\rangle$  is the higher-energy state and  $|0\rangle$  is the lower-energy state.

Consider the two-level system discussed in Example 2, with Hamiltonian

$$H = \frac{E}{2}\sigma^z + \Omega\sigma^x, \quad (8.127)$$

and spontaneous-emission jump operator

$$L = \sqrt{\Gamma}\sigma^-, \quad \sigma^- = |0\rangle\langle 1|. \quad (8.128)$$

The master equation is

$$\dot{\rho}(t) = -i[H, \rho] + \Gamma \left( \sigma^- \rho \sigma^+ - \frac{1}{2} \{ \sigma^+ \sigma^-, \rho \} \right), \quad (8.129)$$

and in vectorized form

$$\frac{d}{dt} \|\rho(t)\rangle\rangle = \tilde{\mathcal{L}} \|\rho(t)\rangle\rangle. \quad (8.130)$$

Use the row-stacking vectorization adapted to the basis ordering  $\{|1\rangle, |0\rangle\}$ :

$$\|\rho\rangle\rangle = \begin{pmatrix} \rho_{11} \\ \rho_{10} \\ \rho_{01} \\ \rho_{00} \end{pmatrix}. \quad (8.131)$$

#### 1. Derivation of the Liouvillian.

Starting from the Lindblad equation and the vectorization identity

$$\text{vec}(A\rho B) = (A \otimes B^T) \text{vec}(\rho),$$

show all steps needed to derive the  $4 \times 4$  Liouvillian matrix

$$\tilde{\mathcal{L}} = \begin{pmatrix} -\Gamma & i\Omega & -i\Omega & 0 \\ i\Omega & -iE - \Gamma/2 & 0 & -i\Omega \\ -i\Omega & 0 & iE - \Gamma/2 & i\Omega \\ \Gamma & -i\Omega & i\Omega & 0 \end{pmatrix}. \quad (8.132)$$

**2. Spectral analysis: pure decay.**

Set

$$\Gamma = 0.2, \quad \Omega = 0, \quad E = 1.$$

For this case:

- (a) Compute all eigenvalues of  $\tilde{\mathcal{L}}$ .
- (b) Compute the right eigenvectors and left eigenvectors.
- (c) Normalize them biorthogonally if possible.
- (d) Identify the eigenvalue associated with the steady state.
- (e) Comment on why this case is especially simple.

This is a good first problem because the matrix becomes simple enough to analyze analytically.

**3. Population dynamics for pure decay: second rate.**

Set

$$\Gamma = 0.2, \quad \Omega = 0, \quad E = 1,$$

and take the initial state

$$\rho(0) = |1\rangle\langle 1|, \quad \rho_{11}(0) = 1.$$

Plot  $\rho_{11}(t)$  and  $\rho_{00}(t)$  as functions of time. Compare your numerical result with the analytical solution.

**4. Population dynamics for pure decay: first rate.**

Repeat the previous item for

$$\Gamma = 0.1, \quad \Omega = 0, \quad E = 1,$$

again with

$$\rho(0) = |1\rangle\langle 1|, \quad \rho_{11}(0) = 1.$$

Plot  $\rho_{11}(t)$  and  $\rho_{00}(t)$  as functions of time. Compare your numerical result with the analytical solution. Compare the time scale of relaxation with the previous case.

**5. Driven and dissipative dynamics.**

Now consider

$$\Gamma = 0.2, \quad \Omega = 0.5, \quad E = 0.$$

To make the coherent dynamics more interesting, use the initial pure superposition

$$|\psi(0)\rangle = \frac{|1\rangle + |0\rangle}{\sqrt{2}}, \quad \rho(0) = |\psi(0)\rangle\langle\psi(0)|. \quad (8.133)$$

Plot  $\rho_{11}(t)$  and  $\rho_{00}(t)$ , and explain physically why the dynamics is no longer a simple exponential relaxation.

**6. Coherences: generation and decay.****(a) No driving: decay of existing coherences.**

Consider the case

$$\Omega = 0, \quad \Gamma = 0.2, \quad E = 1,$$

with initial state

$$|\psi(0)\rangle = \frac{|1\rangle + |0\rangle}{\sqrt{2}}, \quad \rho(0) = |\psi(0)\rangle \langle \psi(0)|.$$

- i. Plot  $\rho_{10}(t)$  and  $\rho_{01}(t)$ . If there are real and imaginary parts, show the curves for each one.
- ii. Explain why coherences decay in time.
- iii. Does the Hamiltonian contribute to the dynamics of the coherences in this case?

**(b) Driving and decay: competition between generation and damping.**

Now consider

$$\Omega = 0.1, \quad \Gamma = 0.2, \quad E = 1,$$

with the same initial state.

- i. Plot  $\rho_{10}(t)$  and  $\rho_{01}(t)$ . If there are real and imaginary parts, show the curves for each one.
- ii. Explain why coherences are now continuously generated.
- iii. Describe qualitatively the competition between coherent driving and dissipation.
- iv. Do the coherences vanish at long times, or do they approach a finite value?

**7. Purity.**

For the three parameter sets

$$(\Gamma, \Omega, E) = (0.1, 0, 1), \quad (0.2, 0, 1), \quad (0.2, 0.5, 0),$$

compute and plot the purity

$$\mathcal{P}(t) = \text{Tr}[\rho^2(t)].$$

Use the same initial state for all cases:

$$|\psi(0)\rangle = \frac{|1\rangle + |0\rangle}{\sqrt{2}}, \quad \rho(0) = |\psi(0)\rangle \langle \psi(0)|.$$

Discuss the following points:

- (a) Why is  $\mathcal{P}(0) = 1$  for this initial state?
- (b) Does the purity necessarily decrease monotonically?
- (c) What is the long-time value of the purity in each case, and why?

