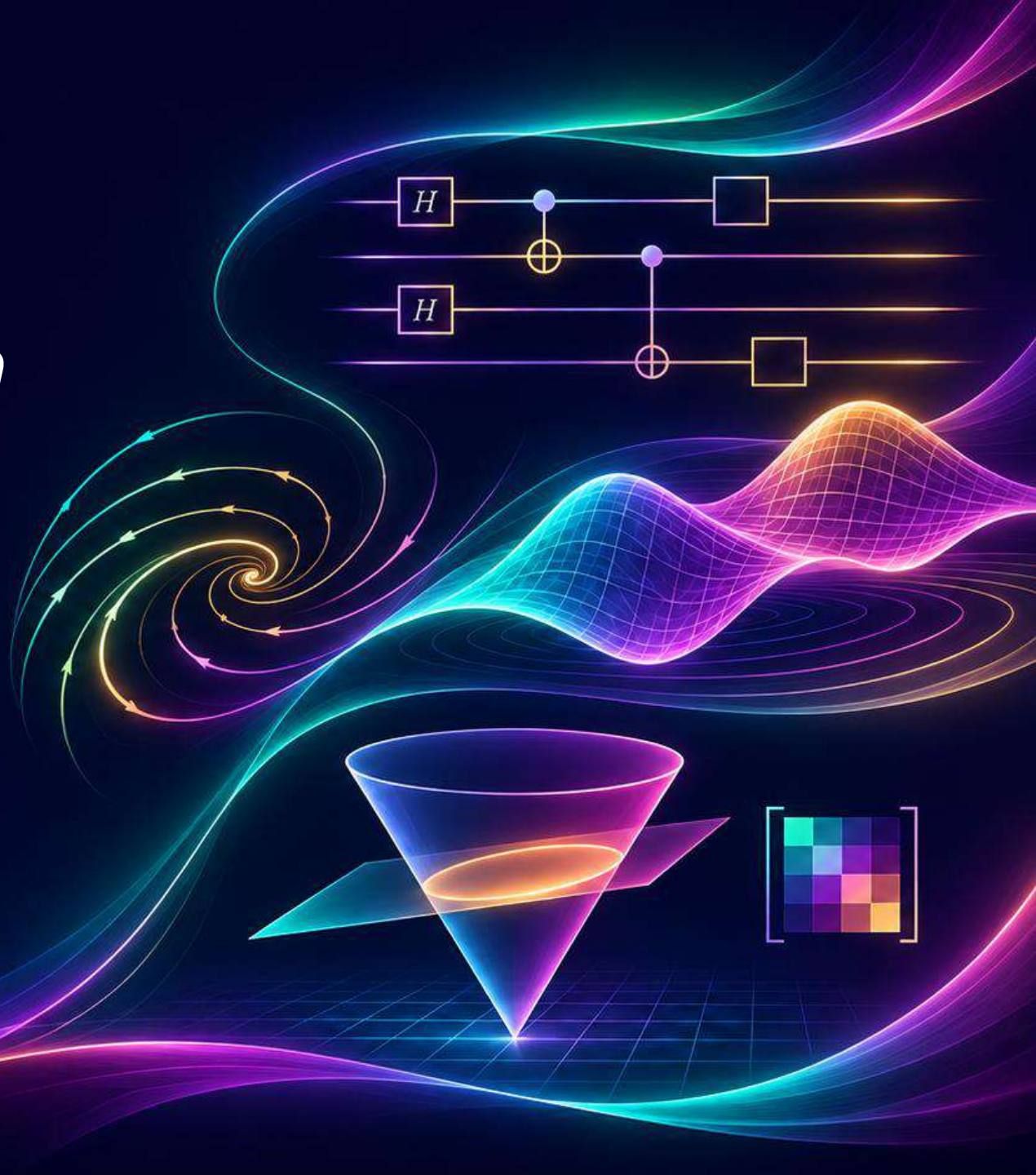
Quantum algorithms for scientific computing: *viewpoint from quantum dynamics*



Nana Liu
Shanghai Jiao Tong University
3rd Quantum Computing School
Sao Paulo, November 2026

Scientific computing:

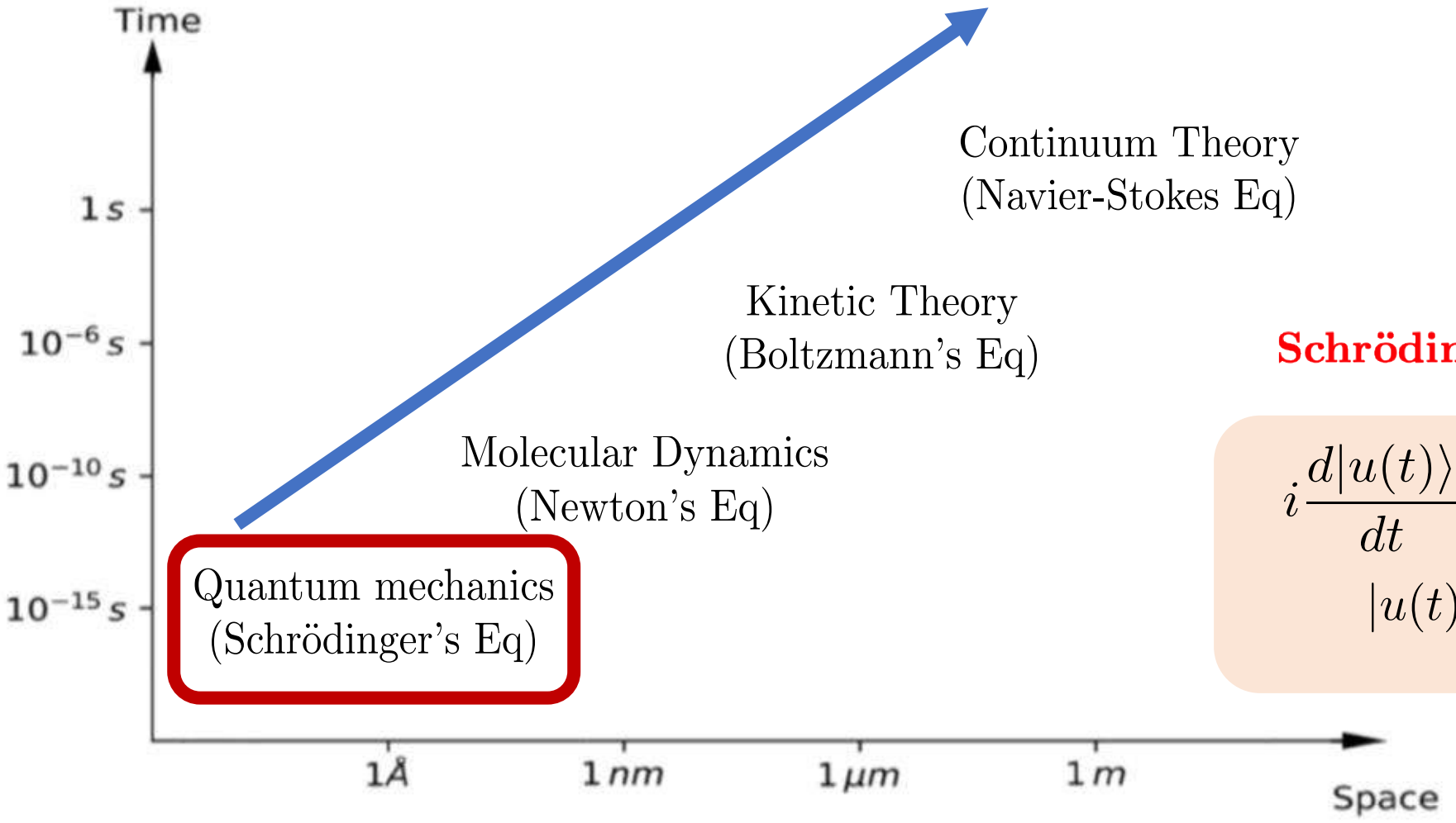
a dynamical viewpoint

- Linear algebra
- Ordinary differential equations (ODEs)
- Partial differential equations (PDEs)
- Optimisation
- Machine learning

All of these can be mapped to *dynamical processes*!

What happens when that dynamics becomes quantum?

Dynamical processes are described by ordinary and partial differential equations:



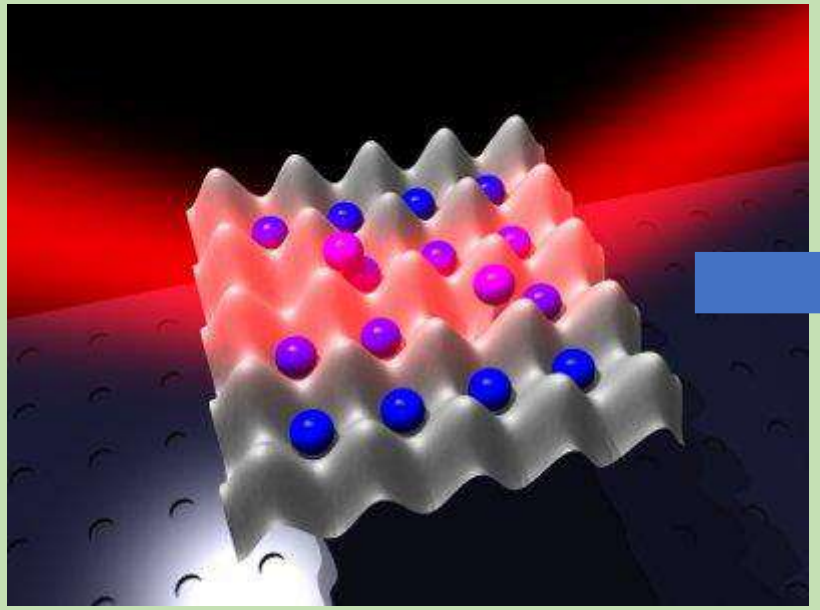
Schrödinger's equation

$$i\frac{d|u(t)\rangle}{dt} = \mathbf{H}(t)|u(t)\rangle$$

$$|u(t)\rangle = U(t)|u(0)\rangle$$

Quantum simulation

Quantum simulations can efficiently simulate quantum systems



After a certain time?

$$|u(0)\rangle \rightarrow U(t)|u(0)\rangle = |u(t)\rangle$$

$U(t)$ is unitary: $U(t)^\dagger U(t) = \mathbf{1}$

Today we are reaching beyond the limit of what classical computers can easily simulate:

Quantum computers:
O(100) 'quite good' qubits

Quantum simulators with continuous-variables:
O(1000000) qumodes

N 2-level systems (qubits)
Classical vector: 2^N entries

Linear ODEs/PDEs

$$\frac{du}{dt} = -A(t)u \rightarrow i\frac{d\psi}{dt} = H(t)\psi$$

Nonlinear ODEs/PDEs (e.g. fluid dynamics, optimal control, machine learning)

$$\frac{du}{dt} = F(u,t)$$

Steady-state solutions (e.g. linear algebra and optimisation)

$$\frac{dY}{dt} = f(Y,t) = 0$$

Thermal states (e.g. sampling, machine learning and optimisation)

$$\frac{du}{dt} = -Hu, \qquad u(t=\beta) \propto e^{-\beta H}$$

Quantum simulation of ODEs and PDEs

D ODEs

$$\frac{dX^{[k]}(t)}{dt} = F(X^{[k]}(t)), \qquad X^{[k]} \in \mathbb{R}^D$$
$$X^{[k]}(0) = X_0^{[k]}, \qquad k = 1, \cdots, M$$

Molecular dynamics, particle swarm, electrical networks...etc

$(d+1)$-dim PDEs

$$\frac{\partial u^{[k]}}{\partial t} + F(u^{[k]}, \nabla u^{[k]}, \nabla^2 u^{[k]}, ...) = 0 \quad u^{[k]} \in \mathbb{R}^d$$

Fluid dynamics, financial market behaviour, machine learning...etc

To put onto quantum hardware:

How to map onto Schrodinger's equation in a *simple* way?

Schrodingerisation!

Overview of school lectures

PART I: Basics of quantum algorithms for ordinary and partial differential equations (using Schrodingerisation)

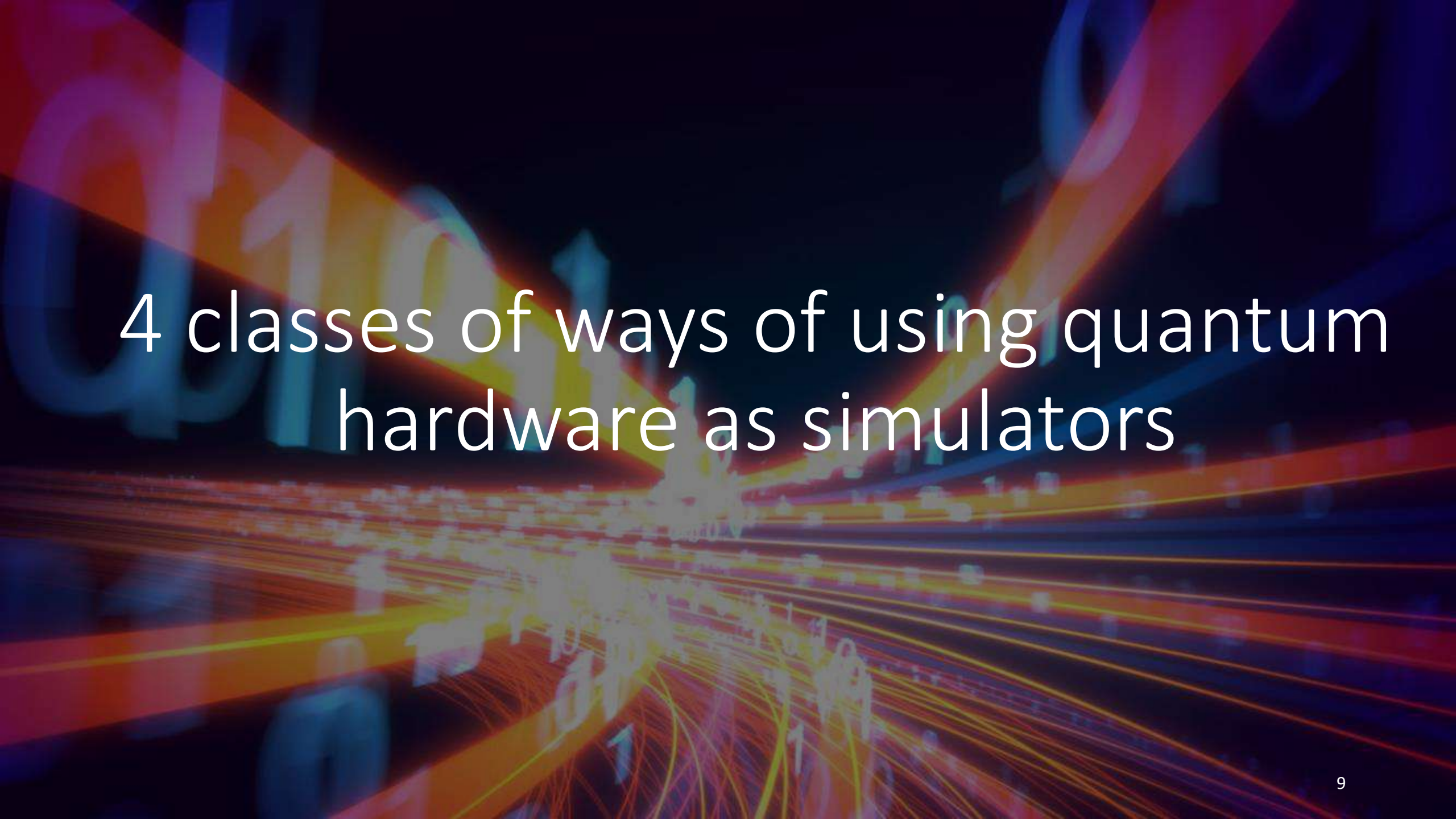
Flexible method for mapping linear ODEs or PDEs to a corresponding Schrodinger equation in one higher dimension

- Continuous space and time formulation (analogue)
- Discrete space formulation (digital)
- Homogeneous
- Inhomogeneous
- Higher-order time derivatives
- Ill-posed linear PDEs
- Boundary conditions
- Improving algorithm with respect to precision

Overview of autumn lectures on Schrodingerisation

PART II: Special topics

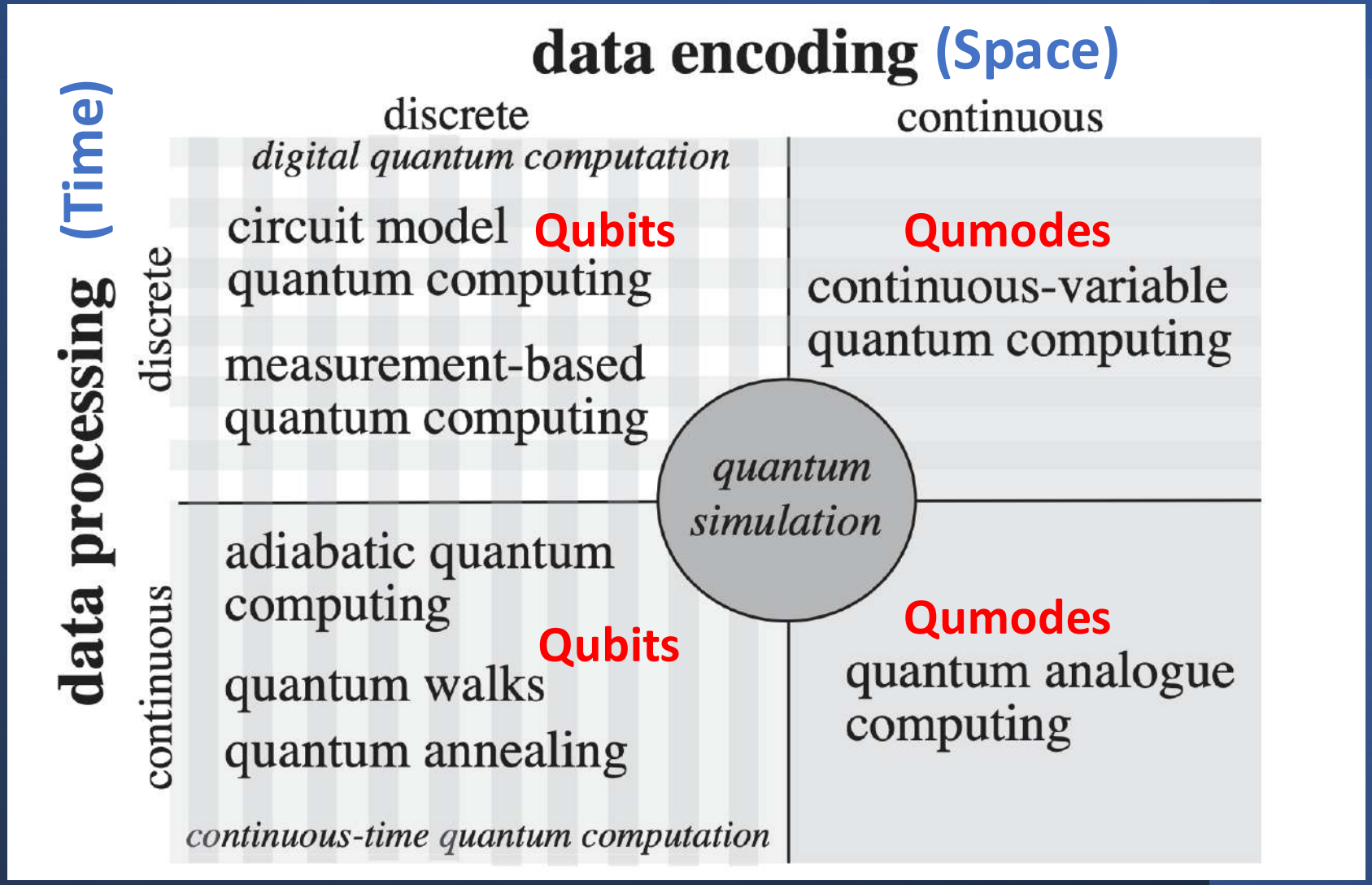
- **Introducing UnitaryLab: software for quantum algorithms for scientific computing**
- **Optimisation: semidefinite programming**
- **If there's time: uncertain ODEs/PDEs; nonlinear PDEs; iterative linear algebra, non-autonomous mapped to autonomous PDEs; applications to machine learning**


4 classes of ways of using quantum hardware as simulators

Formulation of differential equations versus linear algebra

Mathematical language	Time	Space
Partial differential equation	Continuous	Continuous
Ordinary differential equation	Continuous	Discrete
Linear algebra	Discrete	Discrete

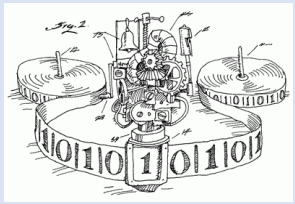
Do we choose space and time to be continuous or discrete during simulation? Depends on the quantum platform!

