Open Floquet systems

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In this chapter we will derive a master equation for open Floquet systems, following

D. Hone, R. Ketzmerick, W. Kohn, PRE 79, 051129 (2009)

The derivation generalizes the standard Born-Markov theory to time-periodically driven (i.e. Floquet) systems. Such a theory was developed already in earlier works for specific systems (see references in Hone et al. 2009).

We will, moreover, discuss the properties of the quasi-steady (i.e. time periodic) solution $\varrho^{[0]}(t) = \varrho^{[0]}(t+T)$ of the equation, to which the system relaxes in the long-time limit. Special focus will lie on the Floquet "pointer" basis, $\{|v_i(t)\rangle\}$, i.e. the instantaneous eigenstates of $\varrho^{[0]}(t)$,

$$\varrho^{[0]}(t) = \sum_i p_i \; |v_i(t)\rangle\langle v_i(t)| \; .$$

While for ultraweak coupling, it corresponds to the basis of exact Floquet states, $|u_i(t)\rangle$, the $|v_i\rangle$ approach approximate Floquet states $|u_i^{\mathrm{HF}}(t)\rangle$ as they result from a high-frequency approximation (even beyond the regime where it is valid in closed systems).

A) Open Systems

The textbook idealization of an isolated quantum system described by the Schrödinger equation

$$i\,|\dot{\psi}(t)\rangle = H(t)\,|\psi(t)\rangle$$

| We use units with $\hbar = 1$

for a pure state $|\psi(t)\rangle$, or the equivalent von Neumann equation **

$$\dot{\rho}(t) = \frac{1}{i}\,[H(t), \rho(t)]$$

for mixed states, with density operator * $\rho(t)$, is realized in experiments at most approximately.

* The density operator $\rho(t)$ acts in the state space $\mathcal{H}$ of the system and has the following properties:

(i) Hermitian $\quad \rho^\dagger = \rho$

(ii) normalized $\quad \mathrm{tr}\{\rho\} = 1$

(iii) non-negative $\quad \langle x|\rho|x\rangle \geq 0 \quad \forall\, |x\rangle \in \mathcal{H}$.

With respect to a generic basis of orthonormal states $|i\rangle$ ($\langle i|j\rangle = \delta_{ij}$, $\sum_i |i\rangle\langle i| = \mathbb{1}$) it is represented by the density matrix $\rho_{ij} = \langle i|\rho|j\rangle$,

$$\rho = \sum_{ij} \rho_{ij}\, |i\rangle\langle j| .$$

A special basis is given by its orthonormal eigenstates $|\varphi_k\rangle$,

$$\rho = \sum_k p_k |\varphi_k\rangle\langle\varphi_k|$$

that are found with probability $p_k = \langle\varphi_k|\rho|\varphi_k\rangle \in [0,1]$. For pure states, we have $p_k = \delta_{k,k_0}$, i.e.

$$\rho = |\varphi_{k_0}\rangle\langle\varphi_{k_0}| \equiv |\psi\rangle\langle\psi|.$$

Expectation values of observables A are computed according to the rule

$$\langle A\rangle = \mathrm{tr}\{\rho A\} = \sum_k p_k \langle\varphi_k|\hat{A}|\varphi_k\rangle.$$

Two ways of defining a density operator are the following:

(a) To describe a stochastic process that produces pure states $|\psi_\alpha\rangle$ (which shall be normalized, $\langle\psi_\alpha|\psi_\alpha\rangle = 1$, but are not necessarily orthogonal, $\langle\psi_\alpha|\psi_\beta\rangle \neq 0$), with probabilities π_α ($\pi_\alpha \in [0,1]$, $\sum_\alpha \pi_\alpha = 1$). Then defining

$$\rho = \sum_\alpha \pi_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|.$$

produces precisely the expectation values

$$\langle A \rangle = tr\{\rho A\} = \sum_\alpha \pi_\alpha \langle \psi_\alpha | A | \psi_\alpha \rangle$$

as they should result from such a process.

(b) As reduced density operator

$$\rho = tr_E\{\rho_{tot}\}$$

or, for $\rho_{tot} = |\psi_{tot}\rangle\langle\psi_{tot}|$,

$$\rho = tr_E\{|\psi_{tot}\rangle\langle\psi_{tot}|\},$$

where ρ_{tot} acts in ($|\psi_{tot}\rangle$ is element of) the larger state space $\mathcal{H}_{tot} = \mathcal{H} \otimes \mathcal{H}_E$ of system and environment E. Here $tr_E\{\cdot\}$ denotes the partial trace over the environmental degrees of freedom. This definition allows to compute all expectation values of operators $A \otimes 1\!\!1_E$ that act solely on the system degrees of freedom, namely

$$\langle A \rangle = tr_{tot}\{\rho_{tot}(A \otimes 1\!\!1_E)\} = tr\{\rho A\},$$

where $tr\{\cdot\}$ denotes the trace over the system degrees of freedom and $tr_{tot}\{\circ\} = tr\{tr_E\{\cdot\}\}$ the trace over the total state space of system and environment.

