Quantum simulation of partial differential equations via Schrodingerisation

PART I: Basics for linear PDEs

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Looking beyond classical infrastructure…

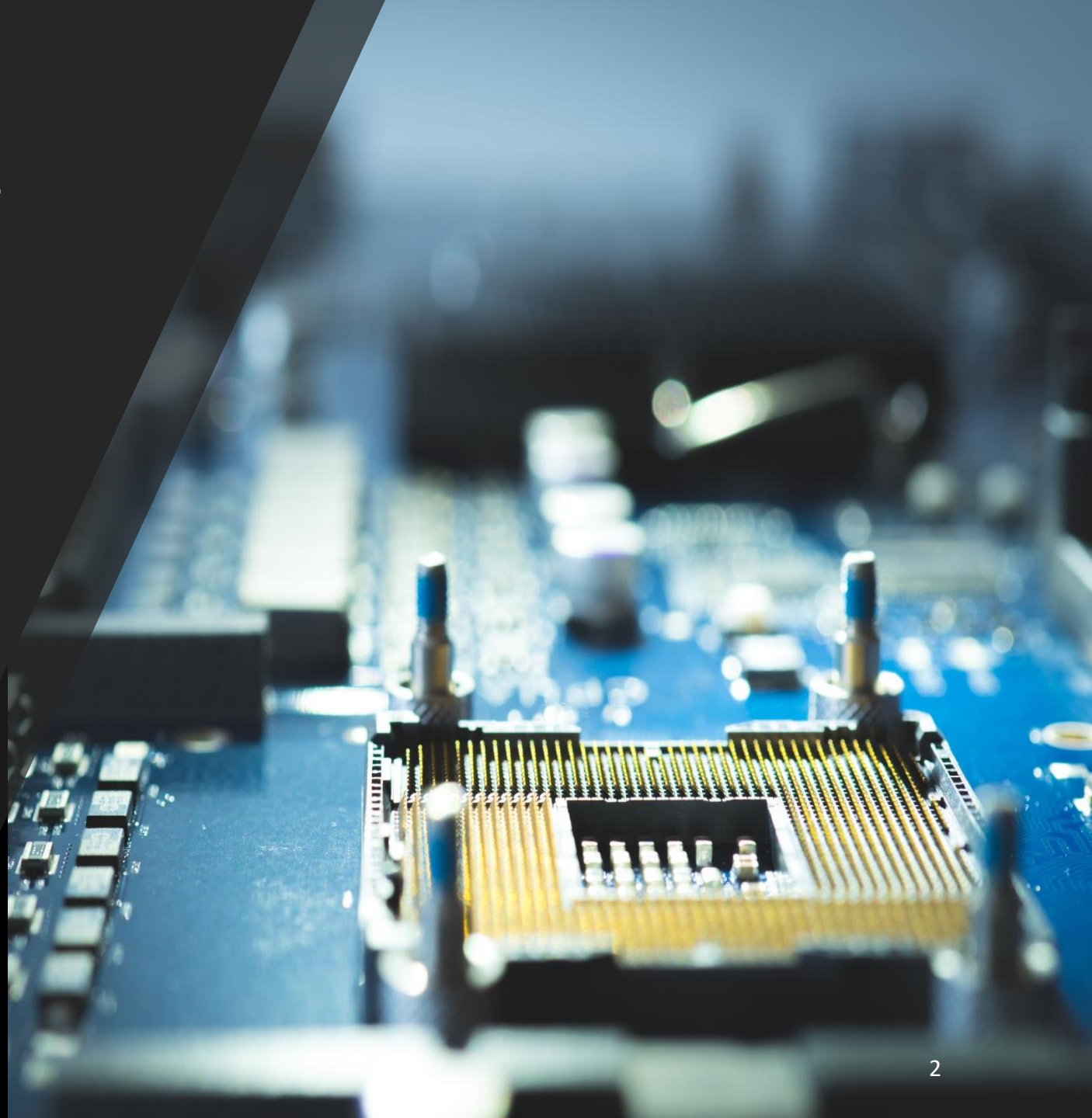
Reaching classical bottlenecks in

- Size of chips (Moore's law)
- Communication (bandwidth)
- Energy cost
- Memory
- Time

KEY MESSAGE:

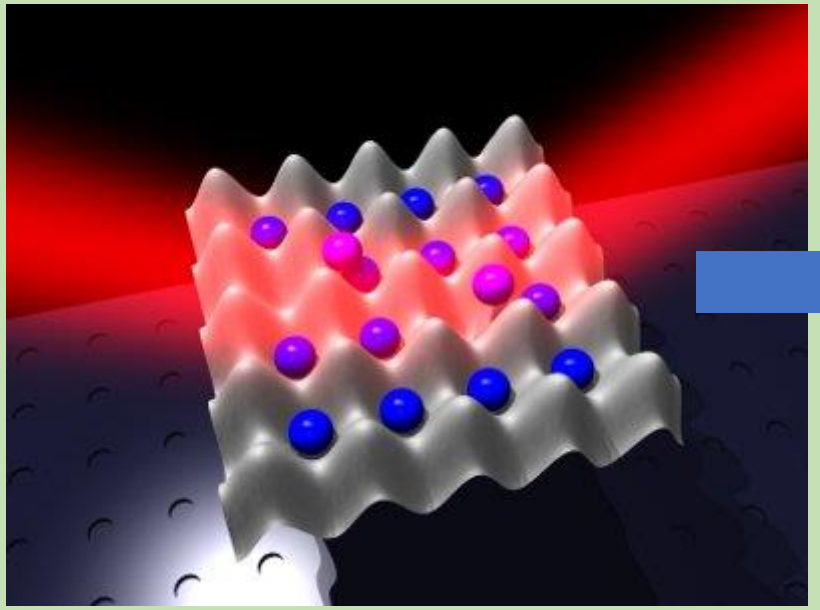
Our computational techniques and mathematical language must change when the underlying physical infrastructure changes!

Furthermore, algorithms should be *as simple as possible*, but no simpler



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

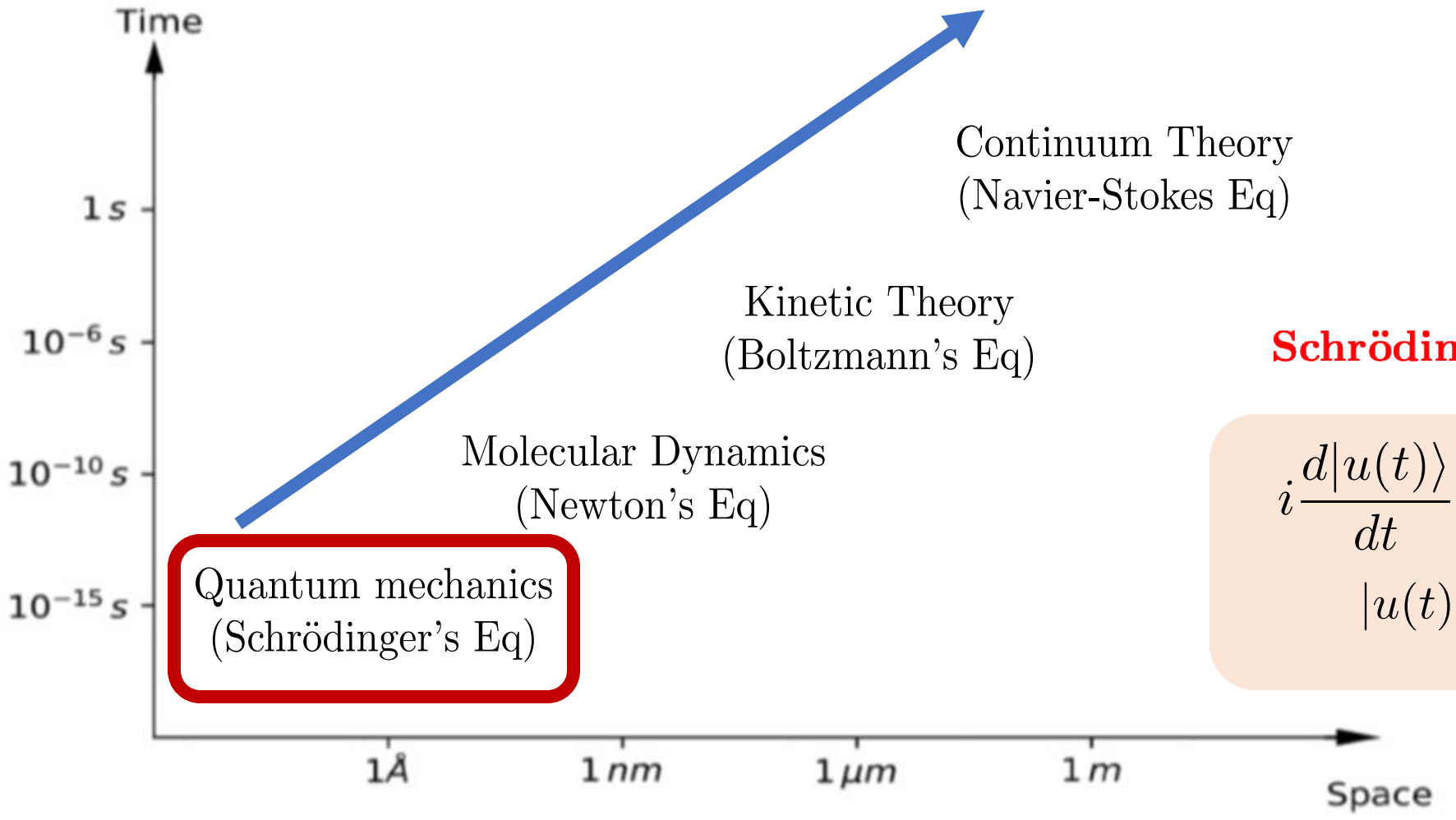
Today we are reaching beyond the limit of what classical computers can easily simulate:

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

Ordinary and partial differential equations across multiple scales



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 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 summer lectures on Schrodingerisation

PART I: Basics of Schrodingerisation (today and tomorrow)

Flexible method for mapping linear 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 summer lectures on Schrodingerisation

PART II: Special topics (tomorrow and day after)

- **Nonlinear ODEs and PDEs**
- **Uncertain ODEs/PDEs**
- **Non-autonomous mapped to autonomous PDEs**
- **Application to linear algebra, ground state and thermal state preparation**

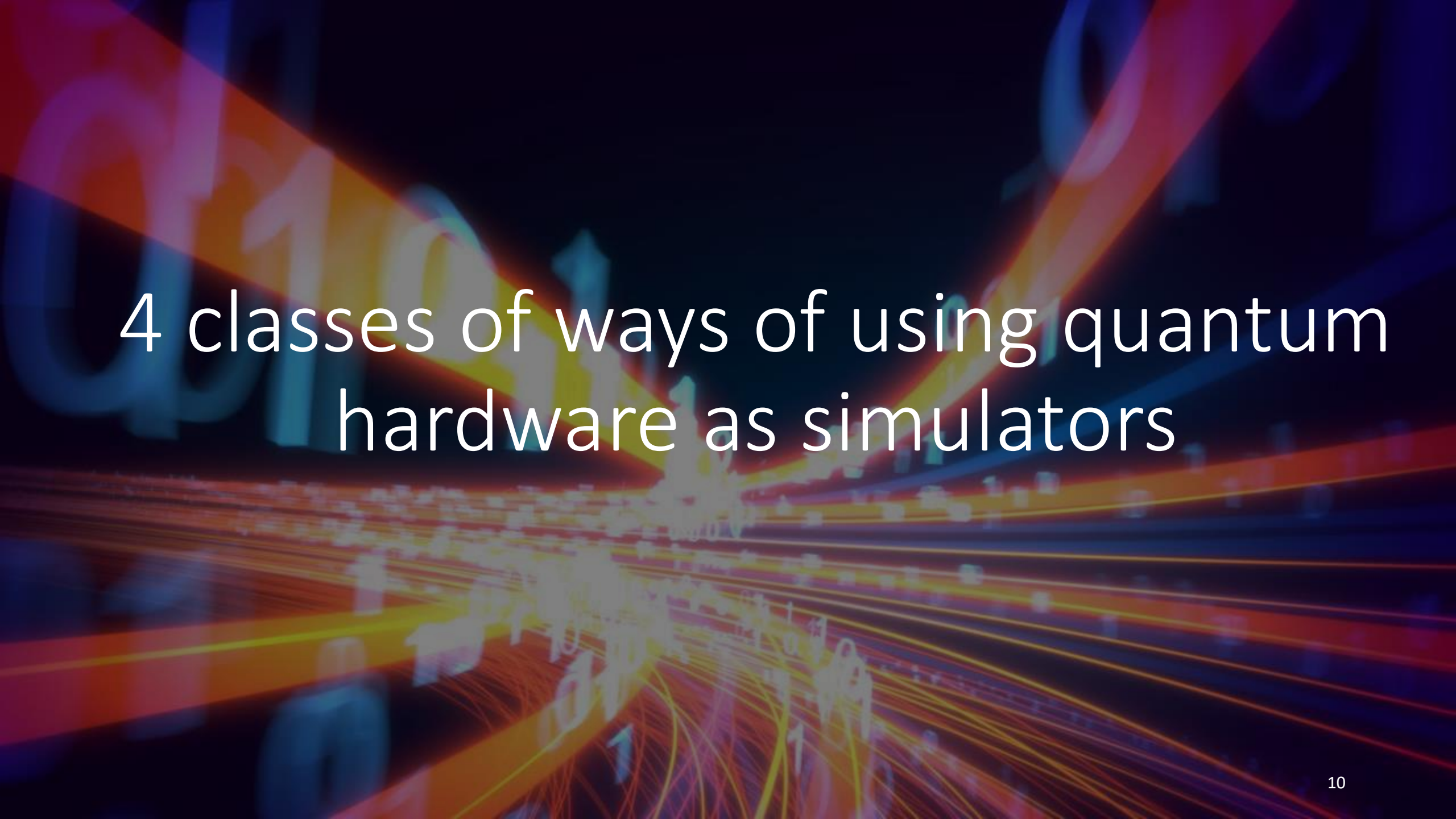
Overview of summer lectures on Schrodingerisation

PART III: Examples session (flexible)!

- **Any of the special topics in Part II in more depth**
- **Going through some examples and explicit circuits**
- **Introducing UnitaryLab: software for quantum simulation for PDEs**
- **Extra topics (a) quantum thermal state preparation for optimization (b) quantum algorithm for algebraic Riccati equation (application to learning problem)**

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



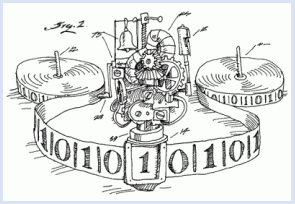
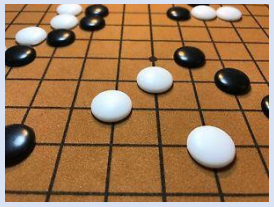
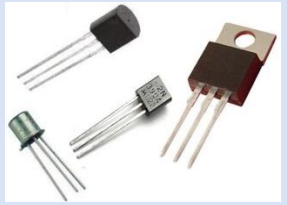
4 classes of ways of using quantum hardware as simulators

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

4 types of simulators/computers	**Continuous/analog**	**Discrete/digital**
Space (data encoding)	*Continuous variable quantum states, qumodes* (infinite dimensional vectors; acted on by operators)	*Qubits, qudits* (finite dimensional vectors; acted on by matrices)
Time (data processing)	*Continuous-time and analogue quantum simulation* (matrix language or operator language, depending on data encoding)	*Digital quantum simulation* (matrix language or operator language, depending on data encoding)

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

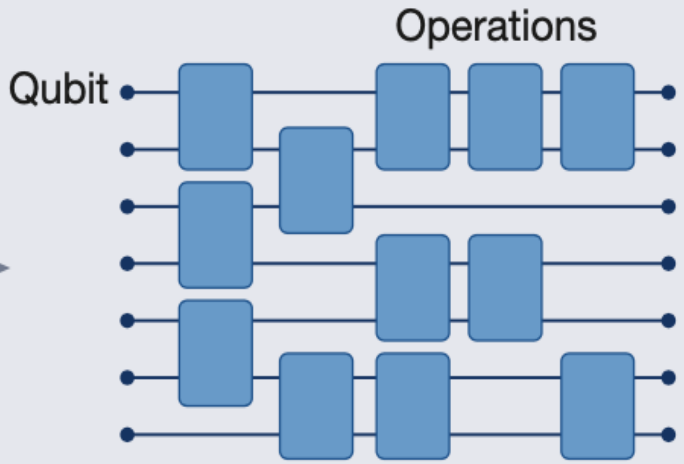
Programmable quantum simulator

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 $\sim t^2/\epsilon$



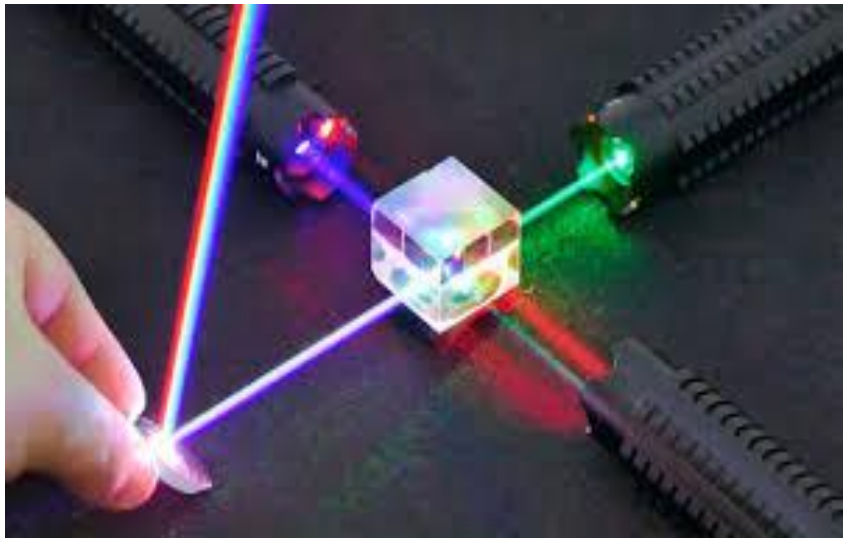
Analogue quantum information: operator language

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

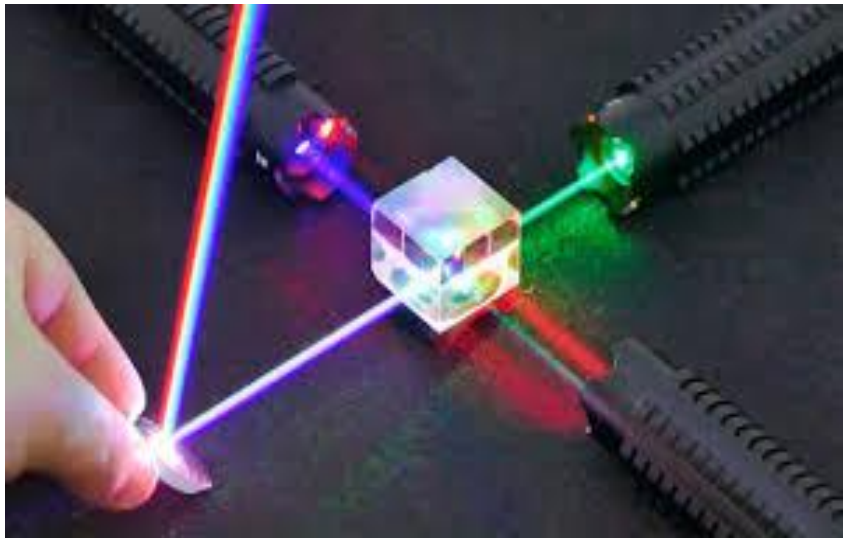
Analogue quantum information: operator language

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

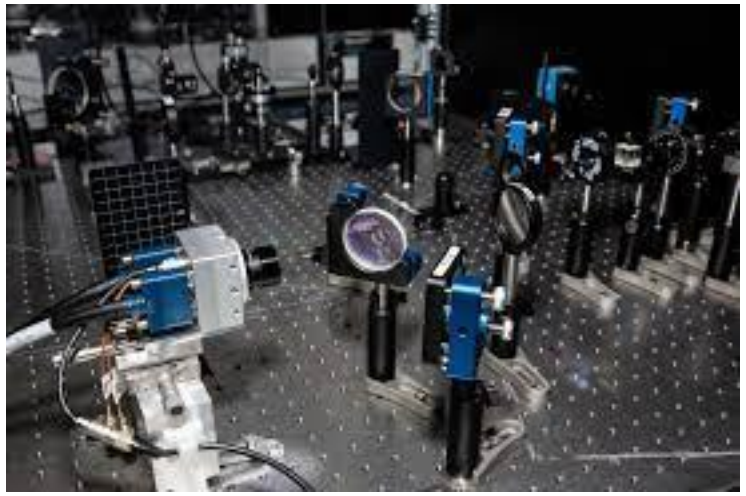
Analogue quantum simulation: evolution in continuous time

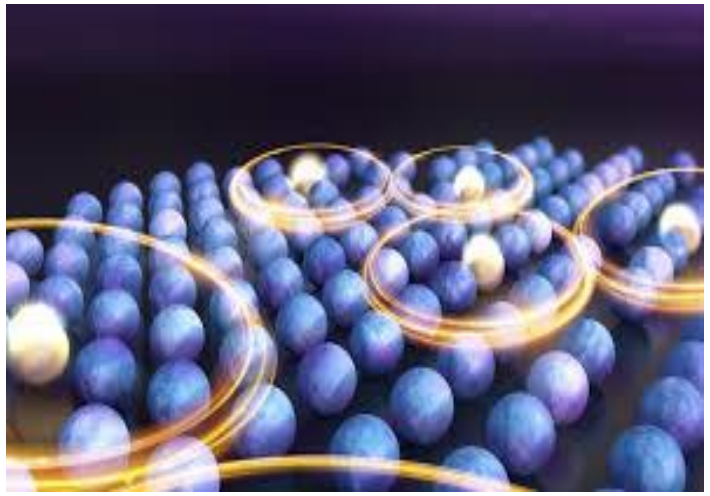
Time evolution through natural dynamics of a quantum system: quantum control of a single Hamiltonian in continuous time

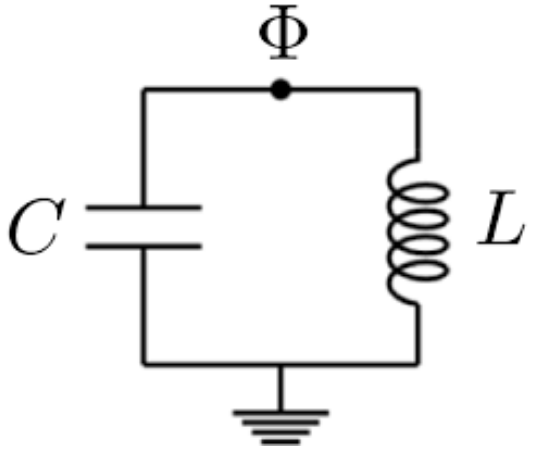
Aim to prepare: $|u(t)\rangle = e^{-iH_{CV}t}|u(0)\rangle$

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

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

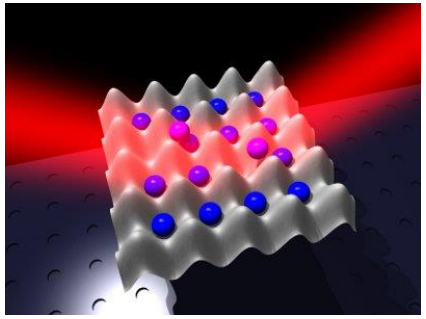
Generating Hamiltonian

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

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

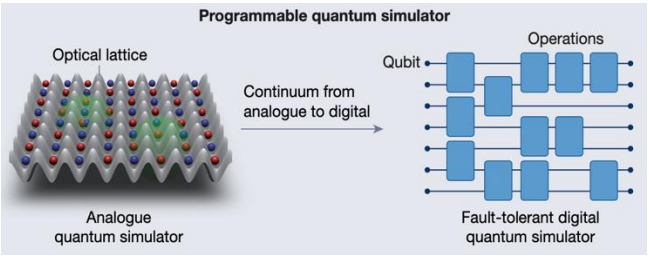
- **Analogue quantum simulation: Nearer-term**

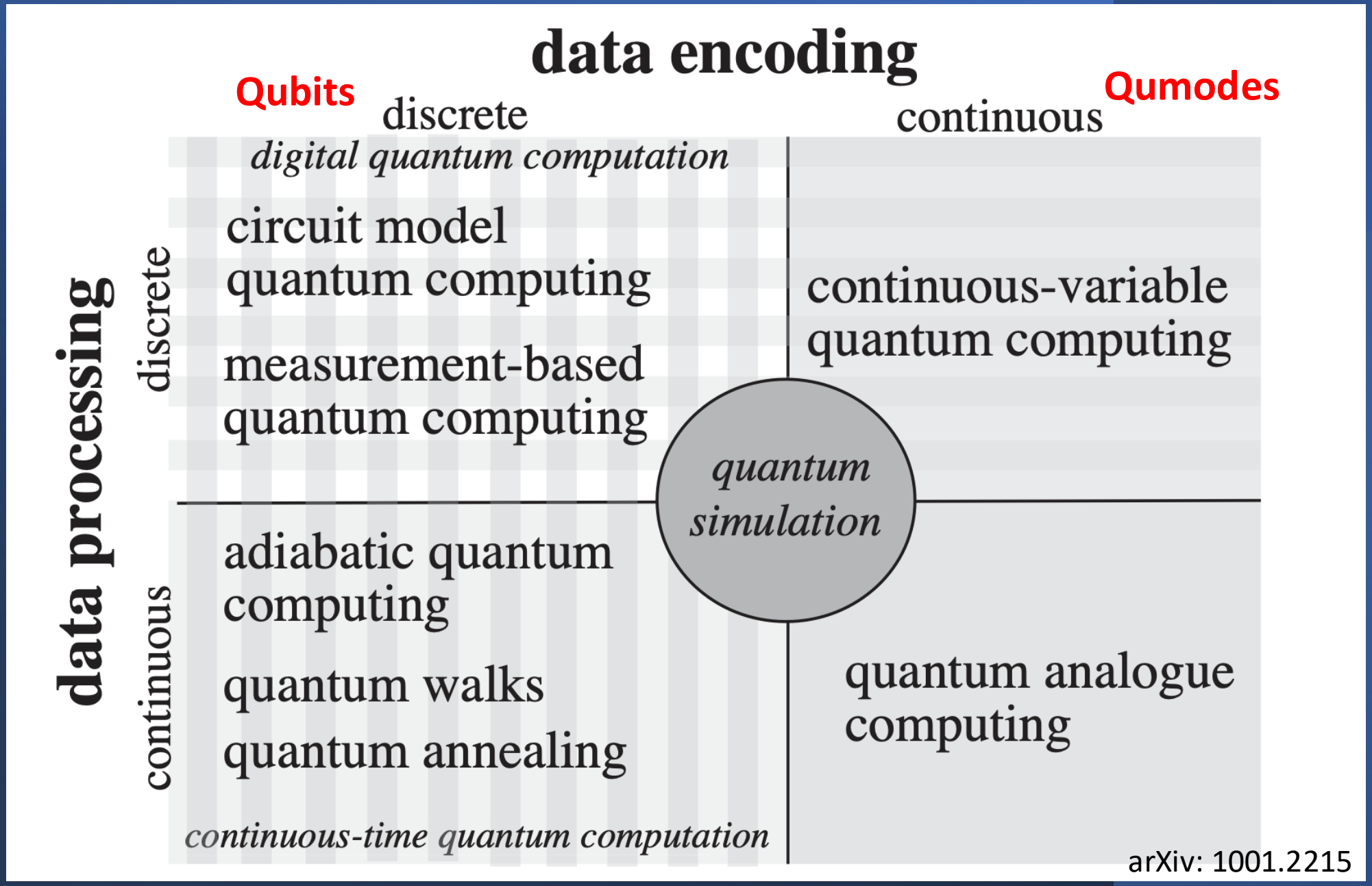
- System evolves naturally *(continuously) in time*
- Can readily scale to large system sizes
- Error limited by accuracy of model used (parameter calibration, noise…etc)
- Continuous spatial degrees of freedom also allowed: analog (or continuous-variable) quantum simulation