## Problem 2: Three spin- $\frac{1}{2}$ particles with XXZ couplings and dissipation

In this problem, use the same convention as in Problem 1:

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \sigma^z|1\rangle = +|1\rangle, \quad \sigma^z|0\rangle = -|0\rangle. \quad (8.134)$$

Thus,  $|1\rangle$  is the higher-energy state and  $|0\rangle$  is the lower-energy state.

Consider three spin- $\frac{1}{2}$  particles with open boundary conditions and Hamiltonian

$$H = J \sum_{i=1}^2 (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z). \quad (8.135)$$

To model local spontaneous relaxation, use the jump operators

$$L_1 = \sqrt{\gamma} \sigma_1^-, \quad L_2 = \sqrt{\gamma} \sigma_2^-, \quad L_3 = \sqrt{\gamma} \sigma_3^-, \quad (8.136)$$

where

$$\sigma^- = |0\rangle\langle 1|.$$

### 1. Hamiltonian and Hilbert-space dimension.

Explain why we now need to consider the full computational basis

$$\{|000\rangle, |001\rangle, |010\rangle, |011\rangle, |100\rangle, |101\rangle, |110\rangle, |111\rangle\}.$$

State the Hilbert-space dimension and the dimension of Liouville space.

### 2. Vectorized Lindbladian.

Construct the Liouvillian superoperator numerically

$$\tilde{\mathcal{L}} = -i(H \otimes \mathbb{I} - \mathbb{I} \otimes H^T) + \sum_{k=1}^3 \left[ L_k \otimes L_k^* - \frac{1}{2} \left( L_k^\dagger L_k \otimes \mathbb{I} + \mathbb{I} \otimes (L_k^\dagger L_k)^T \right) \right].$$

What is the matrix dimension of  $\tilde{\mathcal{L}}$ ?

### 3. Initial state and observables.

Take

$$J = 1, \quad \Delta = 0.8, \quad \gamma = 0.2, \quad \rho(0) = |101\rangle\langle 101|.$$

Integrate the Lindblad equation and plot:

- (a) the site magnetizations  $\langle \sigma_i^z(t) \rangle$ ,  $i = 1, 2, 3$ ,
- (b) the total magnetization  $\langle \sigma_1^z + \sigma_2^z + \sigma_3^z \rangle$ ,

(c) the purity  $\text{Tr}[\rho^2(t)]$ .

**Comment:** The purity initially decreases because the dissipative dynamics introduces statistical mixtures due to different decay processes. However, the steady state of the system is the pure state  $\rho_{\text{ss}} = |000\rangle\langle 000|$ , since all spins eventually relax to the lower-energy state. As time increases, all trajectories converge to this unique pure steady state, and the purity returns to  $\text{Tr}(\rho^2) \rightarrow 1$ . Thus, the purity exhibits non-monotonic behavior: it decreases at intermediate times due to mixing and increases again as the system approaches a pure steady state.

#### 4. Steady state for the relaxation problem.

Identify the steady-state eigenvector(s) for the relaxation case and determine whether the steady state is unique.

Use the steady state to mark the saturation values of the plots in item (3) above.

#### 5. Pure dephasing.

Repeat item (3) with pure-dephasing jump operators

$$L_i = \sqrt{\gamma} \sigma_i^z, \quad i = 1, 2, 3.$$

Compare the dynamics with the relaxation case. In particular, discuss which quantities are most strongly affected in each case.

#### 6. Conceptual question: trivial dephasing dynamics.

Suppose that the jump operators are again

$$L_i = \sqrt{\gamma} \sigma_i^z, \quad i = 1, 2, 3,$$

but now the initial state is

$$\rho(0) = |000\rangle\langle 000|.$$

Before doing any numerics, explain what you would expect for:

- (a) the site magnetizations  $\langle \sigma_i^z(t) \rangle$ ,
- (b) the total magnetization,
- (c) the purity.

Would you expect any nontrivial dynamics? Why or why not?

## Problem 3: Random-matrix Lindbladian and complex spacing ratios

In this problem you will construct a random non-Hermitian open-system model and analyze the complex spectrum of its Liouvillian.

The total Hamiltonian is

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_{\text{TD}} + \frac{\mu}{\sqrt{N}} \hat{\mathcal{H}}_1, \quad (8.137)$$

where  $\hat{\mathcal{H}}_{\text{TD}}$  is a tridiagonal  $N \times N$  Gaussian random matrix and  $\hat{\mathcal{H}}_1$  is full  $N \times N$  GOE random matrix. Dissipation is incorporated through a random jump operator  $\hat{L}$ , which has nonzero real Gaussian random entries only on the first subdiagonal,

$$L_{m+1,m} \neq 0.$$

The corresponding Liouvillian superoperator is

$$\hat{\mathcal{L}} = -i \left[ \hat{\mathcal{H}} \otimes \mathbb{I} - \mathbb{I} \otimes \hat{\mathcal{H}} \right] + \gamma \left( 2\hat{L} \otimes \hat{L}^* - \hat{L}^\dagger \hat{L} \otimes \mathbb{I} - \mathbb{I} \otimes \hat{L}^\text{T} \hat{L}^* \right). \quad (8.138)$$

Use  $N = 60$ . If you have access to stronger computational resources, you may try  $N = 80$  or  $N = 100$ . Fix  $\gamma = 1$ . Consider the four values

$$\mu = 0, \quad \mu = 0.3, \quad \mu = 0.6, \quad \mu = 1.$$

### 1. Complex spacing ratios.

For each eigenvalue  $\lambda_k$ , determine its nearest and next-to-nearest neighbors in the complex plane, and define

$$z_k = \frac{\lambda_k^{\text{NN}} - \lambda_k}{\lambda_k^{\text{NNN}} - \lambda_k} = r_k e^{i\theta_k}.$$

(a) For each value of  $\mu$ , plot  $z_k$  in the plane

(b) Compute

$$\langle r \rangle, \quad -\langle \cos \theta \rangle.$$

Compare your results with the benchmark values

$$\langle r \rangle_{\text{Poi}} = \frac{2}{3}, \quad -\langle \cos \theta \rangle_{\text{Poi}} = 0,$$

and

$$\langle r \rangle_{\text{GinUE}} \approx 0.74, \quad -\langle \cos \theta \rangle_{\text{GinUE}} \approx 0.24.$$

Discuss whether your spectra appear closer to Poisson-like or Ginibre-like behavior as  $\mu$  increases.