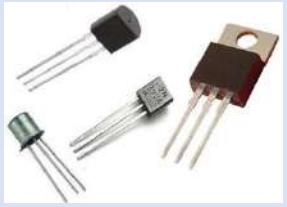


arXiv: 1001.2215

Digital quantum information: matrix language

Bit $|0\rangle$ or $|1\rangle$





Qubit

$|1\rangle$

e.g. 1st excited state

α, β are complex-valued!

$$|u\rangle = \alpha|0\rangle + \beta|1\rangle$$

β

Born's rule:
Probability $|\alpha|^2 + |\beta|^2 = 1$

Energy

Atomic energy level

$|0\rangle$ $|1\rangle$

α

$|0\rangle$

e.g. ground state

N qubits

$$|u\rangle \in \mathcal{H}^{\otimes N}$$

$D = 2^N$ dimensional Hilbert space

Pauli operators: $\hat{\sigma}^{\otimes N}$

Ions, spin systems, superconducting qubits…etc

Typical digital quantum simulation: evolution through digital steps

Time evolution through concatenation of large number of gates

Aim to prepare: $|u(t)\rangle = \sum_j u_j(t)|j\rangle = \exp(-i\mathbf{H}t)|u(0)\rangle$

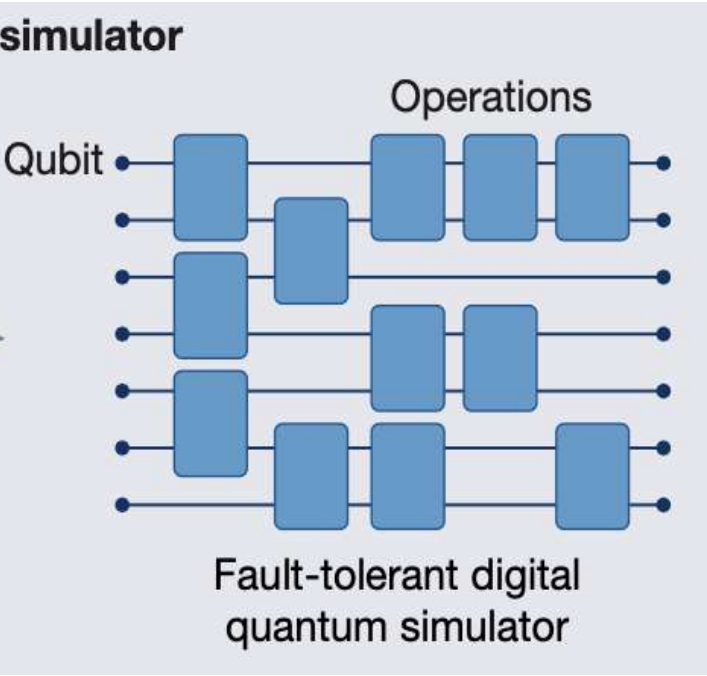
$\mathbf{H}$ Hermitian $D \times D$ matrix

Example: Trotter decomposition

$$\mathbf{H} = \sum_l \mathbf{H}_l$$

$$e^{-i\mathbf{H}t} = \prod_l e^{-i\mathbf{H}_l \Delta t} + O(\Delta t^2)$$

Number of steps $\sim t^2/\epsilon$



Analogue quantum information: operator language

Qumode

(continuous-variable CV)

$$|u\rangle = \int u(x)|x\rangle dx \qquad x \in \mathbb{R}$$

$u(x)$: wavefunction



$$\hat{x}|x\rangle = x|x\rangle \qquad \hat{p}|p\rangle = p|p\rangle$$

$$\int |x\rangle\langle x|dx = \mathbf{1} = \int |p\rangle\langle p|dp$$

$$[\hat{x}, \hat{p}] = i\hbar\mathbf{1}$$

Heisenberg's uncertainty principle

Position and momentum operators don't commute in quantum mechanics

Analogue quantum information: operator language

Qumode

(continuous-variable CV)

$$|u\rangle = \int u(x)|x\rangle dx \qquad x \in \mathbb{R}$$

$u(x)$: wavefunction



$$\langle p|x\rangle = \exp(-ixp)$$

$$\text{Fourier transform: } \mathcal{F}|x\rangle = |p\rangle$$

Important correspondence we will use later:

$$xu(x) \to \hat{x}|u\rangle$$

$$\frac{d}{dx}u(x) \to i\hat{p}|u\rangle$$

Easy to do Fourier transform on optical systems (change of measurement basis)!

Analogue quantum information: operator language

Derivation of correspondence: $xu(x) \rightarrow \hat{x}|u\rangle$

$$\frac{d}{dx}u(x) \rightarrow i\hat{p}|u\rangle$$

The quadrature operators of a qumode are $\hat{x}$ and $\hat{p}$, where $[\hat{x},\hat{p}] = i$. If we let $|x\rangle$ and $|p\rangle$ denote the eigenvectors of $\hat{x}$ and $\hat{p}$ respectively, then $\langle x|p\rangle = \exp(ixp)/\sqrt{2\pi}$. The position and momentum eigenstates each form a complete eigenbasis so $\int dx|x\rangle\langle x| = I = \int dp|p\rangle\langle p|$. Here the quantised momentum operator $\hat{p}$ is also associated with the spatial derivative $\hat{p} \leftrightarrow -i\partial/\partial x$. One can see this easily from the same commutation relation being obeyed $[x, -i\partial/\partial x]u = iu$. Suppose we define the state $|\partial u/\partial x\rangle = \int(\partial u/\partial x)|x\rangle dx$. Then it is straightforward to show $i\hat{p}|u\rangle = |\partial u/\partial x\rangle$. For simplicity, we ignore normalisation constants and it is simple to prove the following. Let $\tilde{u}(p)$ denote the Fourier transform of $u(x)$. Then $i\hat{p}|u\rangle = i\int u(x)\hat{p}|x\rangle dx = i\iint u(x)\hat{p}|p\rangle\langle p|x\rangle dxdp = i\iint u(x)p\exp(-ixp)|p\rangle dxdp = i\int \tilde{u}(p)p|p\rangle dp = i\iint \tilde{u}(p)p|x'\rangle\langle x'|p\rangle dpdx' = i\iint \tilde{u}(p)p\exp(ix'p)|x'\rangle dx'dp = \iint(\partial/\partial x')(\tilde{u}(p)\exp(ix'p))|x'\rangle dx'dp = \int \partial u(x')/\partial x'|x'\rangle dx' = |\partial u/\partial x\rangle$. Similarly $(i\hat{p})^n|u\rangle = |\partial^n u/\partial x^n\rangle$. This simple observation will be important for our simulation of PDEs later.

Analogue quantum information: operator language

Qumode

(continuous-variable CV)

$$|u\rangle = \int u(x)|x\rangle dx \qquad x \in \mathbb{R}$$

$u(x)$: wavefunction



Infinite dimensional Hilbert space

Born's rule

$$\int |u(x)|^2 dx = 1$$

$$N \text{ qumodes: } |u\rangle = \int u(x_1, ..., x_N)|x_1, ..., x_N\rangle dx_1 ... dx_N$$

Lasers, light inside cavities, freely moving atoms…etc

Analogue quantum simulation: evolution in continuous time

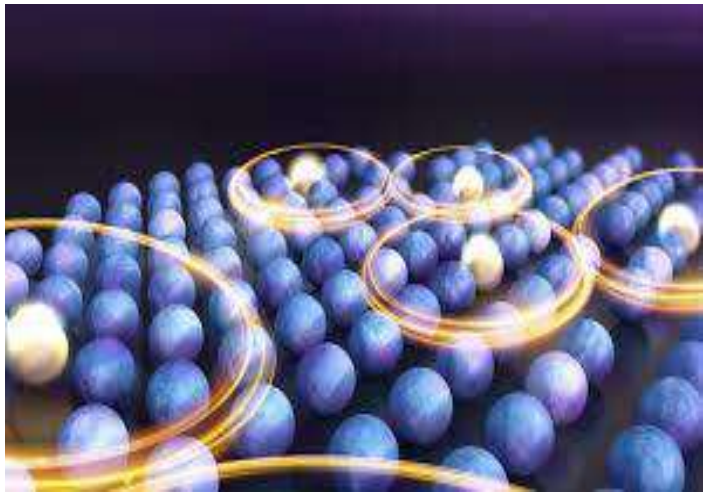
Time evolution through natural dynamics of a quantum system: quantum control of a single Hamiltonian in continuous time

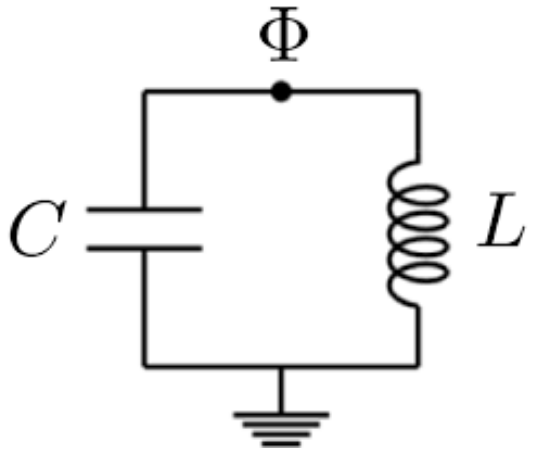
Aim to prepare: $|u(t)\rangle = e^{-iH_{CV}t}|u(0)\rangle$

or $e^{-i\mathbf{H}t}|u(0)\rangle$ without breaking up into many gates

Systems: quantum optomechanics, superconductors, photonics, neutral atoms...etc







Quantum simulation

$$|u(t)\rangle = U(t)|u(0)\rangle$$

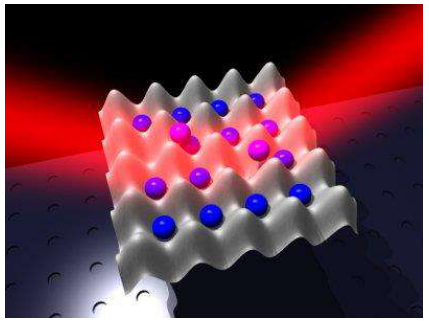
Generating Hamiltonian

$$\mathbf{H}^\dagger = \mathbf{H}$$

$$H_{CV} = H_{CV}^\dagger$$

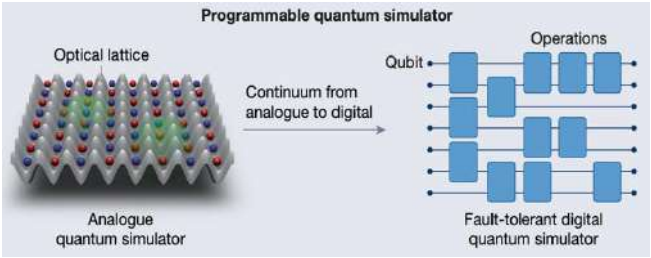
- **Analogue quantum simulation: Nearer-term**

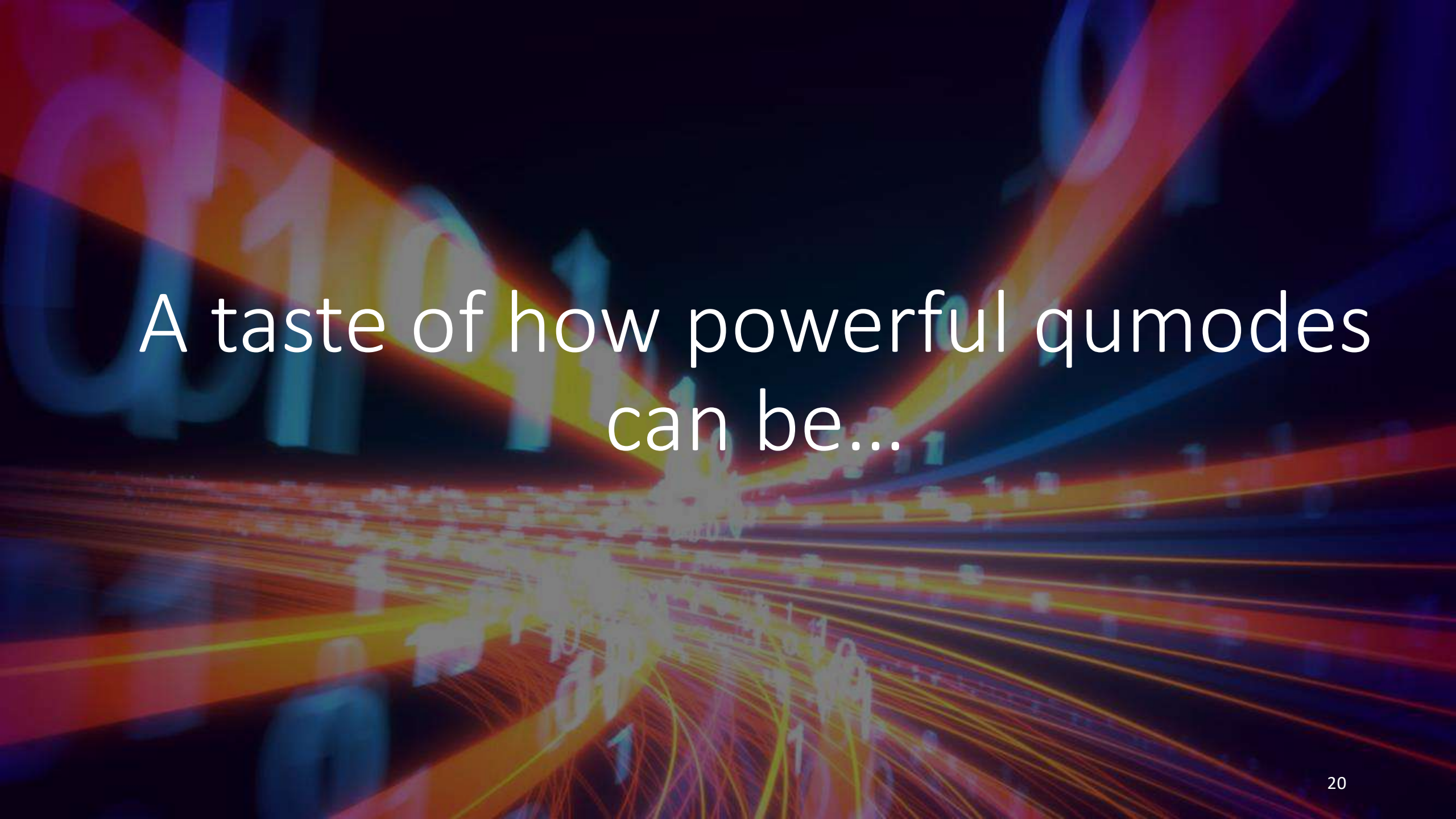
- System evolves naturally *(continuously) in time*
- Can readily scale to large system sizes
- Error limited by accuracy of model used (parameter calibration, noise…etc)
- Continuous spatial degrees of freedom also allowed: analog (or continuous-variable) quantum simulation



- **Digital quantum simulation: Far-term**

- Evolution broken down into elementary gates or easily realisable Hamiltonian evolution
- Error correction and fault tolerance: much larger system sizes required

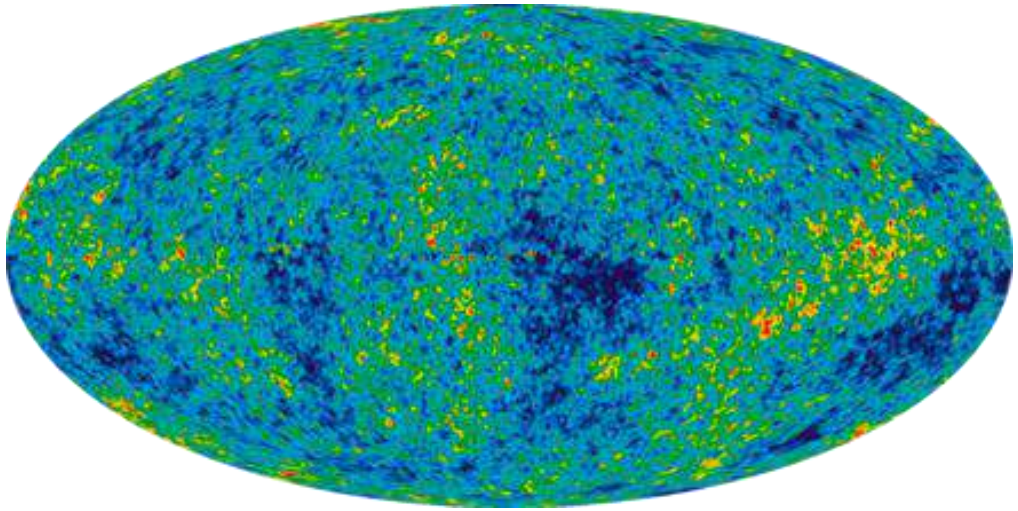



A taste of how powerful qumodes can be…

Shor's algorithm: a quantum algorithm to break RSA requires many perfect qubits…

To factor integer N, run-time for quantum algorithm $\mathcal{O}(\text{poly}\log N)$

Classically to break RSA 2048-bit encryption key would take 3×10^{14} years.
The universe is around 1.4×10^{10} years old.



4099 perfect qubits can break this in 10 seconds

For noisy systems: need 20 million qubits and 8 hours

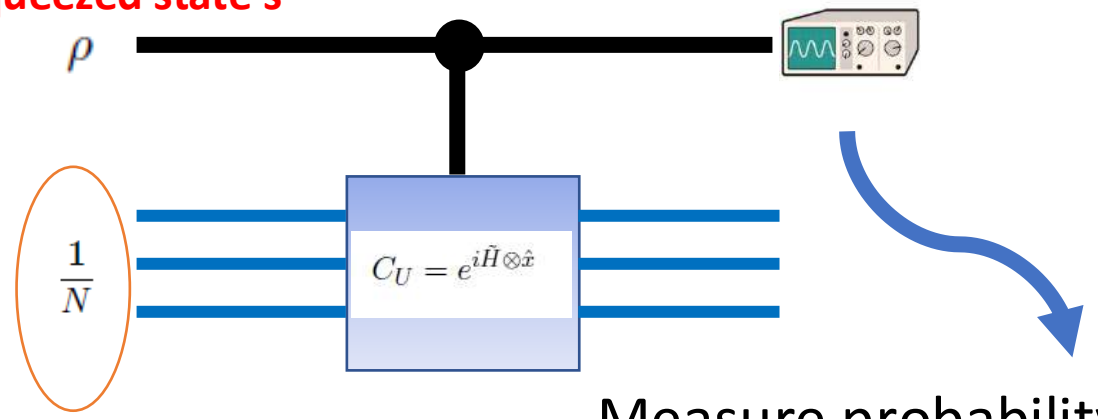
Lots of quantum algorithms based on quantum phase estimation and quantum fourier transforms (crucial part for factoring and other algorithms): https://quantumalgorithmzoo.org/

Factoring can be powered by a *single* clean qumode!

N. Liu et al, `Power of one qumode', PRA, 2016:

Exchanging number of qubits as resource for energy of a qumode

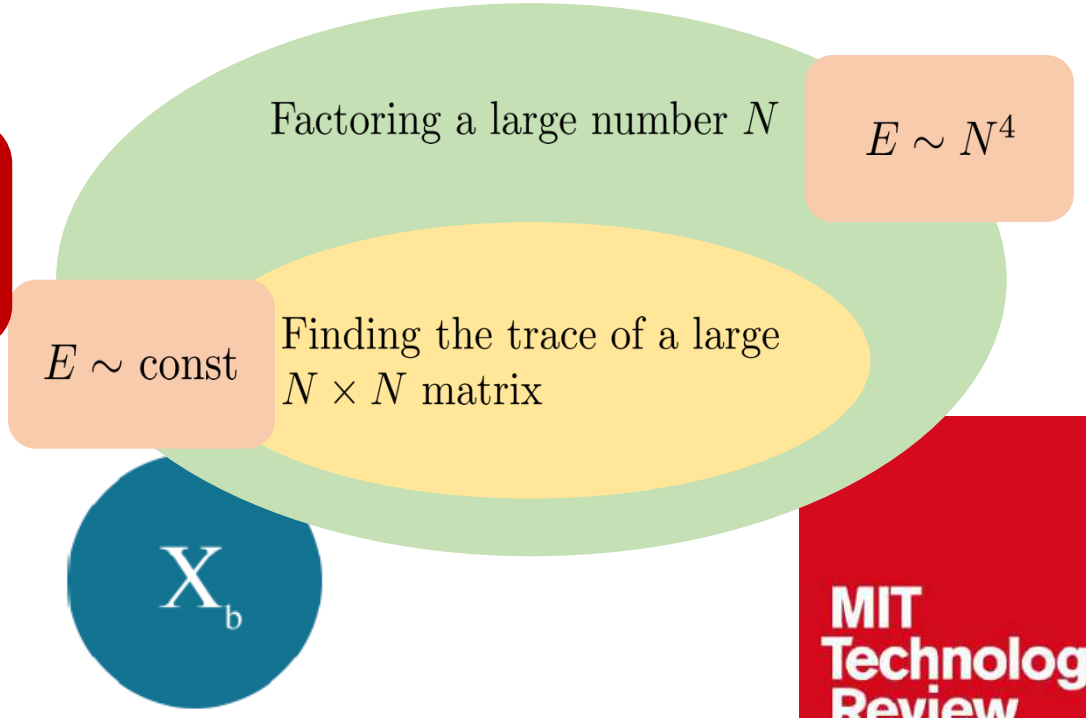
Squeezed state s



Squeezed state input

Measure probability distribution of outcome after running for time $\mathcal{T}$

$$\rho = \frac{1}{\pi^{\frac{1}{4}} s^{\frac{1}{2}}} \int e^{-\frac{x^2}{2s^2}} |x\rangle dx$$



MIT Technology Review

A View from **Emerging Technology from the arXiv**

Squeezed Light and Quantum Clockspeeds

Why do some quantum computations require entanglement while others don't? Squeezed photons may hold the answer, say physicists.