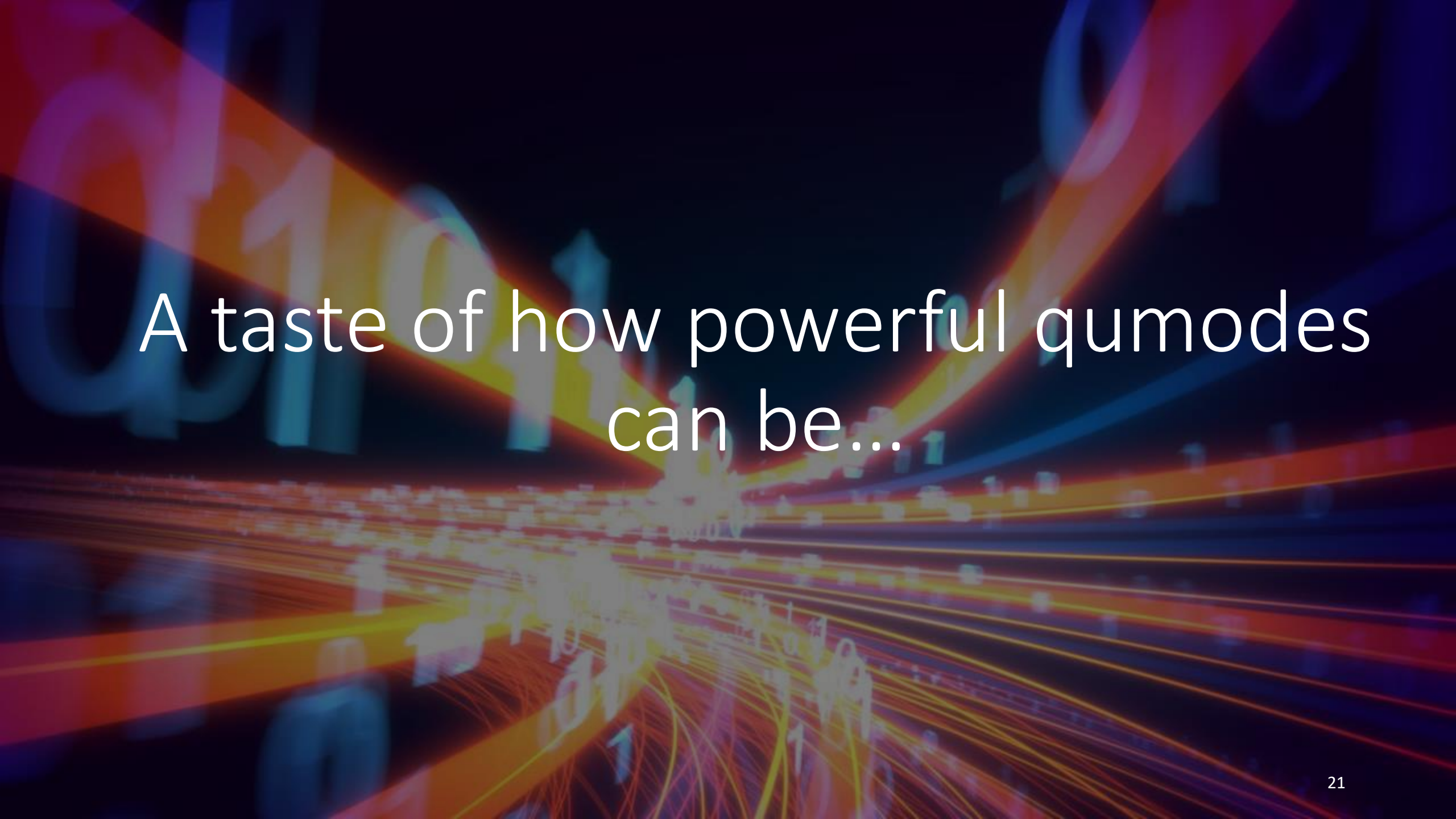
- **Digital quantum simulation: Far-term**

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





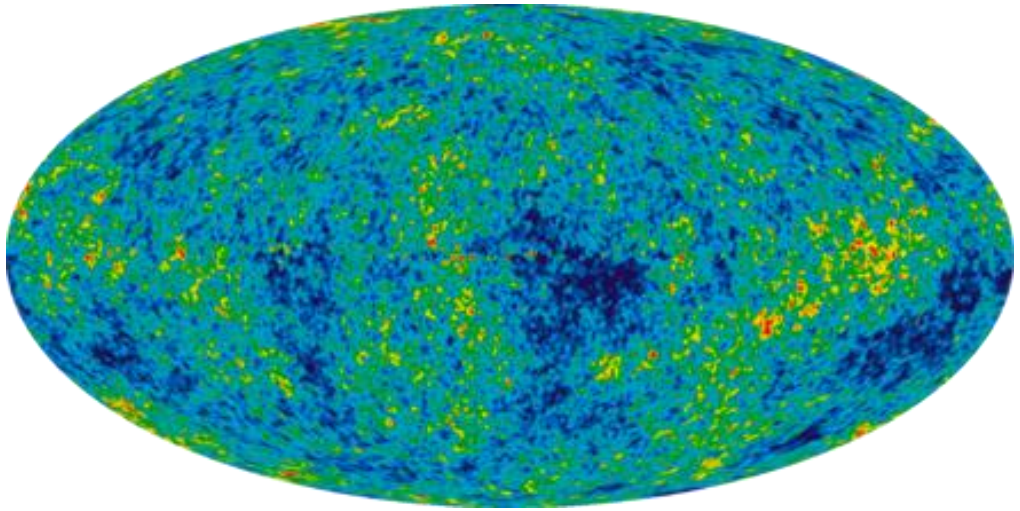
arXiv: 1001.2215


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

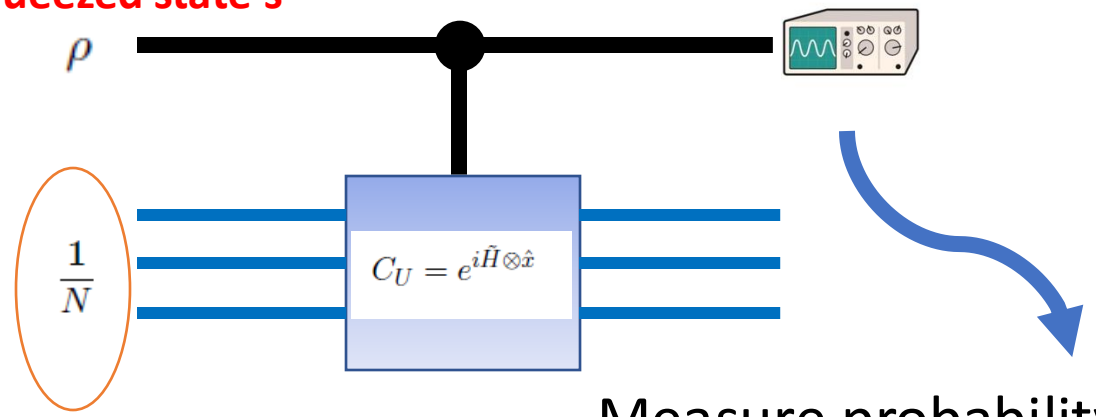
Lots of quantum algorithms based on quantum phase estimation and quantum fourier transforms (crucial part for factoring and other algorithms): https://quantumalgorithmzoo.org/

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

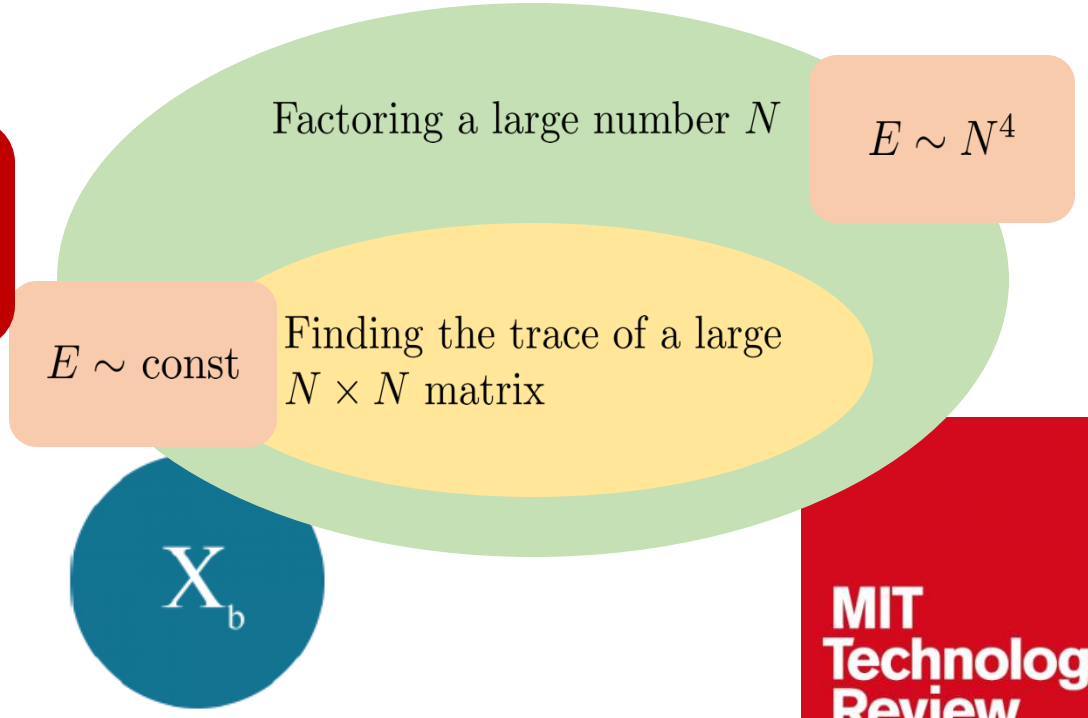
Squeezed state s



Squeezed state input

Measure probability distribution of outcome after running for time τ

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



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

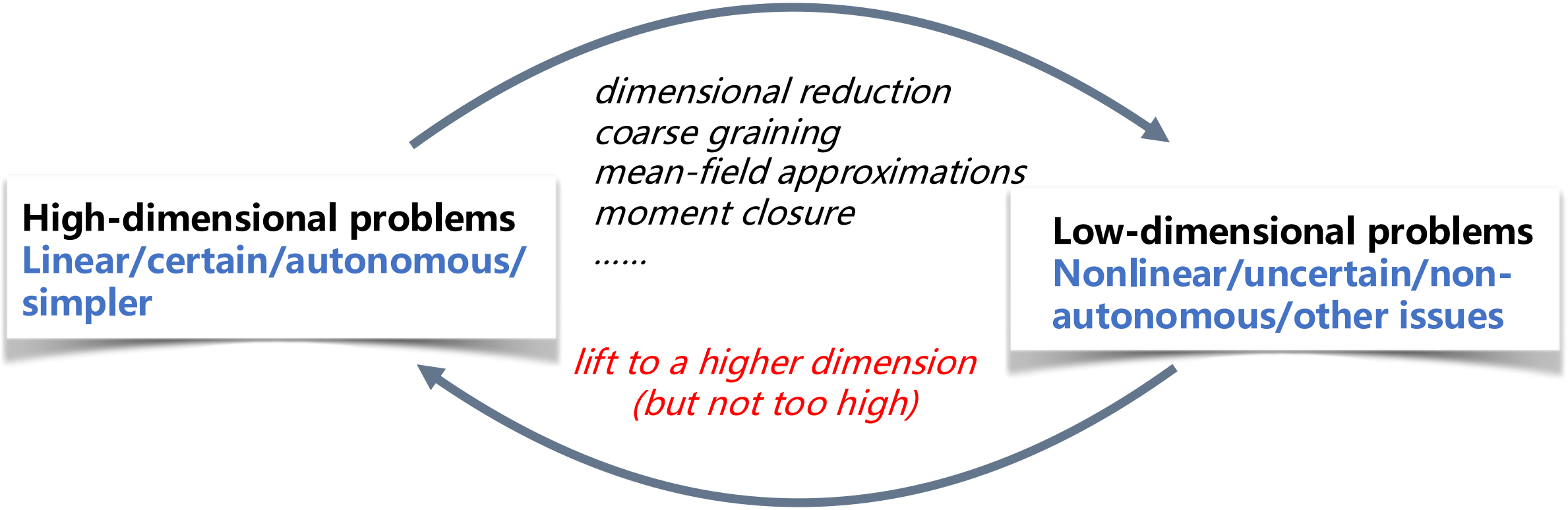
4. Linear non-autonomous systems become linear autonomous

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

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

$Examples:$

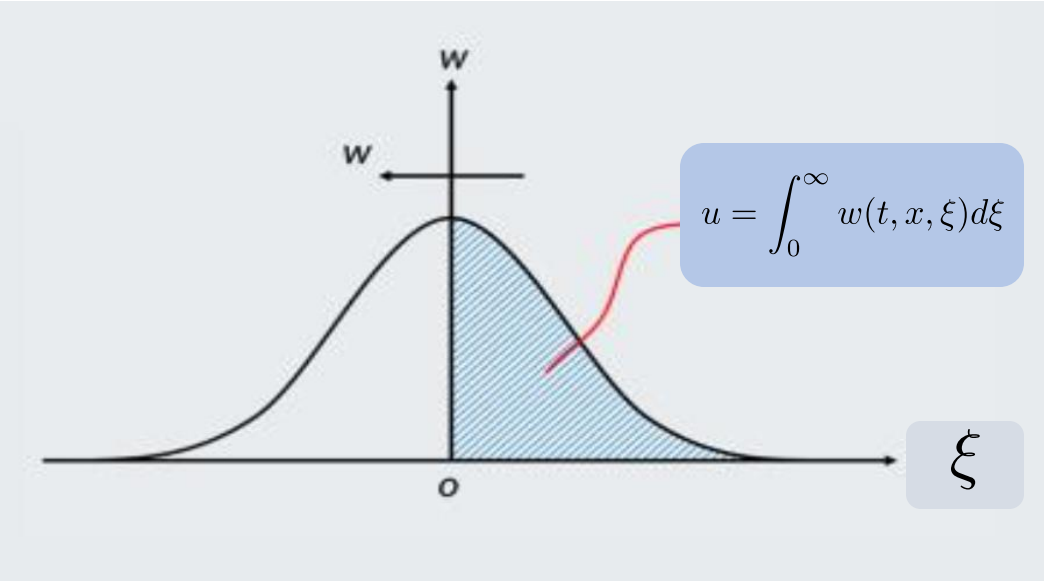
$$\text{Schrodinger: } \mathcal{L} = -i(-\nabla_x^2 + V(x))$$

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

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

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

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

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

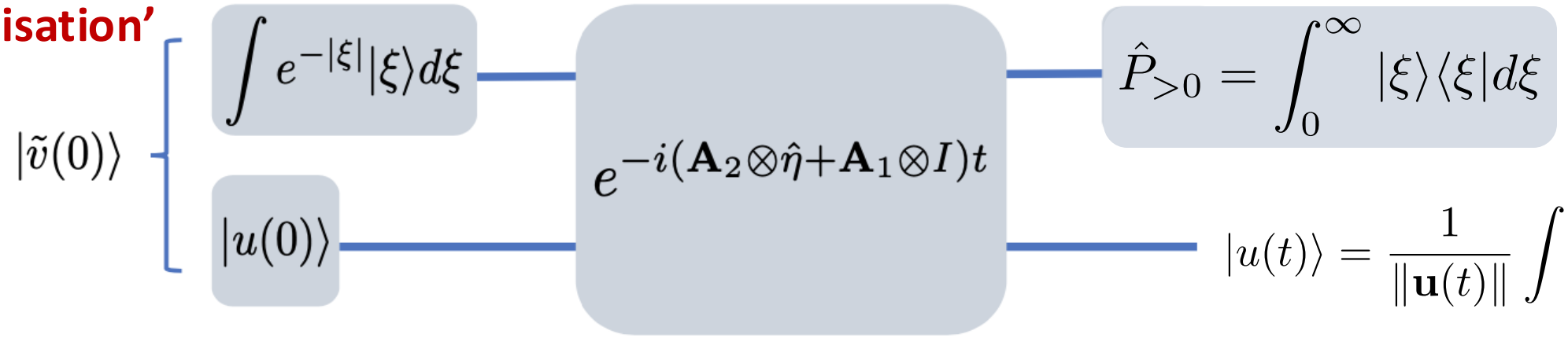
$$\frac{d\tilde{\boldsymbol{v}}(t)}{dt} = -i(\boldsymbol{A}_2 \otimes \hat{\eta} + \boldsymbol{A}_1 \otimes I)\tilde{\boldsymbol{v}}(t) = -i\boldsymbol{H}\tilde{\boldsymbol{v}}(t), \qquad \boldsymbol{H} = \boldsymbol{A}_2 \otimes \hat{\eta} + \boldsymbol{A}_1 \otimes I = \boldsymbol{H}^\dagger,$$

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

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 $\quad |\langle\Xi|G\rangle| \approx 0.986, s \approx 0.925$

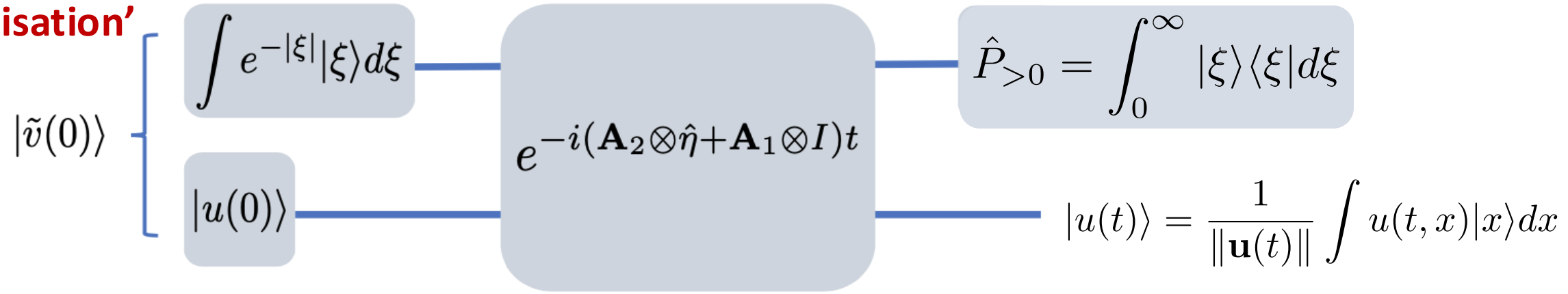
Probability $\frac{\|\mathbf{u}(t)\|^2}{2\|\mathbf{u}(0)\|^2}$

$D+1$ 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 $\quad \dfrac{\partial u}{\partial t} = \sum_k A_k \left(x, \dfrac{\partial^k}{\partial x^k} \right) u$

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

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

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

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:

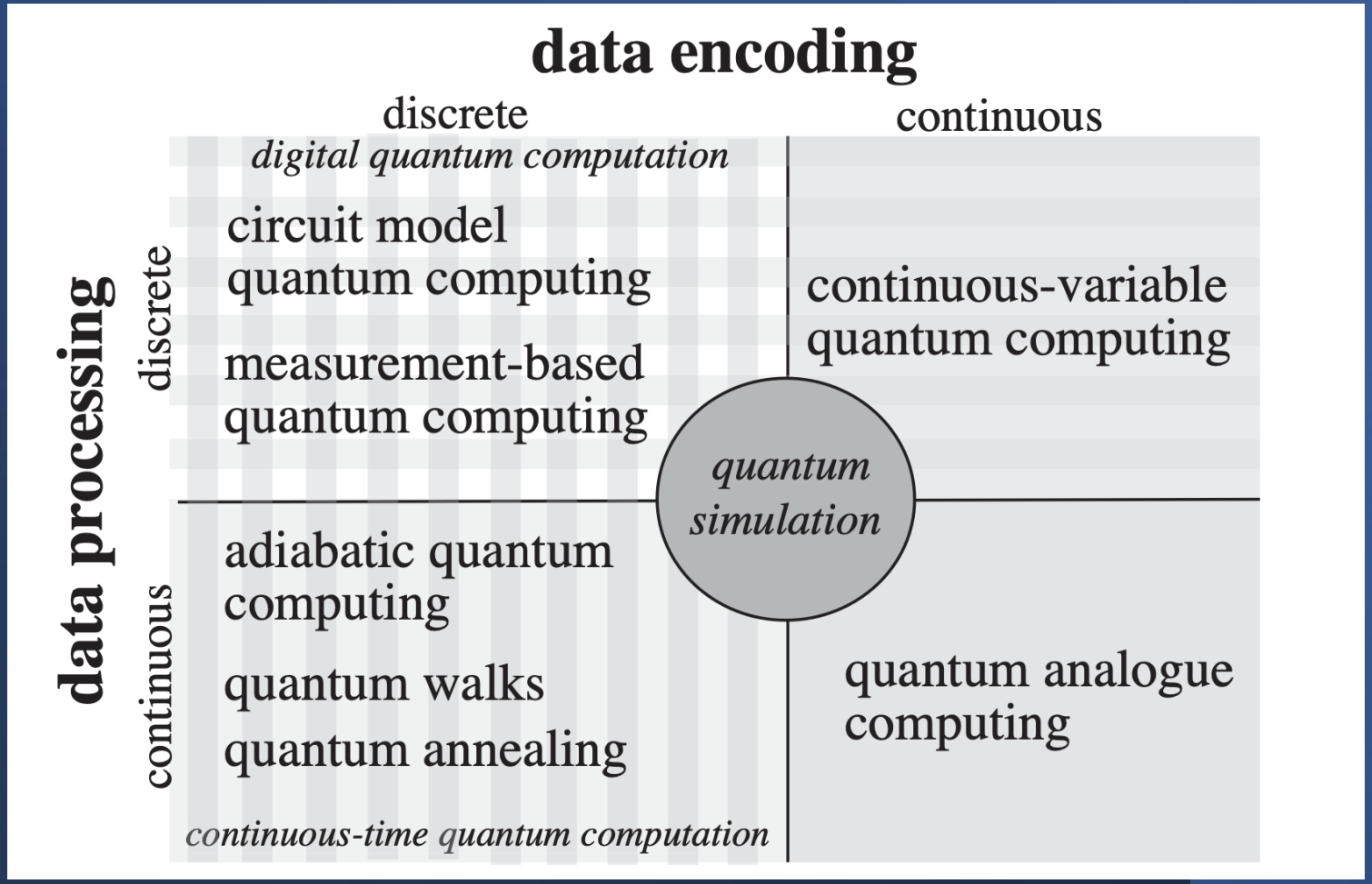
$$\mathbf{H}(t) = \mathbf{A}_2(t) \otimes \hat{\eta} + \mathbf{A}_1(t) \otimes \mathbf{1}$$

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

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

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

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

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

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

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

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:

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

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

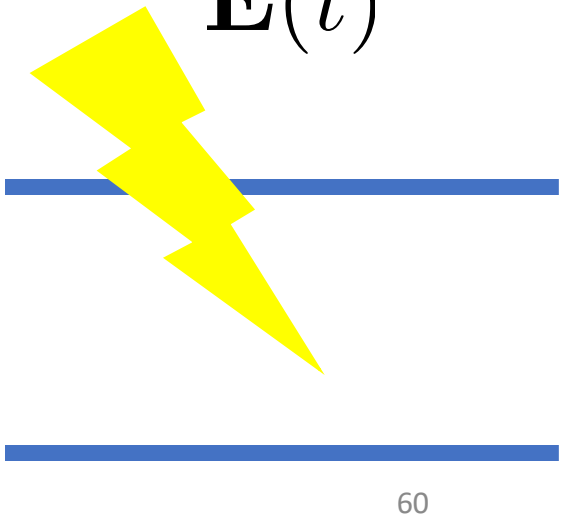
Jaynes-Cummings model

$\mathbf{B}(t)$

Magnetic dipole

Electric dipole

$\mathbf{E}(t)$

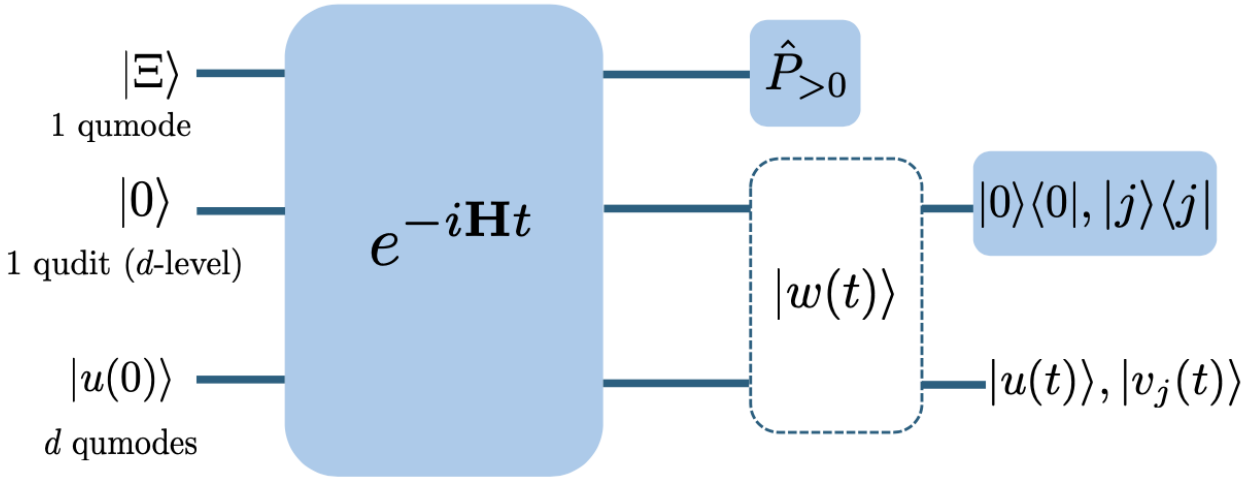


Applications

Applications to:

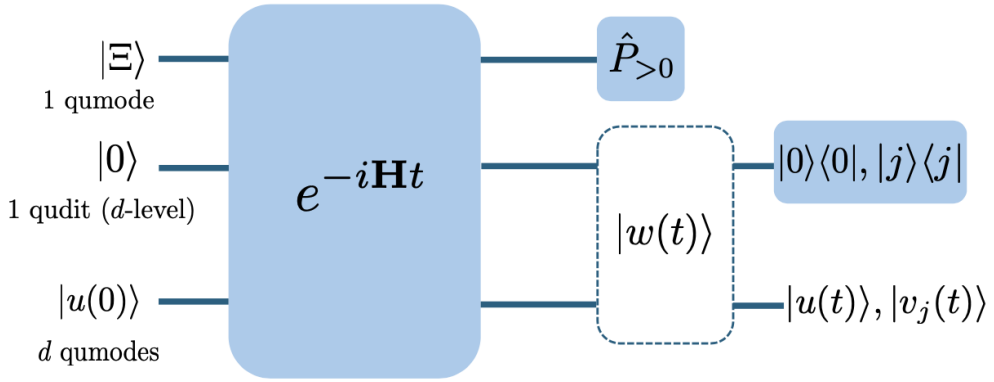
1) **Multidimensional heat equation**
2) **Black-Scholes equation: 1-dimensional (heat) and multidimensional**
3) **Fokker-Planck equations**

….realisable in cavity and circuit QED systems



Applications

Equation	Size of system	Hamiltonian $\boldsymbol{H}$ interaction terms
1D heat	1 qubit and 2 qumodes	$\mathbf{1}_2 \otimes \mathbf{1}_x \otimes \hat{\eta}, \quad \sigma_z \otimes \mathbf{1}_x \otimes \hat{\eta}, \quad \sigma_x \otimes \hat{p}_x \otimes \mathbf{1}_\eta$
1D Black-Scholes	1 qubit and 2 qumodes	$\mathbf{1}_2 \otimes \mathbf{1}_x \otimes \hat{\eta}, \quad \sigma_z \otimes \mathbf{1}_x \otimes \hat{\eta}, \quad \sigma_x \otimes \hat{p}_x \otimes \mathbf{1}_\eta$ $\sigma_z \otimes \hat{p}_x \otimes \mathbf{1}_\eta, \quad \mathbf{1}_2 \otimes \hat{p}_x \otimes \mathbf{1}_\eta$
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	$\lvert j\rangle\langle j\rvert \otimes \mathbf{1}_x \otimes \hat{\eta}, \; (\lvert 0\rangle\langle j\rvert + \lvert j\rangle\langle 0\rvert) \otimes \hat{p}_x \otimes \mathbf{1}_\eta, \lvert 0\rangle\langle 0\rvert \otimes \hat{p}_x \otimes \mathbf{1}_\eta, \; j = 1, \cdots, d$



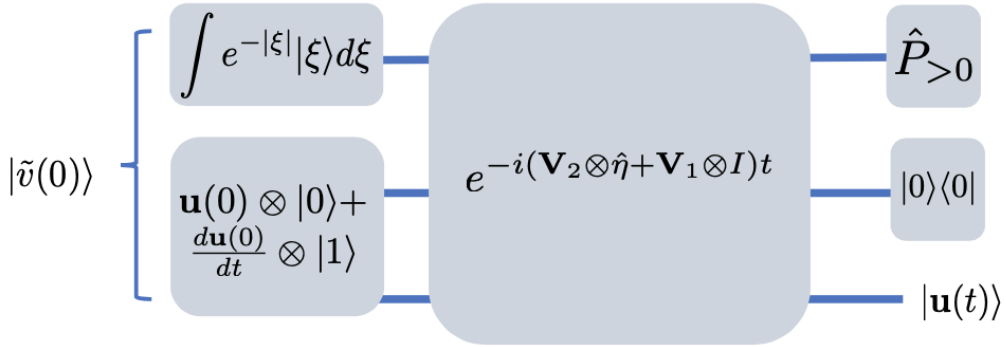
Higher-order time derivatives…second order example

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

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

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

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

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

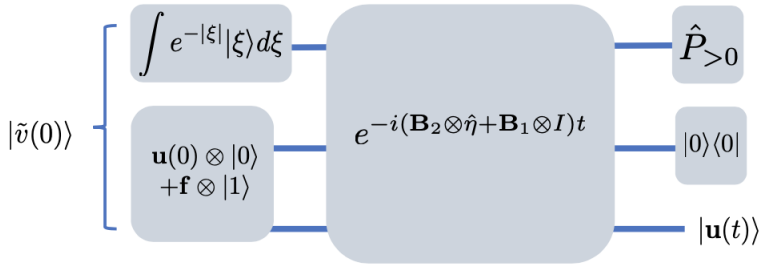
- Backward PDEs

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

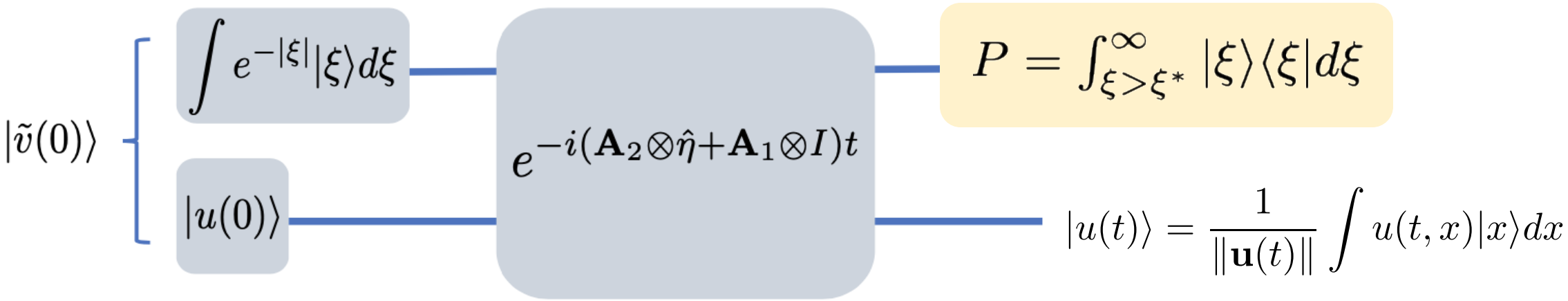
$|\lambda_D|$: interpreted as the maximum speed of the right-moving w solution along ξ

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 $\mathbf{w}$ 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

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

$\hat{p} = -i\dfrac{\partial}{\partial x} \to N \times N$ 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: $\eta \to \eta_i, \quad i = 0, \cdots, M \quad \hat{\eta} \to \mathrm{diag}(-M/2, \cdots, M/2-1)$

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

- 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 $i = 1, \cdots, N$:

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

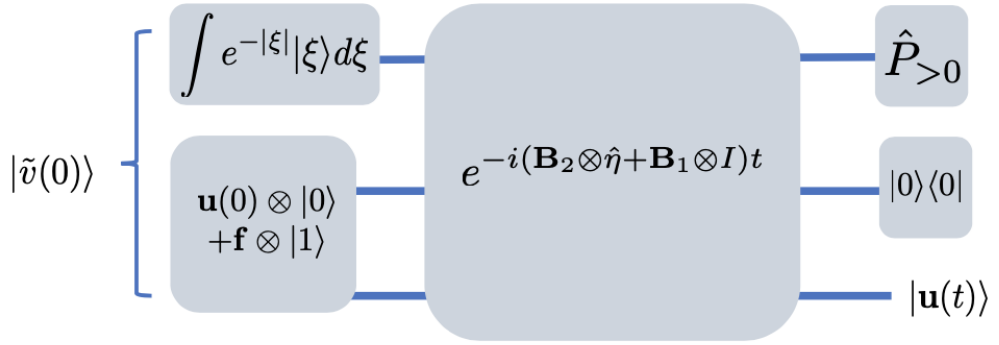
Dirichlet BCs: $u(0, t) = A, \quad u(L, t) = B \Rightarrow u_0 = A, \quad u_{N+1} = B$

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

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

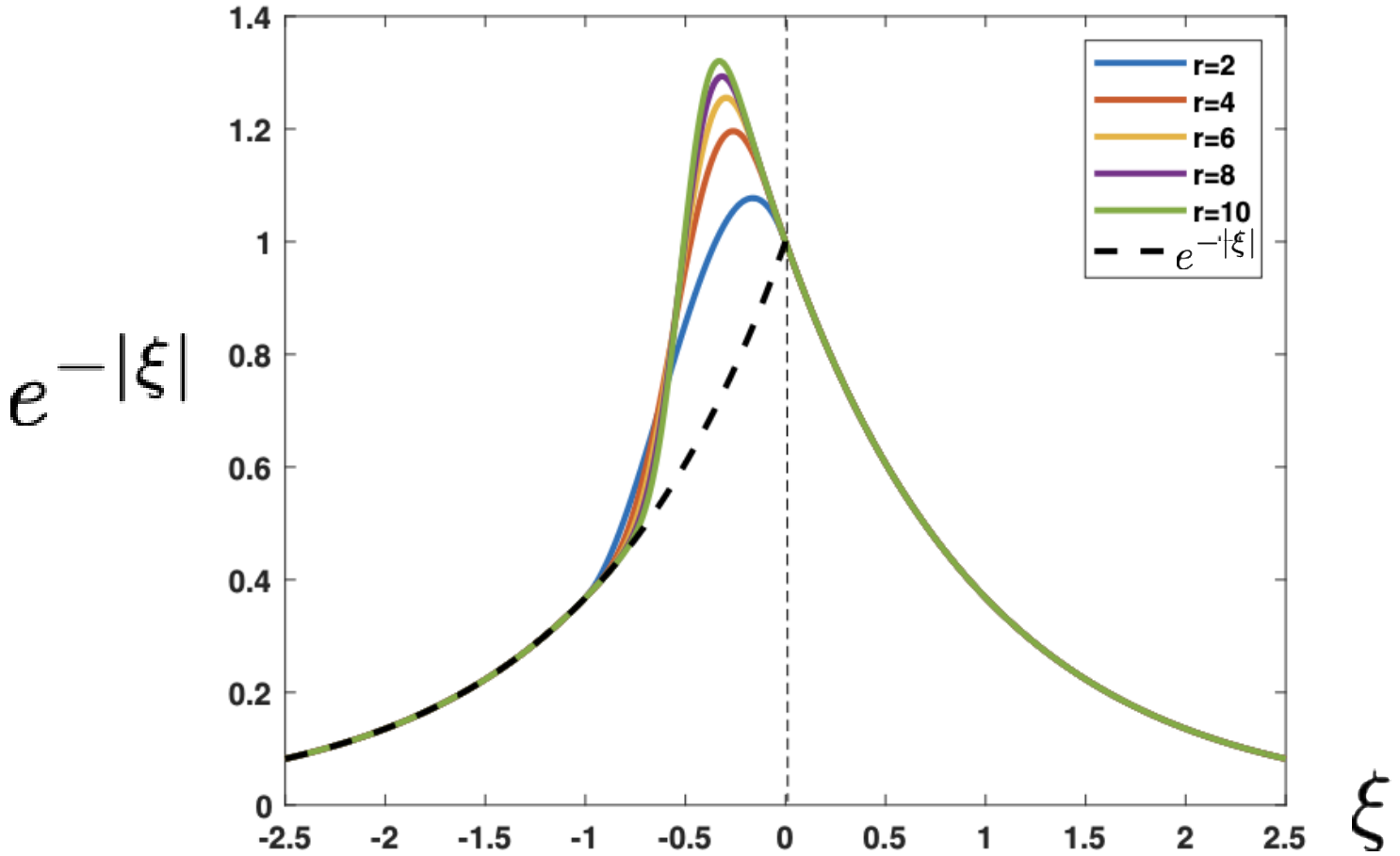
If $\|\psi - \hat{\psi}\| \leq \epsilon \implies N_\xi \sim (R-L)|\psi|_r^{1/r} \epsilon^{-1/r}$

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).

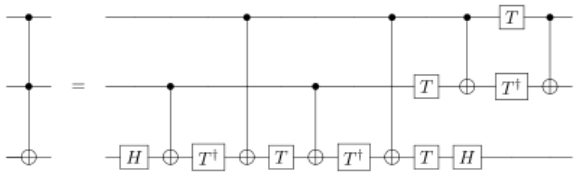
Where is the quantum? Future interesting questions

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



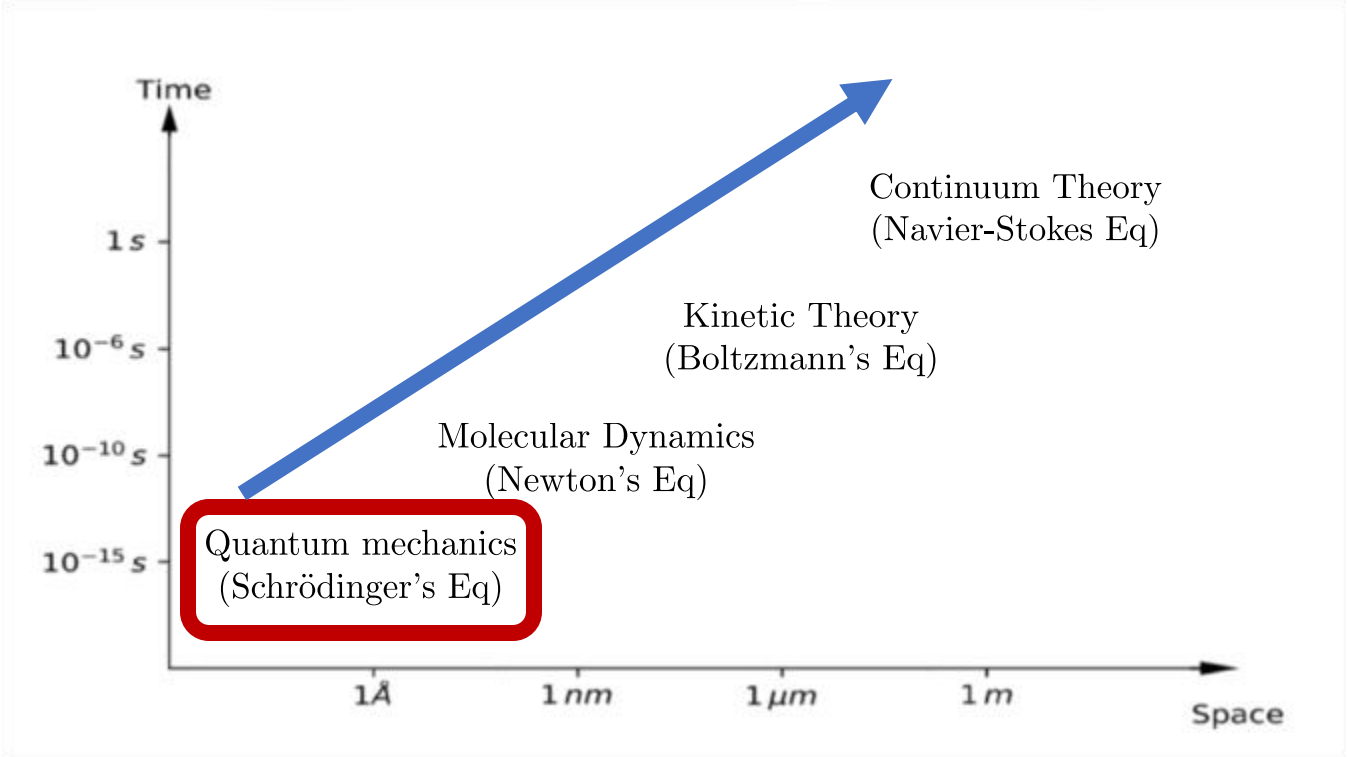
$$T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}$$

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

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

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	$N+1$	$i[Q, F] \otimes \hat{\eta}$, $\{Q, F\} \otimes I$	$O(N)$

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.

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

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

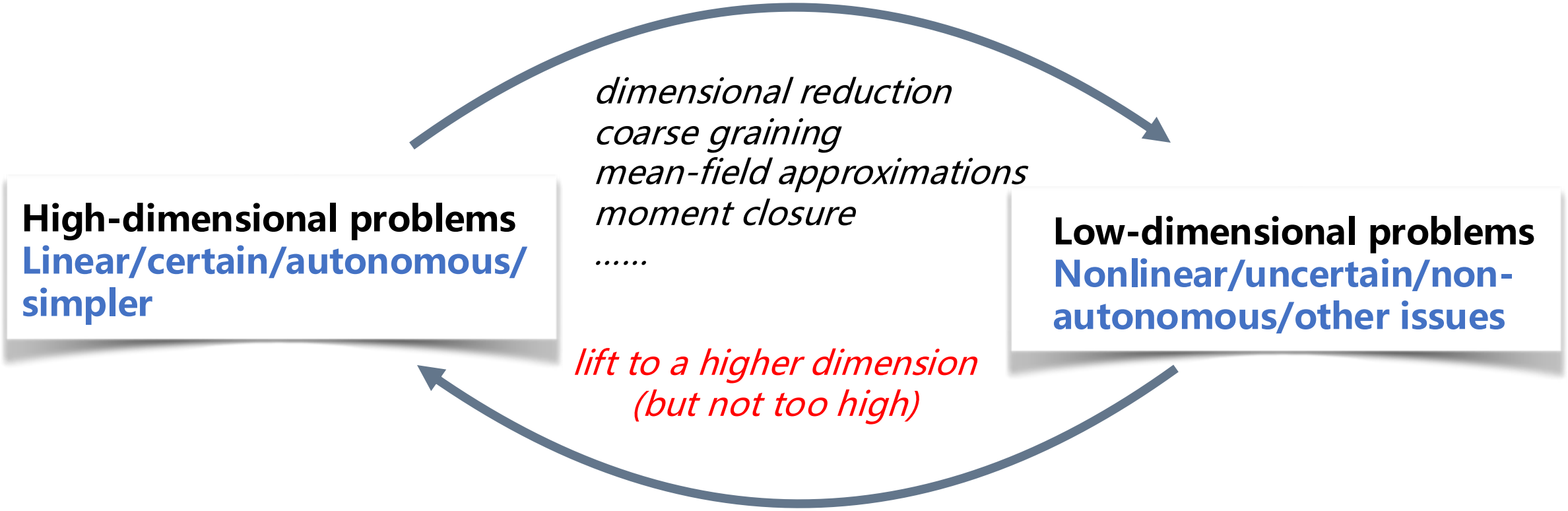
4. Linear non-autonomous systems become linear autonomous

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

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

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)

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Overview of summer lectures on Schrodingerisation

PART II: Special topics

- **Nonlinear ODEs and PDEs**
- **Uncertain ODEs/PDEs**
- **Non-autonomous mapped to autonomous PDEs**
- **Application to linear algebra, ground state and thermal state preparation**

Overview of summer lectures on Schrodingerisation

PART III: Examples session (flexible)!

- **Any of the special topics in Part II in more depth**
- **Going through some examples and explicit circuits**
- **Introducing UnitaryLab: software for quantum simulation for PDEs**
- **Extra topics (a) quantum thermal state preparation for optimization (b) quantum algorithm for algebraic Riccati equation (application to learning problem)**

Preparation for using UnitaryLab software: To install today (available in French)!

https://randbatch.com:8443/unitarylab/index.html

Installing UnitaryLab software

⚠ **Activation required on first launch**

- Copy your Device ID from the pop-up
- Email it to: hjp3268@sjtu.edu.cn with subject: pdeClient Activation Request
- **You'll receive activation code within 24h**
- Paste the code to unlock full features

Installing UnitaryLab software

Installing the software directly:

https://sjtueducn-my.sharepoint.com/:f:/g/personal/hjp3268_sjtu_edu_cn/EuSUbJPRn91DvISg68OquLQBjwY06S-ee8adqxYY5BEoVw

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Institute of Natural Sciences

University of Michigan-Shanghai Jiao Tong Joint Institute

Open postdoc positions available!

Nana.Liu@quantumlah.org

www.nanaliu.weebly.com

Group website:
https://www.quantumquintet.com/

Quantum simulation of partial differential equations via Schrodingerisation

PART II: Special topics Nonlinear PDEs

Nana Liu
Shanghai Jiao Tong University

CEMRACS 15-19 Jul 2025

Overview of summer lectures on Schrodingerisation

PART II: Special topics

- **Nonlinear ODEs and PDEs**
- **Uncertain ODEs/PDEs**
- **Non-autonomous mapped to autonomous PDEs**
- **Application to linear algebra, ground state and thermal state preparation**

II. Nonlinear ODEs and PDEs

``Turning nonlinear ODEs and PDEs into linear PDEs"

Based on:
"Quantum algorithms for nonlinear partial differential equations", (arXiv: 2209.08478), Bulletin de Sciences Mathematiques, Shi Jin, Nana Liu*

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

Nonlinear systems

Applications in fluid dynamics (Navier-Stokes), gas dynamics, molecular dynamics, financial markets, machine learning…etc

Unpredictability: breakdown of perturbative theory (e.g. Bruns: if perturbation theory converges in neighbourhood of one point, at other points it must diverge), chaos…etc

Appearance of discontinuities and shock solutions and singularities

Often statistical methods are employed: to understand ensemble behaviour (e.g. statistical behaviour of fluids)

Is it possible to have quantum advantages in solving nonlinear ODEs and PDEs?

- What do we mean by solve?
- What do we mean by advantage?
- How do we embed the nonlinearity?

Nonlinear ODEs and PDEs with multiple M initial conditions

D ODEs

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

Nonlinear F

$(d+1)$-dim PDEs

$$\frac{\partial u^{[k]}}{\partial t} + F(u^{[k]}, \nabla u^{[k]}, \nabla^2 u^{[k]}, ...) = 0$$
$$u^{[k]} \in \mathbb{R}^d \qquad k = 1, ..., M$$

Nonlinear F

Classical versus quantum solutions

Classical solutions

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

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

Quantum solutions

Typically...

$$\propto \sum_t X^{[k]}(t)|t\rangle$$

$$\propto \sum_{(x,t)} u^{[k]}(x,t)|x,t\rangle$$

Classical versus quantum solutions

Classical solutions

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

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

Quantum solutions

Typically...