### 2. Distribution of $r_k$ .

For each value of  $\mu$ , compute and plot the histogram of  $r_k$  on the interval  $0 \leq r \leq 1$ . Do you find linear or cubic repulsion?

## Problem 4: Dynamics and survival probability

*This problem may take some hours to run. Don't leave it to the last minute.*

Using the same Liouvillian as in Problem 3, study the time evolution of a pure initial state.

**ATTENTION!** To compare the results for different values of  $\mu$ , you need to have fixed the same  $\hat{\mathcal{H}}_{\text{TD}}$  and  $\hat{\mathcal{H}}_{\text{I}}$  and  $L$ .

Choose as initial pure state the column vector

$$|\psi_0\rangle = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad (8.139)$$

where the only nonzero entry is a 1 at position  $m_0 = \lfloor \frac{N}{2} \rfloor$ . The corresponding initial density matrix is

$$\rho(0) = |\psi_0\rangle \langle \psi_0|. \quad (8.140)$$

**Definition of survival probability.** For a pure initial state

$$\rho(0) = |\psi_0\rangle \langle \psi_0|,$$

and **ONLY** in this case, the survival probability is given by

$$SP(t) = \text{Tr}[\rho(t)\rho(0)] = \langle \psi_0 | \rho(t) | \psi_0 \rangle. \quad (8.141)$$

### 1. Time evolution.

For the four values

$$\mu = 0, \quad \mu = 0.3, \quad \mu = 0.6, \quad \mu = 1,$$

compute and plot  $SP(t)$  on the same graph.

### 2. Purity in the random-matrix model.

Also compute and plot

$$\mathcal{P}(t) = \text{Tr}[\rho^2(t)]$$

for the same four cases. Compare its behavior with that of the survival probability.

### 3. Connection with the spectrum.

Discuss qualitatively how the Liouvillian spectrum influences the decay of  $SP(t)$ . In particular, explain why eigenvalues with real parts closest to zero control the long-time dynamics.