Problems become `simpler' by lifting to a higher dimension!

Extra cost in quantum simulation of extra K dimensions costs only O(K) and not exponential in K.

1. Schrodingerisation: Linear non-Schrodinger's equations become Schrodinger-like equations

(e.g. dissipative equations become conservative equations)

JUST ADD ONE DIMENSION

2. . nonlinear problems become linear

DEPENDS ON PDE

3. Linear uncertain problems with L uncertain variables become deterministic

JUST ADD L DIMENSIONS

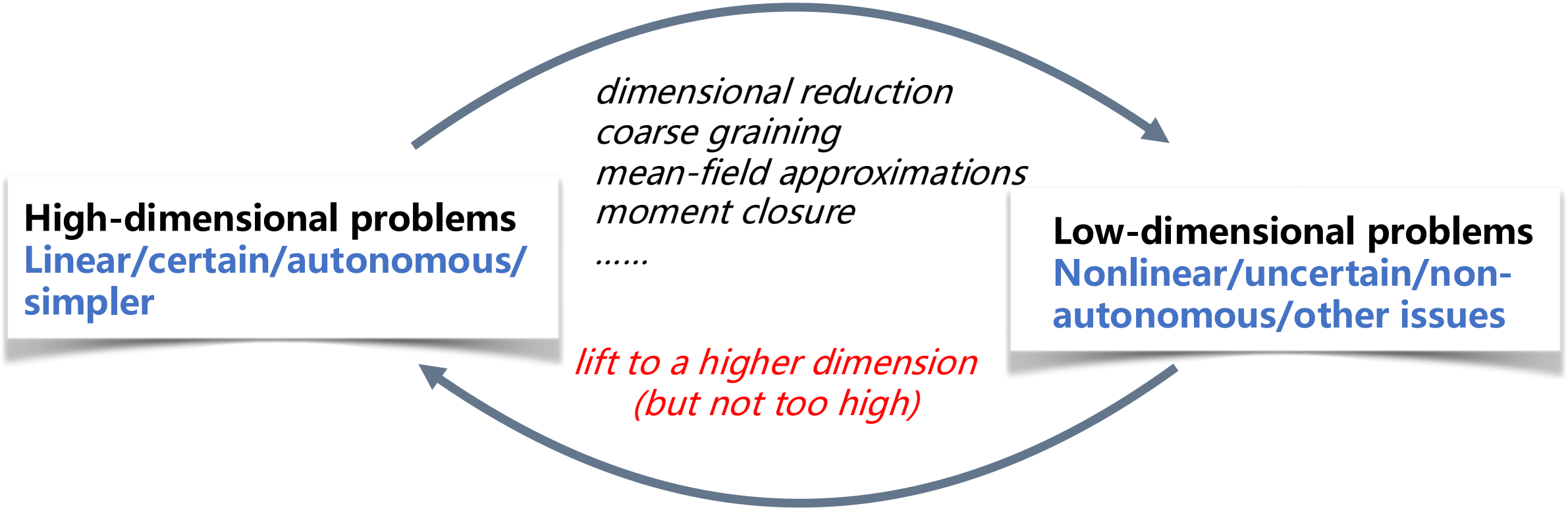
4. Linear non-autonomous systems become linear autonomous

JUST ADD MAX TWO DIMENSIONS

Might be classically more costly…but can potentially be more efficient with quantum simulation!

Our philosophy: problems become simpler by lifting to higher dimension

Classical computation: suffers from curse of dimensionality



Quantum computation: can resolve curse of dimensionality for PDEs

I. Schrodingerisation

``Turning linear non-Schrodinger's equations into Schrodinger's equations"

Based on:

"Quantum simulation of partial differential equations via Schrodingerisation",
Physical Review Letters (arXiv: 2212.13969), Shi Jin, Nana Liu*, Yue Yu
+ technical companion paper Physical Review A (arXiv: 2212.14703), Shi Jin, Nana Liu*, Yue Yu

"Analog quantum simulation of partial differential equations",
Quantum Science and Technology (arXiv: 2308.00646), Shi Jin, Nana Liu*

ODEs and PDEs with multiple M initial conditions: how to map onto equations of Schrodinger's form?

D ODEs

$$\frac{dX^{[k]}(t)}{dt} = F(X^{[k]}(t)), \qquad X^{[k]} \in \mathbb{R}^D$$

$$X^{[k]}(0) = X_0^{[k]}, \qquad k = 1, \cdots, M$$

$(d+1)$-dim PDEs

$$\frac{\partial u^{[k]}}{\partial t} + F(u^{[k]}, \nabla u^{[k]}, \nabla^2 u^{[k]}, ...) = 0$$

$$u^{[k]} \in \mathbb{R}^d \qquad k = 1, ..., M$$

Equations of Schrodinger form –
can use quantum simulation directly when evolution is ***unitary***

D ODEs

$$i\frac{d\mathbf{u}(t)}{dt} = \mathbf{H}\mathbf{u}(t)$$

$\mathbf{H}$ is a $D \times D$ Hermitian matrix

$$|u(t)\rangle = e^{-i\mathbf{H}t}|u(0)\rangle$$

Discrete-variable

Qubits

$(d+1)$-dim PDEs

$$i\frac{\partial u(x,t)}{\partial t} = (-\nabla_x^2 + V(x))u(x,t)$$

$$H_{CV} = \hat{p}^2 + V(\hat{x}) = H_{CV}^\dagger$$

$$\int u(t,x)|x\rangle dx = \exp(-iH_{CV}t)|u(0)\rangle_{CV}$$

Continuous-variable

Qumodes

Classical versus quantum solutions

Classical solutions

$$X^{[k]}(t=T)$$

$$u^{[k]}(t=T, x_1, ..., x_d)$$

Quantum solutions

Amplitude-encoded, typically...

$$\propto \sum_j X_j^{[k]}(t=T)|j\rangle$$

$$\propto \int u^{[k]}(t=T,x)|x\rangle dx$$

$$\propto \sum_{j_1,\cdots,j_d} u^{[k]}(t=T, x_{j_1,\cdots,j_d})|j_1,\cdots,j_d\rangle$$

D+1 qumode quantum evolution solves D-dimensional linear PDE!

	Analogue (A)	**Digital (D)**
Quantum (Q)	PDEs mapped to continuous quantum systems Quantum cost linear in dimension No discretisation necessary	Discretised PDE mapped to qubit dynamics Quantum cost poly in dimension and logarithmic in N
Classical (C)	For PDEs, often need to discretise spatially first into a system of ODEs	For PDEs, can have curse-of-dimensionality

Benefits of analogue quantum simulation for PDEs

- No need to discretise the PDE (derivatives in time, derivatives in space…etc)
- Can potentially utilise existing Hamiltonians without breaking up into many gates, e.g. like in analogue quantum simulation
- Mimicking the history of classical computing…classical computing also evolved from analog to digital before error-correction was well-developed. Today analog is making a comeback in classical computing too
- Touches on foundational questions, more directly, on how one physical system can emulate another
- *Simpler formulation and easier when learning for the first time: good for seeing the structure of the Hamiltonian*

Linear partial differential equations: warm-up example with heat equation

$$\frac{\partial u}{\partial t} = \mathcal{L}u \qquad \text{Linear operator } \mathcal{L}$$

$Examples:$

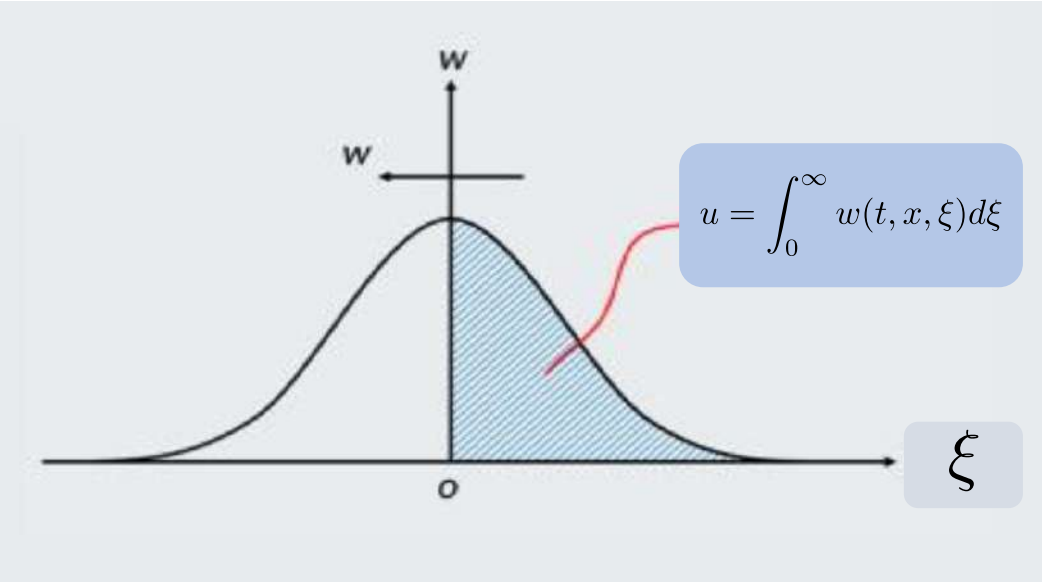
$$\text{Schrodinger: } \mathcal{L} = -i(-\nabla_x^2 + V(x))$$

$$\text{Heat with force term: } \mathcal{L} = -(-\nabla_x^2 + V(x))$$

Schrodingerisation and the warped phase transformation

Increase problem by one dimension ('warped phase space')

Warped phase transformation: $w(t,x,\xi) = e^{-\xi}u(t,x)$ $\xi > 0$



$$\frac{\partial u}{\partial t} = \mathcal{L}u$$

$$\mathcal{L} = -(-\nabla_x^2 + V(x))$$

Recover $u(t,x)$: $u(t,x) = \int_0^\infty w(t,x,\xi)d\xi$

or $u(t,x) = e^{\xi^*}w(t,x,\xi^*)$, $\xi^* > 0$

Heat equation in ‘warped phase space’

$$\frac{\partial w}{\partial t} = (-\nabla_x^2 + V(x))\frac{\partial w}{\partial \xi}$$

$$w(0, x, \xi) = e^{-|\xi|} u(0, x)$$

$$\xi \in (-\infty, \infty)$$

Before we had $w(0, x, \xi) = e^{-\xi} u(0, x)$ for $\xi > 0$. Here w moves from right to left along ξ, so no boundary condition is needed at $\xi = 0$. We can extend the initial data $w(0, x, \xi)$ and w to $\xi < 0$ since the solution does not impact the region $\xi > 0$. This extension to $\xi \in (-\infty, \infty)$ is necessary for the Fourier transform step

Take Fourier transform to make into Schrodinger-like equation

Fourier transform in ξ

$$w(t,x,\xi) = \int e^{-i\xi\eta}\tilde{w}(t,x,\eta)d\eta$$

$$i\frac{\partial \tilde{w}}{\partial t} = \eta(-\nabla_x^2 + V(x))\tilde{w}$$

$$\tilde{w}(0,x,\eta) = 1/(\pi(1+\eta^2))u(0,x)$$

Schrodinger's equations for each Fourier mode η: $t \to \eta t$

Schrodingerisation in continuous-variable implementation

$$i\frac{\partial \tilde{w}}{\partial t} = \eta(-\nabla_x^2 + V(x))\tilde{w}$$
$$\tilde{w}(0,x,\eta) = 1/(\pi(1+\eta^2))u(0,x)$$

$$x \to \hat{x}$$
$$\eta \to \hat{\eta}$$
$$\frac{\partial}{\partial x} \to i\hat{p}$$

$$|\tilde{w}(t)\rangle \propto \iint \tilde{w}(t,x,\eta)|x\rangle|\eta\rangle dx d\eta \propto \exp(-iH_{CV}t)|\tilde{w}(0)\rangle$$

Example: $H_{CV} = (\hat{p}^2 + V(\hat{x})) \otimes \hat{\eta}$

$\hat{\eta}$ can act like any quadrature, e.g. $\hat{\eta} = \hat{x}$

Recovering the state u

Recover $u(t,x)$: $$u(t,x) = \int_0^\infty w(t,x,\xi)d\xi$$

$$\text{or } u(t,x) = e^{\xi^*} w(t,x,\xi^*), \qquad \xi^* > 0$$

Inverse quantum Fourier transform $|\tilde{w}(t)\rangle \to |w(t)\rangle \propto \int\int w(t,x,\xi)|x\rangle|\xi\rangle d\xi$

Recover $|u(t)\rangle \propto \int u(t,x)|x\rangle dx$:

Projective measurement onto $|w(t)\rangle$ using either $P = \int_0^\infty |\xi\rangle\langle\xi| d\xi$
or $P = |\xi^* > 0\rangle\langle\xi^* > 0|$

Probability of success $\propto \|\mathbf{u}(t)\|^2 / \|\mathbf{u}(0)\|^2$
Algorithm has an in-built way to compute normalisation constant!

General methodology

Linear homogeneous PDE

K^{th}-order derivatives, D spatial dimensions

$$\frac{\partial u}{\partial t} + \sum_{k=1}^{K} \sum_{j=1}^{D} a_{k,j}(x_1, ..., x_D) \frac{\partial^k u}{\partial x_j^k} + b(x_1, ..., x_D) u = 0$$

$$a_{k,j} < 0 \text{ for } k \text{ even}$$

$$\mathbf{u}(t) \equiv \int u(t, x) |x\rangle dx$$

$$\frac{d\boldsymbol{u}}{dt} = -i\boldsymbol{A}(\hat{x}_1, ..., \hat{x}_D, \hat{p}_1, ..., \hat{p}_D)\boldsymbol{u}, \qquad \boldsymbol{u}(0)$$

$$\mathbf{A} = \sum_{k=1}^{K} \sum_{j=1}^{D} a_{k,j}(\hat{x}_1, ..., \hat{x}_D) i^{k+3} \hat{p}_j^k - ib(\hat{x}_1, ..., \hat{x}_D)$$

$\mathbf{A}$ can also have explicit time-dependence

$$x_i \rightarrow \hat{x}_i$$

$$\frac{\partial^k}{\partial x_j^k} \rightarrow (i\hat{p}_j)^k$$

General methodology

$$\frac{d\boldsymbol{u}}{dt} = -i\boldsymbol{A}(\hat{x}_1, ..., \hat{x}_D, \hat{p}_1, ..., \hat{p}_D)\boldsymbol{u}, \qquad \boldsymbol{u}(0)$$

$$\boldsymbol{A} = \boldsymbol{A}_1 - i\boldsymbol{A}_2, \qquad \boldsymbol{A}_1 = (\boldsymbol{A} + \boldsymbol{A}^\dagger)/2 = \boldsymbol{A}_1^\dagger, \qquad \boldsymbol{A}_2 = i(\boldsymbol{A} - \boldsymbol{A}^\dagger)/2 = \boldsymbol{A}_2^\dagger$$

Hermitian part of $\mathbf{A}$: Schrödinger-like equation
Anti-Hermitian part of $\mathbf{A}$: heat-like equation

Original system stable if $\mathbf{A}_2 > 0$

General methodology

$$\frac{d\boldsymbol{u}}{dt} = -i\boldsymbol{A}(\hat{x}_1, ..., \hat{x}_D, \hat{p}_1, ..., \hat{p}_D)\boldsymbol{u}, \qquad \boldsymbol{u}(0)$$

$$\boldsymbol{A} = \boldsymbol{A}_1 - i\boldsymbol{A}_2, \qquad \boldsymbol{A}_1 = (\boldsymbol{A} + \boldsymbol{A}^\dagger)/2 = \boldsymbol{A}_1^\dagger, \qquad \boldsymbol{A}_2 = i(\boldsymbol{A} - \boldsymbol{A}^\dagger)/2 = \boldsymbol{A}_2^\dagger$$

$$\tilde{\mathbf{v}}(t) \equiv \iint \tilde{w}(t, x, \eta)|x\rangle|\eta\rangle dx d\eta$$

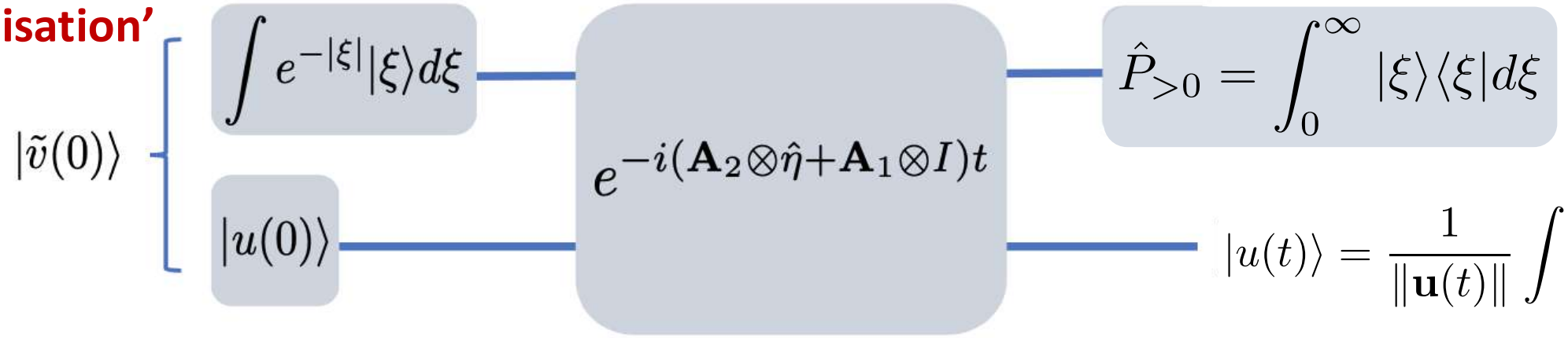
$$\frac{d\tilde{\boldsymbol{v}}(t)}{dt} = -i(\boldsymbol{A}_2 \otimes \hat{\eta} + \boldsymbol{A}_1 \otimes I)\tilde{\boldsymbol{v}}(t) = -i\boldsymbol{H}\tilde{\boldsymbol{v}}(t), \qquad \boldsymbol{H} = \boldsymbol{A}_2 \otimes \hat{\eta} + \boldsymbol{A}_1 \otimes I = \boldsymbol{H}^\dagger,$$

$$\tilde{\boldsymbol{v}}(0) = \int \frac{2}{1+\eta^2}|\eta\rangle d\eta \boldsymbol{u}(0) = \int e^{-|\xi|}|\xi\rangle d\xi \boldsymbol{u}(0) = |\Xi\rangle \boldsymbol{u}(0), \qquad |\Xi\rangle = \int e^{-|\xi|}|\xi\rangle d\xi.$$

Implementation scheme

Just add one qumode:

`Qumodisation'



Initial ancilla state preparation

$$|\Xi\rangle = \int e^{-|\xi|}|\xi\rangle d\xi \qquad |G\rangle = \frac{1}{\sqrt{s}\pi^{1/4}}\int e^{-\xi^2/2s^2}|\xi\rangle d\xi$$

Close to Gaussian state $\quad |\langle\Xi|G\rangle| \approx 0.986, s \approx 0.925$

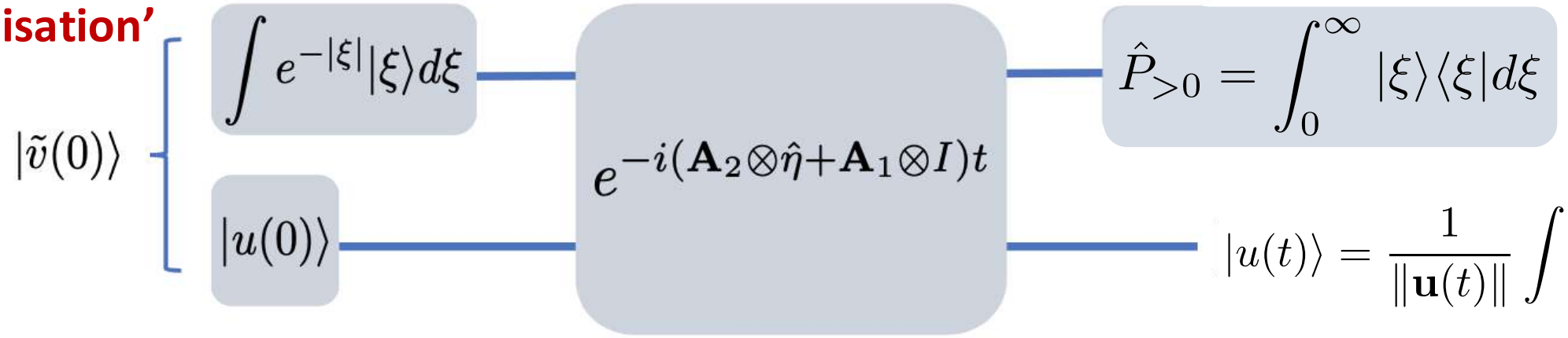
Probability $\frac{\|\mathbf{u}(t)\|^2}{2\|\mathbf{u}(0)\|^2}$

$D+1$ qumodes

Implementation scheme

Just add one qumode:

`Qumodisation'



Probability $\frac{\|\mathbf{u}(t)\|^2}{2\|\mathbf{u}(0)\|^2}$

Initial state preparation

$|u(0)\rangle \propto \int u(0,x)|x\rangle dx$ can in principle be prepared for any boundary condition in x and $t = 0$ so long as $u(0,x)$ is ' smooth' and $\lim_{x\to\infty} u(0,x) \to 0$ and $\|\mathbf{u}(0)\| < \infty$