$$\propto \sum_t X^{[k]}(t)|t\rangle$$

$$\propto \sum_{(x,t)} u^{[k]}(x,t)|x,t\rangle$$

Compare observables only

Classical versus quantum cost

Classical cost

Numerical steps

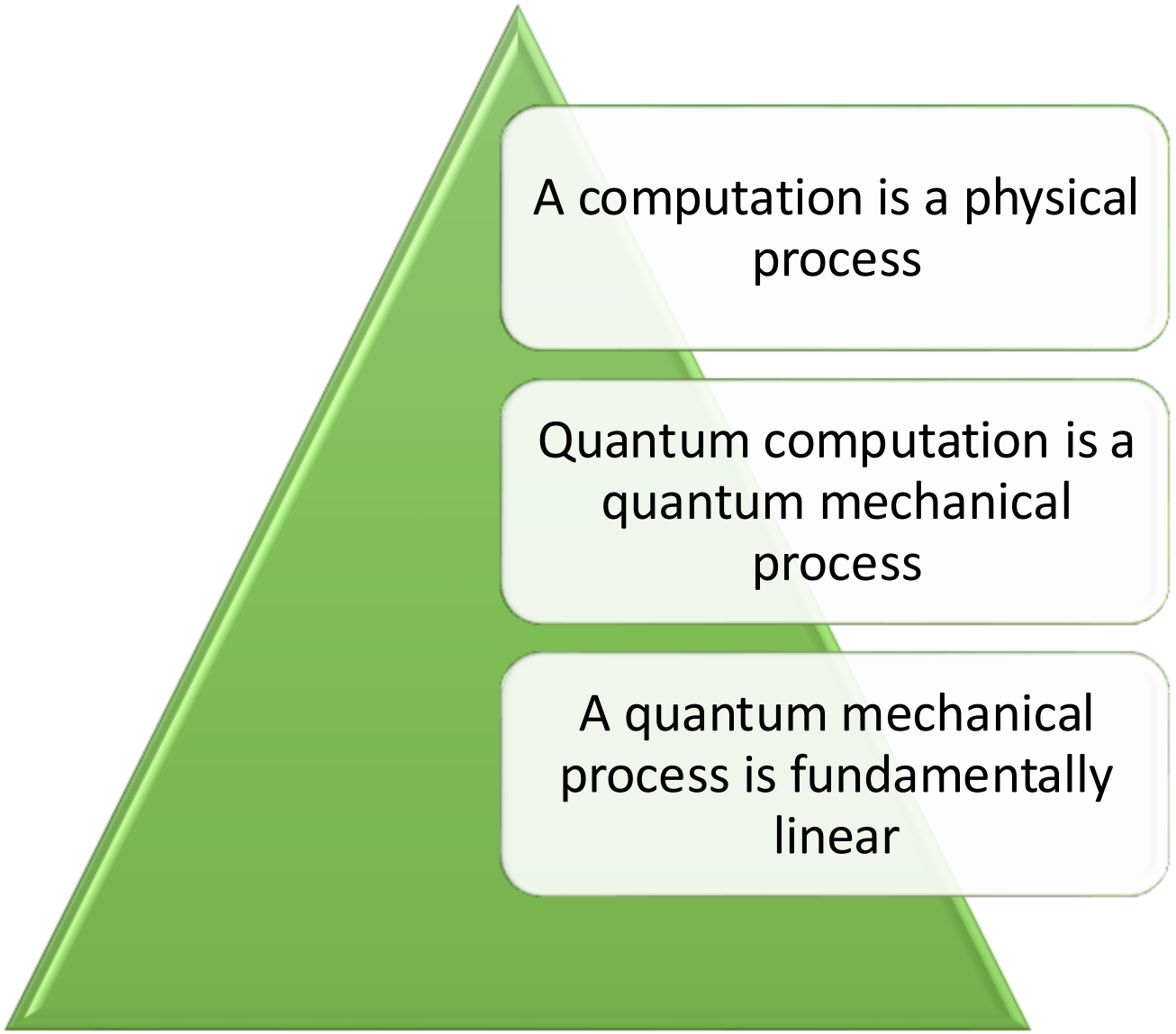
Quantum cost

Query complexity

Gate complexity

Parameters: d, D, ϵ, T, M

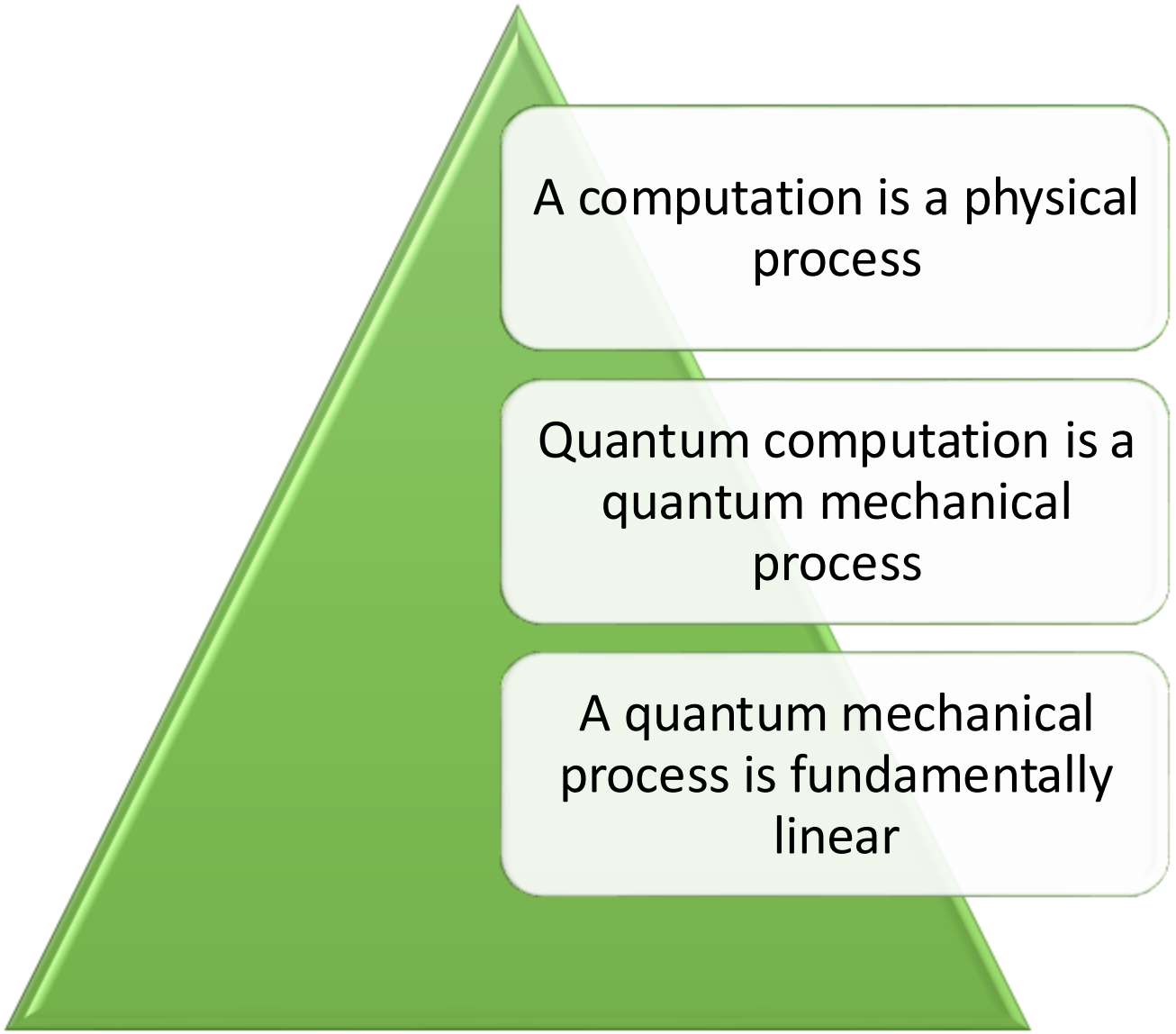
Are nonlinear problems suitable for quantum computation?



Two routes:

1) Make the problem look linear

2) Don’t use fundamental quantum mechanics

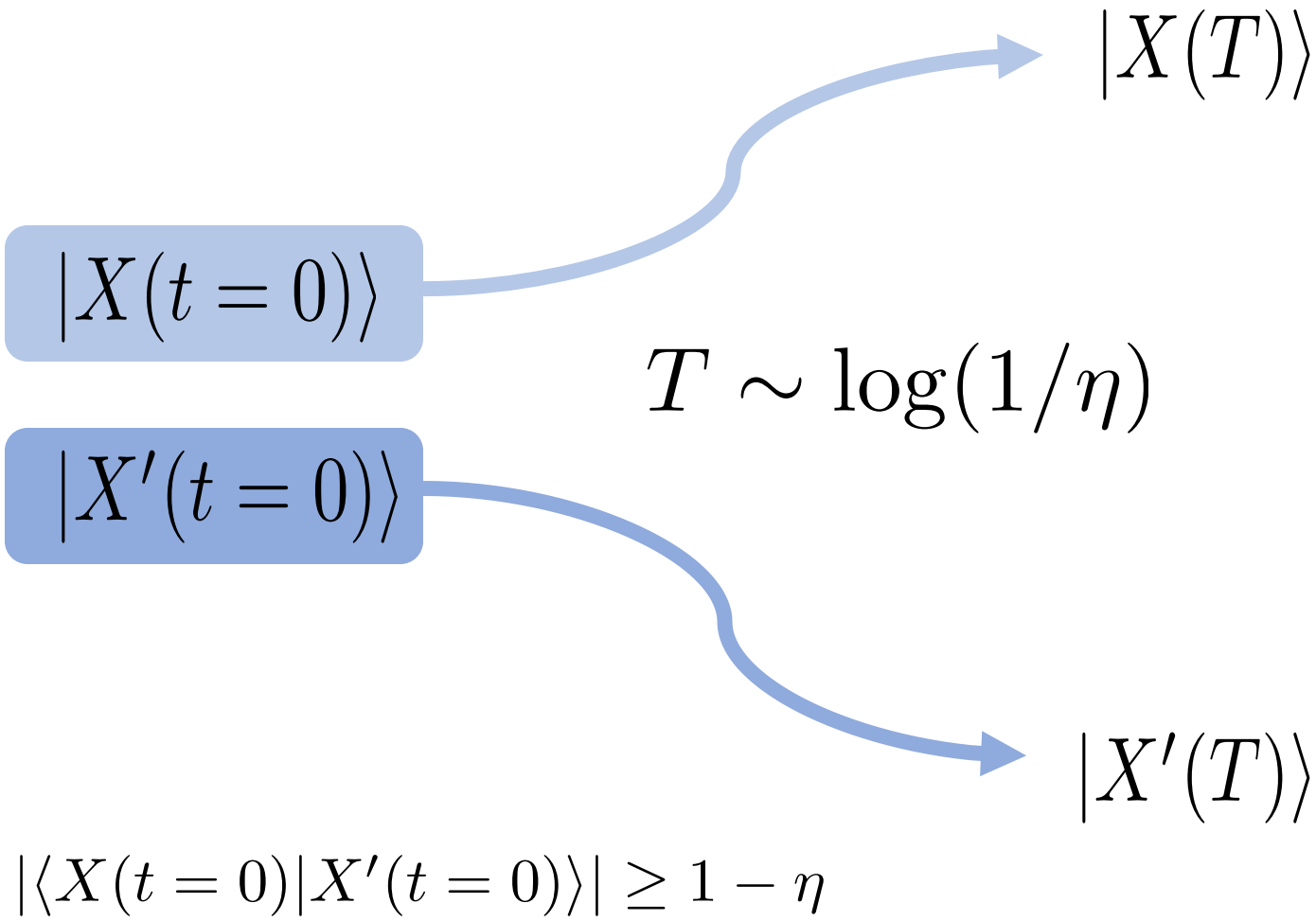


Two routes:

1) Make the problem look linear

2) Don't use fundamental quantum mechanics

Nonlinear quantum mechanics

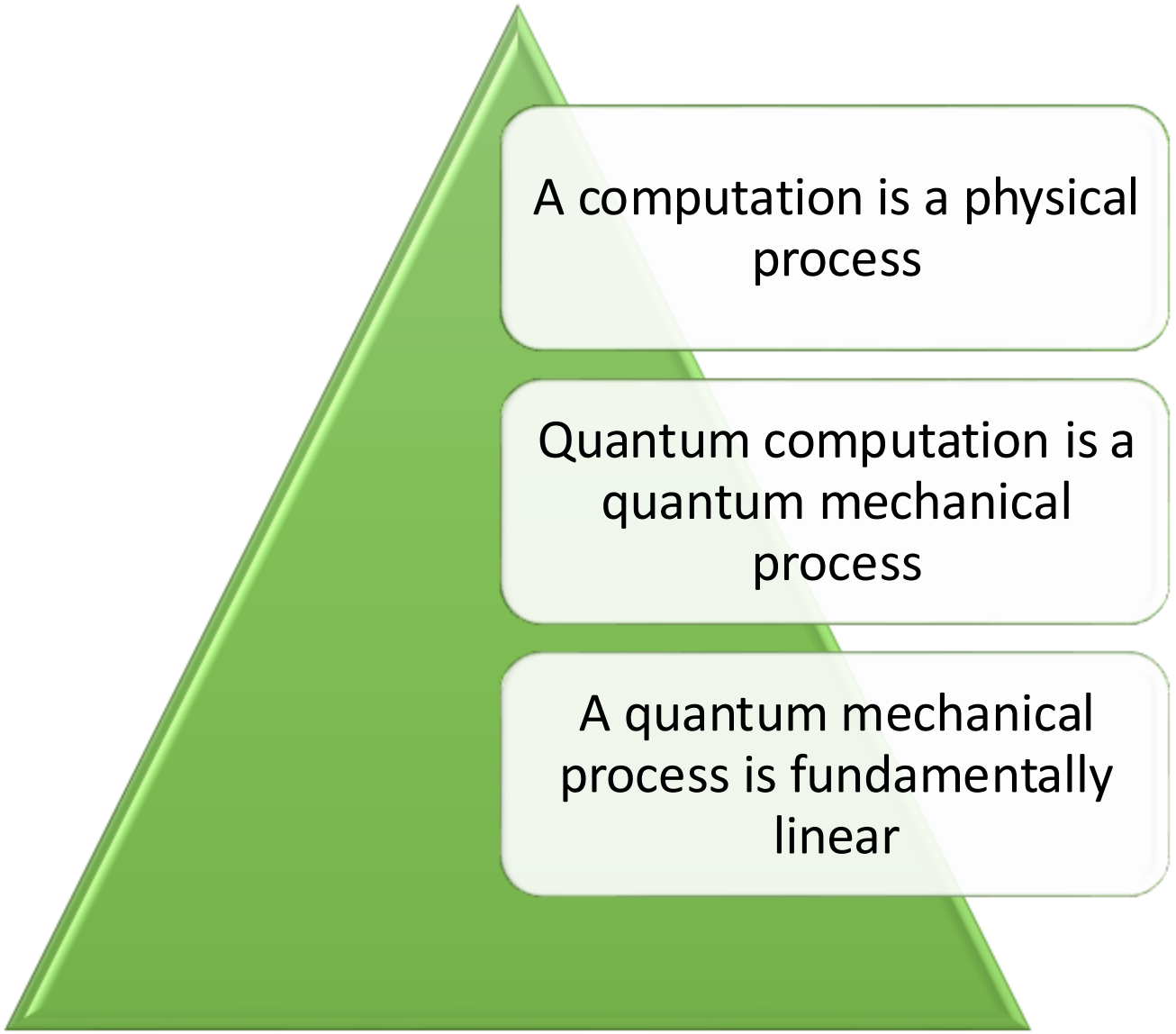


$$|\langle X(t=0)|X'(t=0)\rangle| \geq 1-\eta$$

Two routes:

1) Make the problem look linear

2) Don’t use fundamental quantum mechanics

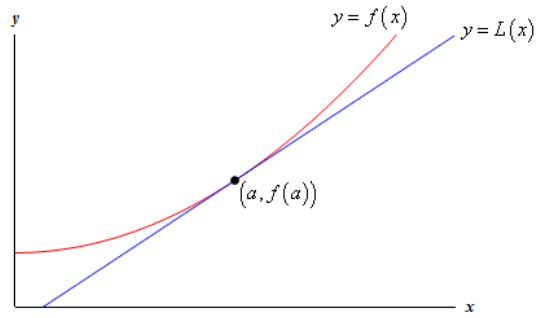


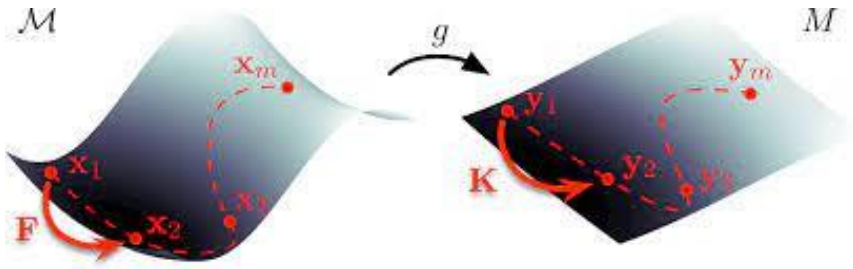
Making nonlinear problem look linear

Approximations

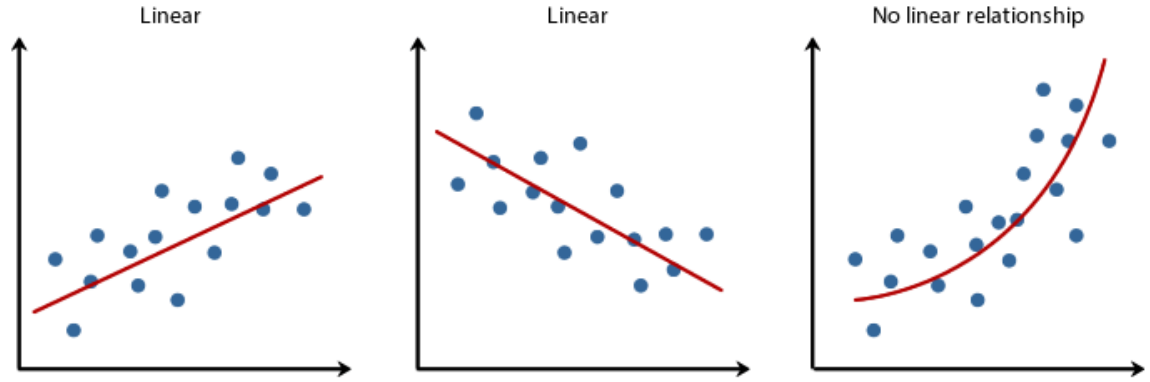
Exact mapping

Making nonlinear problem look linear

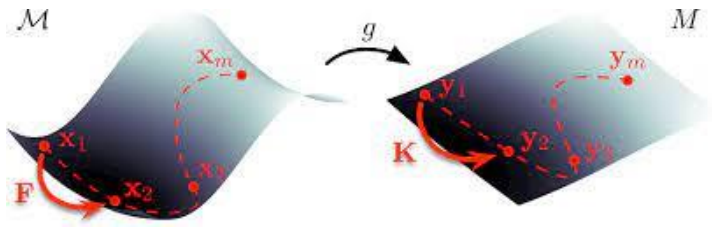




Approximations

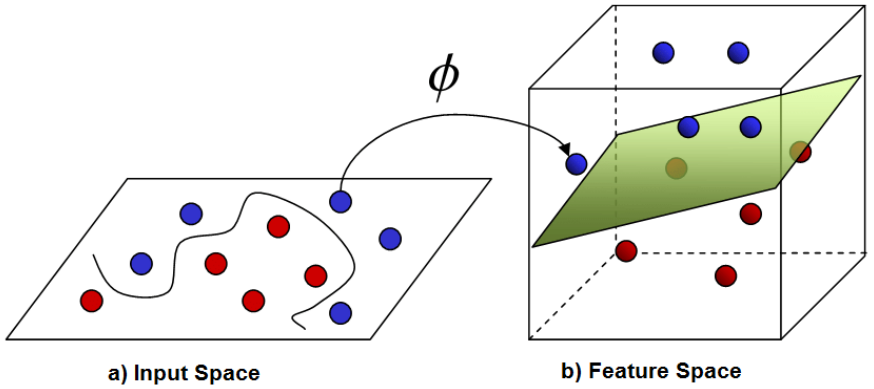


Making nonlinear problem look linear



Can map to finite-dimensional system & capture *any* nonlinearity?

Sometimes ∞-dimensional space



Exact mapping

Making nonlinear problem look linear

2D Burgers' Equation

- Exact solution
- Use Cole-Hopf transformation

$$\bar{u} = \frac{-2\nu \dfrac{\partial \bar{\Phi}}{\partial x}}{\bar{\Phi}}, \quad \bar{v} = \frac{-2\nu \dfrac{\partial \bar{\Phi}}{\partial y}}{\bar{\Phi}}$$

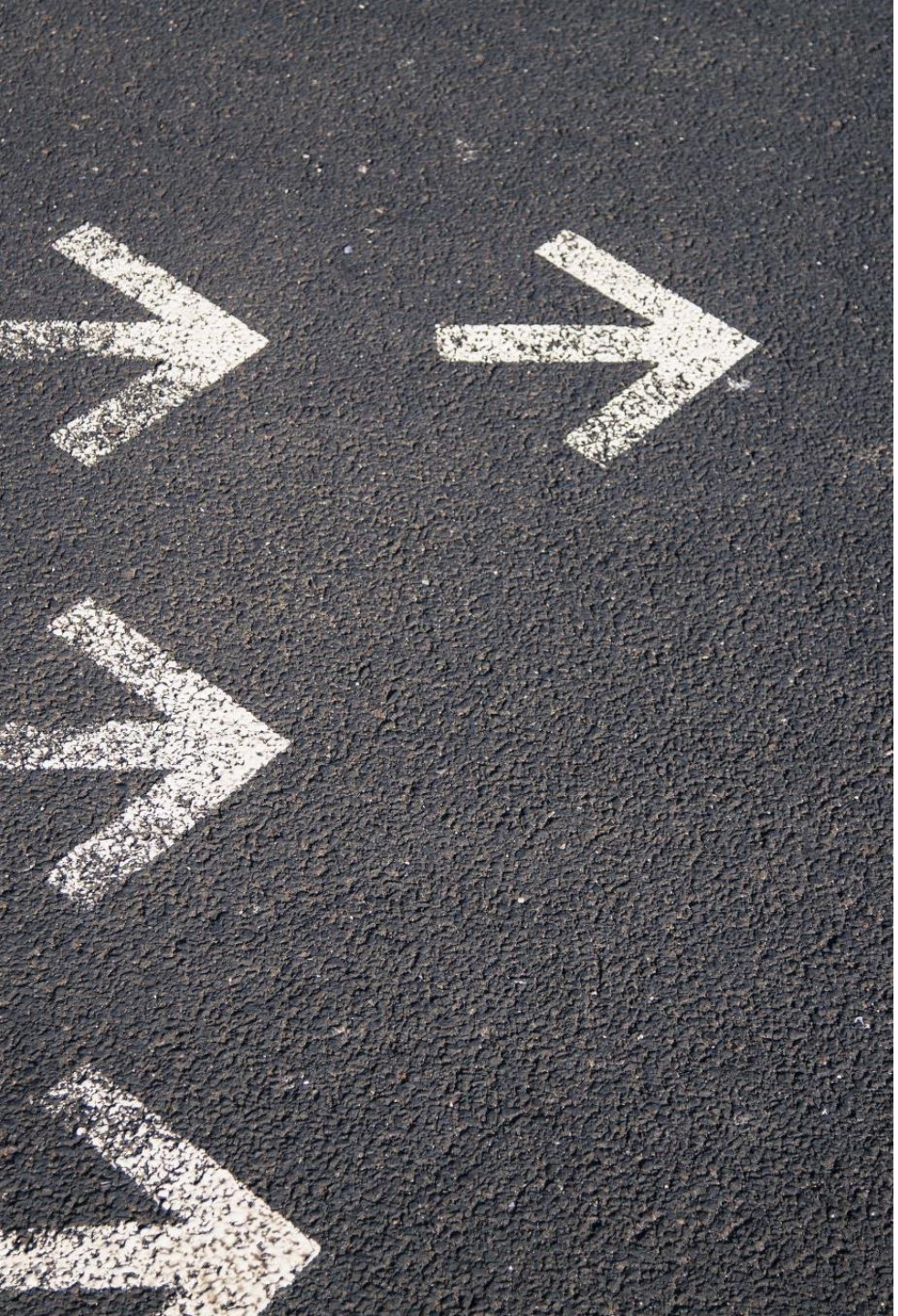
- Transform the 2D Burgers' equation into one single equation – **2D diffusion equation**

$$\frac{\partial \bar{\Phi}}{\partial t} - \left(\frac{\partial^2 \bar{\Phi}}{\partial x^2} + \frac{\partial^2 \bar{\Phi}}{\partial y^2} \right) = 0$$

Can map to finite-dimensional system & capture *any* nonlinearity?

Special cases of finite-dimensional projection: Cole-Hopf transformation

Exact mapping



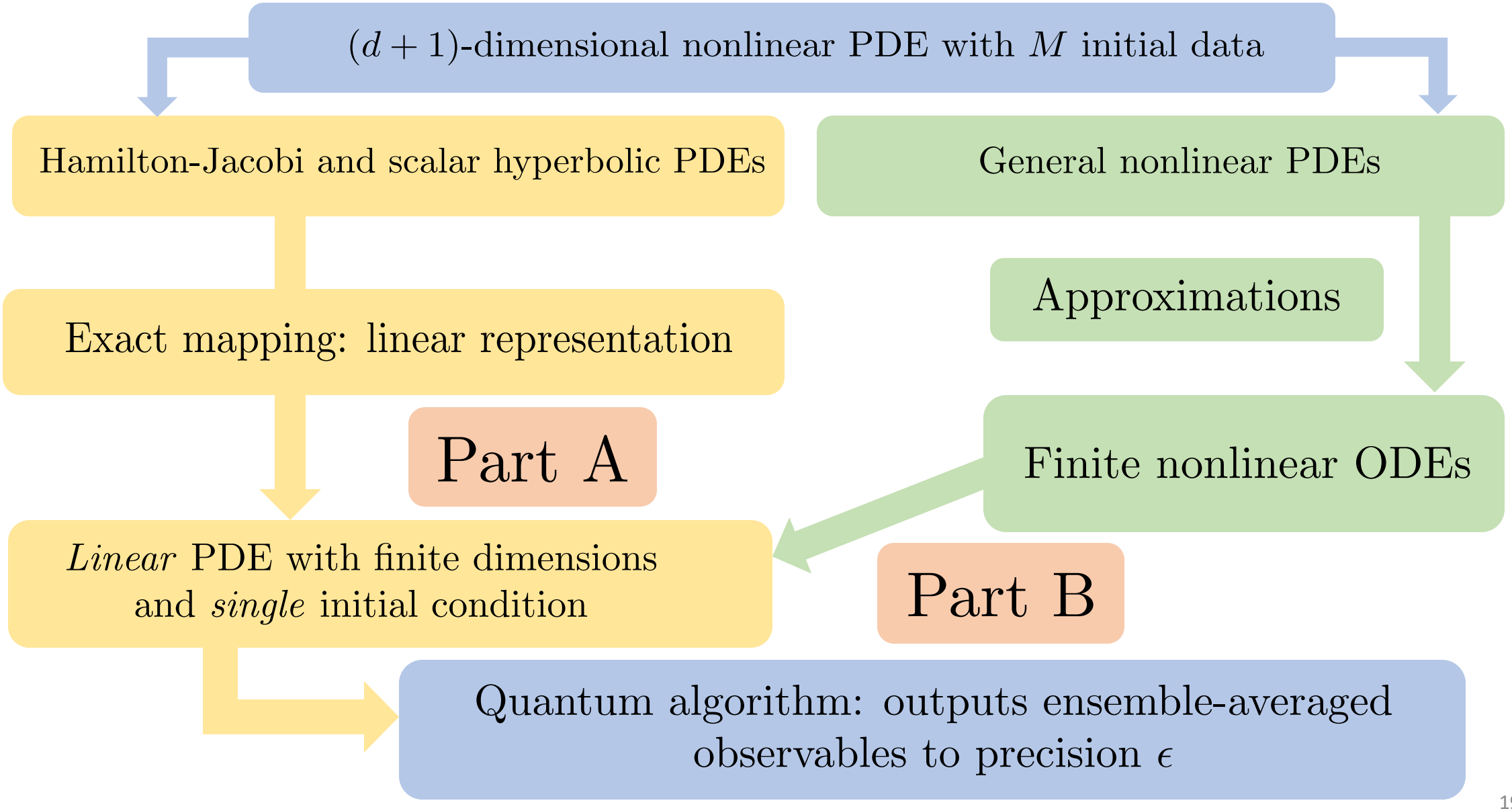
Basic roadmap:

Making nonlinear problem look linear

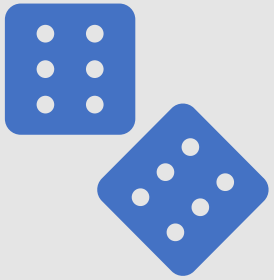
Approximations

Exact mapping

Basic roadmap:



Part A: Hamilton-Jacobi and hyperbolic PDEs



$(d+1)$-dimensional nonlinear PDE with M initial conditions

General:

$$\frac{\partial u^{[k]}}{\partial t} + F(u^{[k]}, \nabla u^{[k]}, \nabla^2 u^{[k]}, \cdots) = 0, \quad t \in \mathbb{R}^+, x \in \mathbb{R}^d, u^{[k]} \in \mathbb{R}^d, k = 1, ..., M$$

Here $t \geq 0$ is time, x is the spatial variable, while F is a nonlinear function or functional.