## 8.11.1 Sketches of the solutions

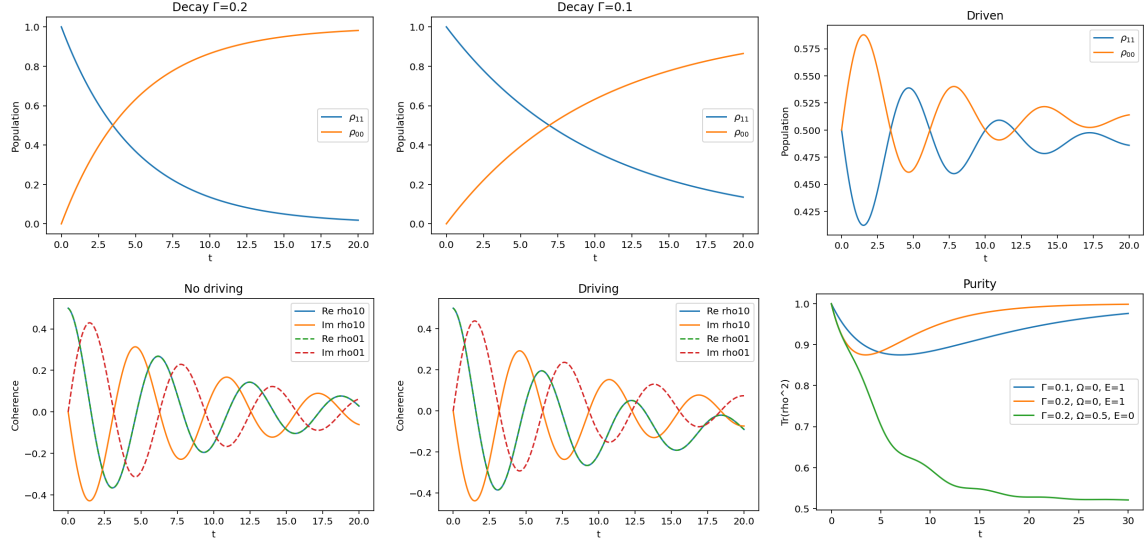


Figure 8.3: Problem 1

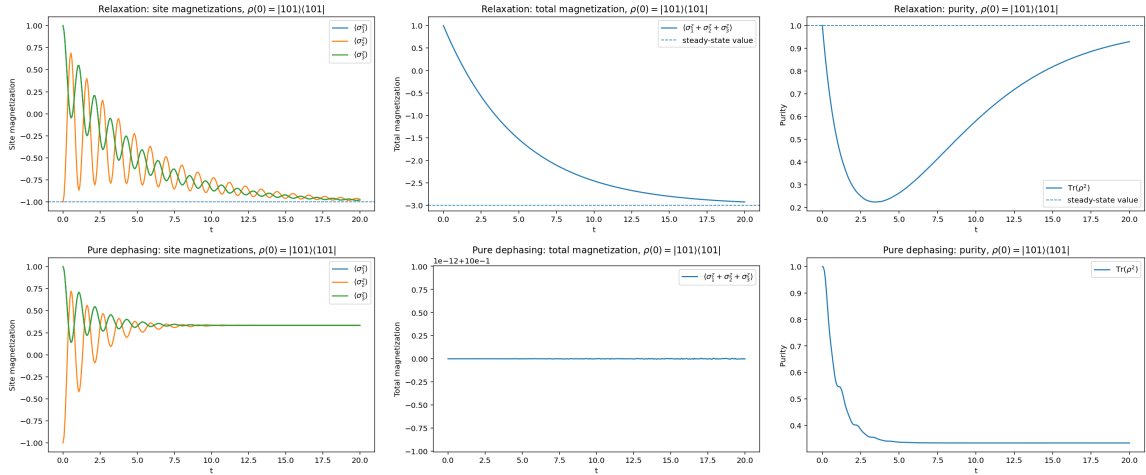


Figure 8.4: Problem 2

| $\mu$ | $\langle r \rangle$ | $-\langle \cos \theta \rangle$ |
|-------|---------------------|--------------------------------|
| 0.0   | 0.674964            | -0.014401                      |
| 0.3   | 0.694942            | 0.054401                       |
| 0.6   | 0.711280            | 0.155301                       |
| 1.0   | 0.730236            | 0.157516                       |

Table 8.1: Table for Problem 3: Average complex spacing ratio  $\langle r \rangle$  and angular statistic  $-\langle \cos \theta \rangle$  for different values of  $\mu$ .

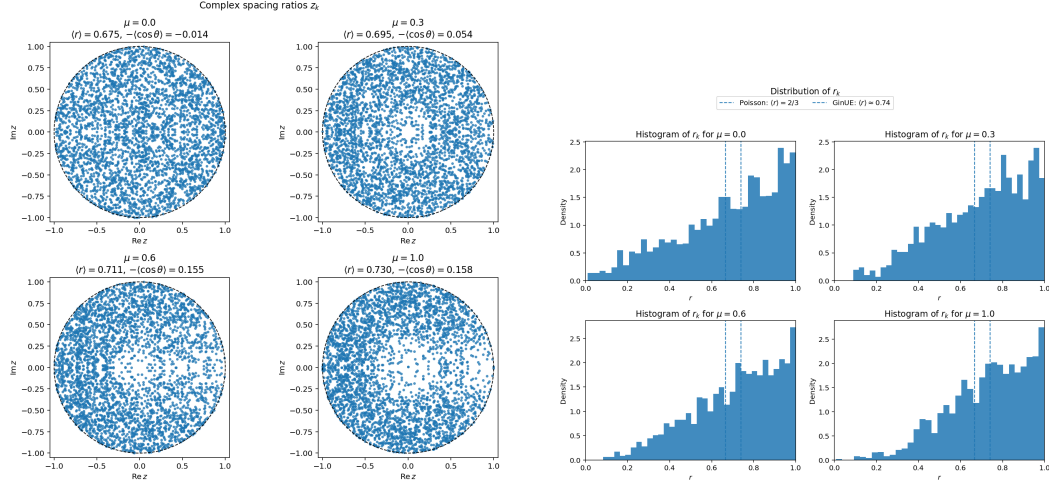


Figure 8.5: Problem 3.

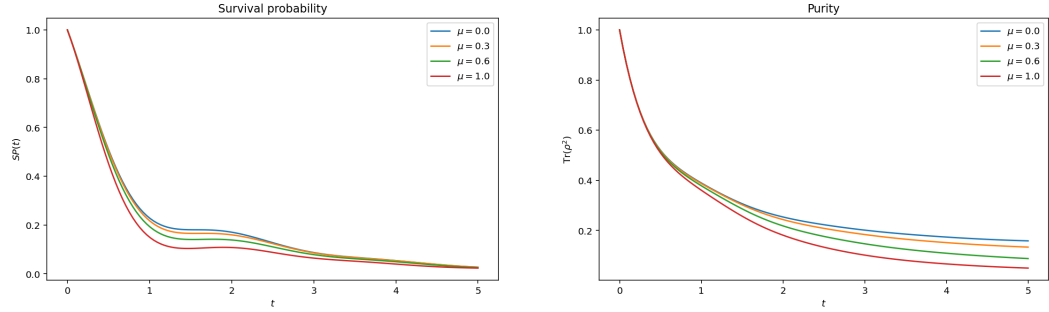


Figure 8.6: Problem 4.

## 8.12 Derivation of the Lindblad equation

Following Eq. (8.16)... **Reduced dynamics.** Taking the partial trace over the environment,

$$\frac{d\hat{\rho}_S(t)}{dt} = -\alpha^2 \int_0^t ds \operatorname{Tr}_E \left( [\hat{H}_I(t), [\hat{H}_I(s), \hat{\rho}_T(s)]] \right), \quad (8.142)$$

where we have assumed

$$\operatorname{Tr}_E ([\hat{H}_I(t), \hat{\rho}_T(0)]) = 0,$$

which can always be enforced by redefining the interaction Hamiltonian.

This redefinition can always be satisfied without changing the physics. To see this, write the interaction Hamiltonian as

$$H_I = \sum_i S_i \otimes E_i,$$

and decompose the environment operators as

$$E_i = (E_i - \langle E_i \rangle) + \langle E_i \rangle, \quad \langle E_i \rangle = \operatorname{Tr}_E (E_i \rho_E).$$

Then the interaction Hamiltonian becomes

$$H_I = \sum_i S_i \otimes (E_i - \langle E_i \rangle) + \sum_i \langle E_i \rangle S_i \otimes \mathbb{1}.$$

The second term acts only on the system and can be absorbed into a redefinition of the system Hamiltonian,

$$H'_S = H_S + \alpha \sum_i \langle E_i \rangle S_i,$$

while the new interaction Hamiltonian is

$$H'_I = \sum_i S_i \otimes (E_i - \langle E_i \rangle).$$

By construction, the environment operators in  $H'_I$  have zero average,

$$\text{Tr}_E(E_i \rho_E) = 0,$$

which ensures that the first-order contribution vanishes. This redefinition does not change the total Hamiltonian, but simplifies the derivation by isolating the fluctuating part of the environment responsible for dissipation.