$D + 1$ qumodes

Linear PDE $\frac{\partial u}{\partial t} = \sum_k A_k \left(x, \frac{\partial^k}{\partial x^k}\right) u$

$$\mathbf{A} = \mathbf{A}_1 - i\mathbf{A}_2$$

$$\mathbf{A}_1 = (1/2)(\mathbf{A} + \mathbf{A}^\dagger)$$

$$\mathbf{A}_2 = (i/2)(\mathbf{A} - \mathbf{A}^\dagger)$$

Embed into qumodes

$$u \to \mathbf{u} \equiv \int u(t,x)|x\rangle dx$$

$$x \to \hat{x}$$

$$\frac{\partial^k}{\partial x^k} \to (i\hat{p})^k$$

$$\sum_k A_k \to -i\mathbf{A}$$

$$\frac{d\mathbf{u}}{dt} = -i\mathbf{A}\mathbf{u}$$

Initial condition $\mathbf{u}(0)$

Schrödingerisation

$$\frac{d\tilde{\mathbf{v}}}{dt} = -i\mathbf{H}\tilde{\mathbf{v}}$$

Initial condition

$$\tilde{\mathbf{v}}(0) = \int e^{-|\xi|}|\xi\rangle d\xi \mathbf{u}(0)$$

$$\mathbf{H} = \mathbf{A}_2 \otimes \hat{\eta} + \mathbf{A}_1 \otimes I = \mathbf{H}^\dagger$$

Also applicable to time-dependent (non-autonomous) systems

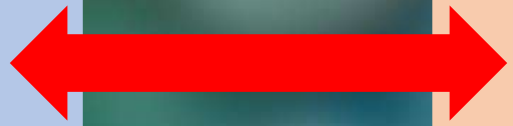
Schrodingerisation formulation:
any linear PDE becomes a Schrodinger-like equation in *one* higher dimension in a very simple way

Any linear system of ODEs or PDE

$$\frac{d\mathbf{u}(t)}{dt} = -\mathbf{A}(t)\mathbf{u}(t)$$

$$\mathbf{A}_1 = (1/2)(\mathbf{A} + \mathbf{A}^\dagger) = \mathbf{A}_1^\dagger$$

$$\mathbf{A}_2 = (i/2)(\mathbf{A} - \mathbf{A}^\dagger) = \mathbf{A}_2^\dagger$$



Simulated on quantum device:

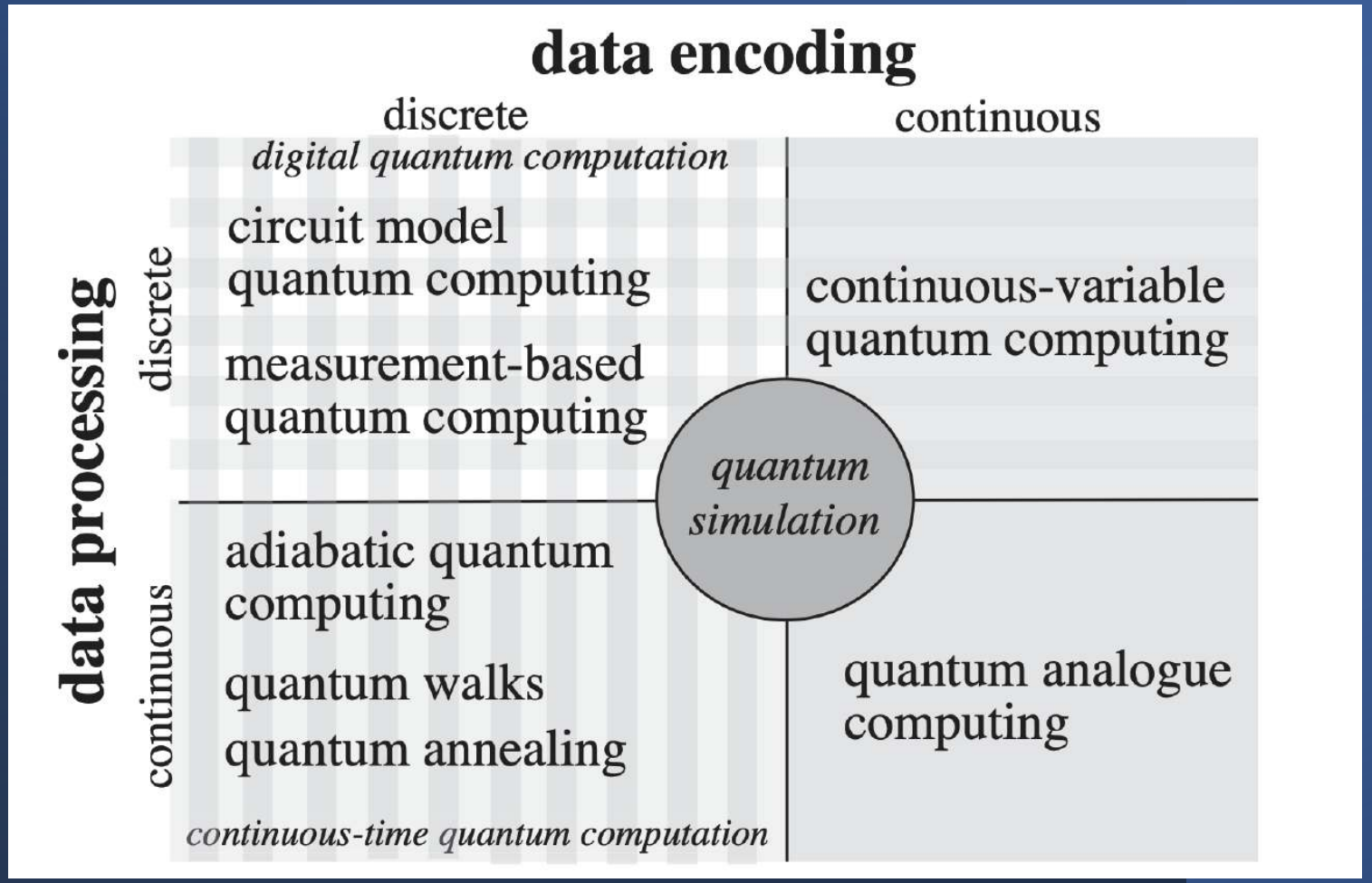
$$\mathbf{H}(t) = \mathbf{A}_2(t) \otimes \hat{\eta} + \mathbf{A}_1(t) \otimes \mathbf{1}$$

$$\mathbf{H}(t) = \mathbf{H}(t)^\dagger$$

$$\hat{\eta} \to \mathrm{diag}(-M/2, \cdots, M/2 - 1)$$

We provide *a simple recipe*: Given any linear system of ODEs or PDE we find the corresponding quantum system; and given any quantum system, can find corresponding linear ODE/PFE

Schrodingerisation is easily applicable to not only the four main classes of quantum devices, but also hybrid qubit-qumode devices



Examples of scalar homogeneous PDEs

Simplest example

D-dimensional convection equation

$$\frac{\partial u}{\partial t} - \sum_{j=1}^{D} a_j \frac{\partial u}{\partial x_j} = 0, \qquad u(0,x) = u_0(x), \qquad x_j \in \mathbb{R}^D, \qquad a_j \in \mathbb{R}$$

Only displacement required

$$\frac{d\boldsymbol{u}}{dt} = -i\mathbf{H}\boldsymbol{u}, \qquad \mathbf{H} = \sum_{j=1}^{D} \mathbf{H}_j, \qquad \mathbf{H}_j = a_j \hat{p}_j, \qquad \boldsymbol{H}_j = \boldsymbol{H}_j^{\dagger}$$

D qumodes

In general, simulation of PDEs require entangling operations and will go beyond Gaussian operations

Simplest example

Analog photonic simulator for large-scale transport

Mengyu Zhao,[1,*] Xuezhi Zhu,[1,*] Nikita Guseynov,[2,*] Yewei Yuan,[2,*] Na Wang,[1] Meihong Wang,[1,3] Yunyun Cao,[1] Shi Jin,[4,5] Nana Liu,[2,4,5,†] Changde Xie,[1] Kunchi Peng,[1] and Xiaolong Su[1,3,‡]

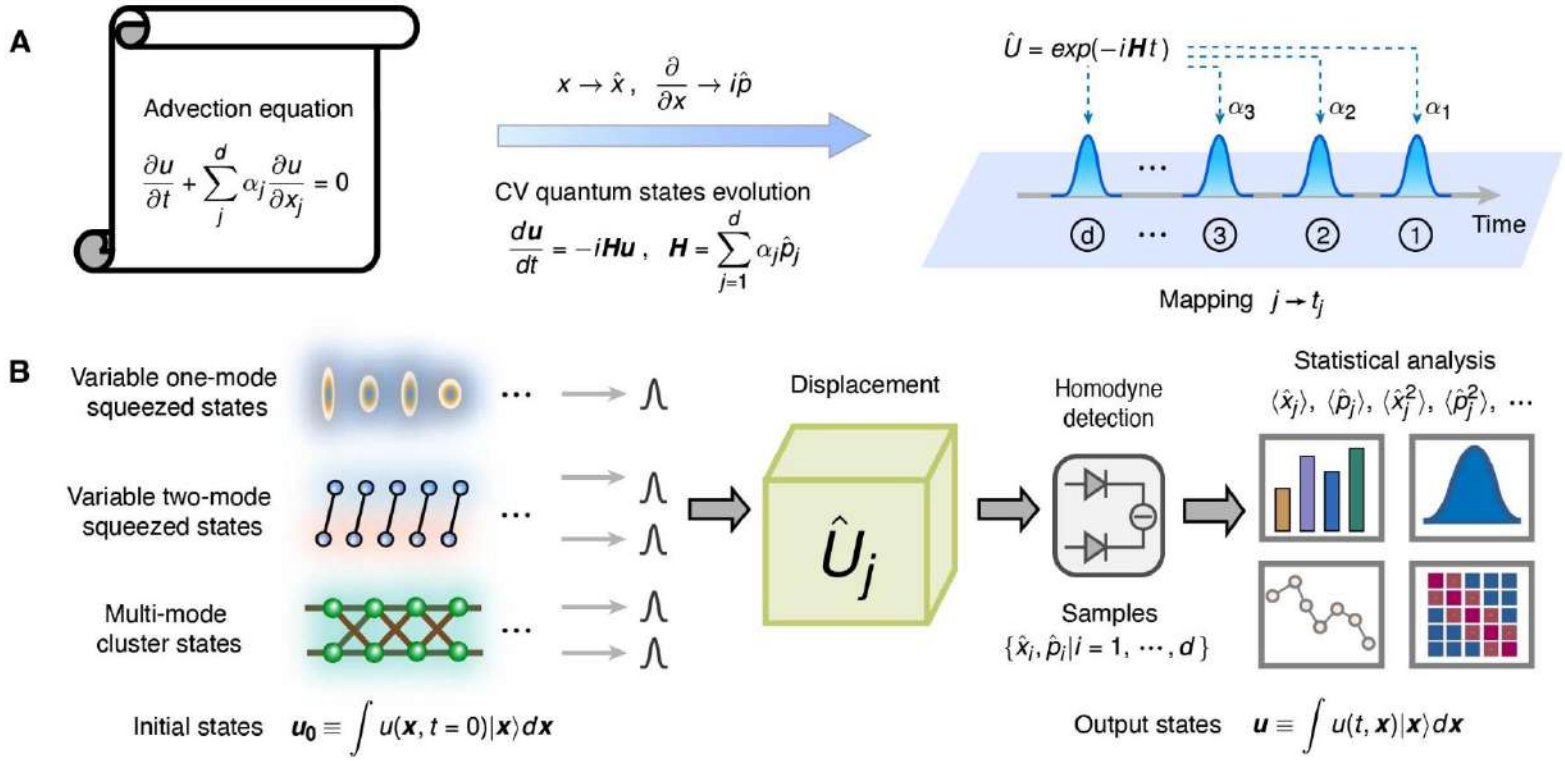
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arXiv: 2606.00581

Simplest example

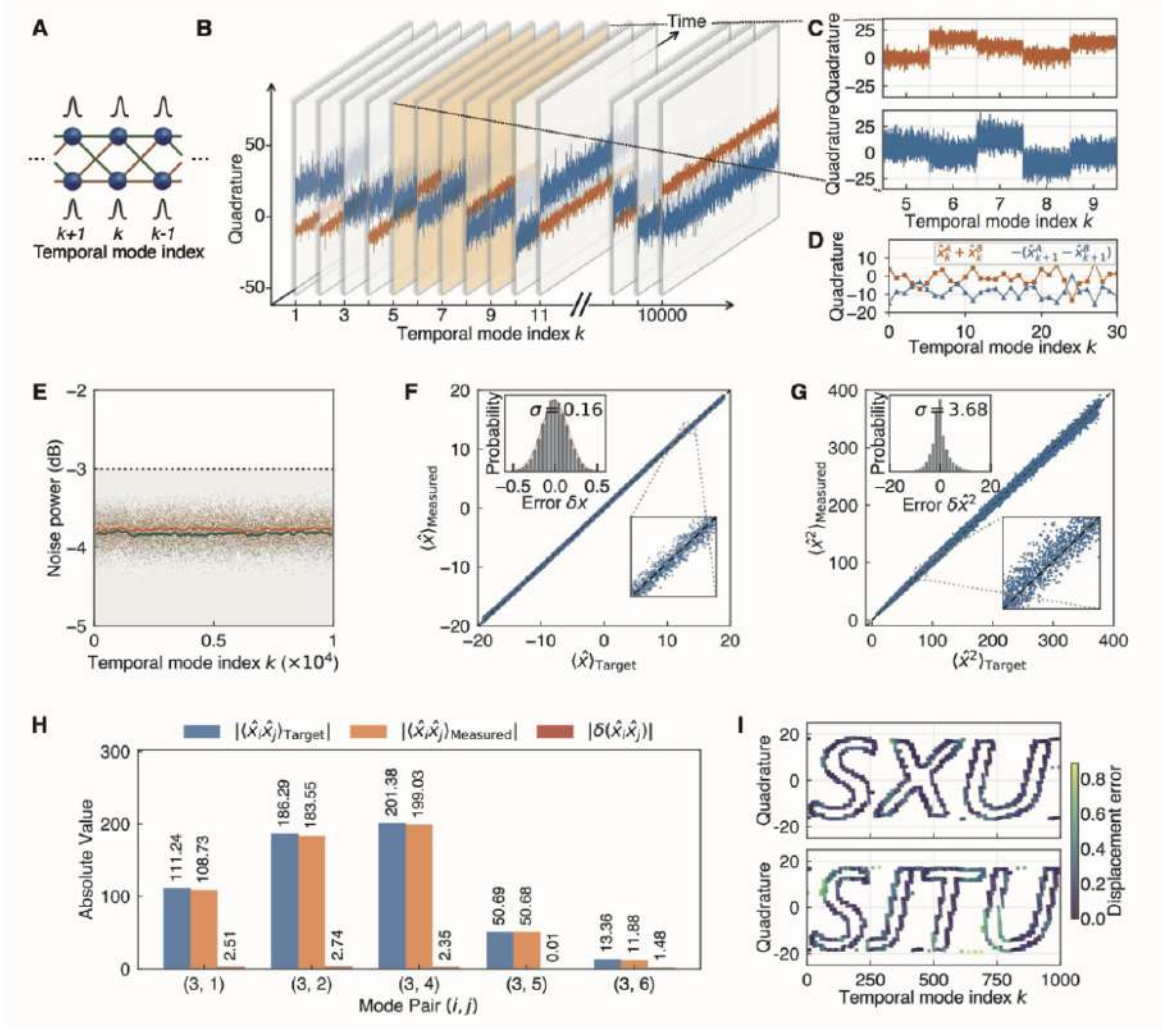


Figure 4: **Results of the analog photonic simulation with CV cluster state.** (A) Graphical representation of the CV cluster state. (B) The quadrature output after displacement crosses 10,000 temporal modes. The green and orange lines correspond to the amplitude quadrature of the two rails. (C) Amplitude quadrature values measured by BHD A and B over five consecutive temporal modes. (D) Amplitude quadrature combination evolution within one time bin. (E) $\langle(\hat{x}_k^A + \hat{x}_k^B + \hat{x}_{k+1}^A - \hat{x}_{k+1}^B)^2\rangle$ before and after displacement. The green and orange scatter points represent the experimental data before and after displacement, respectively. Solid lines represent the corresponding moving averages. (F) Displacement error of first-moment $\langle\hat{x}_j\rangle$ across 20,000 uniformly random displacements. The experimental data (blue scatter points) agree well with the target (black dashed line). The lower right inset provides a magnified view. The upper left insert displays the probability distribution of the displacement error δx—defined as the difference between the target displacement and the measured displacement, which presents the standard deviation error of $\sigma \approx 0.16$. (G) Displacement error of second-moment $\langle\hat{x}_j^2\rangle$ across 20,000. (H) Correlations $\langle\hat{x}_i\hat{x}_j\rangle$ and absolute errors $|\delta\langle\hat{x}_i\hat{x}_j\rangle|$ for representative mode pairs involving $i = 3$. (I) Amplitude quadrature values

Example for physical platform

Quantum optomechanical system

$$\mathbf{H} \supset \Delta(\hat{x}^2 + \hat{p}^2) \otimes I + g_1 \hat{x} \otimes \hat{x} + g_2(\hat{p} \otimes I)$$

$$\frac{\partial u}{\partial t} = i\frac{\partial^2 u}{\partial x^2} + g_2\frac{\partial u}{\partial x} - (g_1 x + i\Delta x^2)u$$

Complex potential and convection term

Linear first-order PDEs

$$\frac{\partial u}{\partial t} + \sum_{j=1}^{D} a_j(x_1, ..., x_D)\frac{\partial u}{\partial x_j} + b(x_1, ..., x_D)u = 0, \qquad a_j \in \mathbb{R}, b \in \mathbb{C}.$$

$$\frac{d\boldsymbol{u}}{dt} = -i\boldsymbol{A}\boldsymbol{u}, \qquad \boldsymbol{A} = \sum_{j=1}^{D} a_j(\hat{x}_1, ..., \hat{x}_D)\hat{p}_j - ib(\hat{x}_1, ..., \hat{x}_D), \qquad \boldsymbol{A} = \boldsymbol{A}_1 - i\boldsymbol{A}_2$$

$$\frac{d\tilde{\boldsymbol{v}}}{dt} = -i\boldsymbol{H}\tilde{\boldsymbol{v}}, \qquad \boldsymbol{H} = \boldsymbol{A}_2 \otimes \hat{\eta} + \boldsymbol{A}_1 \otimes I = \boldsymbol{H}^{\dagger}$$

$$\mathbf{A}_1 = \frac{1}{2}\sum_{j=1}^{D}\{\hat{p}_j, a_j\} + \frac{i}{2}(b^* - b)$$

$$\mathbf{A}_2 = \frac{i}{2}\sum_{j=1}^{D}[\hat{p}_j, a_j] + \frac{1}{2}(b^* + b)$$

Gaussian operations $D + 1$ qumodes

$\hat{\Theta} \equiv (1/2)\sum_{jk}\alpha_{jk}(\hat{x}_j\hat{p}_k + \hat{p}_k\hat{x}_j) \bar{\otimes} I$

	$a_j = \text{constant}$	$a_j = \sum_{k=1}^{D}\alpha_{jk}x_k$
$b = \text{constant}$	$\text{Re}(b)I \otimes \hat{\eta} + \sum_j a_j\hat{p}_j \otimes I$	$\hat{\Theta}$
$b = \sum_{j=1}^{D}\beta_j x_j$	$\sum_j \text{Re}(\beta_j)\hat{x}_j \otimes \hat{\eta}$	$\sum_j \text{Re}(\beta_j)\hat{x}_j \otimes \hat{\eta} + \hat{\Theta}$
$b = \sum_{j,k=1}^{D}\gamma_{jk}x_j x_k$	$\sum_{j,k}\text{Re}(\gamma_{jk})\hat{x}_j\hat{x}_k \otimes \hat{\eta} - \sum_{jk}\text{Im}(\gamma_{jk})\hat{x}_j\hat{x}_k \otimes I$	$\sum_{jk}\text{Re}(\gamma_{jk})\hat{x}_k\hat{p}_j \otimes \hat{\eta} - \sum_{jk}\text{Im}(\gamma_{jk})\hat{x}_j\hat{x}_k \otimes I + \hat{\Theta}$

Liouville equation

$$\frac{\partial u}{\partial t} + \sum_{j=1}^{D} a_j(x_1, ..., x_D) \frac{\partial u}{\partial x_j} = 0$$

$$\frac{d\boldsymbol{u}}{dt} = -i\boldsymbol{A}\boldsymbol{u}, \qquad \boldsymbol{A} = \sum_{j=1}^{D} a_j(\hat{x}_1, ..., \hat{x}_D)\hat{p}_j \qquad \boldsymbol{A} = \boldsymbol{A}_1 - i\boldsymbol{A}_2$$

$$\frac{d\tilde{\boldsymbol{v}}}{dt} = -i\boldsymbol{H}\tilde{\boldsymbol{v}}, \qquad \boldsymbol{H} = \boldsymbol{A}_2 \otimes \hat{\eta} + \boldsymbol{A}_1 \otimes I = \boldsymbol{H}^{\dagger}$$

$$\mathbf{A}_1 = \tfrac{1}{2} \sum_{j=1}^{D} \{a_j, \hat{p}_j\}$$
$$\mathbf{A}_2 = \tfrac{i}{2} \sum_{j=1}^{D} [\hat{p}_j, a_j]$$