Hamilton-Jacobi:

$$F = H(\nabla u^{[k]}, x)$$

Hyperbolic:

$$F = \nabla H(u^{[k]}, x)$$

Some applications

Optimal control

Machine learning

Semiclassical limit of the Schrodinger equation

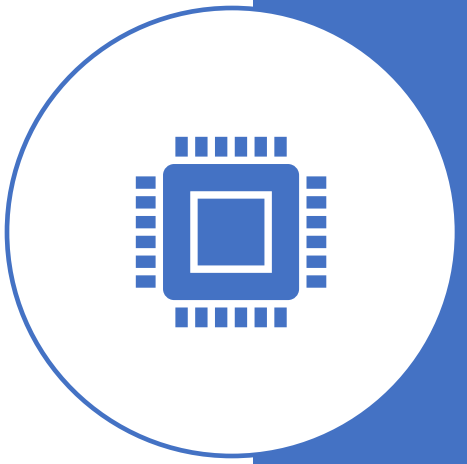
Geometric optics

Mean-field games

Front propagation

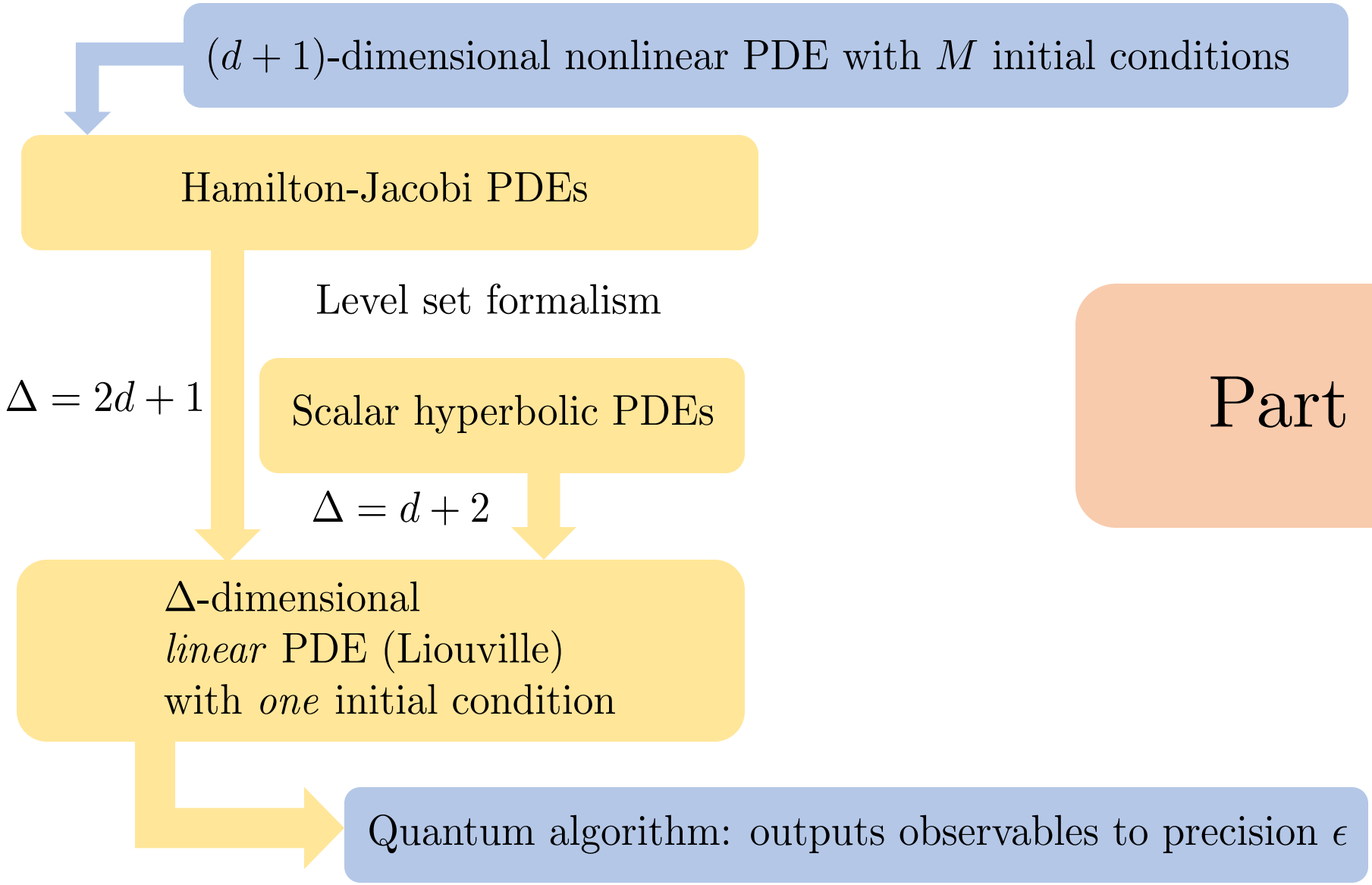
Sticky particles or pressureless gases

KPZ equations



Types of methods

Solution and method	Advantages	Disadvantages
Viscosity solution (direct numerical substitution)	Weaker notion of solution	Not valid when linear superposition principle not obeyed (e.g. high frequency limit of wave equations)
Multivalued solution (Ray tracing)	Simplicity: solving ODEs	Numerical accuracy not easily guaranteed
Multivalued solution (Moment methods)	N/A	Not easy to derive for high-dimensional systems
Multivalued solution (Level set methods)	Globally valid solution	Curse of dimensionality


$(d+1)$-dimensional nonlinear PDE with M initial conditions
Hamilton-Jacobi PDEs
Level set formalism
$\Delta = 2d+1$
Scalar hyperbolic PDEs
$\Delta = d+2$
Δ-dimensional
linear PDE (Liouville)
with *one* initial condition
Quantum algorithm: outputs observables to precision ϵ

Part A

Level set mapping

The level set function $\phi_i^{[k]}(t, x, p)$ can be defined by

$$\phi_i^{[k]}(t, x, p = u^{[k]}(t, x)) = 0$$

Level set function lives in a space with ~twice the dimension

[5] S. Osher and J. Sethian, 1988; S. Jin and S. Osher 2003

Level set mapping

The level set function $\phi_i^{[k]}(t,x,p)$ can be defined by

$$\phi_i^{[k]}(t,x,p=u^{[k]}(t,x))=0$$

Level set function lives in a space with ~twice the dimension

Then $\phi^{[k]}=(\phi_1^{[k]},...,\phi_d^{[k]})$ solves the *linear* PDE

$$\partial_t\phi^{[k]}+\nabla_p H\cdot\nabla_x\phi^{[k]}-\nabla_x H\cdot\nabla_p\phi^{[k]}=0.$$

Want to compute the observable instead

Level set mapping

Instead solve for ψ

$$\psi(t,x,p) = \frac{1}{M}\sum_{k=1}^{M} \delta(\phi^{[k]}(t,x,p))\,.$$

Want to compute the observable instead

Level set mapping

Instead solve for ψ

$$\psi(t,x,p) = \frac{1}{M}\sum_{k=1}^{M}\delta(\phi^{[k]}(t,x,p))\,.$$

Analytical solution to *linear* PDE problem

$$\partial_t\psi + \nabla_p H\cdot\nabla_x\psi - \nabla_x H\cdot\nabla_p\psi = 0$$

$$\psi(0,x,p) = \frac{1}{M}\sum_{k=1}^{M}\prod_{i=1}^{d}\delta(p_i - u_i^{[k]}(0,x)).$$

Want to compute the observable instead

$$\partial_t \psi + \nabla_p H \cdot \nabla_x \psi - \nabla_x H \cdot \nabla_p \psi = 0$$

Level set mapping

$$\psi(0, x, p) = \frac{1}{M} \sum_{k=1}^{M} \prod_{i=1}^{d} \delta(p_i - u_i^{[k]}(0, x)).$$

$$\mathbf{\Psi} = \int \int \psi(t, x, p) |x\rangle |p\rangle dx dp$$

$$\frac{d\mathbf{\Psi}}{dt} = -i\boldsymbol{H}\mathbf{\Psi}, \qquad \boldsymbol{H} = i \sum_{j=1}^{D} (\hat{\zeta}_j H(\hat{x}_1, ..., \hat{x}_D, \hat{p}_1, ..., \hat{p}_D) \hat{p}_j - \hat{p}_j H(\hat{x}_1, ..., \hat{x}_D, \hat{p}_1, ..., \hat{p}_D) \hat{\zeta}_j) = \boldsymbol{H}^{\dagger}$$

Physical observables

Given any function $G : \mathbb{R}^d \to \mathbb{R}$

$$\langle G(t,x)\rangle \equiv \int_{\mathbb{R}^d} G(p)\psi(t,x,p)dp = \frac{1}{M}\sum_{k=1}^{M}\int_{\mathbb{R}^d} G(p)\delta(\phi^{[k]}(t,x,p))dp$$

ψ acts like the Wigner function
for nonlinear HJE in WKB approx

$\langle G(t,x)\rangle$ are the moments

Physical observables

Given any function $G : \mathbb{R}^d \to \mathbb{R}$

$$\langle G(t,x)\rangle \equiv \int_{\mathbb{R}^d} G(p)\psi(t,x,p)dp = \frac{1}{M}\sum_{k=1}^{M}\int_{\mathbb{R}^d} G(p)\delta(\phi^{[k]}(t,x,p))dp$$

ψ acts like the Wigner function
for nonlinear HJE in WKB approx

Example:

$$i\hbar\partial_t\Psi = -\frac{\hbar^2}{2}\Delta\Psi + V(x)\Psi\,, \qquad \Psi(0,x) = A_0(x)e^{i\frac{S_0(x)}{\hbar}}$$

S satisfies HJ PDE with nonlinear $H = (1/2)|\nabla S|^2 + V(x)$

Physical observables

Given any function $G : \mathbb{R}^d \to \mathbb{R}$

$$\langle G(t,x)\rangle \equiv \int_{\mathbb{R}^d} G(p)\psi(t,x,p)dp = \frac{1}{M}\sum_{k=1}^{M}\int_{\mathbb{R}^d} G(p)\delta(\phi^{[k]}(t,x,p))dp$$

ψ acts like the Wigner function
for nonlinear HJE in WKB approx

Example: $w \leftrightarrow \psi$

$$\partial_t w + \nabla_p H \cdot \nabla_x w - \nabla_x H \cdot \nabla_p w = 0$$

$$w(0,x,p) = |A_0(x)|^2 \delta(p - \nabla S_0(x))$$

Physical observables

Given any function $G : \mathbb{R}^d \to \mathbb{R}$

$$\langle G(t,x)\rangle \equiv \int_{\mathbb{R}^d} G(p)\psi(t,x,p)dp = \frac{1}{M}\sum_{k=1}^{M}\int_{\mathbb{R}^d} G(p)\delta(\phi^{[k]}(t,x,p))dp$$

ψ acts like the Wigner function
for nonlinear HJE in WKB approx

Example: $G(p) = 1, p, |p|^2$

$$\rho(t,x) = \int w\,dp\,, \quad \rho(t,x)u(t,x) = \int pw\,dp\,, \quad \frac{1}{2}\rho(t,x)u^2(t,x) = \int \frac{|p|^2}{2} w\,dp$$

Physical observables

Given any function $G : \mathbb{R}^d \to \mathbb{R}$

$$\langle G(t,x)\rangle \equiv \int_{\mathbb{R}^d} G(p)\psi(t,x,p)dp = \frac{1}{M}\sum_{k=1}^{M}\int_{\mathbb{R}^d} G(p)\delta(\phi^{[k]}(t,x,p))dp$$

ψ acts like the Wigner function
for nonlinear HJE in WKB approx

Example: $G(p) = 1, p, |p|^2$

$$\rho(t,x) = \int w\,dp\,, \quad \rho(t,x)u(t,x) = \int pw\,dp\,, \quad \frac{1}{2}\rho(t,x)u^2(t,x) = \int \frac{|p|^2}{2} w\,dp$$

First 3 moments give classical limits to
density, momentum and kinetic energy

$$|\Psi|^2, \hbar \mathrm{Im}(\bar{\Psi}\nabla\Psi), (\hbar^2/2)|\nabla\Psi|^2$$

Physical observables

Given any function $G : \mathbb{R}^d \to \mathbb{R}$

$$\langle G(t,x)\rangle \equiv \int_{\mathbb{R}^d} G(p)\psi(t,x,p)dp = \frac{1}{M}\sum_{k=1}^{M}\int_{\mathbb{R}^d} G(p)\delta(\phi^{[k]}(t,x,p))dp$$

ψ acts like the Wigner function
for nonlinear HJE in WKB approx

Compute inner products via inner product algorithm (e.g. swap-test)

Many other examples:

High-frequency limits of general hyperbolic systems

1) Geometric optics
2) Maxwell equations in isotropic medium
3) Elastic waves
4) Dirac equation
5) …etc

Physical observables

Given any function $G : \mathbb{R}^d \to \mathbb{R}$

$$\langle G(t,x)\rangle \equiv \int_{\mathbb{R}^d} G(p)\psi(t,x,p)dp = \frac{1}{M}\sum_{k=1}^{M}\int_{\mathbb{R}^d} G(p)\delta(\phi^{[k]}(t,x,p))dp$$

$$\langle G(t,x)\rangle \equiv \int_{\mathbb{R}^d} G(p)\psi(t,x,p)dp = \frac{1}{M}\sum_{k=1}^{M}\int_{\mathbb{R}^d} G(p)\delta(\phi^{[k]}(t,x,p))dp = \frac{1}{M}\sum_{k=1}^{M}\sum_{\gamma=1}^{J_k}\frac{G(u_\gamma^{[k]}(t,x))}{\mathcal{J}_\gamma^{[k]}}$$

$$Jacobian\ \mathcal{J}_\gamma^{[k]} \equiv \left|\det\left(\partial\phi^{[k]}/\partial p\right)\right|_{p=u_\gamma^{[k]}(t,x)}$$

Level-set encoding is important: Amplitude-encoded solution in *u* requires the extra computation of the Jacobian, but level-set solution takes this into account automatically!

D dimensional nonlinear scalar hyperbolic PDE with M initial conditions

$$\frac{\partial u^{[k]}}{\partial t} - \sum_{j=1}^{D} F_j(u^{[k]}) \frac{\partial u^{[k]}}{\partial x_j} + Q(x_1, ..., x_D, u^{[k]}) = 0, \qquad u^{[k]}(0, x) = u_0^{[k]}(x), \quad k = 1, ..., M$$

Level set mapping

Level set function lives in a space with one more dimension

We introduce a level set function $\phi(t, x_1, ..., x_D, \chi)$, where $\chi \in \mathbb{R}$

$$\phi^{[k]}(t, x_1, ..., x_D, \chi) = 0 \quad \text{at} \quad \chi = u^{[k]}(t, x_1, ..., x_D)$$

$$\Psi(t, x_1, ..., x_D, \chi) = \frac{1}{M} \sum_{k=1}^{M} \delta(\phi^{[k]}(t, x_1, ..., x_D, \chi))$$

$D + 1$ dimensional *linear* PDE

$$\frac{\partial \Psi^{[k]}}{\partial t} - \sum_{j=1}^{D+1} \frac{\partial}{\partial X_j}(a_j(X)\Psi^{[k]}) = 0$$

$$X = (x_1, ..., x_D, \chi), \; a_j = F_j(\chi) \text{ for } j = 1, ..., D$$

$$a_{D+1} = -Q(x_1, ..., x_D, \chi)$$

$$\Psi^{[k]}(0, x_1, ..., x_D, \chi) = \frac{1}{M} \sum_{k=1}^{M} \delta(\chi - u_0^{[k]}(x_1, ..., x_D))$$

Level set mapping

$$\boldsymbol{\Psi}(t) \equiv \int dX \Psi(t, X)|X\rangle$$

$$\frac{d\boldsymbol{\Psi}}{dt} = -i\boldsymbol{A}\boldsymbol{\Psi}, \qquad \boldsymbol{A} = \sum_{j=1}^{D+1} \hat{P}_j a_j(\hat{X}) = \sum_{j=1}^{D} \hat{p}_j F_j(\hat{\chi}) - \hat{\zeta} Q(\hat{x}_1, ..., \hat{x}_D, \hat{\chi})$$

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

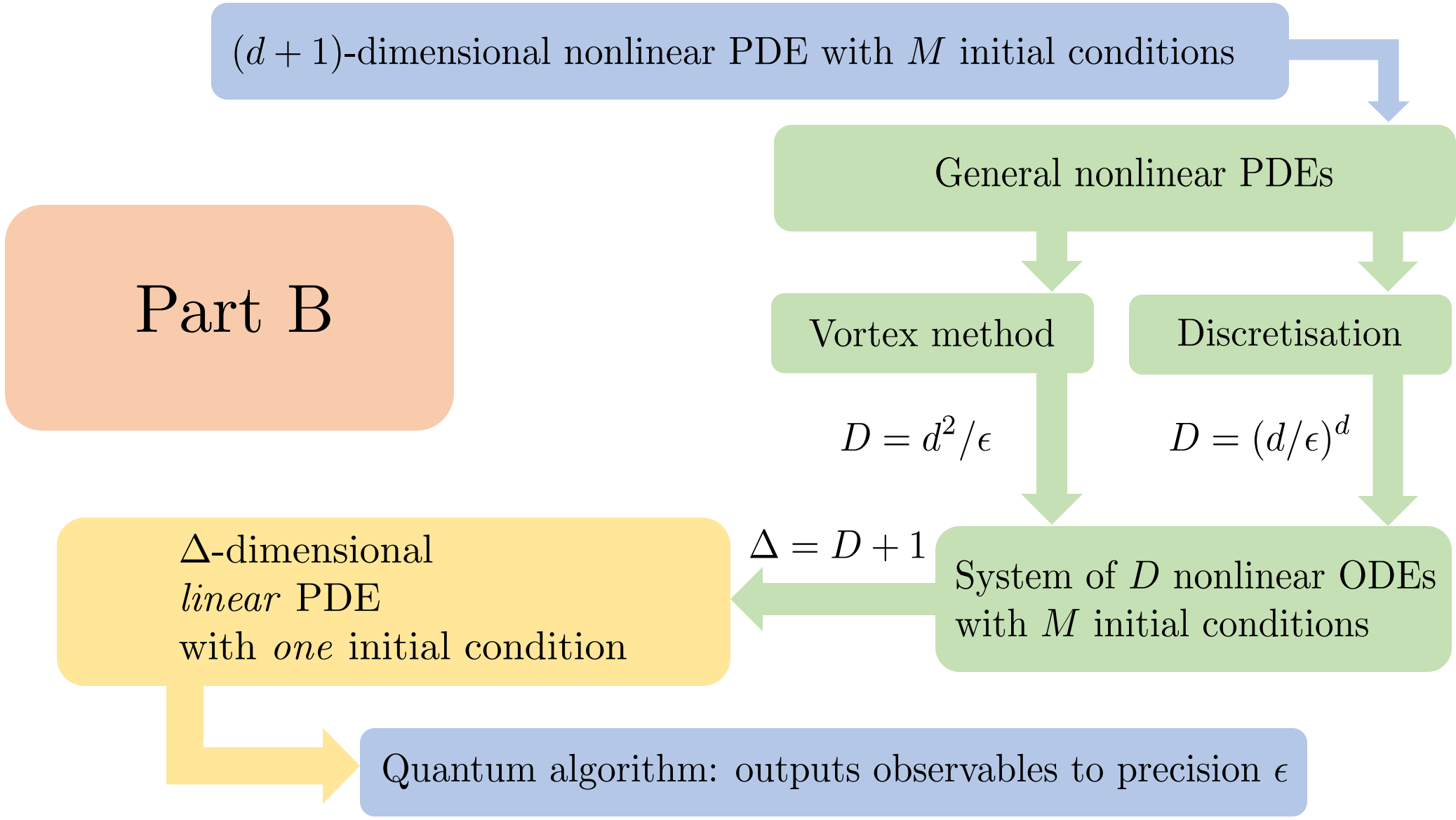
$$\mathbf{A}_1 = \sum_{j=1}^{D} \hat{p}_j F_j(\hat{\chi}) - \frac{1}{2} \sum_{j=1}^{D} \{\hat{\zeta}, Q\}$$

$$\mathbf{A}_2 = \frac{i}{2} \sum_{j=1}^{D} [Q, \hat{\zeta}]$$

Quick observations for $Q = 0$:

1. Direct simulation without Schrodingerisation is already sufficient
2. Linear hyperbolic PDEs require only Gaussian operations
3. Nonlinear hyperbolic PDEs require non-Gaussian operations

Part B: General nonlinear PDEs


$(d+1)$-dimensional nonlinear PDE with M initial conditions
General nonlinear PDEs
Part B
Vortex method
Discretisation
$D = d^2/\epsilon$
$D = (d/\epsilon)^d$
Δ-dimensional
linear PDE
with *one* initial condition
$\Delta = D + 1$
System of D nonlinear ODEs
with M initial conditions
Quantum algorithm: outputs observables to precision ϵ

System of N nonlinear ODEs

Nonlinear mapping

$$\frac{d\gamma_n(t)}{dt} = -F_n(\gamma_0, ..., \gamma_{N-1}, t), \qquad n = 0, ..., N-1$$

$$\Phi(t, q_0, ..., q_{N-1}) = \prod_{n=0}^{N-1} \delta(q_n - \gamma_n(t)), \qquad q_n \in \mathbb{R}$$

$N+1$ dimensional *linear* PDE

$$\frac{\partial \Phi(t, q_0, ..., q_{N-1})}{\partial t} - \sum_{n=0}^{N-1} \frac{\partial}{\partial q_n}(F_n(q_0, ..., q_{N-1})\Phi(t, q_0, ..., q_{N-1})) = 0$$

$$\boldsymbol{\Phi}(t) \equiv \int \Phi(t, q_0, ..., q_{N-1}) |q_0, ..., q_{N-1}\rangle dq_0 ... dq_{N-1} \qquad \frac{d\boldsymbol{\Phi}(t)}{dt} = -i\boldsymbol{A}\boldsymbol{\Phi}(t), \qquad \boldsymbol{A} = \sum_{n=0}^{N-1} \hat{Q}_n F_n(\hat{q}_0, ..., \hat{q}_{N-1})$$

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

$$\mathbf{A}_1 = \tfrac{1}{2}\sum_{n=0}^{N-1}\{\hat{Q}_n, F_n\}$$

$$\mathbf{A}_2 = \tfrac{1}{2}\sum_{n=0}^{N-1}[\hat{Q}_n, F_n]$$

$$[\hat{q}_n, \hat{Q}_n] = i$$

If F is nonlinear (i.e. nonlinear ODE)
then we must go beyond Gaussian operations

System of D nonlinear ODEs

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

Observable

$$A(t) = \frac{1}{M}\sum_{k=1}^{M} A(X^{[k]}(t))$$

Exact mapping: Linear representation:
$(d+1)$-dimensional *linear* PDE

Compute

$$\frac{\partial \Phi(t,q)}{\partial t} + \nabla_q \cdot [F(q)\Phi(t,q)] = 0$$
$$\Phi(0,q) = \frac{1}{M}\sum_{k=1}^{M} \delta(q - X_0^{[k]}).$$

Solution

$$\Phi(t,q) = \frac{1}{M}\sum_{k=1}^{M} \delta(q - X^{[k]}(t))$$

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	$D+1$	$[a_{K,j}, \hat{p}_j^K] \otimes \hat{\eta}, \quad b \otimes \hat{\eta}$	$O(DK)$
Inhomogeneous IV A	Add 1 more qubit	$[a_{K,j}, \hat{p}_j^K] \otimes \hat{\eta} \otimes \sigma, \quad b \otimes \hat{\eta} \otimes \sigma$	$O(DK)$
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	$D+1$	$i[\hat{p}, L] \otimes \hat{\eta}, \quad \{\hat{p}, L\} \otimes I$	$O(D)$
Heat V B 1	$D+1$	$\{\hat{p}\mathrm{D}, \hat{p}\} \otimes \hat{\eta}, \quad V \otimes \hat{\eta}$	$O(D+1)$
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	$\{a, \hat{p}^2\} \otimes \hat{\eta} \otimes \sigma, \quad V \otimes \eta \otimes \sigma, \quad i[a, \hat{p}^2] \otimes I \otimes \sigma$	$O(D)$
Maxwell ($D=3$) V B 5	4 qumodes + 4 qubits	See Section V B 5	30
Uncertain linear PDE VI Convection	$D+L+1$	$i[c, \hat{p}] \otimes \hat{\eta}, \quad \{c, \hat{p}\} \otimes I$	$O(DL)$
Nonlinear			
Scalar hyperbolic VII A	$D+1$	$i[Q, \hat{\zeta}] \otimes \hat{\eta}, \quad \{Q, \hat{\zeta}\} \otimes I$	$O(D)$
Hamilton-Jacobi VII A	$2D$	$[\hat{\zeta}H, \hat{p}]$	$O(D)$
N nonlinear ODEs VII B	$N+1$	$i[Q, F] \otimes \hat{\eta}, \quad \{Q, F\} \otimes I$	$O(N)$

arXiv: 2308.00646

Reference list for Part II: Nonlinear PDEs

Nonlinear PDEs:

- *Analog quantum simulation of partial differential equations,* Shi Jin, Nana Liu*, arXiv: 2308.00646, Quantum Science and Technology, Vol 9, 035047, 2024>> for nonlinear PDE and ODE algorithms based on the techniques introduced in the following papers (written prior to Schrodingerisation):

- *Quantum algorithms for computing observables of nonlinear partial differential equations,* Shi Jin, Nana Liu*, arXiv: 2022.07834, Bulletin des Sciences Mathematiques, Vol 194, 103457, 2024

- *Time complexity analysis of quantum algorithms via linear representations for nonlinear ordinary and partial differential equations*, Shi Jin, Nana Liu, Yue Yu*, Journal of Computational Physics, Vol 487, 112149, 2023