Equation (8.142) is still exact but not closed, since it depends on the full density matrix  $\hat{\rho}_T(t)$ . The Lindblad equation emerges after a sequence of approximations (Born, Markov, and secular) that allow us to obtain a closed equation for  $\rho_S(t)$  alone. It is important to understand what each approximation means physically.

### 1. Weak-coupling (Born) expansion

The coupling constant  $\alpha$  is assumed small. This allows us to expand the exact equation perturbatively and truncate at second order in the interaction. Physically, the system is influenced by the environment, but not so strongly that high-order processes must be kept.

### 2. Initially factorized state

One assumes

$$\rho_T(0) = \rho_S(0) \otimes \rho_E,$$

so that system and environment are initially uncorrelated. This is not exact in all situations, but it is a natural starting point when the coupling is switched on at  $t = 0$  or when pre-existing correlations are negligible.

### 3. Stationary environment

The environment is usually taken to be in a thermal or otherwise stationary state,

$$\rho_E \propto e^{-H_E/T},$$

so its statistical properties do not change in time. One also shifts operators so that the environment averages  $\langle E_i \rangle$  vanish, absorbing any constant bias into the system Hamiltonian.

#### 4. Born approximation (second order)

Equation (8.142) is not closed because it depends on the full state  $\hat{\rho}_T(s)$ . Under the assumption of weak coupling, one neglects system–environment correlations and approximates

$$\hat{\rho}_T(s) \approx \hat{\rho}_S(s) \otimes \rho_E,$$

where  $\rho_E$  is a fixed bath state. This substitution is performed inside the memory integral, yielding

$$\frac{d\hat{\rho}_S(t)}{dt} = -\alpha^2 \int_0^t ds \operatorname{Tr}_E \left( [\hat{H}_I(t), [\hat{H}_I(s), \hat{\rho}_S(s) \otimes \rho_E]] \right).$$

This approximation is consistent to second order in the coupling constant  $\alpha$ , since corrections to  $\hat{\rho}_T(s)$  would contribute only at higher order.

This approximation implies that correlations generated during the evolution are assumed weak enough to be neglected when computing the dissipative kernel. This means that the system is affected by the bath, but the bath is so large that it hardly notices the system. In that sense, the bath acts like a reservoir with fixed statistical properties.

#### 5. Markov approximation

Let us do the change of integration variable

$$u = t - s \Rightarrow s = t - u \quad du = -ds.$$

We get

$$\frac{d\hat{\rho}_S(t)}{dt} = -\alpha^2 \int_t^0 (-du) \operatorname{Tr}_E \left( [\hat{H}_I(t), [\hat{H}_I(t-u), \hat{\rho}_S(t-u) \otimes \rho_E]] \right).$$

The idea of the Markov approximation is that the environment correlation time is very short, so the kernel in the integral is appreciable only for small  $u$ . Over such a short memory time, the system state changes very little, so one replaces

$$\hat{\rho}_S(t-u) \approx \hat{\rho}_S(t).$$

Note: A kernel is the function or operator that appears inside an integral and weights the contribution from past times.

*Physical idea.* The bath is said to have a short memory if its correlation functions decay on a very short time scale  $\tau_B$ . This means that the bath quickly “forgets” any disturbance caused by the system. If  $\tau_B \ll \tau_S$ , where  $\tau_S$  is the typical time scale of the system evolution, then the system does not depend significantly on its past history. In this case, the dominant contribution to the integral comes from short times  $u \lesssim \tau_B$ , and the dependence on  $\rho_S(t-u)$  can be approximated by  $\rho_S(t)$ . [Note that we cannot do the same approximation to the interaction part of the Hamiltonian,  $\hat{H}_I(t-u) \approx \hat{H}_I(t)$ , because the operators involved in it typically contain fast oscillations.]

*Mathematical step.* Since the bath correlations vanish for  $u \gg \tau_B$ , extending the upper limit of integration from  $t$  to  $\infty$  introduces only a negligible error:

$$\int_0^t du (\dots) \longrightarrow \int_0^\infty du (\dots).$$

*Interpretation.* This step removes the explicit dependence on the past history of the system and leads to a *time-local* equation: the rate of change of  $\rho_S(t)$  depends only on its value at time  $t$ . This is what is meant by a *Markovian* (memoryless) evolution.

**Result: Born–Markov (Redfield) equation.**

Applying the Born approximation (weak coupling) together with the Markov approximation leads to a time-local master equation for the reduced density matrix. In the interaction picture, it takes the form

$$\frac{d\hat{\rho}_S(t)}{dt} = -\alpha^2 \int_0^\infty ds \operatorname{Tr}_E \left( [\hat{H}_I(t), [\hat{H}_I(t-s), \hat{\rho}_S(t) \otimes \rho_E]] \right), \quad (8.143)$$

where we have used the Markov approximation to replace  $\rho_S(s) \rightarrow \rho_S(t)$  and extended the upper limit of the integral to infinity.

This equation is often referred to as the *Redfield equation*. More precisely, the Redfield equation is obtained after evaluating the environmental correlation functions and expressing the result explicitly in terms of system operators. In general, this equation is not guaranteed to preserve complete positivity. Additional approximations (such as the secular or rotating-wave approximation) are typically required to obtain the Lindblad (GKSL) form.