** For an isolated system, the von Neumann equation follows immediately from interpretation (a). After the ensemble has been realized, the states $|\psi_i\rangle$ evolve according to the Schrödinger equation, i.e.

$$|\psi_i(t)\rangle = U(t)\,|\psi_i\rangle$$

with time-evolution operator $U(t)$ of the system from time 0 to time t, which obeys the Schrödinger equation

$$i\,\dot{U}(t) = H(t)\,U(t) \quad \text{with} \quad U(0) = \mathbb{1}.$$

Thus the density operator evolves like

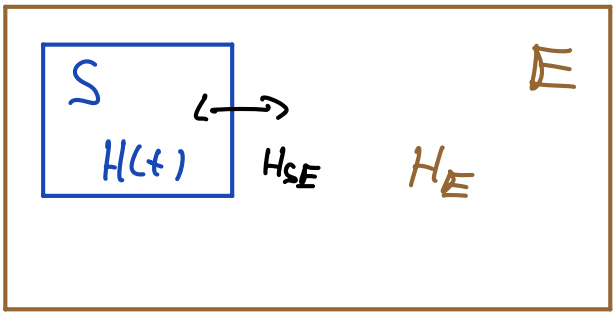
$$\begin{aligned} \rho(t) &= \sum_i \pi_i\, |\psi_i(t)\rangle\langle\psi_i(t)| \\ &= \sum_i \pi_i\, U(t)\,|\psi_i(0)\rangle\langle\psi_i(0)|\,U^\dagger(t) \end{aligned}$$

where the probabilities π_i are time independent. Taking the time derivative

$$\begin{aligned} \dot{\rho}(t) &= \sum_i \pi_i \Big(\underbrace{\dot{U}(t)}_{\frac{1}{i}H(t)U(t)}\,|\psi_i(0)\rangle\langle\psi_i(0)|\,U^\dagger(t) \\ &\qquad + U(t)\,|\psi_i(0)\rangle\langle\psi_i(0)|\,\underbrace{\dot{U}^\dagger(t)}_{-\frac{1}{i}U^\dagger(t)H(t)} \Big) \\ &= \frac{1}{i}\Big(\underbrace{H(t)\rho(t) - \rho(t)H(t)}_{[H,\rho]}\Big) \end{aligned}$$

corresponding to the von Neumann equation.

Generally, the system will interact with its environment E, so that the total system, given by system and environment, is described by the total Hamiltonian



$$H_{tot} = \underbrace{H \otimes \mathbb{1}_E}_{\equiv H} + H_{SB} + \underbrace{\mathbb{1} \otimes H_E}_{\equiv H_E},$$

acting in the product space $\mathcal{H}_{tot} = \mathcal{H} \otimes \mathcal{H}_E$ (we omit the label S for the system, instead we label the environment with "E" and the total system with "tot").

The system-bath coupling generally takes the form

$$H_{SB} = \sum_n A_n \otimes B_n$$

with system operators $A_n = A_n^\dagger$, bath operators $B_n = B_n^\dagger$ and coupling strengths $\gamma_n = \gamma_n^*$. For simplicity and for the sake of a lighter notation, we assume from now on

$$H_{SB} = A \otimes B = AB,$$

Reintroducing the sum $\sum_n$ is rather straightforward (and can be done as an exercise).

often we are neither interested in the state of the environment, nor able to practically compute it. The theory of open quantum systems, thus, aims for an effective description that focuses on the system degrees of freedom and treats the environment in a minimal fashion, either by reducing it to a few auxiliary degrees of freedom or by integrating it out completely. The latter gives rise to a master equation

$$\dot{s} = \mathcal{L}[s]$$

with (effective) Liouvillian $\mathcal{L}$, possibly being a functional of s as a function of time or a time-local superoperator.

Deriving a master equation almost always involves approximations. In the following we will describe such an approximative derivation of a master equation for open Floquet systems.

B) Redfield equation for time-dependent Hamiltonians

Let us now generalize the Born-Markov-approximation to the case of time-dependent system Hamiltonians $H(t)$, with unitary time evolution operator $U(t,t_0) = \mathcal{T}\exp(-i\int_{t_0}^{t} dt' H(t'))$, solving

$$i\partial_t U(t,t') = H(t)U(t,t') \quad \text{with} \quad U(t',t') = 1,$$

we also use the short-hand $U(t) \equiv U(t,0)$.
For simplicity, we assume the environment Hamiltonian H_E time-independent, with evolution operator $U_E(t,t') = \exp(-i(t-t')H_E) \equiv U_E(t-t')$.
The coupling operator might be time-dependent in the system operator A, $H_{SE}(t) = A(t)B$.

We assume the initial state to be uncorrelated

$$\tilde{\rho}_{tot}(0) = \underbrace{\rho_{tot}(0)}_{U_0(0)=0} = \rho(0)\otimes\rho_E(0),$$

and the environment to be in equilibrium

$$\rho_E(0) = \frac{1}{Z_E} e^{-\beta H_E}$$

with inverse temperature β and partition function $Z_E = \mathrm{tr}_E\{e^{-\beta H_E}\}$.