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

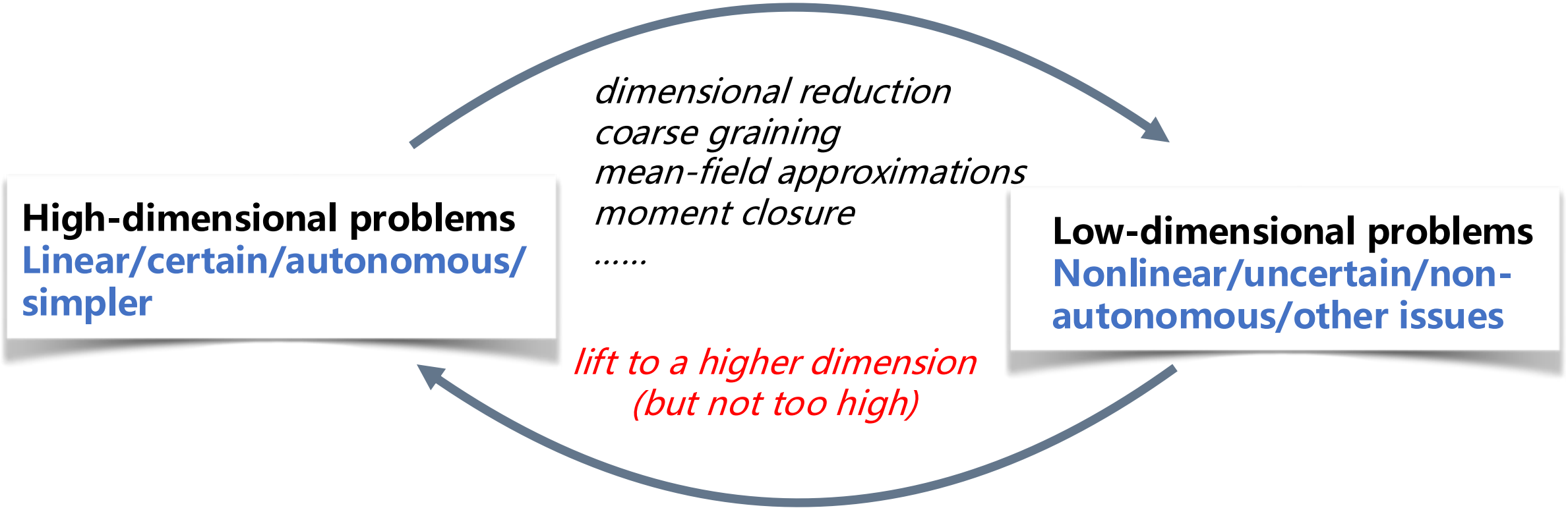
4. Linear non-autonomous systems become linear autonomous

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

Reference list for Part II: Nonlinear ODEs/PDEs

Nonlinear PDEs:

- See << *Analog quantum simulation of partial differential equations,* Shi Jin, Nana Liu*, arXiv: 2308.00646, Quantum Science and Technology, Vol 9, 035047, 2024>> for nonlinear PDE and ODE algorithms based on the techniques introduced in the following papers (written prior to Schrodingerisation):

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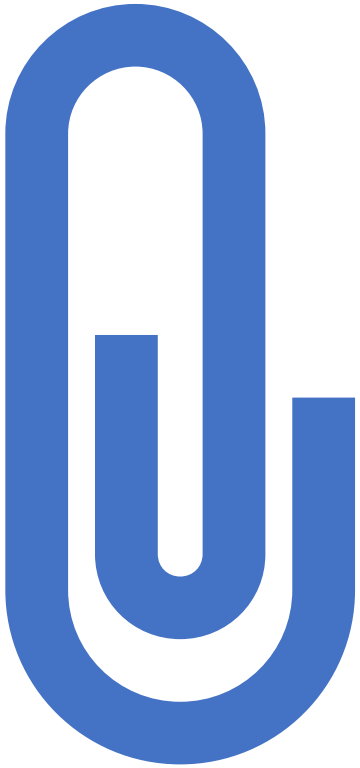
- Time complexity analysis of quantum algorithms via linear representations for nonlinear ordinary and partial differential equations, Shi Jin, Nana Liu, Yue Yu*, Journal of Computational Physics, Vol 487, 112149, 2023

Overview of summer lectures on Schrodingerisation

PART II: Special topics

- **Nonlinear ODEs and PDEs**
- **Uncertain ODEs/PDEs**
- **Non-autonomous mapped to autonomous PDEs**
- **Application to linear algebra, ground state and thermal state preparation**



Appendix Slides

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

Block-encoding method

Computing physical observable

Given any function $G : \mathbb{R}^d \to \mathbb{R}$

$$\langle G(t,x)\rangle \equiv \int_{\mathbb{R}^d} G(p)\psi(t,x,p)dp = \frac{1}{M}\sum_{k=1}^{M}\int_{\mathbb{R}^d} G(p)\delta(\phi^{[k]}(t,x,p))dp$$

Discretising ψ and the delta function

$$\psi^{\omega}_{0,\boldsymbol{j},\boldsymbol{l}} = \frac{1}{M}\sum_{k=1}^{M}\prod_{i=1}^{d}\delta_{\omega}(l_i h - u_i^{[k]}(n=0,h\boldsymbol{j})).$$

$$\begin{pmatrix}\mathbf{0}\\ \psi_{n,\boldsymbol{j},\boldsymbol{l}}\end{pmatrix} = \mathcal{M}^{-1}\begin{pmatrix}\psi_{0,\boldsymbol{j},\boldsymbol{l}}\\ \mathbf{0}\end{pmatrix}$$

Computing physical observable

Given any function $G : \mathbb{R}^d \to \mathbb{R}$

$$\langle G(t,x)\rangle \equiv \int_{\mathbb{R}^d} G(p)\psi(t,x,p)dp = \frac{1}{M}\sum_{k=1}^{M}\int_{\mathbb{R}^d} G(p)\delta(\phi^{[k]}(t,x,p))dp$$

Estimate with a quantum algorithm:

$$\langle G(t,x)\rangle \approx$$

$$\langle G^{\omega}_{n,\boldsymbol{j}}\rangle \equiv \frac{1}{N^d}\sum_{\boldsymbol{l}}^{N} G_{\boldsymbol{l}}\psi_{n,\boldsymbol{j},\boldsymbol{l}}.$$

Computing physical observable

Estimate with a quantum algorithm:

$$\langle G^{\omega}_{n,\boldsymbol{j}} \rangle \equiv \frac{1}{N^d} \sum_{\boldsymbol{l}}^{N} G_{\boldsymbol{l}} \psi_{n,\boldsymbol{j},\boldsymbol{l}}.$$

Main players:

$$|\psi_0\rangle = \frac{1}{N_{\psi_0}} \sum_{\boldsymbol{j}^N} \sum_{\boldsymbol{l}}^{N} \psi_{0,\boldsymbol{j},\boldsymbol{l}} |\boldsymbol{j}\rangle |\boldsymbol{l}\rangle |n=0\rangle$$

$$|G_{n,\boldsymbol{j}}\rangle \equiv \frac{1}{N_G} \sum_{\boldsymbol{l}}^{N} G^{*}_{\boldsymbol{l}} |\boldsymbol{l}\rangle |\boldsymbol{j}\rangle |n\rangle$$

$$\mathcal{G} = |G_{n,\mathbf{j}}\rangle\langle G_{n,\mathbf{j}}|$$

$\mathcal{M}$: sparse oracle access

Computing physical observable

Estimate with a quantum algorithm:

$$\langle G^{\omega}_{n,\boldsymbol{j}} \rangle \equiv \frac{1}{N^d} \sum_{\boldsymbol{l}}^{N} G_{\boldsymbol{l}} \psi_{n,\boldsymbol{j},\boldsymbol{l}}.$$

$$\langle G^{\omega}_{n,\boldsymbol{j}} \rangle \equiv \frac{1}{N^d} \sum_{\boldsymbol{l}=1}^{N} G_{\boldsymbol{l}} \psi_{n,\boldsymbol{j},\boldsymbol{l}} = \frac{1}{N^d} N_{\psi_0} N_G |\sqrt{\Upsilon}| = n_{\psi_0} n_G |\sqrt{\Upsilon}|$$

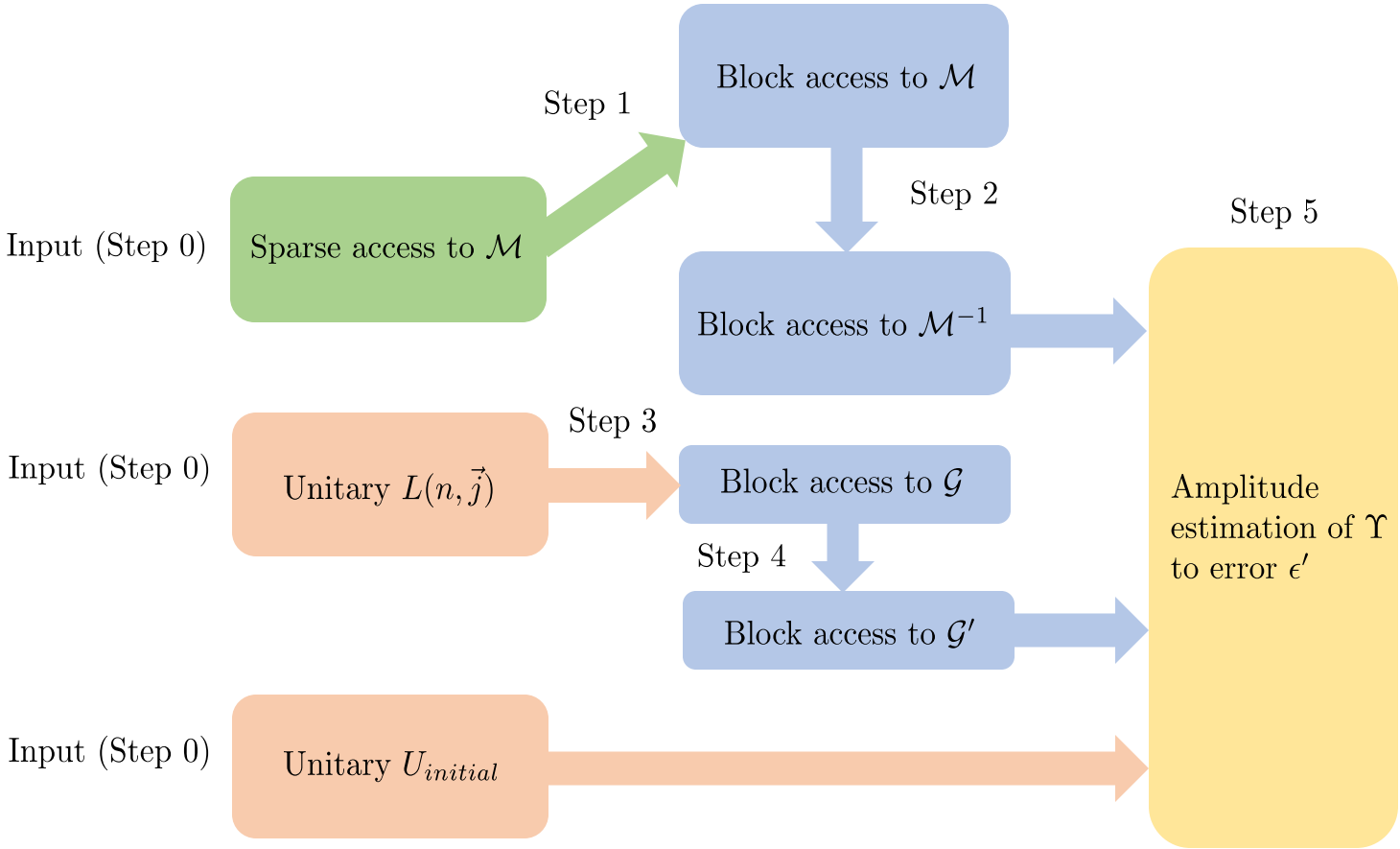
$$\Upsilon \equiv \langle \psi_0 | (\mathcal{M}^{-1})^{\dagger} \mathcal{G} \mathcal{M}^{-1} | \psi_0 \rangle$$

To design quantum algorithm for this...

Computing physical observable

To design quantum algorithm for this...

$$\Upsilon \equiv \langle \psi_0 | (\mathcal{M}^{-1})^\dagger \mathcal{G} \mathcal{M}^{-1} | \psi_0 \rangle$$



Theorem: Computing observables of nonlinear Hamilton-Jacobi PDEs

A quantum algorithm that takes sparse access $(s = O(d), \|\mathcal{M}\|_{max} = O(1), O_M, O_F)$ *to* $\mathcal{M}$*, where* $\|\mathcal{M}\| = O(1)$*, and access to the unitaries* $L(t_n, \boldsymbol{j}/N)$*, where* $L(t_n, \boldsymbol{j}/N)|0\rangle = |G_{n,\boldsymbol{j}}\rangle$ *and* $U_{initial}$*, where* $U_{initial}|0\rangle = |\psi_0\rangle$*, is able to estimate the ensemble average* $\langle G(T,x)\rangle$ *at time* $T = t_n$*, with* M *initial data, to precision* ϵ *with an upper bound on the query complexity* $\mathcal{Q}$

$$\mathcal{Q} = \mathcal{O}\left(\frac{n_{\psi_0}^2 d^7 T^3}{\epsilon^{10}} \log\left(\frac{n_{\psi_0}^2 d^4 T^2}{\epsilon^7}\right)\right)$$

and the same order of additional 2-qubit gates, where we suppress all $O(1)$ *terms except* $T = O(1)$ *and* $n_{\psi_0} \geq O(1)$*.*

$$\text{Compare to } \mathcal{C} = O\left(MTd^2\left(\frac{d}{\epsilon}\right)^{d+1}\right)$$

Theorem: Computing observables of scalar hyperbolic PDEs

A quantum algorithm that takes sparse access $(s = O(d), \|\mathcal{M}\|_{max} = O(1), O_{\mathcal{M}}, O_F)$ *to* $\mathcal{M}$ *with* $\|\mathcal{M}\| = O(1)$ *and access to the unitaries* $l(t_n, \boldsymbol{j}/N)$ *where* $l(t_n, \boldsymbol{j}/N)|0\rangle = |g_{n,\boldsymbol{j}}\rangle$, *and* $U_{initial}$ *where* $U_{initial}|0\rangle = |\psi_0'\rangle$, *is able to estimate the ensemble average* $\langle g(T, \boldsymbol{j}/N)\rangle$ *at time* T, *with* M *initial data, to precision* ϵ *with an upper bound on the query complexity* $\mathcal{Q}$

$$\mathcal{Q} = \mathcal{O}\left(\frac{(n'_{\psi_0})^2 d^7 T^3}{\epsilon^{10}} \log\left(\frac{(n'_{\psi_0})^2 d^4 T^2}{\epsilon^7}\right)\right)$$

and the same order of additional 2-qubit gates, where we suppress all $O(1)$ *terms except* $T = O(1)$ *and* $n'_{\psi_0} \geq O(1)$.

$$\text{Compare to } \mathcal{C} = O\left(MTd^3\left(\frac{d}{\epsilon}\right)^{d+1}\right)$$

Level-set encoded solution can give observables that amplitude-encoded solutions cannot

Level-set encoding: $\rightarrow \sum_{n,j,k} \psi_{n,j,k} |n\rangle |j\rangle |k\rangle$

Amplitude encoding: $\rightarrow \sum_{n,j} u_{n,j} |n\rangle |k\rangle$

Level-set encoded solution can give observables that amplitude-encoded solutions cannot

Level-set encoding: $\rightarrow \sum_{n,j,k} \psi_{n,j,k} |n\rangle |j\rangle |k\rangle$

Amplitude encoding: $\rightarrow \sum_{n,j} u_{n,j} |n\rangle |k\rangle$

$$\langle G(t,x) \rangle \equiv \int_{\mathbb{R}^d} G(p)\psi(t,x,p)dp = \frac{1}{M}\sum_{k=1}^{M} \int_{\mathbb{R}^d} G(p)\delta(\phi^{[k]}(t,x,p))dp = \frac{1}{M}\sum_{k=1}^{M}\sum_{\gamma=1}^{J_k} \frac{G(u_\gamma^{[k]}(t,x))}{\mathcal{J}_\gamma^{[k]}}$$

Amplitude-encoded solution requires the extra computation of the Jacobian

$$Jacobian\ \mathcal{J}_\gamma^{[k]} \equiv |\det(\partial\phi^{[k]}/\partial p)|_{p=u_\gamma^{[k]}(t,x)}$$

but level-set solution takes this into account automatically!

Theorem: Computing observables of nonlinear ODEs

The worst-case total query complexity $\mathcal{Q}$ to estimate the observable $\langle A(t_n)\rangle$ to precision ϵ on a quantum algorithm that takes sparse access $(s = O(D), \|\mathcal{M}\|_{max} = O(1), O_M, O_F)$ to $\mathcal{M}_{ODE}$, access to the unitaries $J(n)$ where $J(n)|0\rangle = |A^n\rangle$ and U_{Φ_0} where $U_{\Phi_0}|0\rangle = |\Phi_0\rangle$, is

$$\mathcal{Q} = \mathcal{O}\left(\frac{n_{\Phi_0}^2 D^7 T^3}{\epsilon^{10}} \log\left(\frac{n_{\Phi_0}^2 D^4 T^2}{\epsilon^7}\right)\right)$$

where all constant terms $O(1)$ are suppressed except $T = O(1)$ and $n_{\Phi_0} = O(1)$. This complexity is independent of M.

Compare to $\mathcal{C}\left(\frac{M D^3 T}{\epsilon}\right)$

TABLE I. Quantum ($\mathcal{Q}$) and classical ($\mathcal{C}$) cost comparison in computing observables at time T and $\Lambda = O(N^{ad})$ spatial points to precision ϵ

$$\text{PDE: } \mathcal{O}\left(\frac{\mathcal{C}}{\mathcal{Q}}\right) = \tilde{O}\left(\frac{M}{T^2} d^{r_1} \left(\frac{1}{\epsilon}\right)^{r_2}\right)$$

$$\text{ODE: } \mathcal{O}\left(\frac{\mathcal{C}}{\mathcal{Q}}\right) = \tilde{O}\left(\frac{M}{T^2} D^{r_1} \left(\frac{1}{\epsilon}\right)^{r_2}\right)$$

Nonlinear equations (M initial data)	r_1	r_2	b range (initial data-dependent)	Quantum advantage (possible)
$(d+1)$-dimensional Hamilton-Jacobi PDE	$(1-a)d-4-b$	$(1-3a)d-9-3b$	$b \in [0, \frac{(1-3a)d}{3} - 3)$	M, d, ϵ
$(d+1)$-dimensional hyperbolic PDE	$(1-a)d-5-b$	$(1-3a)d-9-3b$	$b \in [0, \frac{(1-3a)d}{3} - 3)$	M, d, ϵ
System of D ODEs	-5	-9	$b=0$	M
$(d+1)$-dimensional general PDE (Lagrangian discretisation)	$-7-ad$	$-13-ad$	$b=0$	M
$(d+1)$-dimensional general PDE (Eulerian discretisation)	$-(4+a)d$	$-9-(4+a)d$	$b=0$	Large M

Advantage with respect to number of initial conditions

1. Using the linear representation method: will get quantum advantage with respect to number of initial conditions. Classical algorithm is linear in this number and quantum algorithm is independent of this number!

2. Applications:

Running numerical simulations with many differential initial data: e.g. Monte-Carlo, Stochastic collocation, Rayleigh-Taylor instability

Uncertainty quantification

Quantum simulation of partial differential equations via Schrodingerisation

PART II: Special topics
Uncertain and stochastic ODEs/PDEs

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CEMRACS 15-19 Jul 2025

Overview of summer lectures on Schrodingerisation

PART II: Special topics

- **Nonlinear ODEs and PDEs**
- **Uncertain ODEs/PDEs**
- **Non-autonomous mapped to autonomous PDEs**
- **Application to linear algebra, ground state and thermal state preparation**

II. Uncertain ODEs and PDEs

``Turning uncertain PDEs into certain PDEs"

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

"Quantum algorithms for uncertainty quantification: applications to partial differential Equations" (arXiv: 2209.1120), Francoise Golse, Shi Jin, Nana Liu*

"Quantum algorithms for stochastic differential equations: a Schrodingerisation approach", Shi Jin, Nana Liu, Wei Wei*, arXiv:2412.14868, 2024, Journal of Scientific Computing, Vol 104, no. 56, 2025

Uncertain PDE: Method 1

- have knowledge of the distribution where stochastic variables are sampled

Uncertainty quantification

- One of the most active areas in scientific computing, applied mathematics and data science
- Our PDE problem: coefficients are modelled stochastically
- Many samples M needed to get an ensemble average
- Classically can be intractable if M is high and the number of stochastic variables can also be high
- Is there a way of directly capturing ensemble-averaged quantities without solving PDE multiple M times?

Quantum stochastic galerkin method

- Would like a method that does not require the cost of implementation to scale exponentially with the number of stochastic variables L: preferably only linearly.
- If in addition we have knowledge of the actual underlying distribution itself, we want to the method to be independent of the number of samples M of the underlying distribution
- Want a method that is 'natural' for implementation on physical systems

Example: convection equation with stochastic coefficients

$$\frac{\partial u}{\partial t} + \sum_{j=1}^{D} c_j(z_1, ..., z_L, x_1, ..., x_D)\frac{\partial u}{\partial x_j} = 0, \qquad z_1, ..., z_L \sim W(z_1, ..., z_L) = \prod_{l=1}^{L} w(z_l) = \prod_{l=1}^{L} \frac{\exp(-z_l^2)}{\sqrt{\pi}}, \qquad c_j \in \mathbb{R}$$

Can always make expansion $$u(t, z_1, ..., z_L, x_1, ..., x_D) = \sum_{\boldsymbol{n} \in \mathbb{N}_0^L} u_{\boldsymbol{n}}(t, x_1, \cdots, x_D) P_{\boldsymbol{n}}(z_1, ..., z_L)$$

arXiv: 2308.00646

Quantum stochastic galerkin method

Here the weights obey the normalisation condition:

$$\int P_{\boldsymbol{n}}(z_1,...,z_L)P_{\boldsymbol{m}}(z_1,...,z_L)W(z_1,...,z_L)dz_1...dz_L = \delta_{\boldsymbol{nm}}$$

$\{|\boldsymbol{n}\rangle\}_{\boldsymbol{n}\in\mathbb{N}_0^L}$ as the Fock or number basis, so $\sum_{\boldsymbol{n}\in\mathbb{N}_0^L} |\boldsymbol{n}\rangle\langle\boldsymbol{n}| = I$

Natural basis for physical systems like photonics!

$$P_{\boldsymbol{n}}(z) = \frac{\langle z_1...z_L|\boldsymbol{n}\rangle}{W^{1/2}(z_1,...,z_L)} = \prod_{l=1}^{L} P_{n_l} = \prod_{l=1}^{L} \frac{\langle z_l|n_l\rangle}{w^{1/2}(z_l)} = \prod_{l=1}^{L} \frac{H_{n_l}(z_l)}{\sqrt{2^{n_l}n_l!}}, \qquad w(z_l) = \frac{\exp(-z_l^2)}{\sqrt{\pi}}$$

$H_{n_l}(z_l)$ are the one-dimensional Hermite polynomials

Quantum stochastic galerkin method

$$\frac{\partial u}{\partial t} - \sum_{j=1}^{D} c_j(z_1, ..., z_L, x_1, ..., x_D)\frac{\partial u}{\partial x_j} = 0, \qquad z_1, ..., z_L \sim W(z_1, ..., z_L) = \prod_{l=1}^{L} w(z_l) = \prod_{l=1}^{L} \frac{\exp(-z_l^2)}{\sqrt{\pi}}, \qquad c_j \in \mathbb{R}$$

Observables are independent of z:

$$u_{\mathbf{0}}(t, x_1, ..., x_D) = \int u(t, z_1, ..., z_L, x_1, ..., x_D) w(z_1)...w(z_L) dz_1...dz_L \equiv \mathbb{E}_{z_1,...,z_L}(u)$$

$$\mathrm{Var}_z(u) \equiv \int u^2(t, z_1, ..., z_L, x_1, ..., x_D) w(z_1)...w(z_l) dz_1...dz_L - \mathbb{E}^2_{z_1,...,z_L}(u) = \sum_{\boldsymbol{n} \in \mathbb{N}_0^L, |n| \geq 1} u^2_{\boldsymbol{n}}(t, x_1, ..., x_D)$$

Quantum stochastic galerkin method

$$u(t, z_1, \ldots, z_L, x_1, \ldots, x_D) = \sum_{\boldsymbol{n} \in \mathbb{N}_0^L} u_{\boldsymbol{n}}(t, x_1, \ldots, x_D) P_{\boldsymbol{n}}(z_1, \ldots, z_L)$$

$$\Longrightarrow \quad \frac{\partial}{\partial t} u_{\boldsymbol{n}}(t, x_1, \ldots, x_D) + \sum_{j=1}^{D} \sum_{\boldsymbol{m} \in \mathbb{N}_0^L} \Lambda_{j\boldsymbol{n}\boldsymbol{m}}(x_1, \ldots, x_D) \frac{\partial}{\partial x_j} u_{\boldsymbol{n}}(t, x_1, \ldots, x_D) = 0,$$

$$\Lambda_{j\boldsymbol{n}\boldsymbol{m}}(x_1, \ldots, x_D) = \int c_j(z_1, \ldots, z_L, x_1, \ldots, x_D) w(z_1) \ldots w(z_L) P_{\boldsymbol{n}}(z_1, \ldots, z_L) P_{\boldsymbol{m}}(z_1, \ldots, z_L) \, \mathrm{d}z_1, \ldots, \mathrm{d}z_L$$

where the coefficients of the PDE are now completely *independent* of z!