Example: $a_j(x_1, ..., x_D) = a_j \hat{x}_j,\ a_j \in \mathbb{R}$

$$\mathbf{A}_1 = \tfrac{1}{2} \sum_{j=1}^{D} a_j (\hat{x}_j \hat{p}_j + \hat{p}_j \hat{x}_j)$$

$$\mathbf{A}_2 = \sum_{j=1}^{D} a_j I$$

$D + 1$ qumodes

Black-Scholes equation

$$\frac{\partial u}{\partial t} + \frac{1}{2}\sigma^2 x^2 \frac{\partial^2}{\partial x^2} + rx\frac{\partial u}{\partial x} - ru = 0$$

$$\frac{d\boldsymbol{u}}{dt} = -i\boldsymbol{A}\boldsymbol{u}, \qquad \boldsymbol{A} = \frac{1}{2}\sigma^2\hat{x}^2\hat{p}^2 + ir\hat{x}\hat{p} + rI$$

$$\frac{d\tilde{\boldsymbol{v}}}{dt} = -i\boldsymbol{H}\tilde{\boldsymbol{v}}, \qquad \boldsymbol{H} = \boldsymbol{A}_2 \otimes \hat{\eta} + \boldsymbol{A}_1 \otimes I = \boldsymbol{H}^\dagger$$

$$\boldsymbol{A}_1 = -\left(\sigma^2 + \frac{r}{2}\right)(\hat{x}\hat{p} + \hat{p}\hat{x}), \qquad \boldsymbol{A}_2 = \frac{1}{4}\sigma^2(\hat{x}^2\hat{p}^2 + \hat{p}^2\hat{x}^2) - \frac{r}{2}I$$

2 qumodes

Heat equation

$$\frac{\partial u}{\partial t} + \sum_{i=1}^{D} \frac{\partial}{\partial x_i} \left(\sum_{j=1}^{D} D_{ij}(x_1, ..., x_D) \frac{\partial u}{\partial x_j} \right) = 0$$

$$D_{ij} < 0$$

$$D_{ij} = D_{ji}$$

$$\frac{d\boldsymbol{u}}{dt} = -i\boldsymbol{A}\boldsymbol{u}, \qquad \boldsymbol{A} = i \sum_{i,j=1} \hat{p}_i D_{ij}(\hat{x}_1, ..., \hat{x}_D) \hat{p}_j$$

$$\frac{d\tilde{\boldsymbol{v}}}{dt} = -i\boldsymbol{H}\tilde{\boldsymbol{v}}, \qquad \boldsymbol{H} = \boldsymbol{A}_2 \otimes \hat{\eta} + \boldsymbol{A}_1 \otimes I = \boldsymbol{H}^\dagger$$

$$\boldsymbol{A}_1 = 0$$

$$\boldsymbol{A}_2 = \sum_{i,j=1}^{D} \hat{p}_i D_{ij}(\hat{x}_1, ..., \hat{x}_D) \hat{p}_j + V(\hat{x}_1, ..., \hat{x}_D)$$

$D + 1$ qumodes

Fokker-Planck equation

$$\frac{\partial u}{\partial t} + \sum_{j=1}^{D} \frac{\partial}{\partial x_j}(\mu_j(x_1, ..., x_D)u) - \sum_{j=1}^{D} \frac{\partial^2}{\partial x_j^2}(D_j(x_1, ..., x_D)u) = 0,$$

$$D_j > 0$$

$$\frac{d\boldsymbol{u}}{dt} = -i\boldsymbol{A}\boldsymbol{u}, \qquad \boldsymbol{A} = \sum_{j=1}^{D} \hat{p}_j \mu_j(\hat{x}_1, ..., \hat{x}_D) - i \sum_{j=1}^{D} \hat{p}_j^2 D_j(\hat{x}_1, ..., \hat{x}_D).$$

$$\frac{d\tilde{\boldsymbol{v}}}{dt} = -i\boldsymbol{H}\tilde{\boldsymbol{v}}, \qquad \boldsymbol{H} = \boldsymbol{A}_2 \otimes \hat{\eta} + \boldsymbol{A}_1 \otimes I = \boldsymbol{H}^\dagger$$

$$\boldsymbol{A}_1 = \frac{1}{2} \sum_{j=1}^{D} \{\hat{p}_j, \mu_j(\hat{x}_1, ..., \hat{x}_D)\} - \frac{i}{2} \sum_{j=1}^{D} [\hat{p}_j^2, D_j(\hat{x}_1, ..., \hat{x}_D)]$$

$$\boldsymbol{A}_2 = \frac{i}{2} \sum_{j=1}^{D} [\mu_j(\hat{x}_1, ..., \hat{x}_D), \hat{p}_j] - \frac{1}{2} \sum_{j=1}^{D} \{\hat{p}_j^2, D_j(\hat{x}_1, ..., \hat{x}_D)\}$$

Example: linear drift and additive noise

$\mu_j = c_j \hat{x}_j$, $c_j \in \mathbb{R}$, $D_j = a_j \in \mathbb{R}^+$

$$\boldsymbol{H} = \frac{1}{2} \sum_{j=1}^{D} \left(c_j I - a\hat{p}_j^2\right) \otimes \hat{\eta} + \frac{1}{2} \sum_{j=1}^{D} c_j (\hat{x}_j \hat{p}_j + \hat{p}_j \hat{x}_j) \otimes I.$$

$D + 1$ qumodes

D+1 qumode quantum evolution solves D-dimensional linear PDE!

	Analogue (A)	**Digital (D)**
Quantum (Q)	PDEs mapped to continuous quantum systems Quantum cost linear in dimension No discretisation necessary	Discretised PDE mapped to qubit dynamics Quantum cost poly in dimension and logarithmic in N
Classical (C)	For PDEs, often need to discretise spatially first into a system of ODEs	For PDEs, can have curse-of-dimensionality

Systems of linear PDEs

Systems of linear PDEs

There are at least five different reasons to consider systems of linear PDEs and this requires either hybrid qumode-qubit systems or qubit-based systems:

- **The application itself naturally** has multiple variables obeying a coupled PDE
- **A scalar PDE solution can be approximated by a system of PDEs** which can be more experimentally accessible (using analogue quantum simulation)
- **Higher-order time derivatives**
- **Inhomogeneous PDEs** which can arise either

- naturally from source terms or
- through boundary conditions (in qubit-based formalism)

Example: Hyperbolic heat equation approach

The one-dimensional heat equation for $\tilde{u}(t,x)$ is a second-order PDE

$$\frac{\partial \tilde{u}}{\partial t} = k\frac{\partial^2 \tilde{u}}{\partial x^2}, \qquad x \in \mathbb{R}, \qquad k > 0,$$

Hyperbolic heat equation

Goldstein-Taylor

$$\frac{\partial u}{\partial t} = -\frac{1}{\epsilon}\frac{\partial v}{\partial x}$$
$$\frac{\partial v}{\partial t} = -\frac{1}{\epsilon}\frac{\partial u}{\partial x} - \frac{1}{k\epsilon^2}v, \qquad 0 < \epsilon \ll 1$$

Hyperbolic heat equation solution approximates heat equation solution

Lemma 1. *Let $u(x,t)$ be the solution of Eqs. (11) and (12) with given initial conditions $u(0,x)$, and arbitrary initial data $v(0,x)$ (e.g. one can choose $v(0,x)=0$ without losing generality). Let $\tilde{u}(t,x)$ be the solution of the heat equation $\partial\tilde{u}(t,x)/\partial t = k\partial^2\tilde{u}(t,x)/\partial x^2$ with initial condition $\tilde{u}(0,x) = u(0,x)$. Then $\|\tilde{u}(t,x) - u(t,x)\| \leq O(e^{-2kt}\epsilon^2)$ for $t >> O(\epsilon^2 \ln(1/\epsilon))$.*

$$\frac{\partial u}{\partial t} = -\frac{1}{\epsilon}\frac{\partial v}{\partial x} \tag{11}$$

$$\frac{\partial v}{\partial t} = -\frac{1}{\epsilon}\frac{\partial u}{\partial x} - \frac{1}{k\epsilon^2}v, \qquad 0 < \epsilon \ll 1 \tag{12}$$

Quantum simulation of hyperbolic heat equation

Define the infinite-dimensional vectors and their corresponding quantum states:

$$\boldsymbol{u}(t) = \int u(t,x)|x\rangle dx, \qquad \boldsymbol{v}(t) = \int v(t,x)|x\rangle dx$$

$$\boldsymbol{w}(t) = \begin{pmatrix} \boldsymbol{u}(t) \\ \boldsymbol{v}(t) \end{pmatrix} = |0\rangle \otimes \boldsymbol{u}(t) + |1\rangle \otimes \boldsymbol{v}(t) \qquad w(t,x) = (u(t,x), v(t,x))^T$$

$$|u(t)\rangle = \frac{\boldsymbol{u}(t)}{\|\boldsymbol{u}(t)\|}, \qquad |v(t)\rangle = \frac{\boldsymbol{v}(t)}{\|\boldsymbol{v}(t)\|}, \qquad |w(t)\rangle = \frac{\boldsymbol{w}(t)}{\|\boldsymbol{w}(t)\|} = |0\rangle \otimes |u(t)\rangle \frac{\|\boldsymbol{u}(t)\|}{\|\boldsymbol{w}(t)\|} + |1\rangle \otimes |v(t)\rangle \frac{\|\boldsymbol{v}(t)\|}{\|\boldsymbol{w}(t)\|},$$

$$\|\boldsymbol{w}(t)\|^2 = \|\boldsymbol{u}(t)\|^2 + \|\boldsymbol{v}(t)\|^2.$$

$$\frac{\partial w(t,x)}{dt} = \begin{pmatrix} 0 & -\frac{1}{\epsilon} \\ -\frac{1}{\epsilon} & 0 \end{pmatrix} \frac{\partial w(t,x)}{\partial x} + \begin{pmatrix} 0 & 0 \\ 0 & -\frac{1}{k\epsilon^2} \end{pmatrix} w(t,x)$$

Quantum simulation of hyperbolic heat equation

$$\frac{\partial w(t,x)}{dt} = \begin{pmatrix} 0 & -\frac{1}{\epsilon} \\ -\frac{1}{\epsilon} & 0 \end{pmatrix} \frac{\partial w(t,x)}{\partial x} + \begin{pmatrix} 0 & 0 \\ 0 & -\frac{1}{k\epsilon^2} \end{pmatrix} w(t,x)$$

Our first step is to simulate $|w(t)\rangle$. From Lemma 1, without losing generality, we can begin with the initial conditions $u(0,x)$, $v(0,x) = 0$, which requires the initial state preparation

$$|w(0)\rangle = |0\rangle \otimes |u(t)\rangle.$$

$$\frac{d\boldsymbol{w}(t)}{dt} = \left(-i\frac{1}{\epsilon}\sigma_x \otimes \hat{p}_x - \frac{1}{k\epsilon^2}|1\rangle\langle 1| \otimes \mathbf{1}_x \right) \boldsymbol{w}(t) = -i\boldsymbol{A}\boldsymbol{w}(t)$$

$$\boldsymbol{A} = \boldsymbol{A}_1 - i\boldsymbol{A}_2 = \frac{1}{\epsilon}\sigma_x \otimes \hat{p}_x - \frac{i}{k\epsilon^2}|1\rangle\langle 1| \otimes \mathbf{1}_x,$$

$$\boldsymbol{A}_1 = \frac{1}{\epsilon}\sigma_x \otimes \hat{p}_x = \boldsymbol{A}_1^\dagger, \qquad \boldsymbol{A}_2 = \frac{1}{k\epsilon^2}|1\rangle\langle 1| \otimes \mathbf{1}_x = \boldsymbol{A}_2^\dagger.$$

Already experimentally accessible in analog quantum simulation

Apply Schrödingerisation:

$$\boldsymbol{H} = \boldsymbol{A}_2 \otimes \hat{\eta} + \boldsymbol{A}_1 \otimes \mathbf{1}_\eta = \frac{1}{k\epsilon^2}|1\rangle\langle 1| \otimes \mathbf{1}_x \otimes \hat{\eta} + \frac{1}{\epsilon}\sigma_x \otimes \hat{p}_x \otimes \mathbf{1}_\eta$$

$$= \frac{1}{2k\epsilon^2}\mathbf{1}_2 \otimes \mathbf{1}_x \otimes \hat{\eta} - \frac{1}{2k\epsilon^2}\sigma_z \otimes \mathbf{1}_x \otimes \hat{\eta} + \frac{1}{\epsilon}\sigma_x \otimes \hat{p}_x \otimes \mathbf{1}_\eta.$$

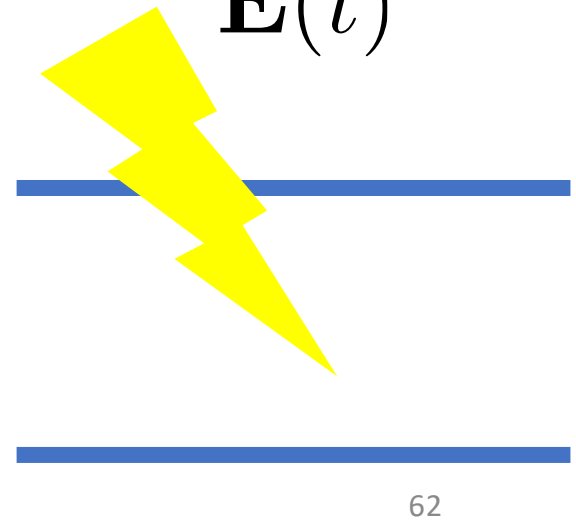
Jaynes-Cummings model

$\mathbf{B}(t)$

Magnetic dipole

Electric dipole

$\mathbf{E}(t)$

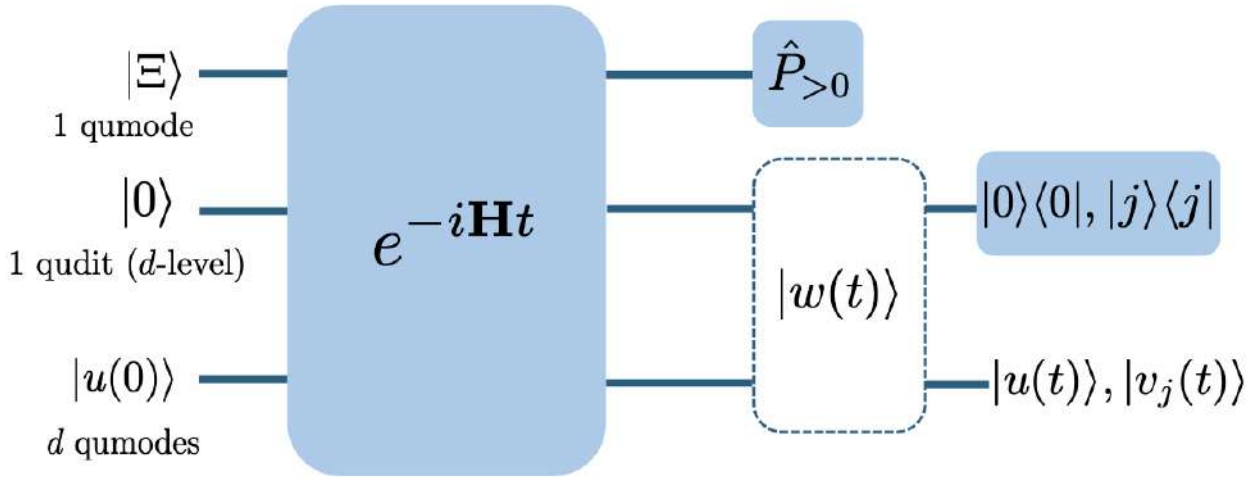


Applications

Applications to:

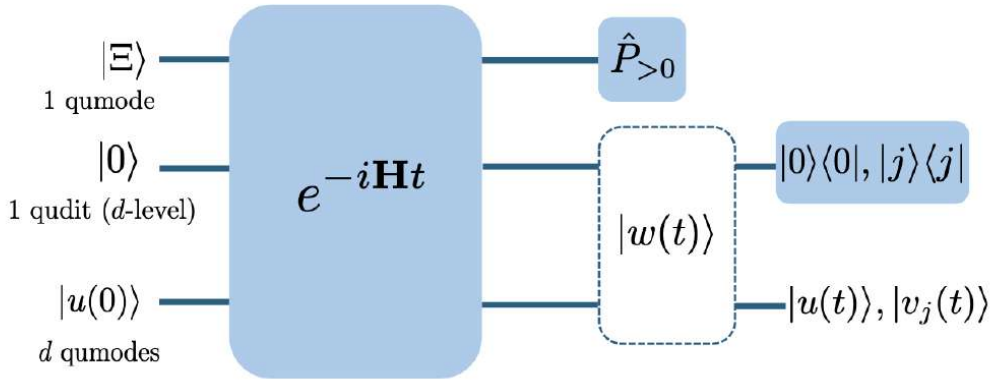
1) **Multidimensional heat equation**
2) **Black-Scholes equation: 1-dimensional (heat) and multidimensional**
3) **Fokker-Planck equations**

….realisable in cavity and circuit QED systems



Applications

Equation	Size of system	Hamiltonian $\boldsymbol{H}$ interaction terms
1D heat	1 qubit and 2 qumodes	$\mathbf{1}_2 \otimes \mathbf{1}_x \otimes \hat{\eta}, \quad \sigma_z \otimes 1_x \otimes \hat{\eta}, \quad \sigma_x \otimes \hat{p}_x \otimes \mathbf{1}_\eta$
1D Black-Scholes	1 qubit and 2 qumodes	$\mathbf{1}_2 \otimes \mathbf{1}_x \otimes \hat{\eta}, \quad \sigma_z \otimes 1_x \otimes \hat{\eta}, \quad \sigma_x \otimes \hat{p}_x \otimes \mathbf{1}_\eta$ $\sigma_z \otimes \hat{p}_x \otimes \mathbf{1}_\eta, \quad \mathbf{1}_2 \otimes \hat{p}_x \otimes 1_\eta$
1D Fokker-Planck	1 qubit and 2 qumodes	Same interaction terms as 1D Black-Scholes, different coefficients
2D heat	1 qudit (3 levels, qutrit) and 3 qumodes	$\lvert j\rangle\langle j\rvert \otimes \mathbf{1}_x \otimes \hat{\eta}, \quad (\lvert 0\rangle\langle j\rvert + \lvert j\rangle\langle 0\rvert) \otimes \hat{p}_j \otimes \mathbf{1}_\eta, \quad j = 1, 2$
2D Fokker-Planck	1 qutrit and 3 qumodes	$\lvert j\rangle\langle j\rvert \otimes \mathbf{1}_x \otimes \hat{\eta}, \quad (\lvert 0\rangle\langle j\rvert + \lvert j\rangle\langle 0\rvert) \otimes \hat{p}_x \otimes \mathbf{1}_\eta, \lvert 0\rangle\langle 0\rvert \otimes \hat{p}_x \otimes \mathbf{1}_\eta, \quad j = 1, 2$
3D heat	1 qudit (4 levels, ququart) and 4 qumodes	$\lvert j\rangle\langle j\rvert \otimes \mathbf{1}_x \otimes \hat{\eta}, \quad (\lvert 0\rangle\langle j\rvert + \lvert j\rangle\langle 0\rvert) \otimes \hat{p}_j \otimes \mathbf{1}_\eta, \quad j = 1, 2, 3$
3D Fokker-Planck	1 ququart and 4 qumodes	$\lvert j\rangle\langle j\rvert \otimes \mathbf{1}_x \otimes \hat{\eta}, \quad (\lvert 0\rangle\langle j\rvert + \lvert j\rangle\langle 0\rvert) \otimes \hat{p}_x \otimes \mathbf{1}_\eta, \lvert 0\rangle\langle 0\rvert \otimes \hat{p}_x \otimes \mathbf{1}_\eta, \; j = 1, 2, 3$
d-dim heat	1 qudit d levels and d+1 qumodes	$\lvert j\rangle\langle j\rvert \otimes \mathbf{1}_x \otimes \hat{\eta}, \quad (\lvert 0\rangle\langle j\rvert + \lvert j\rangle\langle 0\rvert) \otimes \hat{p}_j \otimes \mathbf{1}_\eta, \quad j = 1, \cdots, d$
d-dim Fokker-Planck	1 qudit d levels and d+1 qumodes	$\lvert j\rangle\langle j\rvert \otimes \mathbf{1}_x \otimes \hat{\eta}, \; (\lvert 0\rangle\langle j\rvert + \lvert j\rangle\langle 0\rvert) \otimes \hat{p}_x \otimes \mathbf{1}_\eta, \lvert 0\rangle\langle 0\rvert \otimes \hat{p}_x \otimes \mathbf{1}_\eta, \; j = 1, \cdots, d$