## 6. Decomposition of the interaction Hamiltonian

We write the interaction Hamiltonian as

$$\hat{H}_I(t) = \sum_i \hat{S}_i(t) \otimes \hat{E}_i(t), \quad (8.144)$$

where  $\hat{S}_i(t)$  and  $\hat{E}_i(t)$  act on the system and environment Hilbert spaces, respectively.

Substituting into Eq. (8.143) and tracing over the environment yields terms involving the bath correlation functions,

$$C_{ij}(s) = \operatorname{Tr}_E (\hat{E}_i(t) \hat{E}_j(t-s) \rho_E). \quad (8.145)$$

For a stationary environment,  $C_{ij}(s)$  depends only on the time difference  $s$ .

## 7. Expansion in Bohr frequencies

We now decompose the system operators into eigenoperators of the system Hamiltonian  $H_S$ ,

$$\hat{S}_i(t) = \sum_\omega e^{-i\omega t} S_i(\omega), \quad (8.146)$$

where

$$S_i(\omega) = \sum_{\epsilon' - \epsilon = \omega} |\epsilon\rangle \langle \epsilon| S_i |\epsilon'\rangle \langle \epsilon'|. \quad (8.147)$$

These operators describe transitions between energy eigenstates with energy difference  $\omega$ .

## 8. Time integration and spectral densities

Inserting the above decomposition into Eq. (??), one encounters integrals of the form

$$\int_0^\infty ds e^{i\omega s} C_{ij}(s). \quad (8.148)$$

We define the bath spectral density matrix,

$$\Gamma_{ij}(\omega) = \int_0^\infty ds e^{i\omega s} C_{ij}(s). \quad (8.149)$$

In general,  $\Gamma_{ij}(\omega)$  is a complex matrix. Its real part determines dissipative processes, while its imaginary part leads to a Hamiltonian renormalization (Lamb shift).

## 9. Rotating wave (secular) approximation

After inserting all terms, the master equation contains oscillatory factors of the form

$$e^{i(\omega-\omega')t}. \quad (8.150)$$

The rotating wave (or secular) approximation consists of neglecting rapidly oscillating terms with  $\omega \neq \omega'$ , retaining only energy-conserving contributions with  $\omega = \omega'$ .

This yields a master equation of the form

$$\frac{d\rho_S(t)}{dt} = \sum_{\omega, i, j} \Gamma_{ij}(\omega) \left( S_j(\omega) \rho_S(t) S_i^\dagger(\omega) - \frac{1}{2} \{ S_i^\dagger(\omega) S_j(\omega), \rho_S(t) \} \right) - i[H_{\text{LS}}, \rho_S(t)], \quad (8.151)$$

where  $H_{\text{LS}}$  is the Lamb-shift Hamiltonian arising from the imaginary part of  $\Gamma_{ij}(\omega)$ .

## 10. Diagonalization and Lindblad operators

For each frequency  $\omega$ , the matrix  $\Gamma_{ij}(\omega)$  is positive semidefinite. We diagonalize it as

$$\Gamma_{ij}(\omega) = \sum_k u_{ik}(\omega) \gamma_k(\omega) u_{jk}^*(\omega), \quad (8.152)$$

where  $\gamma_k(\omega) \geq 0$  are eigenvalues.

We define the Lindblad (jump) operators as

$$L_k(\omega) = \sqrt{\gamma_k(\omega)} \sum_i u_{ik}(\omega) S_i(\omega). \quad (8.153)$$

## 11. Final Lindblad form

The master equation then takes the standard Gorini–Kossakowski–Sudarshan–Lindblad form,

$$\frac{d\rho_S(t)}{dt} = -i[H_S + H_{\text{LS}}, \rho_S(t)] + \sum_{\omega, k} \left( L_k(\omega) \rho_S(t) L_k^\dagger(\omega) - \frac{1}{2} \{ L_k^\dagger(\omega) L_k(\omega), \rho_S(t) \} \right). \quad (8.154)$$

The operators  $S_i(\omega)$  describe transitions between system energy eigenstates with frequency  $\omega$ , while the coefficients  $\gamma_k(\omega)$  encode the strength of the coupling to the environment at those frequencies. The Lindblad operators  $L_k(\omega)$  therefore represent the effective dissipative channels induced by the environment.

part of what is below will be incorporated above...

## 6. Secular or rotating-wave approximation (RWA)

Recall that the interaction Hamiltonian has the form

$$H_I = \sum_i S_i \otimes E_i,$$

where  $S_i$  act on the system and  $E_i$  act on the environment. In the interaction picture,

$$\hat{S}_i(t) = e^{iH_S t} S_i e^{-iH_S t}, \quad \hat{E}_i(t) = e^{iH_E t} E_i e^{-iH_E t}.$$

*Decomposition into Bohr frequencies.* To proceed, we express the system operators  $S_i$  in terms of the eigenbasis of the system Hamiltonian  $H_S$ ,

$$H_S |n\rangle = E_n |n\rangle.$$

We define the Bohr frequencies  $\omega = E_n - E_m$  and decompose

$$S_i = \sum_{\omega} S_i(\omega), \quad S_i(\omega) = \sum_{E_n - E_m = \omega} |n\rangle \langle n| S_i |m\rangle \langle m|. \quad (8.155)$$

These operators satisfy

$$[H_S, S_i(\omega)] = -\omega S_i(\omega),$$

so in the interaction picture they evolve as

$$\hat{S}_i(t) = \sum_{\omega} e^{-i\omega t} S_i(\omega).$$

Substituting this decomposition into Eq. (8.143), one finds terms of the form

$$e^{-i\omega t} e^{i\omega'(t-s)} = e^{i(\omega' - \omega)t} e^{-i\omega' s}.$$

After performing the integral over  $s$ , the evolution equation contains oscillating terms proportional to

$$e^{i(\omega' - \omega)t}.$$

**RWA:** If  $|\omega - \omega'|$  is large compared with the typical relaxation rates of the system, these oscillating terms average to zero over the coarse-grained time scale of the dynamics. The *RWA or secular approximation* consists of neglecting all such rapidly oscillating terms and keeping only the resonant contributions with

$$\omega = \omega'.$$

This approximation removes interference between transitions associated with different energy gaps of the system. Each Bohr-frequency channel then evolves independently.