Rewrite coefficients:

$$\Lambda_{j\boldsymbol{n}\boldsymbol{m}} = \int c_j(z_1, \ldots, z_L, x_1, \ldots, x_D) \langle \boldsymbol{m} | z_1, \ldots, z_L \rangle \langle z_1, \ldots, z_L | \boldsymbol{n} \rangle \mathrm{d}z_1, \ldots, \mathrm{d}z_L$$

$$= \langle \boldsymbol{m} | \int c_j(x_1, \ldots, x_D, \hat{z}_1, \ldots, \hat{z}_L) | z_1, \ldots, z_L \rangle \langle z_1, \ldots, z_L | \boldsymbol{n} \rangle \mathrm{d}z_1 \ldots \mathrm{d}z_L = \langle \boldsymbol{m} | c_j(x_1, \ldots, x_D, \hat{z}_1, \ldots, \hat{z}_L) | \boldsymbol{n} \rangle$$

Quantum stochastic galerkin method

Instead of solving the original z-dependent PDE multiple times for every sample of $z_1, \cdots, z_L$, we can now solve a z-independent equation

Define:

$$\boldsymbol{u}(t) \equiv \int \sum_{\boldsymbol{n} \in \mathbb{Z}_0^L} u_{\boldsymbol{n}}(t, x_1, \ldots, x_D) \, |\boldsymbol{n}\rangle |x_1, \ldots, x_D\rangle \mathrm{d}x$$

$$\Longrightarrow \qquad \frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} = -\mathrm{i}\boldsymbol{A}\boldsymbol{u}, \qquad \boldsymbol{A} = \sum_{j=1}^{D} c_j(\hat{z}_1, \ldots, \hat{z}_L, \hat{x}_1, \ldots, \hat{x}_D)\, \hat{p}_j,$$

$$\boldsymbol{u}(0) = \int \sum_{\boldsymbol{n} \in \mathbb{N}_0^L} u_{\boldsymbol{n}}(0, x_1, \ldots, x_D) \, |\boldsymbol{n}\rangle |x_1, \ldots, x_D\rangle \mathrm{d}x_1 \ldots \mathrm{d}x_D$$

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

Quantum stochastic galerkin method

$$\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} = -\mathrm{i}\boldsymbol{A}\boldsymbol{u}, \qquad \boldsymbol{A} = \sum_{j=1}^{D} c_j(\hat{z}_1,\ldots,\hat{z}_L,\hat{x}_1,\ldots,\hat{x}_D)\,\hat{p}_j,$$

$$\boldsymbol{u}(0) = \int \sum_{\boldsymbol{n}\in\mathbb{N}_0^L} u_{\boldsymbol{n}}(0,x_1,\ldots,x_D)\,|\boldsymbol{n}\rangle|x_1,\ldots,x_D\rangle \mathrm{d}x_1\ldots\mathrm{d}x_D$$

We can easily Schrödingerise this equation

$$\frac{\mathrm{d}\tilde{\boldsymbol{v}}}{\mathrm{d}t} = -\mathrm{i}\boldsymbol{H}\tilde{\boldsymbol{v}}, \qquad \boldsymbol{H} = \boldsymbol{A}_2\otimes\hat{\eta} + \boldsymbol{A}_1\otimes I, \qquad \tilde{\boldsymbol{v}}(0) = |\Xi\rangle\boldsymbol{u}(0),$$

$$\boldsymbol{A}_1 = \frac{1}{2}\sum_{j=1}^{D}\left\{c_j(\hat{z}_1,\ldots,\hat{z}_L,\hat{x}_1,\ldots,\hat{x}_D),\hat{p}_j\right\},$$

$$\boldsymbol{A}_2 = \frac{\mathrm{i}}{2}\sum_{j=1}^{D}\left[c_j(\hat{z}_1,\ldots,\hat{z}_L,\hat{x}_1,\ldots,\hat{x}_D),\hat{p}_j\right].$$

Note that when c_j does not depend on $\hat{x}_j$, then $[c_j,\hat{p}_j] = 0 = \boldsymbol{A}_2$, thus $\boldsymbol{A} = \boldsymbol{A}^\dagger$ and we can directly use Hamiltonian simulation and no Schrödingerisation is needed.

Quantum stochastic galerkin method

$$\frac{\mathrm{d}\tilde{\boldsymbol{v}}}{\mathrm{d}t} = -\mathrm{i}\boldsymbol{H}\tilde{\boldsymbol{v}}, \qquad \boldsymbol{H} = \boldsymbol{A}_2 \otimes \hat{\eta} + \boldsymbol{A}_1 \otimes I, \qquad \tilde{\boldsymbol{v}}(0) = |\Xi\rangle \boldsymbol{u}(0),$$

$$\boldsymbol{A}_1 = \frac{1}{2}\sum_{j=1}^{D} \left\{ c_j(\hat{z}_1, \ldots, \hat{z}_L, \hat{x}_1, \ldots, \hat{x}_D), \hat{p}_j \right\},$$

$$\boldsymbol{A}_2 = \frac{\mathrm{i}}{2}\sum_{j=1}^{D} \left[c_j(\hat{z}_1, \ldots, \hat{z}_L, \hat{x}_1, \ldots, \hat{x}_D), \hat{p}_j \right].$$

$\hat{z}_i$ are purely deterministic operators now, not stochastic

Information about the underlying distribution only enters through the initial condition:

$$\boldsymbol{u}(0) = \iint u(0, z_1, \ldots, z_L, x_1, \ldots, x_D)\, w^{1/2}(z_1) \ldots w^{1/2}(z_L)\, |z_1, \ldots, z_L\rangle |x_1, \ldots, x_D\rangle \mathrm{d}z_1 \ldots \mathrm{d}z_L \mathrm{d}x_1 \ldots \mathrm{d}x_D,$$

$$w(z_l) = \frac{\mathrm{e}^{-z_l^2}}{\sqrt{\pi}}.$$

Another interesting observation is that here it is the probability amplitude of the distribution of z_l, i.e. $w^{1/2}(z_l)$ rather than $w(z_l)$, that is embedded in the amplitude of the pure quantum state $|u(0)\rangle$, which is a uniquely quantum way of embedding the probability distribution

New method naturally suited to particle number measurements! Sufficient for these measurements to recover statistics

$$\boldsymbol{u}(t) \equiv \int dx \sum_{\boldsymbol{n}\in\mathbb{Z}_0^L} u_{\boldsymbol{n}}(t, x_1, ..., x_D)|\boldsymbol{n}\rangle|x_1, ..., x_D\rangle$$

$$|\mathbf{n}\rangle\langle\mathbf{n}|$$

projective measurements

Solve instead for $\mathbf{u_n}$

$$\mathbf{u}_0 = \mathbb{E}_z(u)$$

$$\sum_{\mathbf{n}} \mathbf{u}_{\mathbf{n}}^2 = \mathrm{Var}_z(u)$$

Given the output $\boldsymbol{u}(t)$, if one can measure in the number basis $|\boldsymbol{n}\rangle\langle\boldsymbol{n}|$, one is able to retrieve a state $\propto \int u_{\boldsymbol{n}}(t, x_1, \ldots, x_D)|x_1, \ldots, x_D\rangle \mathrm{d}x_1 \ldots \mathrm{d}x_D$, whose amplitudes correspond to already ensemble-averaged physically important quantities. The choice of $\boldsymbol{n} = \mathbf{0}$ for example can give the state whose amplitudes approximate $\mathbb{E}_{z_1,\ldots,z_L}(u)$.

Typically, for smooth, say C^∞, functions u, the coefficients in the above expansion in n_l decays exponentially in n_l, so only small n_l values need to be kept in the expansion, which can be used to retrieve accurately physically meaningful quantities. Suppose we keep terms in the expansion to $n_l = n_{\max}$ for each of the L modes. Then it is known that the error in approximating u with an expansion in u_{n_l} scales like $\sim 1/n_{\max}^m$, where m is the regularity of u, i.e. all derivatives up to $\partial^m u/\partial z_l^m$ exist and are bounded, but no higher derivatives exist. Thus, to capture most of the ensemble information about u, we only need to meausure n_l up to $n_{\max}$ which can be small, typically $n_{\max} \sim 3 - 5$ will be enough, for smooth functions u.

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	$D+1$	$[a_{K,j}, \hat{p}_j^K] \otimes \hat{\eta}, \quad b \otimes \hat{\eta}$	$O(DK)$
Inhomogeneous IV A	Add 1 more qubit	$[a_{K,j}, \hat{p}_j^K] \otimes \hat{\eta} \otimes \sigma, \quad b \otimes \hat{\eta} \otimes \sigma$	$O(DK)$
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	$D+1$	$i[\hat{p}, L] \otimes \hat{\eta}, \quad \{\hat{p}, L\} \otimes I$	$O(D)$
Heat V B 1	$D+1$	$\{\hat{p}\mathrm{D}, \hat{p}\} \otimes \hat{\eta}, \quad V \otimes \hat{\eta}$	$O(D+1)$
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	$\{a, \hat{p}^2\} \otimes \hat{\eta} \otimes \sigma, \quad V \otimes \eta \otimes \sigma, \quad i[a, \hat{p}^2] \otimes I \otimes \sigma$	$O(D)$
Maxwell ($D=3$) V B 5	4 qumodes + 4 qubits	See Section V B 5	30
Uncertain linear PDE VI Convection	$D+L+1$	$i[c, \hat{p}] \otimes \hat{\eta}, \quad \{c, \hat{p}\} \otimes I$	$O(DL)$
Nonlinear			
Scalar hyperbolic VII A	$D+1$	$i[Q, \hat{\zeta}] \otimes \hat{\eta}, \quad \{Q, \hat{\zeta}\} \otimes I$	$O(D)$
Hamilton-Jacobi VII A	$2D$	$[\hat{\zeta}H, \hat{p}]$	$O(D)$
N nonlinear ODEs VII B	$N+1$	$i[Q, F] \otimes \hat{\eta}, \quad \{Q, F\} \otimes I$	$O(N)$

L stochastic variables

Uncertain PDE: Method 2

- do not know the distribution from which the stochastic variables are sampled

New method 2: related to warped phase transformation

Warm-up example: heat equation with uncertain diffusion

$$\begin{cases} \partial_t u - a(x,z)\Delta u = 0 \\ u(0,x,z) = u_0(x,z) \end{cases}$$

Assume:

$$a(x,z) = \sum_{i=1}^{L} a_i(z) b_i(x) \tag{1}$$

where $x \in \mathbb{R}^d$ is the space variable, and z is the (possibly high-dimensional) random or deterministic parameters that model uncertainties. Without loss of generality, we assume $a_i(z) > 0$ for all i (since otherwise one can absorb the negative sign into $b_i(x)$), and

$$\sum_{i=1}^{L} a_i^2(z) \leq C \tag{2}$$

for some C independent of L. This already covers a fairly general class of inhomogeneous and uncertain coefficients.

arXiv: 2209.1120

Uncertain heat equation

$$\begin{cases} \partial_t u - a(x,z)\Delta u = 0 \\ u(0,x,z) = u_0(x,z) \end{cases}$$

Let $p = (p_1, \cdots, p_L)^T$, with $p_i \in (-\infty, \infty)$ for all $i = 1, ..., L$. We introduce the transformation

$$U(t,x,z,p) = \frac{1}{2}\prod_{i=1}^{L} a_i(z) e^{-a_i(z)|p_i|} u(t,x,z),$$

from which one can recover u from U via

$$u(t,x,z) = \int_{(-\infty,\infty)^L} U(t,x,z,p)dp = 2\int_{(0,\infty)^L} U(t,x,z,p)dp.$$

A simple computation shows that U solves

$$\partial_t U + \sum_{i=1}^{L} \text{sign}(p_i) b_i(x) \Delta \partial_{p_i} U = 0,$$

Stochastic term disappears!

in which the coefficients of the equation are *independent* of z!

Uncertain heat equation

To work with M samples $\{z_m\}$, $m = 1, ..., M$, we now define

$$V(t, x, p) = \frac{1}{M} \sum_{m=1}^{M} U(t, x, z_m, p)$$

for $p_i \in (-\infty, \infty)$, $i = 1, \cdots, L$, which solves

$$\begin{cases} \partial_t V + \sum_{i=1}^{L} \operatorname{sign}(p_i) b_i(x) \Delta \partial_{p_i} V = 0 \\ V(0, x, p) = \frac{1}{M} \sum_{m=1}^{M} \prod_{i=1}^{L} a_i(z_m) e^{-a_i(z_m)|p_i|} u(0, x, z_m) \,. \end{cases}$$

This is the linear PDE we will solve, which has *certain* coefficients and a *single* initial condition. Now the average of the solutions of the original problem, Eq. (5), can be recovered from $V(t, x, p)$ using

$$\overline{u}(t, x) = \frac{1}{M} \sum_{m=1}^{M} u(t, x, z_m) = \int V(t, x, p) \, dp \,.$$

Thus, in solving for V, the computational cost is clearly *independent of* M!

TABLE I. Quantum ($\mathcal{Q}$) and classical ($\mathcal{C}$) cost comparison for r^{th}-order approximations in computing ensemble averaged solutions, at Λ final meshpoints, over M samples, when $n_0^2\Lambda = O(N^b)$, where n_0^2 is a normalisation of the initial state. Quantum advantages are possible when $\gamma_i > 0$ for the corresponding parameters. We also give the sufficient range of b where quantum advantage is possible. In the table $M_{heat} \equiv O(L^{2+(d+L+3)/c}(d/\epsilon)^{(L+1)/3})$, $M_{Boltz} \equiv O(L^{(2d+L+1)/c}\max(L,d)(d/\epsilon)^{L/c}/d)$, $M_{adv} \equiv O(L^{(d+2L+3)/c+2}(d/\epsilon)^{(2L+2)/c})$ and $M_{Schr} \equiv O((d+L)^{(d+2L+2)/c+2}/(d^{(d+2)/c+2}\epsilon^{2L/r}))$.

$$\mathcal{O}\left(\frac{\mathcal{C}}{\mathcal{Q}}\right) = \tilde{O}\left(M^{\gamma_1} d^{\gamma_2} L^{\gamma_3} (d+L)^{\gamma_4} \left(\frac{1}{\epsilon}\right)^{\gamma_5}\right)$$

$(d+1)$-dim PDE (M initial data)	γ_1	γ_2	γ_3	γ_4	γ_5	b range	Parameters with advantage (possible)
Linear heat							
$M < M_{heat}$	1	$\frac{d-7-b}{r} - 1$	$-4 - \frac{9+b}{r}$	0	$\frac{d-7-b}{r}$	$[0, d-7-r]$	M, d, ϵ
$M > M_{heat}$	0	$\frac{d+L-6-b}{r} - 2$	$\frac{d+L-6-b}{3}$	0	$\frac{d+L-6-b}{r} - 1$	$[0, d+L-6-2r]$	L, d, ϵ
Linear Boltzmann							
$M < M_{Boltz}$	1	$\frac{d-2-b}{r} + 1$	$-1 - \frac{3+d+b}{r}$	-3	$\frac{d-2-b}{r} - 1$	$[0, d-2-2r]$	M, d, ϵ
$M > M_{Boltz}, L > d$	0	$\frac{d+L-2-b}{r}$	$\frac{d+L-2-b}{r}$	-3	$\frac{d+L-2-b}{r} - 1$	$[0, d+L-2-2r]$	L, d, ϵ
$M > M_{Boltz}, L < d$	0	$\frac{d+L-2-b}{r} + 1$	$\frac{d+L-2-b}{r} - 1$	-3	$\frac{d+L-2-b}{r} - 1$	$[0, d+L-2-2r]$	L, d, ϵ
Linear advection							
$M < M_{adv}$	1	$\frac{d-8-b}{r} - 2$	$-4 - \frac{9}{r}$	0	$\frac{d-8-b}{r} - 1$	$[0, d-8-2r]$	M, d, ϵ
$M > M_{adv}$	0	$\frac{d+2L-6-b}{r} - 2$	$\frac{d+2L-6-b}{r} - 2$	0	$\frac{d+2L-6-b}{r} - 1$	$[0, d+2L-6-2r]$	L, d, ϵ
Schrödinger							
$M < M_{Schr}$	1	$\frac{d+2}{r} + 2$	0	$-4 - \frac{6+b}{r}$	$\frac{d-4-b}{r} - 1$	$[0, d-4-r]$	M, d, ϵ
$M > M_{Schr}$	0	0	0	$\frac{d+2L-4-b}{r} - 2$	$\frac{d+2L-4-b}{r} - 1$	$[0, d+2L-4-2r]$	L, d, ϵ

TABLE II. Here $\mathcal{Q}_{orig}$ and $\mathcal{Q}$ are the respective quantum costs for r^{th}-order methods in computing ensemble averaged observables, over M samples, based on solving the original equation ($\mathcal{Q}_{orig}$) versus the phase space representation ($\mathcal{Q}$). Here s and κ are the sparsity and condition numbers corresponding to $\mathcal{M}$ of the original $(d+1)$-dimensional PDE and the phase space PDE. However, there are more oracle assumptions needed for $\mathcal{Q}_{orig}$ and when these assumptions are not obeyed, the phase space method is always preferable.

PDE	s	κ	$\mathcal{Q} < \mathcal{Q}_{orig}$
Linear heat	d	$(d/\epsilon)^{2/r}$	$M > \tilde{\mathcal{O}}(L^{4+9/r} d^3 (d/\epsilon)^{3/r})$
Phase space linear heat	Ld	$Ld(Ld/\epsilon)^{3/r}$	
Linear Boltzmann	$(d/\epsilon)^{d/r}$	$d(d/\epsilon)^{1/r}$	$M > \tilde{\mathcal{O}}(L^{1+(3+d)/r} (d/\epsilon)^{2/r}/(d\epsilon))$
Phase space linear Boltzmann	$L(Ld/\epsilon)^{d/r}$	$(d+L)(Ld/\epsilon)^{1/r}$	
Linear advection	d	$d(d/\epsilon)^{1/r}$	$M > \tilde{\mathcal{O}}(L^{4+9/r} d^2 (d/\epsilon)^{8/r})$
Phase space linear advection	Ld	$Ld(Ld/\epsilon)^{3/r}$	
Schrödinger	d	$(d/\epsilon)^{2/r}$	$M > \tilde{\mathcal{O}}((d+L)^3 (1+L/d)^{1+2/r} ((L+d)/\epsilon)^{4/r})$
Phase space Schrödinger	$d+L$	$(d+L)((d+L)/\epsilon)^{2/r}$	

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

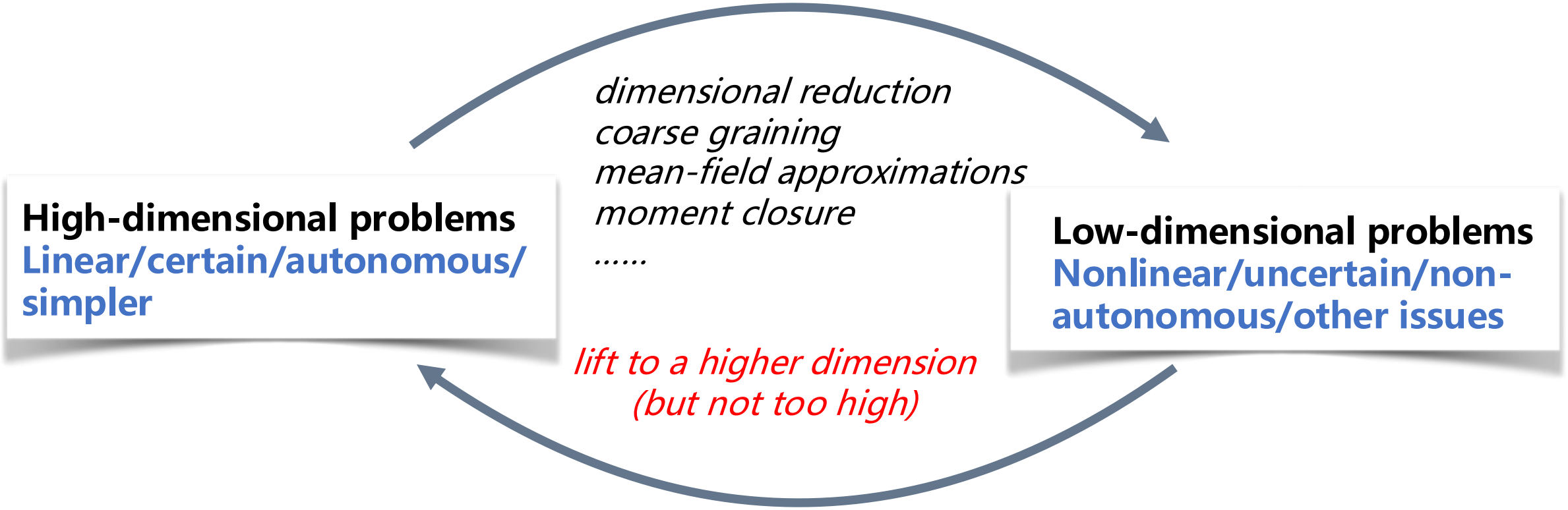
4. Linear non-autonomous systems become linear autonomous

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

Reference list for Part II: Uncertain PDEs

Uncertain PDEs:

- Section 6 in << *Analog quantum simulation of partial differential equations,* Shi Jin, Nana Liu*, arXiv: 2308.00646, Quantum Science and Technology, Vol 9, 035047, 2024>>

- Quantum algorithms for uncertainty quantification: application to partial differential equations, Francoise Golse, Shi Jin, Nana Liu*, arXiv: 2022.112200, SCIENCE CHINA Physics, Mechanics & Astronomy (SCPMA) (accepted 2025)
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Overview of summer lectures on Schrodingerisation

PART II: Special topics

- **Nonlinear ODEs and PDEs**
- **Uncertain ODEs/PDEs**
- **Non-autonomous mapped to autonomous PDEs**
- **Application to linear algebra, ground state and thermal state preparation**

Quantum simulation of partial differential equations via Schrodingerisation

PART II: Special topics
Non-autonomous PDEs

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Overview of summer lectures on Schrodingerisation

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- **Nonlinear ODEs and PDEs**
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- **Non-autonomous mapped to autonomous PDEs**
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II. Non-autonomous PDEs

``Turning linear non-autonomous PDEs into linear autonomous PDEs"

Based on:
"Quantum simulation for time-dependent Hamiltonian – with applications to non-autonomous ordinary and partial differential equations," Journal of Physics A (arXiv: 2312.02817),
Yu Cao, Shi Jin, Nana Liu*

+ using above scheme to unify different quantum simulation schemes for non-autonomous PDEs
"A unifying framework for quantum simulation algorithms for time-dependent Hamiltonian dynamics," arXiv:2411.03180, Yu Cao, Shi Jin, Nana Liu*

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:

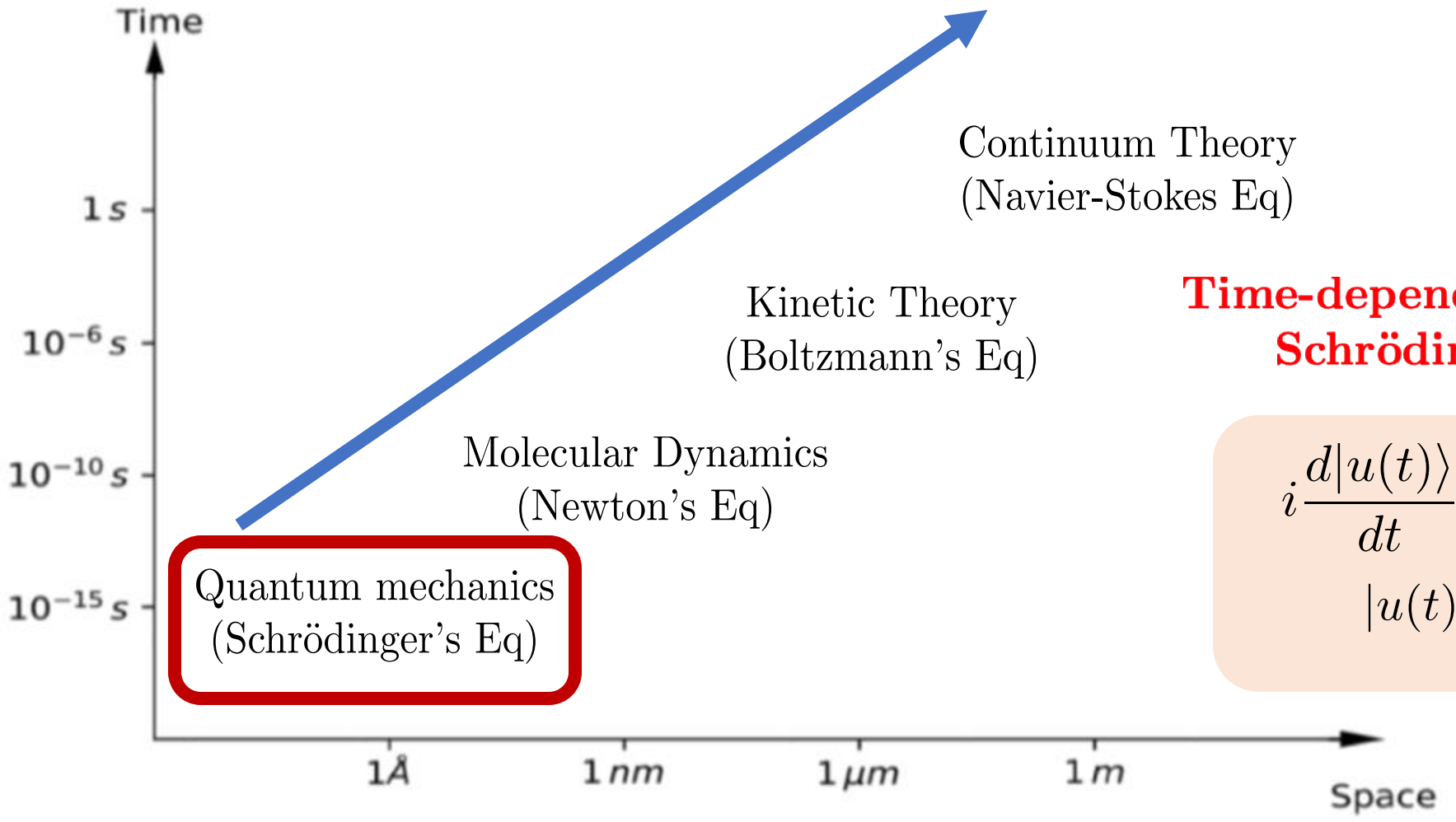
$$\mathbf{H}(t) = \mathbf{A}_2(t) \otimes \hat{\eta} + \mathbf{A}_1(t) \otimes \mathbf{1}$$

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

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

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

Ordinary and partial differential equations across multiple scales



Time-dependent Hamiltonian Schrödinger's equation

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

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

General applications of time-dependent Hamiltonian simulation

Adiabatic Quantum

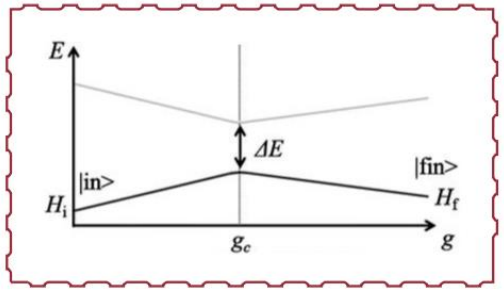


Photo from J. Necaise

Quantum control

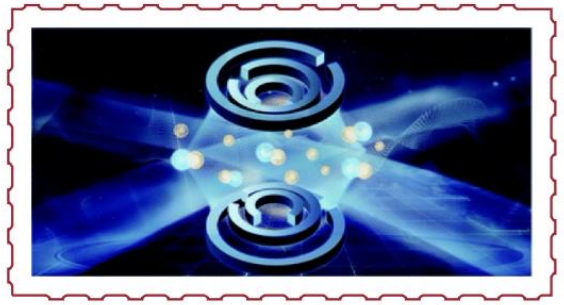
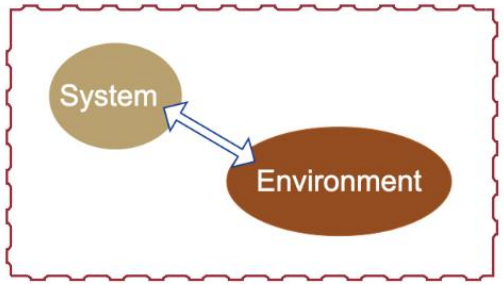