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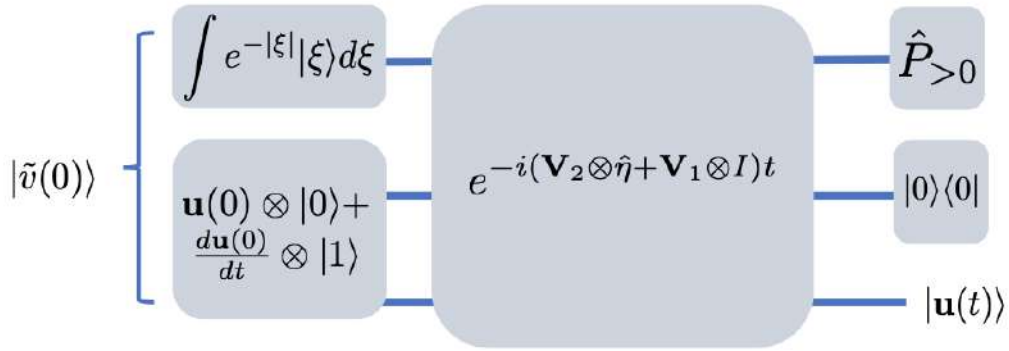
Higher-order time derivatives…second order example

$$\frac{d^2\boldsymbol{u}}{dt^2}+\boldsymbol{\Gamma}\frac{d\boldsymbol{u}}{dt}+i\boldsymbol{A}\boldsymbol{u}=0,\qquad \boldsymbol{\Gamma}\equiv\boldsymbol{c}_0-i\sum_{j=1}^{D}\boldsymbol{c}_j(I^{\otimes j-1}\otimes\hat{p}_j\otimes I^{\otimes D-j}),\qquad \boldsymbol{\Gamma}=\boldsymbol{\Gamma}_1-i\boldsymbol{\Gamma}_2$$

$$\boldsymbol{\Gamma}_1=(\boldsymbol{\Gamma}+\boldsymbol{\Gamma}^\dagger)/2=\boldsymbol{\Gamma}_1^\dagger,\boldsymbol{\Gamma}_2=i(\boldsymbol{\Gamma}-\boldsymbol{\Gamma}^\dagger)/2=\boldsymbol{\Gamma}_1^\dagger,$$

$$\boldsymbol{A}=-i\left(\sum_{l=1}^{L}\sum_{j=1}^{D}a_{j,l}(\hat{x}_1,...,\hat{x}_D)(i\hat{p}_j)^l+b(\hat{x}_1,...,\hat{x}_D)\right)$$

We can dilate the system $\boldsymbol{u}\rightarrow\boldsymbol{y}=\boldsymbol{u}\otimes|0\rangle+(d\boldsymbol{u}/dt)\otimes|1\rangle$



$$\frac{d\boldsymbol{y}}{dt}=\begin{pmatrix}d\boldsymbol{u}/dt\\ d^2\boldsymbol{u}/dt^2\end{pmatrix}=-i\boldsymbol{V}\boldsymbol{y},\qquad \boldsymbol{V}=\begin{pmatrix}0 & iI\\ \boldsymbol{A} & -i\boldsymbol{\Gamma}\end{pmatrix},\qquad \boldsymbol{V}=\boldsymbol{V}_1-i\boldsymbol{V}_2,\qquad \boldsymbol{A}=\boldsymbol{A}_1-i\boldsymbol{A}_2$$

$$\boldsymbol{V}_1=(\boldsymbol{V}+\boldsymbol{V}^\dagger)/2=\boldsymbol{V}_1^\dagger,\boldsymbol{V}_2=i(\boldsymbol{V}-\boldsymbol{V}^\dagger)/2=\boldsymbol{V}_2^\dagger,\qquad \boldsymbol{A}_1=(\boldsymbol{A}+\boldsymbol{A}^\dagger)/2=\boldsymbol{A}_1^\dagger,\boldsymbol{A}_2=i(\boldsymbol{A}-\boldsymbol{A}^\dagger)/2=\boldsymbol{A}_2^\dagger,$$

$$\boldsymbol{V}_1=\frac{1}{2}\begin{pmatrix}0 & \boldsymbol{A}^\dagger+iI\\ \boldsymbol{A}-iI & -i(\boldsymbol{\Gamma}-\boldsymbol{\Gamma}^\dagger)\end{pmatrix}=\boldsymbol{A}_1\otimes\sigma_x+\boldsymbol{A}_2\otimes\sigma_y-\frac{I}{2}\otimes\sigma_y+\boldsymbol{\Gamma}_2\otimes\frac{1}{2}(I-\sigma_z),$$

$$\boldsymbol{V}_2=\frac{1}{2i}\begin{pmatrix}0 & -\boldsymbol{A}^\dagger+iI\\ \boldsymbol{A}+iI & -i(\boldsymbol{\Gamma}+\boldsymbol{\Gamma}^\dagger)\end{pmatrix}=\boldsymbol{A}_2\otimes\sigma_x-\boldsymbol{A}_1\otimes\sigma_y+\frac{I}{2}\otimes\sigma_x-\boldsymbol{\Gamma}_1\otimes\frac{1}{2}(I-\sigma_z).$$

$$\frac{d\tilde{\boldsymbol{v}}}{dt}+i(\boldsymbol{V}_2\otimes\hat{\eta}+\boldsymbol{V}_1\otimes I)\tilde{\boldsymbol{v}}=\frac{d\tilde{\boldsymbol{v}}}{dt}=-i\boldsymbol{H}\tilde{\boldsymbol{v}},\qquad \boldsymbol{H}=\boldsymbol{V}_2\otimes\hat{\eta}+\boldsymbol{V}_1\otimes I=\boldsymbol{H}^\dagger$$

Wave equation

$$\frac{\partial^2 u}{\partial t^2} - \sum_{j=1}^{D} a_j \frac{\partial^2 u}{\partial x_j^2} = -Vu$$

$$\frac{d^2\boldsymbol{u}}{dt^2} = -i\boldsymbol{A}\boldsymbol{u}, \qquad \boldsymbol{A} = -i\left(\sum_{j=1}^{D} a_j(\hat{x}_1, ..., \hat{x}_D)\hat{p}_j^2 + V(\hat{x}_1, ..., \hat{x}_D)\right)$$

$$\mathbf{A}_1 = \frac{i}{2}\sum_{j=1}^{D}[\hat{p}_j^2, a_j]$$

$$\frac{d\tilde{\boldsymbol{v}}}{dt} = -i\boldsymbol{H}\tilde{\boldsymbol{v}}, \qquad \boldsymbol{H} = \boldsymbol{V}_2 \otimes \hat{\eta} + \boldsymbol{V}_1 \otimes I,$$

$$\mathbf{A}_2 = \frac{1}{2}\sum_{j=1}^{D}\{a_j, \hat{p}_j^2\} + V$$

$$\boldsymbol{V}_1 = \boldsymbol{A}_1 \otimes \sigma_x + \left(\boldsymbol{A}_2 - \frac{I}{2}\right) \otimes \sigma_y, \qquad \boldsymbol{V}_2 = -\boldsymbol{A}_1 \otimes \sigma_y + \left(\boldsymbol{A}_2 + \frac{I}{2}\right) \otimes \sigma_x$$

$D + 1$ qumodes $+1$ qubit

Quantum simulation cost is only linear in dimension…and if use qubits is also logarithmic in discretization size!

Equation	Number of qumodes	Max order term in $\boldsymbol{H}$	Number of terms in $\boldsymbol{H}$
General linear PDEs			
Homogeneous IV 1st-order time derivative	$D+1$	$[a_{K,j}, \hat{p}_j^K] \otimes \hat{\eta}$, $b \otimes \hat{\eta}$	$O(DK)$
Inhomogeneous IV A	Add 1 more qubit	$[a_{K,j}, \hat{p}_j^K] \otimes \hat{\eta} \otimes \sigma$, $b \otimes \hat{\eta} \otimes \sigma$	$O(DK)$
n-th order time derivative IV B	Add $\log_2(n)$ more qubits	Similar terms to 1st-order $\otimes\, \sigma^{\otimes \log_2 n}$	$O(DK)$
Examples			
Liouville V A	$D+1$	$i[\hat{p}, L] \otimes \hat{\eta}$, $\{\hat{p}, L\} \otimes I$	$O(D)$
Heat V B 1	$D+1$	$\{\hat{p}\mathrm{D}, \hat{p}\} \otimes \hat{\eta}$, $V \otimes \hat{\eta}$	$O(D+1)$
Fokker-Planck V B 2	$D+1$	$\{\hat{p}^2, \mathrm{D}\} \otimes \hat{\eta}, i[\mu, \hat{p}] \otimes \hat{\eta}, \{\hat{p}, \mu\} \otimes I, i[\hat{p}^2, \mathrm{D}] \otimes I$	$O(D)$
Black-Scholes V B 3	2	$(\hat{x}^2\hat{p}^2 + \hat{p}^2\hat{x}^2) \otimes \hat{\eta}$	5
Wave V B 4	$D+1$ + one qubit	$\{a, \hat{p}^2\} \otimes \hat{\eta} \otimes \sigma$, $V \otimes \eta \otimes \sigma$, $i[a, \hat{p}^2] \otimes I \otimes \sigma$	$O(D)$
Maxwell ($D=3$) V B 5	4 qumodes + 4 qubits	See Section V B 5	30
Uncertain linear PDE VI Convection	$D+L+1$	$i[c, \hat{p}] \otimes \hat{\eta}$, $\{c, \hat{p}\} \otimes I$	$O(DL)$
Nonlinear			
Scalar hyperbolic VII A	$D+1$	$i[Q, \hat{\zeta}] \otimes \hat{\eta}$, $\{Q, \hat{\zeta}\} \otimes I$	$O(D)$
Hamilton-Jacobi VII A	$2D$	$[\hat{\zeta}H, \hat{p}]$	$O(D)$
N nonlinear ODEs VII B	$N+1$	$i[Q, F] \otimes \hat{\eta}$, $\{Q, F\} \otimes I$	$O(N)$

Unstable dynamical systems: more general inhomogeneous PDEs and backward-in-time dissipative linear PDEs

Unstable dynamical modes

$$\frac{d\mathbf{y}}{dt} = -i\mathbf{B}_1\mathbf{y} - \mathbf{B}_2\mathbf{y}$$

What if some eigenvalues of $\mathbf{B}_2$ are negative?

This has applications in

- Inhomogeneous PDEs that arise
- from natural source terms
- Inclusion of boundary conditions

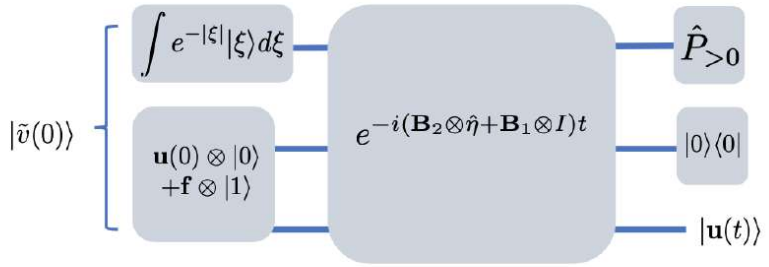
- Backward PDEs

- Iterative algorithms for linear algebra

Inhomogeneous linear PDE

$$\frac{d\boldsymbol{u}}{dt} = -i\boldsymbol{A}(\hat{x}_1, ...\hat{x}_D, \hat{p}_1, ..., \hat{p}_D)\boldsymbol{u} + \boldsymbol{f}(\hat{x}_1, ..., \hat{x}_D)$$

By dilating the system $\boldsymbol{u} \to \boldsymbol{y} = \boldsymbol{u}\otimes|0\rangle + \boldsymbol{f}\otimes|1\rangle$



$$\frac{d\boldsymbol{y}}{dt} = \frac{d}{dt}\begin{pmatrix}\boldsymbol{u}\\ \boldsymbol{f}\end{pmatrix} = -i\boldsymbol{B}\boldsymbol{y}, \qquad \boldsymbol{B} = \begin{pmatrix}\boldsymbol{A} & iI\\ 0 & 0\end{pmatrix}, \qquad \boldsymbol{A} = \boldsymbol{A}_1 - i\boldsymbol{A}_2, \qquad \boldsymbol{B} = \boldsymbol{B}_1 - i\boldsymbol{B}_2,$$

$$\boldsymbol{B}_1 = (\boldsymbol{B} + \boldsymbol{B}^\dagger)/2 = \boldsymbol{B}_1^\dagger, \qquad \boldsymbol{B}_2 = i(\boldsymbol{B} - \boldsymbol{B}^\dagger)/2 = \boldsymbol{B}_2^\dagger,$$

$$\boldsymbol{B}_1 = \begin{pmatrix}\boldsymbol{A}_1 & iI/2\\ -iI/2 & 0\end{pmatrix} = \boldsymbol{A}_1 \otimes \frac{1}{2}(I + \sigma_z) + \frac{I}{2}\otimes\sigma_y, \qquad \boldsymbol{B}_2 = \begin{pmatrix}\boldsymbol{A}_2 & -I/2\\ -I/2 & 0\end{pmatrix} = \boldsymbol{A}_2 \otimes \frac{1}{2}(I + \sigma_z) - \frac{I}{2}\otimes\sigma_x.$$

$$\frac{d\tilde{\boldsymbol{v}}}{dt} = -i\boldsymbol{H}\tilde{\boldsymbol{v}}, \qquad \boldsymbol{H} = \boldsymbol{B}_2\otimes\hat{\eta} + \boldsymbol{B}_1\otimes I = \boldsymbol{H}^\dagger$$

Using the Schrödingerisation introduced so far:
For stability of the new dynamical system $\mathbf{y}$, need $\mathbf{B}_2 > 0$
What if not all eigenvalues of $\mathbf{B}_2$ are positive?

Unstable dynamics

$$\frac{d\mathbf{y}}{dt} = -i\mathbf{B}_1\mathbf{y} - \mathbf{B}_2\mathbf{y}$$

Let $\mathbf{B}_2$ contain D real eigenvalues ordered as $\lambda_1 \geq \lambda_2 \cdots \geq \lambda_D$

Assume there exists $\lambda_i < 0$ for some i between 1 and D so there are some unstable modes (initial value problem is ill-posed)

$$w(0,\xi) = e^{-\xi}y(0), \qquad \xi > 0$$

$$\frac{\partial w(t,\xi)}{\partial t} = -\mathbf{B}_2\frac{\partial w(t,\xi)}{\partial \xi} - i\mathbf{B}_1 w(t,\xi)$$

Unstable dynamics

Theorem. The solution $y(t)$ can be recovered from $w(t,\xi)$ using

$$y(t) = e^{\xi} w(t,\xi), \qquad \text{for any } \xi \geq \xi^* \tag{1}$$

or

$$y(t) = e^{\xi^*} \int_{\xi^*}^{\infty} w(t,\xi) d\xi, \tag{2}$$

where $\xi^* = \max\{|\lambda_D| t, 0\}$

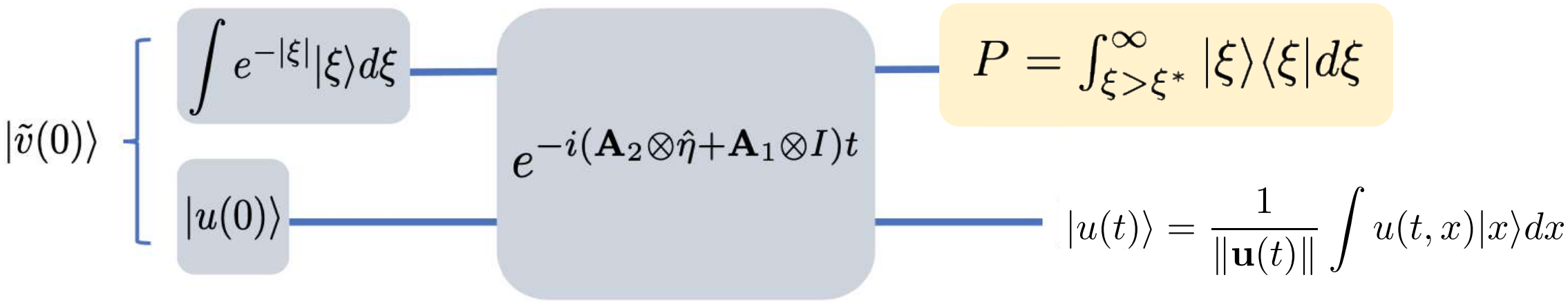
$|\lambda_D|$: interpreted as the maximum speed of the right-moving w solution along ξ

Recovers previous Schrödingerisation formalism $\xi^* = 0$ when $\lambda(\mathbf{B}_2) > 0$

Modified Schrodingerisation

Identical to previous Schrödingerisation except in final measurement procedure we post-select on $|\xi > \xi^*\rangle$

Recover $|y(t)\rangle$, use projective measurement $P = |\xi > \xi^*\rangle\langle\xi < \xi^*|$ with probability of success $\propto \|y(t)\|^2/\|y(0)\|^2$



Backward PDEs

Recall the forward heat equation: $\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \qquad u(0,x) = u_0(x)$

Applying the warped phase transformation $w = e^{-\xi} u = -\frac{\partial w}{\partial \xi}$

Then $\frac{\partial w}{\partial t} = -\frac{\partial^2}{\partial x^2}\frac{\partial w}{\partial \xi} \rightarrow \frac{\partial \mathbf{w}}{\partial t} - \hat{p}^2 \frac{\partial \mathbf{w}}{\partial \xi} = 0$

This means **w** moves from the right to the left along the ξ dimension, so only a boundary condition on the right is needed.

Backward PDEs

Backward heat equation can be written in terms of $v(t,x) = u(T-t,x)$ where

$$\frac{\partial v}{\partial t} = -\frac{\partial^2 v}{\partial x^2}, \qquad v(0,x) = u(T,x)$$

Using warped phase transformation $w = e^{-\xi} v$ we have $\frac{\partial \mathbf{w}}{\partial t} + \hat{p}^2 \frac{\partial \mathbf{w}}{\partial \xi} = 0$

$$\frac{d\mathbf{w}}{dt} = -\mathbf{B}_2 \mathbf{w}$$

This means that all the motion along ξ is going from left to right and the eigenvalues of $\mathbf{B}_2 = -\hat{p}^2 < 0$

Backward PDEs

To use our theorem for unstable dynamics, need $|\lambda(\mathbf{B}_2)| < \infty$ hence need to impose $\max|\lambda_D| = p_{max}^2$ and choose $\xi^* = p_{max}^2 T$ in the following

Theorem. The solution $y(t)$ can be recovered from $w(t,\xi)$ using

$$y(t) = e^{\xi} w(t,\xi), \qquad \text{for any } \xi \geq \xi^* \tag{1}$$

or

$$y(t) = e^{\xi^*} \int_{\xi^*}^{\infty} w(t,\xi) d\xi, \tag{2}$$

where $\xi^* = \max\{|\lambda_D|t, 0\}$

Possible strategies:

(1) Input data (fourier transform) has compact support, so corresponding $|p_{max}| < \infty$. If $u(T,x)$ is smooth in x, the Fourier mode decays rapidly and truncation in momentum is possible.

(2) Numerical discretisation of x then discretise its derivative, so $|\lambda_D| < O(1/(\Delta x)^2)$

Discretisation of qumodes

Discretising qumodes

Possible qumodes to discretise:

- We can choose to discrete only the qumodes for spatial degrees of freedom for the PDE
- We can choose to discretise only the ancilla qumode
- We can discretise all the qumodes

Different numerical schemes

$$\mathbf{H}(t) = \mathbf{A}_2(t) \otimes \hat{\eta} + \mathbf{A}_1(t) \otimes \mathbf{1}$$

Discretising main qumodes: discretising $\mathbf{A}_1, \mathbf{A}_2$ operators

$\hat{x} \to \text{diag}(-N/2, \cdots, N/2-1)$

$\hat{p} = -i\dfrac{\partial}{\partial x} \to N \times N$ matrix representation dependent on numerical scheme

Note: $\hat{p}^2 = -\frac{\partial^2}{\partial x^2}$ discretised in matrix form does not necessarily correspond to the square of previous matrix

Discretising ancilla qumode: $\eta \to \eta_i, \quad i = 0, \cdots, M \quad \hat{\eta} \to \text{diag}(-M/2, \cdots, M/2-1)$

Different numerical schemes: finite difference methods examples

$$u(x = x_i) = u_i$$

$$i = (i_1, \cdots, i_D), \qquad i_j = 0, \cdots, N-1, \qquad N = O(1/\Delta x), \qquad j = 1, \cdots, D$$

Type	Der. order	Acc. order	Formula
Backward	First	First	$\frac{\partial u}{\partial x}\Big\|_{x=x_i} \approx \frac{u_i - u_{i-1}}{\Delta x} + \mathcal{O}(\Delta x)$
Forward	First	Second	$\frac{\partial u}{\partial x}\Big\|_{x=x_i} \approx \frac{-u_{i+2} + 4u_{i+1} - 3u_i}{2\Delta x} + \mathcal{O}((\Delta x)^2)$
Central	First	Second	$\frac{\partial u}{\partial x}\Big\|_{x=x_i} \approx \frac{u_{i+1} - u_{i-1}}{2\Delta x} + \mathcal{O}((\Delta x)^2)$
Backward	Second	First	$\frac{\partial^2 u}{\partial x^2}\Big\|_{x=x_i} \approx \frac{u_i - 2u_{i-1} + u_{i-2}}{(\Delta x)^2} + \mathcal{O}(\Delta x)$
Central	Second	Second	$\frac{\partial^2 u}{\partial x^2}\Big\|_{x=x_i} \approx \frac{u_{i-1} - 2u_i + u_{i+1}}{(\Delta x)^2} + \mathcal{O}((\Delta x)^2)$
Forward	Second	Second	$\frac{\partial^2 u}{\partial x^2}\Big\|_{x=x_i} \approx \frac{2u_i - 5u_{i+1} + 4u_{i+2} - u_{i+3}}{(\Delta x)^2} + \mathcal{O}((\Delta x)^2)$

Costs: simulating 1D advection equation to fidelity 0.9

Table I: Quantum Gate Requirements for Different Qubit Numbers for the Hamiltonian simulation task (2) fo the 1 dimension case. The terminate fidelity of $e^{iHt}|u(0)\rangle$ and the classical solution $F = 0.9$.