After the secular approximation, the generator of the dynamics acquires the Lindblad (GKSL) form, which guarantees complete positivity of the density matrix. Without this step, the Redfield equation does not, in general, preserve positivity.

## 7. Lamb shift

In the microscopic derivation of the master equation, after applying the Born and Markov approximations and performing the secular approximation, the reduced dynamics naturally separates into two contributions:

- *Dissipative terms*, responsible for decay and dephasing;
- *Coherent corrections*, which modify the system Hamiltonian.

The latter take the form of an additional Hamiltonian,

$$H_{LS},$$

called the *Lamb shift Hamiltonian*. The effective system Hamiltonian becomes

$$H_{\text{eff}} = H_S + H_{LS}.$$

Mathematically, the Lamb shift arises from the *imaginary part* of time integrals over bath correlation functions, while the *real part* gives rise to the dissipative terms.

*Physical meaning.* The environment not only induces irreversible processes, but also renormalizes the energy levels of the system. This can be understood as arising from virtual processes in which the system interacts with the bath without exchanging real excitations. This effect is named after the Lamb shift observed in atomic hydrogen, where interactions with the electromagnetic vacuum lead to small but measurable shifts of energy levels.

In the final master equation, the Lamb shift is included in the Hamiltonian term. That is, the  $H$  appearing in the commutator

$$-i[H, \rho]$$

should be understood as the effective Hamiltonian

$$H = H_S + H_{LS}.$$

In practice, when using phenomenological Lindblad models, the Hamiltonian is typically written without an explicit Lamb shift term. In such cases, any environment-induced energy renormalization is either negligible or implicitly absorbed into the parameters of the system Hamiltonian.



# Chapter 9

## Ideas for projects and practice questions:

### 9.1 Ideas for Projects

1. **Extreme eigenvalue statistics:** Study of the distribution of the lowest (highest) energy level. Extreme-value statistics concerns the study of rare events, such as tsunamis, floods, earthquakes, and large variations in the stock market.
2. **Multifractality:** Study of the scaling properties and spatial structure of eigenstates. Multifractality is commonly associated with critical points of localization-delocalization transitions, such as the Anderson transition. This study can be done in the context of random matrices models, such as the powerlaw banded random matrices, or for physical models with disorder.
3. **Scaling Analysis:** How does the transition to chaos depend on the system size? Can we get hints for this transition by analyzing the Hamiltonian matrix and its components before diagonalization?
4. **Many-body localization:** When we add onsite disorder to systems with interactions, we may transition from a chaotic regime to a localized regime.
5. **From few- to many-body interactions:** How many interacting particles (excitations) are needed for a system to be considered many body?
6. **Timescales for saturation:** How does the time to reach equilibrium depend on the energy of the initial state, on the model, and on the observables considered?
7. **Beyond spin-1/2 chains:** You can explore several variations of the systems that we have considered, such as
  - ⇒ spin-1 models (or larger spins),
  - ⇒ Bose-Hubbard model,
  - ⇒ systems with long-range interactions, and even
  - ⇒ larger dimension, such as 2D or 3D.

8. **Experiments and nonequilibrium dynamics:** You can describe systems in which dynamics and thermalization have been studied and reproduce their numerical results.
9. **Out-of-time ordered correlators and correlation hole:** What are the dynamical signatures of quantum chaos?
10. **Quantum-classical correspondence:** You can compare, for example, the dynamics of quantum spin models with  $S > 1/2$  and their classical counterparts.

You can find some ideas in my own publications:

<https://lea-santos.scholar.uconn.edu/publications-2/publications/>

Have a look at the papers starting in 2010 where I am the first author or where the first and/or second authors are:

- Jonathan Torres-Herrera
- Marco Távora
- Mauro Schiulaz
- Aviva Gubin
- Davida Kollmar
- Guy Zisling
- Karin Wittmann
- Isaías Vallejo-Fabila
- Adway Kumar-Das
- David Zarate
- Soumya K Pal

## 9.2 Practice Questions

### 9.2.1 Chapter 2 – Random Matrix Theory

1. What motivated Wigner to introduce random matrix theory?
2. What distinguishes GOE and GUE?
3. What does the Dyson index  $\beta$  represent physically?
4. What is the level spacing distribution for integrable systems without an excessive number of degeneracies?
5. Why is unfolding necessary when studying level spacing distributions?
6. Why is the ratio of consecutive spacings useful?
7. What does spectral rigidity measure?
8. Show that Poisson statistics gives  $\langle \tilde{r} \rangle = 2 \ln 2 - 1$ , using

$$P(\tilde{r}) = \frac{2}{(1 + \tilde{r})^2}.$$

9. Show that the GOE Wigner surmise

$$P(s) = \frac{\pi}{2} s e^{-\pi s^2/4}$$

satisfies  $P(s) \sim s$  for small  $s$ .

10. For a fully delocalized state  $C_n = 1/\sqrt{N}$ , compute the inverse participation ratio (IPR).
11. For a localized state  $C_k = \delta_{k,k_0}$ , compute the IPR.
12. To construct a GOE random matrix, one may start from an  $N \times N$  real matrix  $M$  with independent Gaussian entries of zero mean and variance  $\sigma^2$ .

A GOE matrix  $H$  can be obtained by symmetrizing  $M$ :

(i)  $H = \frac{1}{2}(M + M^T)$

(ii)  $H = M + M^T$

Both constructions produce a real symmetric matrix.

- What is the ratio between the variances of the diagonal and off-diagonal elements in a GOE matrix?
  - For construction (i): What are the mean values and variances of diagonal and off-diagonal elements?
  - For construction (ii): What are the mean values and variances of diagonal and off-diagonal elements?
13. How do we build GUE random matrices?
14. How are the matrices of the Rosenzweig-Porter ensemble constructed? Which phases does the ensemble have?
15. How are power-law banded random matrices constructed? Which phases does this ensemble have?

## Chapter 3 – Spin-1/2 Models

16. Write down the Hamiltonian for the 1D spin-1/2 XXZ model with open boundary conditions,  $L$  sites, and nearest-neighbor couplings.
17. Write down the Hamiltonian matrix for the 1D spin-1/2 XXZ model with open boundary conditions,  $L = 6$  sites and 2 up-spins.
18. Give at least two examples of symmetries of the XXZ model and explain them.
19. Give at least two examples of what breaks integrability in the XXZ model.

20. Why is the XX model noninteracting in fermionic language?
21. Why does the Ising term represent interaction in fermionic language?
22. What is the equation for the entanglement entropy? What does it measure?
23. Using tensor products, write the matrix representation of a nearest-neighbor term (e.g.  $\hat{S}_1^x \hat{S}_2^x$ ) in a 3-site system.
24. What is the total Hilbert space dimension of an  $L$ -site spin-1/2 chain?
25. What is the dimension in the sector with  $M$  up-spins?
26. Write the Hamiltonian matrix for a spin-1 model with  $M = 1$ .
27. Compute the entanglement entropy of

$$\frac{1}{\sqrt{2}}(|01\rangle + |10\rangle).$$

28. Show that for fermions

$$e^{i\pi\hat{n}} = 1 - 2\hat{n}.$$

29. Write the XX model in fermionic language.
30. Show that adding next-nearest-neighbor terms to the XX model leads to interactions after the Jordan-Wigner transformation.
31. Write the Hamiltonian matrix for the Bose-Hubbard model with 3 sites and 2 bosons.
32. For the Bose-Hubbard model with  $L$  sites and  $N$  bosons, what is the Hilbert space dimension?

## Chapter 4 – Thermalization

33. What is thermalization in an isolated quantum system?
34. Why does the initial state matter?
35. How does ETH justify statistical mechanics?
36. Why do integrable systems not thermalize via ETH?
37. What is diagonal ETH?
38. What is the role of off-diagonal elements?
39. In a strongly chaotic system, what is the distribution of off-diagonal elements? Why?
40. Why is ETH automatic in random matrices?

41. What is the long-time average of an observable in a many-body quantum system without degeneracies?
42. Show that the long-time average is given by the diagonal ensemble:

$$\overline{O} = \sum_n |c_n|^2 O_{nn}.$$

43. Given

$$\langle \hat{O}(t) \rangle = \sum_{n,m} c_n^* c_m e^{i(E_n - E_m)t} O_{nm},$$

separate it into:

- time-independent part
- time-dependent fluctuations

44. Compare the diagonal and microcanonical ensembles:

$$O_{\text{diag}} = \sum_n |c_n|^2 O_{nn}, \quad O_{\text{micro}} = \frac{1}{\mathcal{N}} \sum_{E_n \in [E-\delta, E+\delta]} O_{nn}.$$

Under what conditions are they equal (or better, close)?



# Bibliography

- [1] Richard P. Feynman. Simulating physics with computers. *International Journal of Theoretical Physics*, 21(6–7):467–488, 1982. doi: 10.1007/BF02650179.
- [2] Seth Lloyd. Universal quantum simulators. *Science*, 273(5278):1073–1078, 1996. doi: 10.1126/science.273.5278.1073.
- [3] Iulia Buluta and Franco Nori. Quantum simulators. *Science*, 326(5949):108–111, 2009. doi: 10.1126/science.1177838.
- [4] I. M. Georgescu, S. Ashhab, and Franco Nori. Quantum simulation. *Reviews of Modern Physics*, 86:153–185, 2014. doi: 10.1103/RevModPhys.86.153.
- [5] I. Bloch, J. Dalibard, and W. Zwerger. Many-body physics with ultracold gases. *Rev. Mod. Phys.*, 80:885–964, 2008. doi: 10.1103/RevModPhys.80.885.
- [6] Christian Gross and Immanuel Bloch. Quantum simulations with ultracold atoms in optical lattices. *Science*, 357(6355):995–1001, 2017. doi: 10.1126/science.aal3837.
- [7] Antoine Browaeys and Thierry Lahaye. Many-body physics with individually controlled rydberg atoms. *Nature Physics*, 16:132–142, 2020. doi: 10.1038/s41567-019-0733-z.
- [8] R. Blatt and C. F. Roos. Quantum simulations with trapped ions. *Nat. Phys.*, 8: 277–284, 2012. doi: 10.1038/nphys2252.
- [9] Andrew A. Houck, Hakan E. Türeci, and Jens Koch. On-chip quantum simulation with superconducting circuits. *Nature Physics*, 8:292–299, 2012. doi: 10.1038/nphys2251.
- [10] Markus Greiner and Simon Fölling. Optical lattices. *Nature*, 453(7196):736–738, 2008. doi: 10.1038/453736a.
- [11] M. L. Mehta. *Random Matrices*. Academic Press, Boston, 1991.
- [12] David J. Griffiths and Darrell F. Schroeter. *Introduction to Quantum Mechanics*. Cambridge University Press, Cambridge, UK; New York, NY, USA, 3rd edition, 2018. ISBN 978-1-107-18963-8.