Qubit Number	Number of 1-Qubit Rotations	Number of C-NOTs	Single Gate Fidelity Required
5	6080	4800	$1 - 9.68 \times 10^{-6}$
6	17664	14208	$1 - 3.31 \times 10^{-6}$
7	48384	39424	$1 - 1.20 \times 10^{-6}$
8	126976	104448	$1 - 4.55 \times 10^{-7}$
9	322560	267264	$1 - 1.79 \times 10^{-7}$
10	798720	665600	$1 - 7.20 \times 10^{-8}$

Compare: using qumodes we can already simulate to a 200,000 dimensional problem

Costs: simulating 1D hyperbolic heat equation to fidelity 0.9

Table I: Quantum Gate Requirements for Different Qubit Numbers for the Hamiltonian simulation task (1). We used $\epsilon = 0.1$; and the terminate fidelity of $e^{iHt}|u(0)\rangle$ and the classical solution $F = 0.9$.

Qubit Number	Number of 1-Qubit Operations	Number of C-NOTs	Single Gate Fidelity Required
5	27937725	12642950	$1 - 2.60 \times 10^{-9}$
6	72731830	33302709	$1 - 9.94 \times 10^{-10}$
7	180174053	83433274	$1 - 4.00 \times 10^{-10}$
8	431477111	201882772	$1 - 1.66 \times 10^{-10}$
9	1008194862	476169231	$1 - 7.10 \times 10^{-11}$
10	2312161227	1101341794	$1 - 3.09 \times 10^{-11}$

Compare: using qumodes it is already within experimental possibility to simulate this equation

Boundary conditions and inhomogeneous PDEs

Artificial boundary conditions

Simulating time-dependent quantum dynamics (e.g. emission of electrons) usually would require large computational domains. If one limits the computational domain and allow reflecting boundary conditions, this would cause interference with the solution in the domain, so need suitable boundary conditions to absorb outgoing wave-packets. These are *artificial boundary conditions.* For example using CAP:

Complex absorbing potentials: $i\frac{\partial\psi(t,x)}{\partial t} = H\psi(t,x) + W(x)\psi(t,x) \qquad x \in D$

$W(x)$ is selected so $W(x \in \Omega) = 0$ in computational domain Ω and has a negative imaginary part with magnitude decreasing away from $\partial\Omega$ so wavefunction at absorbing layer $D\backslash\Omega$ boundary can be set to zero.

Other methods (also having computational domain and including a buffer layer): Perfectly matched layers (PML) and Dirichlet-to-Neumann map (DtN)

Physical boundary conditions

Dirichlet and von Neumann (and Robin) boundary conditions turns discretised homogeneous PDEs into inhomogeneous PDEs:

Example $\dfrac{\partial u}{\partial t} = \alpha \dfrac{\partial^2 u}{\partial x^2}, \quad x \in [0, L], \quad t > 0$

- Divide $[0, L]$ into $N + 1$ intervals (i.e., $N + 2$ points)
- Grid points: $x_0 = 0, x_1, \ldots, x_N, x_{N+1} = L$
- Let $u_i(t) \approx u(x_i, t)$

Central difference:

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2}$$



For internal points $i = 1, \cdots, N$:

$$\frac{du_i}{dt} = \frac{\alpha}{(\Delta x)^2}(u_{i+1} - 2u_i + u_{i-1})$$

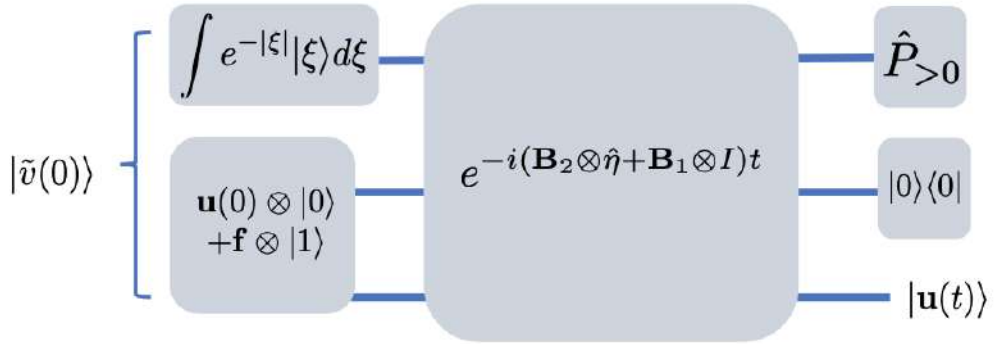
Dirichlet BCs: $u(0, t) = A, \quad u(L, t) = B \Rightarrow u_0 = A, \quad u_{N+1} = B$

$$\Longrightarrow \quad \frac{du_1}{dt} = \frac{\alpha}{(\Delta x)^2}(u_2 - 2u_1 + u_0) = \frac{\alpha}{(\Delta x)^2}(u_2 - 2u_1 + A)$$

Inhomogeneous linear PDE

$$\frac{d\boldsymbol{u}}{dt} = -i\boldsymbol{A}(\hat{x}_1, ...\hat{x}_D, \hat{p}_1, ..., \hat{p}_D)\boldsymbol{u} + \boldsymbol{f}(\hat{x}_1, ..., \hat{x}_D)$$

By dilating the system $\boldsymbol{u} \to \boldsymbol{y} = \boldsymbol{u}\otimes|0\rangle + \boldsymbol{f}\otimes|1\rangle$



$$\frac{d\boldsymbol{y}}{dt} = \frac{d}{dt}\begin{pmatrix}\boldsymbol{u}\\ \boldsymbol{f}\end{pmatrix} = -i\boldsymbol{B}\boldsymbol{y}, \qquad \boldsymbol{B} = \begin{pmatrix}\boldsymbol{A} & iI\\ 0 & 0\end{pmatrix}, \qquad \boldsymbol{A} = \boldsymbol{A}_1 - i\boldsymbol{A}_2, \qquad \boldsymbol{B} = \boldsymbol{B}_1 - i\boldsymbol{B}_2,$$

$$\boldsymbol{B}_1 = (\boldsymbol{B} + \boldsymbol{B}^\dagger)/2 = \boldsymbol{B}_1^\dagger, \qquad \boldsymbol{B}_2 = i(\boldsymbol{B} - \boldsymbol{B}^\dagger)/2 = \boldsymbol{B}_2^\dagger,$$

$$\boldsymbol{B}_1 = \begin{pmatrix}\boldsymbol{A}_1 & iI/2\\ -iI/2 & 0\end{pmatrix} = \boldsymbol{A}_1 \otimes \frac{1}{2}(I + \sigma_z) + \frac{I}{2}\otimes\sigma_y, \qquad \boldsymbol{B}_2 = \begin{pmatrix}\boldsymbol{A}_2 & -I/2\\ -I/2 & 0\end{pmatrix} = \boldsymbol{A}_2 \otimes \frac{1}{2}(I + \sigma_z) - \frac{I}{2}\otimes\sigma_x.$$

$$\frac{d\tilde{\boldsymbol{v}}}{dt} = -i\boldsymbol{H}\tilde{\boldsymbol{v}}, \qquad \boldsymbol{H} = \boldsymbol{B}_2 \otimes \hat{\eta} + \boldsymbol{B}_1 \otimes I = \boldsymbol{H}^\dagger$$

Near-optimal strategies in precision

Schrodingerisation: simplest ancilla initial state

Warped phase transformation: $w(t,x,\xi) = e^{-\xi}u(t,x)$ $\xi > 0$

This in itself does not specify the conditions for $\xi < 0$. Previously we chose the initial condition:

$$w(0,x,\xi) = e^{-|\xi|}u(0,x) \qquad \xi \in (-\infty,\infty)$$

This exhibits first-order convergence in ξ due to the lack of regularity of $\exp(-|\xi|)$

The maximum absolute value among the discrete Fourier modes: $\eta_{max} = O(1/\epsilon)$

Schrodingerisation: improving scaling with precision

The standard error between $\psi(\xi) = \exp(-|\xi|)$ and its approximation using the discrete Fourier transform $\hat{\psi}(\xi)$ is

$$\|\psi - \hat{\psi}\| \lesssim \left(\frac{R-L}{N_\xi}\right)^r |\psi|_r \qquad \psi \in [L, R]$$

ψ has regularity r

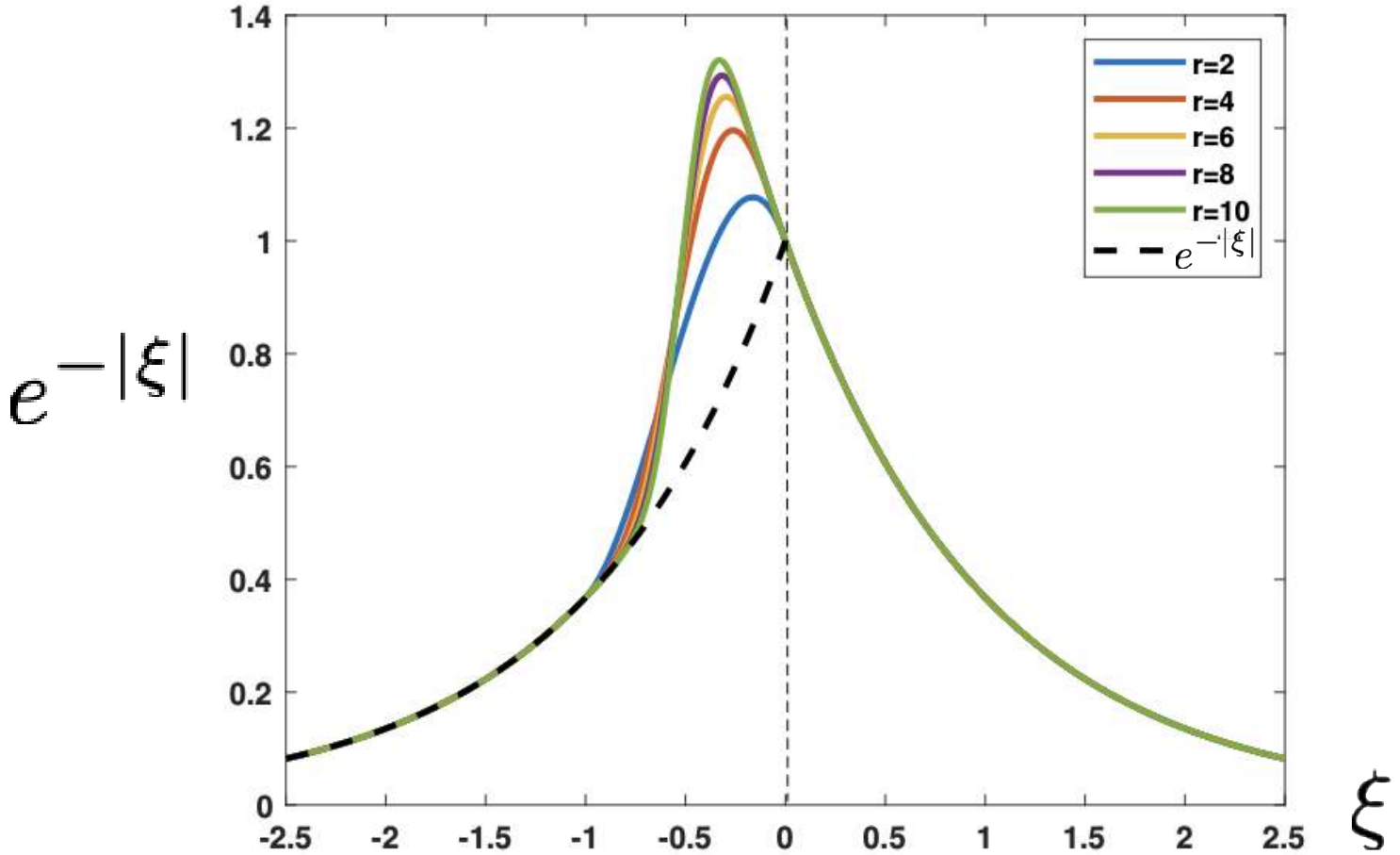
If $\|\psi - \hat{\psi}\| \leq \epsilon \implies N_\xi \sim (R-L)|\psi|_r^{1/r} \epsilon^{-1/r}$

Solving $(1/\epsilon)^{1/r} \sim \log(1/\epsilon)$, one has $N_\xi \sim (R-L)|\psi|_r^{1/r} \log(1/\epsilon)$, if $r \sim \frac{\log(1/\epsilon)}{\log(\log(1/\epsilon))}$

This required regularity for $\psi(\xi)$ gives

$$\eta_{max} = \frac{N_\xi \pi}{R-L} = |\psi|_r^{1/r} \log(1/\epsilon) = O(\log(1/\epsilon))$$

Schrodingerisation: improving scaling with precision



Summary of comparison of methods: for digital quantum algorithms

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{u}(t) = A(t)\boldsymbol{u}(t) & t \in (0,T) \\ \boldsymbol{u}(0) = \boldsymbol{u}_0, \end{cases}$$

Method	Queries to A	Queries to $\boldsymbol{u}_0$
Spectral method [21]	$\widetilde{\mathcal{O}}(\frac{\|\boldsymbol{u}_0\|}{\|\boldsymbol{u}(T)\|}\kappa_V\alpha_A T\mathrm{poly}(\log\frac{1}{\varepsilon}))$	$\widetilde{\mathcal{O}}(\frac{\|\boldsymbol{u}_0\|}{\|\boldsymbol{u}(T)\|}\kappa_V\alpha_A T\mathrm{poly}(\log\frac{1}{\varepsilon}))$
Truncated Dyson [14]	$\widetilde{\mathcal{O}}(\frac{\|\boldsymbol{u}_0\|}{\|\boldsymbol{u}(T)\|}\alpha_A T(\log\frac{1}{\varepsilon})^2)$	$\mathcal{O}(\frac{\|\boldsymbol{u}_0\|}{\|\boldsymbol{u}(T)\|}\alpha_A T\log\frac{1}{\varepsilon})$
Time-marching [17]	$\widetilde{\mathcal{O}}(\frac{\|\boldsymbol{u}_0\|}{\|\boldsymbol{u}(T)\|}\alpha_A^2 T^2\log\frac{1}{\varepsilon})$	$\mathcal{O}(\frac{\|\boldsymbol{u}_0\|}{\|\boldsymbol{u}(T)\|})$
Improved LCHS time-dependent [34]	$\widetilde{\mathcal{O}}(\frac{\|\boldsymbol{u}_0\|}{\|\boldsymbol{u}(T)\|}\alpha_A T(\log\frac{1}{\varepsilon})^{1+1/\beta})$	$\mathcal{O}(\frac{\|\boldsymbol{u}_0\|}{\|\boldsymbol{u}(T)\|})$
Improved LCHS time-independent [34]	$\widetilde{\mathcal{O}}(\frac{\|\boldsymbol{u}_0\|}{\|\boldsymbol{u}(T)\|}\alpha_A T(\log\frac{1}{\varepsilon})^{1/\beta})$	$\mathcal{O}(\frac{\|\boldsymbol{u}_0\|}{\|\boldsymbol{u}(T)\|})$
Schrödingerisation time-dependent	$\widetilde{\mathcal{O}}(\frac{\|\boldsymbol{u}_0\|}{\|\boldsymbol{u}(T)\|}\alpha_A T(\log\frac{1}{\varepsilon})^2)$	$\mathcal{O}(\frac{\|\boldsymbol{u}_0\|}{\|\boldsymbol{u}(T)\|})$
Schrödingerisation time-independent	$\widetilde{\mathcal{O}}(\frac{\|\boldsymbol{u}_0\|}{\|\boldsymbol{u}(T)\|}\alpha_A T\log\frac{1}{\varepsilon})$	$\mathcal{O}(\frac{\|\boldsymbol{u}_0\|}{\|\boldsymbol{u}(T)\|})$

$\alpha_A \geq \|A\|$, T is the evolution time, ε is the error, and $\beta \in (0,1)$

Foundational implications?

Mathematical theory of dilation: Nagy's theorem

A contraction V is an operator on Hilbert space where $\|V\| < 1$
A dilation is an embedding of V into a larger structure U and V is a projection of U onto a particular subspace

Theorem 1 Sz.-Nagy's unitary dilation theorem [1]. *Let V be a contraction on a Hilbert space $\mathcal{H}$, then there exists a Hilbert space $\mathcal{H}_1$ containing $\mathcal{H}$ and a unitary U on $\mathcal{H}_1$, such that*

$$V^k = P_{\mathcal{H}} U^k, \quad \text{for all } k = 0, 1, 2, \ldots$$

Moreover, when $\mathcal{H}_1$ is chosen as the smallest reducing subspace for U that contains $\mathcal{H}$,

$$\mathcal{H}_1 = \bigvee_{k \in \mathbb{Z}} U^k \mathcal{H} := \overline{\text{span}\{U^n \mathcal{H}, n \in \mathbb{Z}\}},$$

$(\mathcal{H}_1, U)$ can be identified as a minimal dilation. These conditions determine U up to an isomorphism.

What are all the possible classes of dilations, that are suitable for different problems?

1. B. S. Nagy, C. Foias, H. Bercovici, and L. Kérchy, *Harmonic analysis of operators on Hilbert space* (Springer Science & Business Media, 2010).

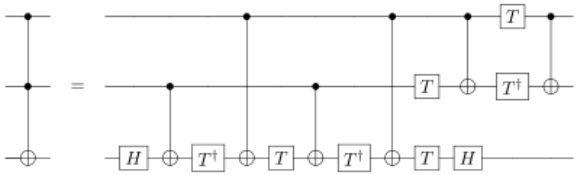
Where is the quantum? Future interesting questions

Foundational question: which PDEs are classically efficiently simulable and which ones are not?

Qubit systems (Gottesman-Knill): Only Clifford gates and projective measurements in computational basis can be efficiently simulated by a classical computer

Hard to see how non-Clifford gates are related to aspects of the PDE. Also difficult to see complementarity for non-Clifford gates

e.g. Toffoli gate is non-Clifford



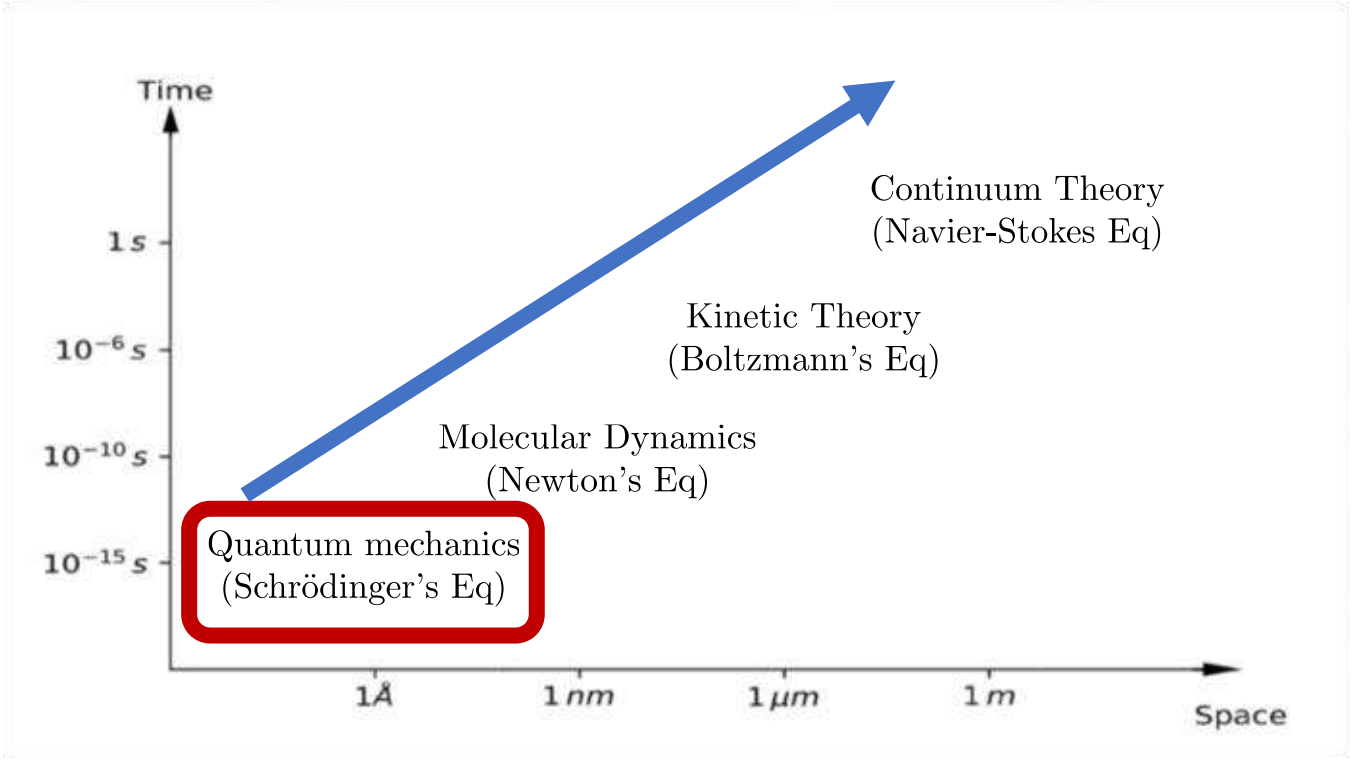
$$T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}$$

Continuous-variable systems (Bartlett-Sanders-Braunstein-Nemoto): Only Gaussian states, gates and measurements can be efficiently simulated by a classical computer

In Schrodingerisation, simple to see exactly which parts of the PDE requires non-Gaussianity

Gaussian gate: H up to quadratic in $\hat{x}, \hat{p}$

A new way to look at the boundary from quantum to classical physics across space and time scales?



Schrödingerisation allows all of classical physics to be captured using quantum mechanical equations (though not necessarily with known quantum advantage for highly nonlinear ODEs/PDEs). So is there a new way of studying the interface between the different physics on different scales using the 'same language'?

Summary

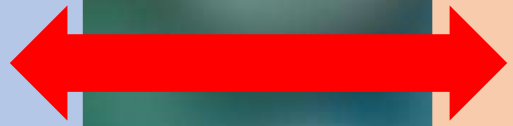
Schrodingerisation formulation:
any linear PDE becomes a Schrodinger-like equation in *one* higher dimension in a very simple way

Any linear system of ODEs or PDE

$$\frac{d\mathbf{u}(t)}{dt} = -\mathbf{A}(t)\mathbf{u}(t)$$

$$\mathbf{A}_1 = (1/2)(\mathbf{A} + \mathbf{A}^\dagger) = \mathbf{A}_1^\dagger$$

$$\mathbf{A}_2 = (i/2)(\mathbf{A} - \mathbf{A}^\dagger) = \mathbf{A}_2^\dagger$$



Simulated on quantum device:

$$\mathbf{H}(t) = \mathbf{A}_2(t) \otimes \hat{\eta} + \mathbf{A}_1(t) \otimes \mathbf{1}$$

$$\mathbf{H}(t) = \mathbf{H}(t)^\dagger$$

$$\hat{\eta} \to \mathrm{diag}(-M/2, \cdots, M/2 - 1)$$

We provide *a simple recipe*: Given any linear system of ODEs or PDE we find the corresponding quantum system; and given any quantum system, can find corresponding linear ODE/PFE

Benefits of Schrodingerisation

Many other methods based on matrix inversion, or block-encoding or LCU: Berry 2014, Berry et al 2015, Costa et al 2019, Linden et al, 2020, Childs et al 2021, An et al 2023 …etc Can ask me later for more references

- Can take advantage of continuous-variable/analog quantum simulation: *no discretisation of PDE is needed*
- No discretisation in time needed: continuous time evolution, even in qubit version; May not need to break up into many gates in the continuous formalism



- Formalism easily adapted to fully digital setting (qubits and discrete time). Here quantum cost can be polylog in discretization size and poly in dimension
- Avoid complications of matrix inversion methods (e.g. condition number dependence) and other methods (e.g. needing square roots of operators in block-encoding, using polynomial expansions)



- Can see explicitly which parts of the PDE (including initial conditions) requires entangling operations and which parts require non-Gaussian operations in the continuous-variable setting



- Formalism is flexible and simple enough for not only continuous-variables and qubits, but also hybrid discrete-continuous variable platforms
- Can get `cost' in D, instead of exponential in D

Cost for discretised scheme

This varies according to:

- Which qumodes one chooses to discretise (ancilla, main, or both?)
- Which numerical scheme one chooses
- Which Hamiltonian simulation protocol one chooses

$$\mathbf{H}(t) = \mathbf{A}_2(t) \otimes \hat{\eta} + \mathbf{A}_1(t) \otimes \mathbf{1}$$

Example:

Theorem 1—Given sparse access to the $M^d \times M^d$ matrix $\boldsymbol{H}$ and the unitary U_{initial} that prepares the initial quantum state $|\boldsymbol{u}(0)\rangle$ to precision ϵ. With the Schrödingerization approach, the state $|\boldsymbol{u}(t)\rangle$ can be prepared with query complexity $\tilde{\mathcal{O}}((\|\boldsymbol{u}(0)\|/\|\boldsymbol{u}(t)\|)st\|\boldsymbol{H}\|_{\max})$ and $\tilde{\mathcal{O}}(\|\boldsymbol{u}(0)\|/\|\boldsymbol{u}(t)\|dst\|\boldsymbol{H}\|_{\max})$ additional two-qubit gates.

Problems become `simpler' by lifting to a higher dimension!

Extra cost in quantum simulation of extra K dimensions costs only O(K) and not exponential in K.

1. Schrodingerisation: Linear non-Schrodinger's equations become Schrodinger-like equations

(e.g. dissipative equations become conservative equations)

JUST ADD ONE DIMENSION

2. . nonlinear problems become linear

DEPENDS ON PDE

3. Linear uncertain problems with L uncertain variables become deterministic

JUST ADD L DIMENSIONS

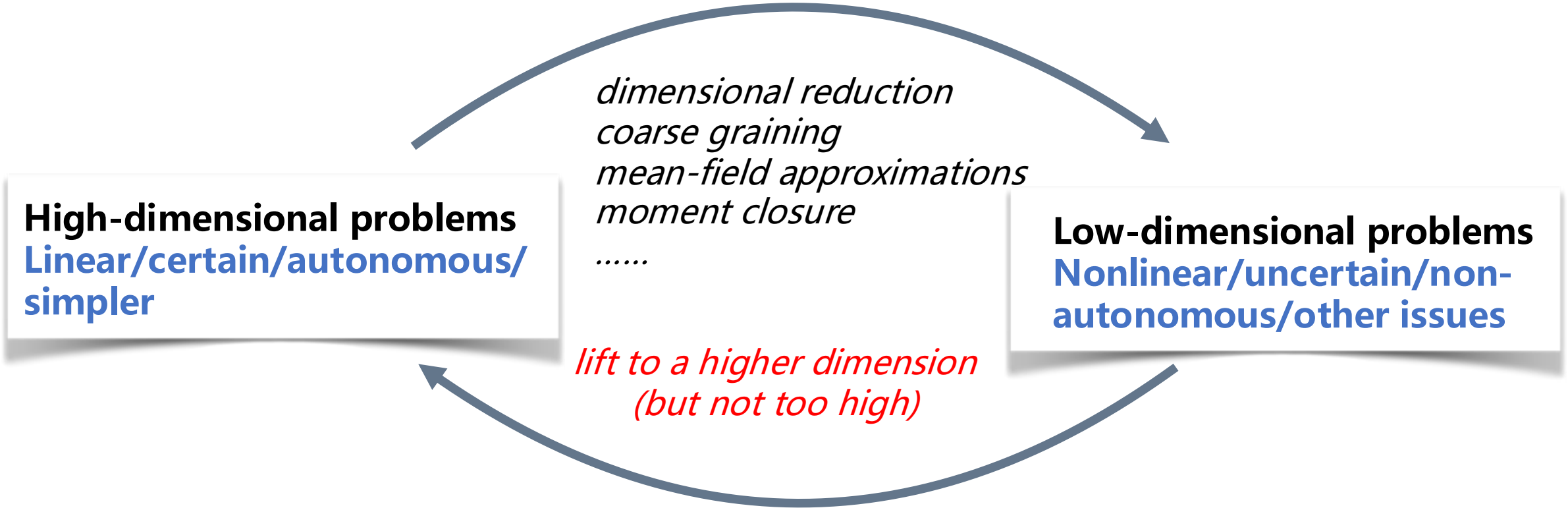
4. Linear non-autonomous systems become linear autonomous

JUST ADD MAX TWO DIMENSIONS

Might be classically more costly…but can potentially be more efficient with quantum simulation!

Our philosophy: problems become simpler by lifting to higher dimension

Classical computation: suffers from curse of dimensionality



Quantum computation: can resolve curse of dimensionality for PDEs

Overview of autumn lectures on Schrodingerisation

PART II: Special topics

- **Introducing UnitaryLab: software for quantum algorithms for scientific computing**
- **Optimisation: semidefinite programming**
- **If there's time: uncertain ODEs/PDEs; nonlinear PDEs; non-autonomous mapped to autonomous PDEs; applications to machine learning**

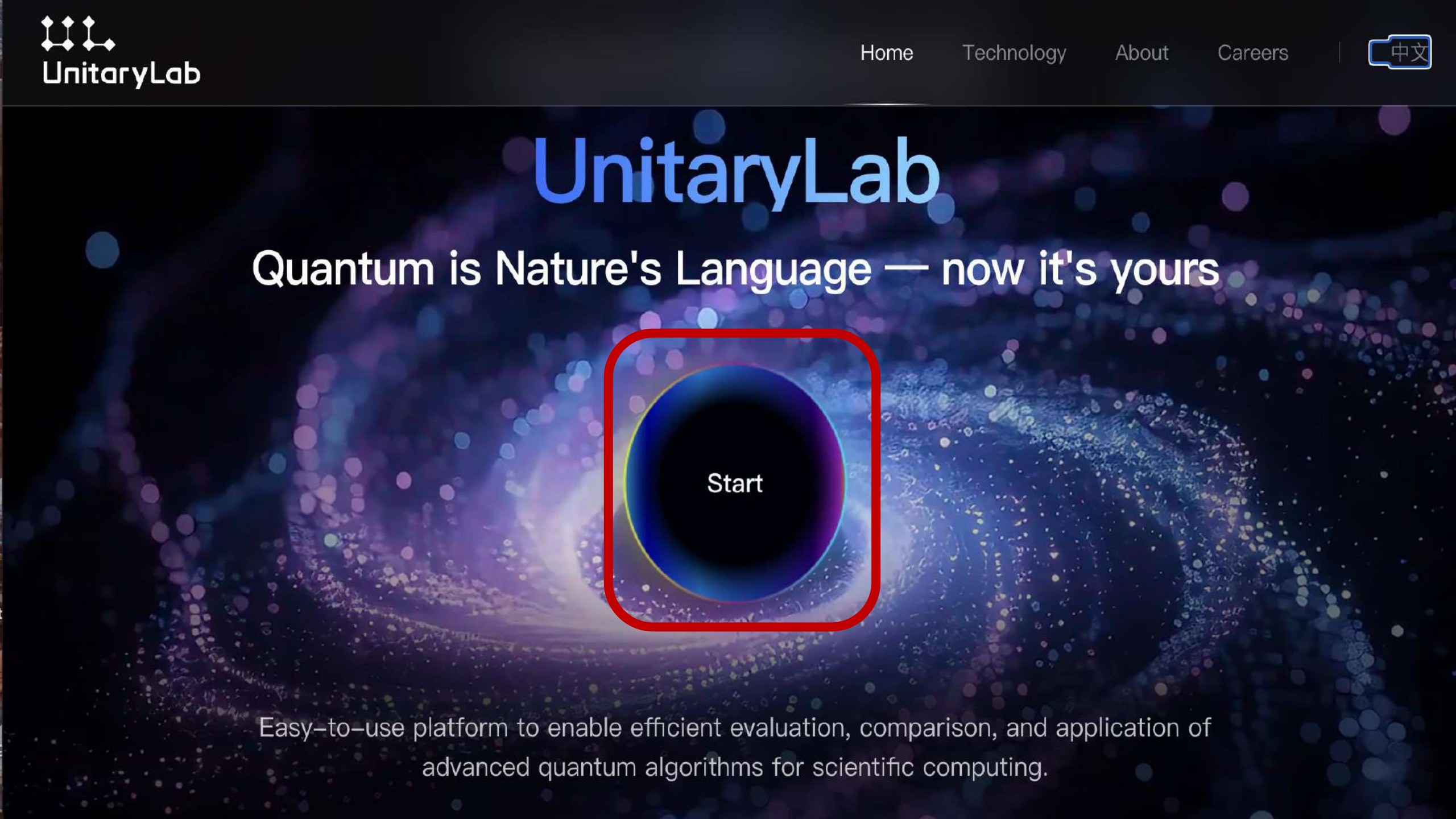
New tools

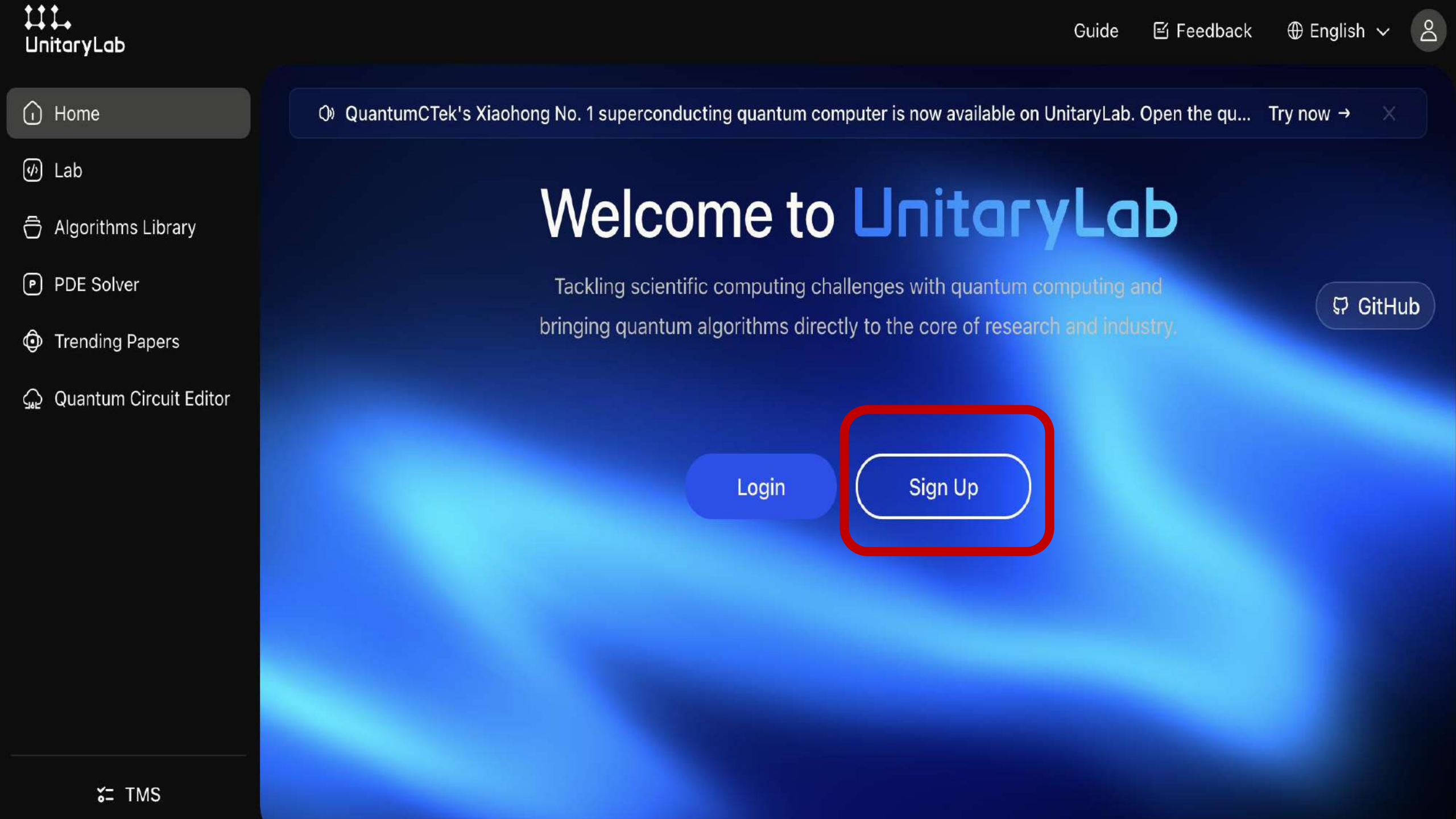
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- Black-Scholes Equation
- Elastic Wave Equation
- Burgers Equation
- Traffic Flow Equation
- Schrödinger Equation
- Helmholtz Equation
- Multiscale Equation

Formula README

Equation Formula

$$\frac{\partial u}{\partial t} = a\frac{\partial^2 u}{\partial x^2}, \quad a > 0$$

Initial Data

$$u(x,0) = u_0(x)$$

Boundary Condition

Parameter Settings

1D Forward heat equation

- Equation
- Boundary
- Initial Data
- Discrete Scheme
- Numerical Method

Job Info Quantum Circuit Results

No data available

Get in touch with us in Shanghai!

Shanghai Jiao Tong University

Open postdoc positions available!

Internship positions in UnitaryLab also available

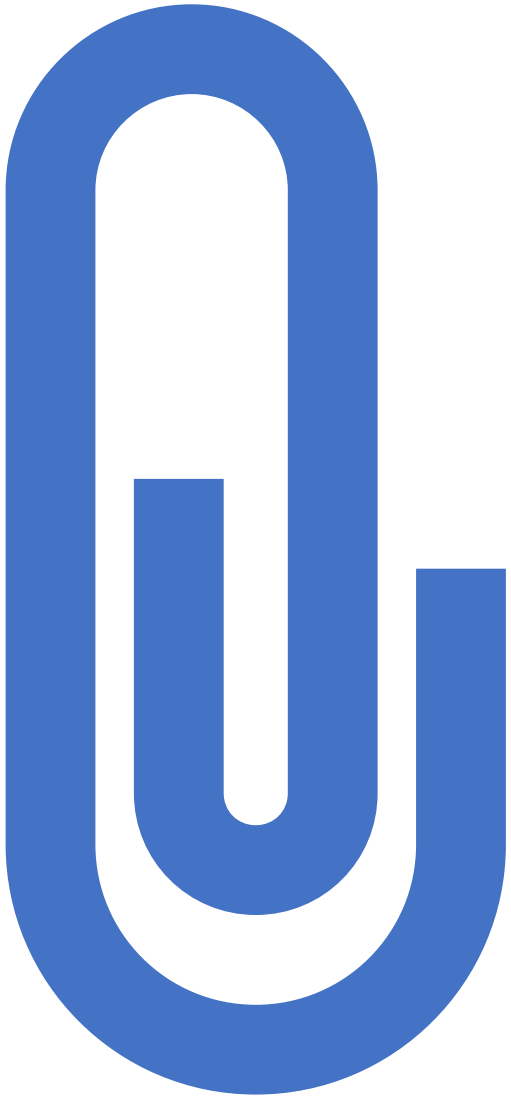
nanaliuquantum@gmail.com







Appendix slides



Reference list for Schrodingerisation (Part I):

Schrodingerisation basics and mathematical theory:

- *Quantum simulation of partial differential equations via Schrodingerisation*, Shi Jin, Nana Liu*, Yue Yu, arXiv: 2212.13969, Physical Review Letters, Vol 133, 230602, 2024

- *Quantum simulation of partial differential equations : applications and detailed analysis*, Shi Jin*, Nana Liu*, Yue Yu*, Physical Review A, Vol 108, 032603, 2023

- *On the Schrodingerisation method for linear non-unitary dynamics with optimal dependence on matrix queries*, Shi Jin, Nana Liu and Chuwen Ma, Yue Yu*, arXiv: 2505.00370, 2025

- *Dilation theorem via Schrodingerisation, with applications to the quantum simulation of differential equations,* Junpeng Hu*, Shi Jin, Nana Liu and Lei Zhang, arXiv: 2309.16262, Studies in Applied Mathematics, Vol 154, No.4, 2025

Reference list for Schrodingerisation (Part I):

Analog quantum simulation for PDEs:

- *Analog quantum simulation of partial differential equations,* Shi Jin, Nana Liu*, arXiv: 2308.00646, Quantum Science and Technology, Vol 9, 035047, 2024

- *Analog quantum simulation of parabolic partial differential equations using Jaynes-Cummings-like models*, Shi Jin, Nana Liu*, arXiv: 2407.01913, 2024

Ill-posed PDEs and inhomogeneous terms:

- *Schrödingerisation-based computationally stable algorithms for ill-posed problems in partial differential equations*, Shi Jin, Nana Liu and Chuwen Ma*, arXiv: 2403.19123, SIAM Journal on Scientific Computing (accepted 2025)

- *On Schrodingerisation based quantum algorithms for linear dynamical systems with inhomogeneous terms,* Shi Jin, Nana Liu and Chuwen Ma*, arXiv: 2402.14696, 2024

Reference list for Schrodingerisation (Part I):

Boundary conditions:

- *Quantum simulation for partial differential equations with physical boundary or interface conditions,* Shi Jin*, Xiantao Li*, Nana Liu*, Yue Yu*, Journal of Computational Physics, Vol 298, 112707, 2024
- *Quantum Simulation for Quantum Dynamics with Artificial Boundary Conditions,* Shi Jin*, Xiantao Li*, Nana Liu*, Yue Yu*, arXiv:*2304.00667*, SIAM Journal on Scientific Computing, Vol 46, Issue 4, B40-B421, 2024
- *Quantum framework for simulating linear PDEs with Robin boundary conditions*, Nikita Guseynov*, Xiajie Huang*, Nana Liu*, arXiv: 2506.20478, 2025

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