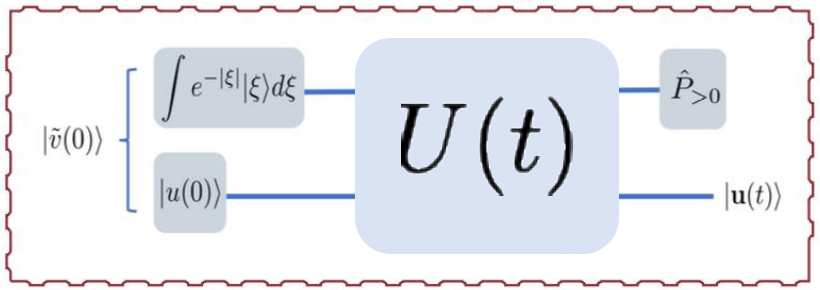
Photo from Chem. Soc. Rev., 2022,51, 1685-1701

Interaction picture



$$\dot{\rho}_I(t) = -i\alpha\left[\hat{H}_{c,I}(t), \rho_I(t)\right]$$

Solving PDEs: Schrödingerisation



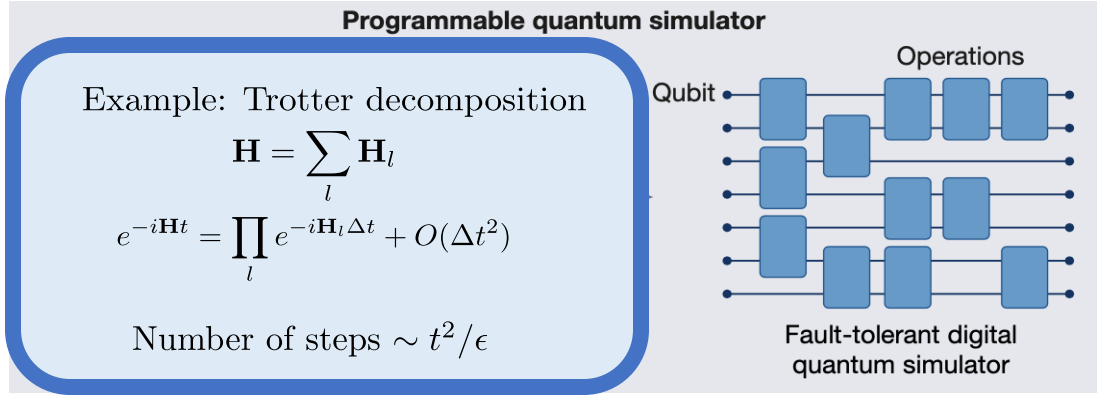
[Jin, Liu, Yu, PRL, 2024]

Time-*independent* Hamiltonian simulation is well-studied

$$U(t) = e^{-iHt}$$

Digital quantum simulation: evolution in discrete time

- Many different well-studied algorithms available



Analogue quantum simulation: evolution in continuous time

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

How to simulate evolution due to a time-dependent Hamiltonian?

$$\frac{\mathrm{d}\boldsymbol{y}(t)}{\mathrm{d}t} = -\mathrm{i}\boldsymbol{H}(t)\boldsymbol{y}(t), \qquad \boldsymbol{H}(t) = \boldsymbol{H}^{\dagger}(t),$$
$$\boldsymbol{y}(0) = \boldsymbol{y}_0.$$

The solution can be written as: $\boldsymbol{y}(t) = \mathcal{U}_{t,0}\boldsymbol{y}_0$

$$\mathcal{U}_{t,s} = \mathcal{T}\mathrm{e}^{-\mathrm{i}\int_s^t \boldsymbol{H}(\tau)\mathrm{d}\tau} = \lim_{N\to\infty} \mathrm{e}^{-\mathrm{i}\boldsymbol{H}(t_N)\Delta t}\cdots\mathrm{e}^{-\mathrm{i}\boldsymbol{H}(t_1)\Delta t}$$
$$= \mathbf{1} + \sum_{n=1}^{\infty}(-\mathrm{i})^n \frac{1}{n!}\int_s^t \mathrm{d}t_1 \cdots \int_s^t \mathrm{d}t_n \mathcal{T}\boldsymbol{H}(t_1)\cdots\boldsymbol{H}(t_n)$$

$\mathcal{T}$ is the chronological time-ordering operator

$[\boldsymbol{H}(t), \boldsymbol{H}(t')] = 0$, then no time-ordering is required

Time-*dependent* Hamiltonian simulation less well-studied

$$U(t) = \mathcal{T} e^{-i \int_0^t H(\tau) d\tau}$$

$$H(t) = \sum_k H_k(t), \qquad H_k(t) = f_k(t) \boldsymbol{h}_k$$

Digital quantum simulation: evolution in discrete time

Approximate $\mathcal{T}\left(e^{-i \int_0^T H(s)\ \mathrm{d}s}\right)$ via many small $e^{-i\alpha \boldsymbol{h}_k}$

Complicated to do time-ordering...

Analogue quantum simulation: evolution in continuous time

Quantum control methods
to tune parameters $f_k(t)$ in time

Changing non-autonomous Schrodinger's equation to autonomous Schrodinger's equation

Theorem 2. *For the non-autonomous system* $\frac{\mathrm{d}\boldsymbol{y}(t)}{\mathrm{d}t} = -\mathrm{i}\boldsymbol{H}(t)\boldsymbol{y}(t)$ *we introduce the following initial-value problem of an autonomous PDE*

$$\begin{aligned} &\frac{\partial \boldsymbol{w}}{\partial t} + \frac{\partial \boldsymbol{w}}{\partial s} = -\mathrm{i}\boldsymbol{H}(s)\boldsymbol{w} \\ &\boldsymbol{w}(0,s) = G(s)\boldsymbol{y}_0, \qquad s \in \mathbb{R}. \end{aligned} \tag{6}$$

The analytical solution to this problem is

$$\boldsymbol{w}(t,s) = G(s-t)\mathcal{U}_{s,s-t}\boldsymbol{y}_0, \qquad \mathcal{U}_{s,s-t} = \mathcal{T}\mathrm{e}^{-\mathrm{i}\int_{s-t}^{s}\boldsymbol{H}(\tau)d\tau} = \mathcal{T}\mathrm{e}^{-\mathrm{i}\int_{0}^{t}\boldsymbol{H}(s-t+\tau)\mathrm{d}\tau}. \tag{7}$$

When $G(s) = \delta(s)$*, one can easily recover* $\boldsymbol{y}(t)$ *in equation (2) from* $\boldsymbol{w}(t,s)$ *using*

$$\boldsymbol{y}(t) = \int_{-\infty}^{\infty} \boldsymbol{w}(t,s)\,\mathrm{d}s. \tag{8}$$

Alternatively, when $G(s) = 1$*,* $\boldsymbol{y}(t)$ *can be recovered with* $\boldsymbol{w}(t, s = t) = \boldsymbol{y}(t)$.

Changing non-autonomous Schrodinger's equation to autonomous Schrodinger's equation

Proof of theorem 2. We will now prove that $\boldsymbol{w}(t,s) = G(\sigma)\mathcal{U}_{s,\sigma}\boldsymbol{y}_0$ solves equation (6) using $\sigma = s - t$. The LHS of equation (6) can be written as

$$\begin{aligned}
\frac{\partial \boldsymbol{w}}{\partial t} + \frac{\partial \boldsymbol{w}}{\partial s} &= \left(\frac{\partial G(\sigma)}{\partial t} + \frac{\partial G(\sigma)}{\partial s}\right)\mathcal{U}_{s,\sigma}\boldsymbol{y}_0 + G(\sigma)\left(\frac{\partial \mathcal{U}_{s,\sigma}}{\partial t} + \frac{\partial \mathcal{U}_{s,\sigma}}{\partial s}\right)\boldsymbol{y}_0 \\
&= G(\sigma)\left(\mathcal{U}_{s,0}\frac{\partial \mathcal{U}_{0,\sigma}}{\partial t} + \frac{\partial \mathcal{U}_{s,0}}{\partial s}\mathcal{U}_{0,\sigma} + \mathcal{U}_{s,0}\frac{\partial \mathcal{U}_{0,\sigma}}{\partial s}\right)\boldsymbol{y}_0 \\
&= G(\sigma)\frac{\partial \mathcal{U}_{s,0}}{\partial s}\mathcal{U}_{0,\sigma}\boldsymbol{y}_0 + G(\sigma)\mathcal{U}_{s,0}\left(\frac{\partial \mathcal{U}_{0,\sigma}}{\partial t} + \frac{\partial \mathcal{U}_{0,\sigma}}{\partial s}\right)\boldsymbol{y}_0 \\
&= -\mathrm{i}\boldsymbol{H}(s)\boldsymbol{w} + G(\sigma)\mathcal{U}_{s,0}\left(\frac{\partial \mathcal{U}_{0,\sigma}}{\partial t} + \frac{\partial \mathcal{U}_{0,\sigma}}{\partial s}\right)\boldsymbol{y}_0 \\
&= -\mathrm{i}\boldsymbol{H}(s)\boldsymbol{w}.
\end{aligned}$$

Here in the first line the first term in brackets is zero, since letting $\sigma = s - t$, clearly $\partial G(\sigma)/\partial s = -\partial G(\sigma)/\partial t$. In the second term we used the expansion $\mathcal{U}_{s,\sigma} = \mathcal{U}_{s,0}\mathcal{U}_{0,\sigma}$. In the third line we used the definition for $\mathcal{U}_{s,0}$ which obeys equation (4) and $G(\sigma)\mathcal{U}_{s,0}\mathcal{U}_{0,\sigma}\boldsymbol{y}_0 = \boldsymbol{w}(t,s)$. The second term in the third line goes to zero since $\partial \mathcal{U}_{0,\sigma}/\partial s = -\partial \mathcal{U}_{0,\sigma}/\partial t$.

- When $G(s) = \delta(s)$, theorem 2 easily follows by integrating $\int \mathrm{d}s\, \boldsymbol{w}(t,s) = \int \mathrm{d}s\, \delta(s - t)\mathcal{U}_{s,s-t}\boldsymbol{y}_0 = \mathcal{U}_{t,0}\boldsymbol{y}_0 = \boldsymbol{y}(t)$.
- When $G(s) = 1$, $\boldsymbol{w}(t,s) = \mathcal{U}_{s,s-t}\boldsymbol{y}_0$, so $\boldsymbol{w}(t, s = t) = \mathcal{U}_{t,0}\boldsymbol{y}_0 = \boldsymbol{y}(t)$.

Non-autonomous unitary evolution can be made equivalent to autonomous unitary evolution in one higher dimension

$$\frac{d\boldsymbol{y}(t)}{dt} = -i\boldsymbol{H}(t)\boldsymbol{u}(t), \qquad \boldsymbol{H}(t) = \boldsymbol{H}^{\dagger}(t)$$
$$\boldsymbol{y}(0) = \boldsymbol{y}_0.$$

Non-autonomous and unitary

Add max 1 dimension

$$\frac{\partial \boldsymbol{w}}{\partial t} + \frac{\partial \boldsymbol{w}}{\partial s} = -i\boldsymbol{H}(s)\boldsymbol{w}$$

Autonomous and unitary

Define: $\bar{\boldsymbol{w}}(t) \equiv \int \mathrm{d}s\, \boldsymbol{w}(t,s)|s\rangle$

Equivalent autonomous unitary evolution with respect to time-independent Hamiltonian $\bar{\mathbf{H}}$:

$$\frac{\mathrm{d}\bar{\boldsymbol{w}}}{\mathrm{d}t} = -\mathrm{i}\bar{\boldsymbol{H}}\bar{\boldsymbol{w}}, \qquad \bar{\boldsymbol{H}} = \mathbf{1} \otimes \hat{p}_s + \boldsymbol{H}(\hat{s}) = \bar{\boldsymbol{H}}^{\dagger}, \qquad \bar{\boldsymbol{w}}(0) = |y_0\rangle \otimes \int \mathrm{d}s\, \boldsymbol{G}(s)\,|s\rangle$$

Sambe-Howland's clock [Sambe, PRA, 1973; Howland, Mathematische Annalen, 1974]

Retrieval of solution for the original non-autonomous Schrodinger equation

Theorem 4. *Given the solution* $\mathbf{y}(t) = \mathcal{U}_{t,0}\mathbf{y}_0$ *to the linear non-autonomous dynamical system* $\frac{\mathrm{d}\mathbf{y}(t)}{\mathrm{d}t} = -\mathrm{i}\boldsymbol{H}(t)\mathbf{y}(t)$ *with initial condition* $\mathbf{y}_0$, $|y(t)\rangle$ *can be simulated via unitary evolution with respect to the time-independent Hamiltonian* $\bar{\boldsymbol{H}}$ *in the following way. We define the quantum state* $\sigma(t)$ *evolving according to*

$$\frac{\mathrm{d}\sigma(t)}{\mathrm{d}t} = -\mathrm{i}\left[\bar{\boldsymbol{H}}, \sigma(t)\right], \qquad \bar{\boldsymbol{H}} = \mathbf{1} \otimes \hat{p}_s + \boldsymbol{H}(\hat{s}),$$

$$\sigma(0) = |y_0\rangle\langle y_0| \otimes \rho_0, \qquad \rho_0 = \iint \mathrm{d}s\,\mathrm{d}s'\, g(s,s')\,|s\rangle\langle s'|, \qquad \int \mathrm{d}s\, g(s,s) = 1,$$

where $\rho_0 = \rho_0^\dagger$ *and* ρ_0 *is also positive semidefinite.*

$$\text{Define:} \quad |y(t)\rangle \equiv \mathbf{y}(t)/\|\mathbf{y}(t)\|$$

Retrieval of solution for the original non-autonomous Schrodinger equation

Theorem continued:

- **(Protocol 1): With the choice of ρ_0 where $g(s,s)=\delta(s)$, then $|y(t)\rangle\langle y(t)| = \mathrm{Tr}_s\big(\sigma(t)\big)$ where the trace is over the $|s\rangle$ mode.**
- **(Protocol 2): Alternatively, with the choice of measuring $\sigma(t)$ in the mode $|s=t\rangle$,** for small $\varepsilon \ll 1$, $|y(t)\rangle\langle y(t)| \approx \frac{\mathrm{Tr}_s((\mathbf{1}\otimes\int_{s'\in[t-\varepsilon,t+\varepsilon]} ds'\ |s=s'\rangle\langle s=s'|)\,\sigma(t))}{\int_{s'\in[-\varepsilon,\varepsilon]} ds'\ g(s',s')}$ which approximately retrieves $|y(t)\rangle$ with success probability $\int_{s'\in[-\varepsilon,\varepsilon]} ds'\ g(s',s')$. The success probability is close to one if the density is $g(s,s)$ localized near $s\approx 0$ (which is essentially the case in Protocol 1).

Imperfect quantum clock register

When implementing the algorithms, one often needs to approximate the Dirac δ-function by a bounded and narrowly supported function δ_ω which becomes zero or vanishingly small outside a domain of $O(\omega)$, for $\omega \ll 1$, namely, we consider

$$\boldsymbol{y}_\omega(t) = \int_{-\infty}^{\infty} \delta_\omega(s-t)\mathcal{U}_{s,s-t}\boldsymbol{y}_0 \, \mathrm{d}s. \tag{10}$$

As conventionally done, we choose δ_ω to be smooth and to satisfy, for $x \in \mathbb{R}^1$,

$$\delta_\omega(x) = 0 \quad \text{if} \quad |x| > \omega; \qquad \int_{|x|\le\omega} \delta_\omega(x)\, dx = 1.$$

One usually approximates δ_ω by the form

$$\delta_\omega(x) = \begin{cases} \frac{1}{\omega}\beta(x/\omega) & |x| \le \omega; \\ 0 & |x| > \omega, \end{cases}$$

where typical choices of $\beta(x)$ include $\beta(x) = 1-|\beta|$ and $\beta(x) = \frac{1}{2}(1+\cos(\pi x))$ [28]. In a discrete-variable formulation, one can choose $\omega = mh$ where m is the number of mesh points within the support of δ_ω, and h is the grid size. For a continuous-variable formulation, one can choose δ_ω to be a Gaussian function

$$\delta_\omega(s-t) = \frac{1}{\sqrt{2\pi\omega^2}} e^{-(s-t)^2/(2\omega^2)},$$

which can give good approximation to $\boldsymbol{y}(t)$ if the width ω is small.

Error estimates

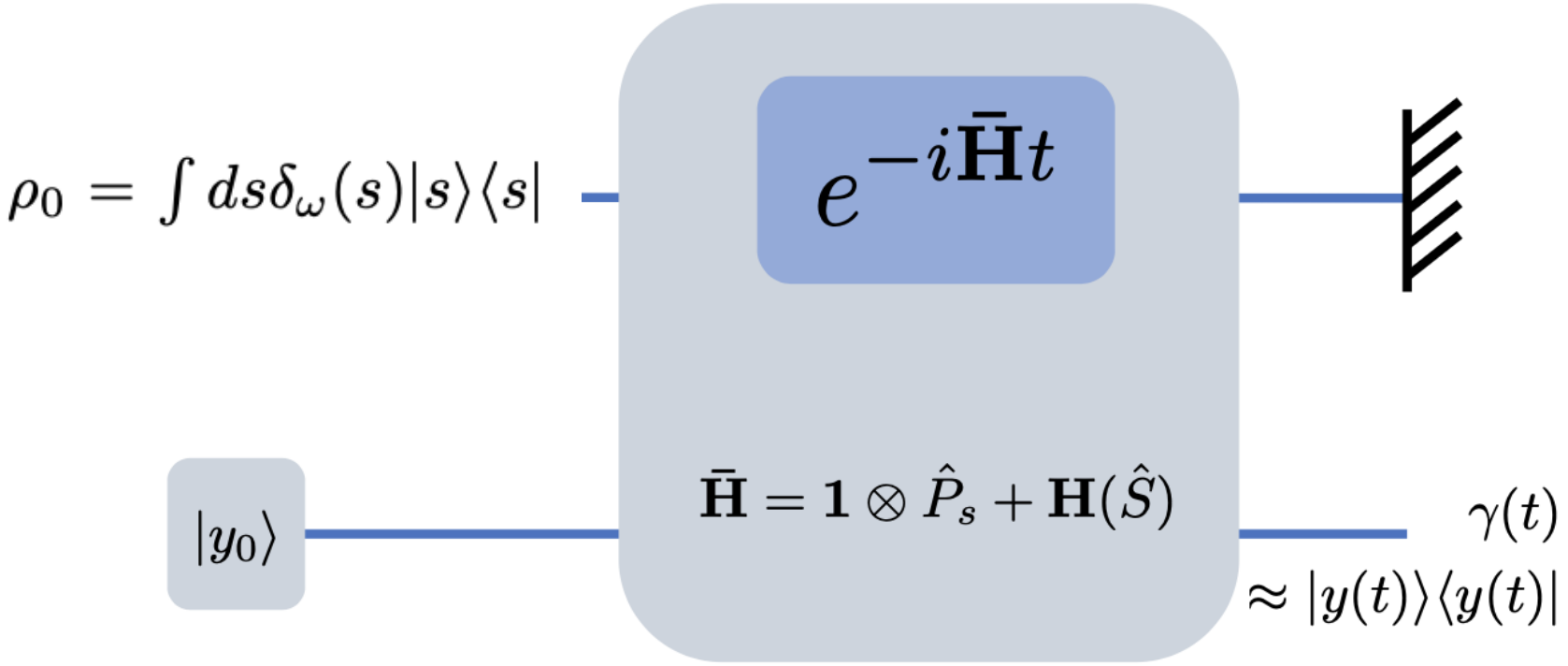
Lemma 3. *Let $\mathbf{y}_\omega(t)$ be given by equation (10) and $\mathbf{y}(t)$ be given by equation (2). Assume $\|\mathbf{y}_0\| = 1$, and the normalised states are expressed as $|y_\omega(t)\rangle = \mathbf{y}_\omega(t)/\|\mathbf{y}_\omega(t)\|$, $|y(t)\rangle = \mathbf{y}(t)/\|\mathbf{y}(t)\| = \mathbf{y}(t)$ where $\|.\|$ is the l_2-norm. Furthermore, Assume that*

(i) *$\delta_w(\cdot)$ is a probability distribution with mean $\mu = o(\omega)$ and second moment ω^2 (presumably $\omega \ll 1$); assume that all its moments equal or larger than three are negligible with scaling $o(\omega^2)$*
(ii) *the Hamiltonian $\boldsymbol{H}(t)$ is continuously differentiable with respect to t.*

Then, in the small ω limit, the quantum fidelity $Fid(.,.)$ between the ideal $|y(t)\rangle$ and the approximated state $|y_\omega(t)\rangle$ is

$$Fid\left(|y_\omega(t)\rangle, |y(t)\rangle\right) := |\langle y_\omega(t)|y(t)\rangle|^2 \equiv \frac{|\langle \mathbf{y}_\omega(t), \mathbf{y}(t)\rangle|^2}{\|\mathbf{y}_\omega(t)\|^2} = 1 + o(\omega^2).$$

Simple quantum protocol: unitary system



General non-autonomous linear PDE

General linear ODE/PDE:

$$\frac{\mathrm{d}\boldsymbol{u}(t)}{\mathrm{d}t} = -\mathrm{i}\boldsymbol{A}(t)\boldsymbol{u}(t) \qquad \boldsymbol{u}(0) = \boldsymbol{u}_0. \qquad \boldsymbol{A}(t) \neq \boldsymbol{A}^{\dagger}(t) \tag{1}$$

Remark 1. While theorem 2 is stated for the unitary dynamics, the same result can also hold for non-unitary dynamics (1) as long as the time-evolution operator for non-unitary case is well-defined.

Remark 2. A conventional way to transform a non-autonomous system to an autonomous ones is to add a new variable representing time

$$\begin{aligned} &\frac{\mathrm{d}\boldsymbol{y}}{\mathrm{d}t} = -\mathrm{i}\boldsymbol{H}(\tau)\boldsymbol{y}(t) \\ &\frac{\mathrm{d}\tau}{\mathrm{d}t} = 1 \\ &\boldsymbol{y}(0) = \boldsymbol{y}_0, \quad \tau(0) = 0. \end{aligned} \tag{9}$$

Note that even if the original system is linear, this new autonomous system becomes *nonlinear*.

Turning general linear non-autonomous system to an autonomous system with unitary dynamics

For a general linear dynamical system

$$\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} = -\mathrm{i}\boldsymbol{A}(t)\boldsymbol{u}, \qquad \boldsymbol{A}(t) \neq \boldsymbol{A}^{\dagger}(t),$$

we use the following decomposition

$$\boldsymbol{A}(t) = \boldsymbol{A}_1(t) - \mathrm{i}\boldsymbol{A}_2(t),$$

where $\boldsymbol{A}_1(t) = \frac{1}{2}\left(\boldsymbol{A}(t) + \boldsymbol{A}^{\dagger}(t)\right) = \boldsymbol{A}_1^{\dagger}(t), \qquad \boldsymbol{A}_2(t) = \frac{i}{2}\left(\boldsymbol{A}(t) - \boldsymbol{A}^{\dagger}(t)\right) = \boldsymbol{A}_2^{\dagger}(t)$

Apply Schrödingerisation $\Longrightarrow$ $\frac{\mathrm{d}\boldsymbol{y}}{\mathrm{d}t} = -\mathrm{i}\boldsymbol{H}(t)\boldsymbol{y}, \qquad \boldsymbol{H}(t) = \hat{\eta} \otimes \boldsymbol{A}_2(t) + \boldsymbol{I}_{\eta} \otimes \boldsymbol{A}_1(t), \qquad \boldsymbol{H}(t) = \boldsymbol{H}^{\dagger}(t)$

Turning general linear non-autonomous system to an autonomous system with unitary dynamics

Schrödingerisation

$$\frac{d\boldsymbol{y}(t)}{dt} = -i\boldsymbol{H}(t)\boldsymbol{u}(t), \qquad \boldsymbol{H}(t) = \boldsymbol{H}^\dagger(t)$$
$$\boldsymbol{y}(0) = \boldsymbol{y}_0.$$

Non-autonomous and unitary

Add max 1 dimension

$$\frac{d\boldsymbol{u}(t)}{dt} = -i\boldsymbol{A}(t)\boldsymbol{u}(t) \qquad \boldsymbol{u}(0) = \boldsymbol{u}_0$$
$$\mathbf{A}^\dagger(t) \neq \mathbf{A}(t)$$

Non-autonomous and non-unitary

Add max 2 dimension

$$\frac{\partial \boldsymbol{w}}{\partial t} + \frac{\partial \boldsymbol{w}}{\partial s} = -i\boldsymbol{H}(s)\boldsymbol{w}$$

Autonomous and unitary

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

Turning general linear non-autonomous system to an autonomous system with unitary dynamics

Theorem 5. *The linear non-autonomous dynamical system* $\frac{d\mathbf{y}}{dt} = -i\boldsymbol{H}(t)\mathbf{y}$ *has a corresponding non-autonomous system* $\mathbf{y}(t)$ *that evolves with respect to the unitary* $\mathcal{U}_{t,0} = \mathcal{T}\exp(-i\int_0^t \boldsymbol{H}(\tau)d\tau)$ *and obeys* $\frac{d\mathbf{y}}{dt} = -i\boldsymbol{H}(t)\mathbf{y}$ *with initial condition* $\mathbf{y}_0 = |\Xi\rangle\boldsymbol{u}_0$, *where* $|\Xi\rangle = \int \exp(-|\xi|)|\xi\rangle d\xi$. *Then* $|u(t)\rangle$ *can be simulated via unitary evolution with respect to the time-independent Hamiltonian* $\bar{\boldsymbol{H}}$ *in the following way. We define the quantum state* $\sigma(t)$ *evolving according to*

$$\frac{d\sigma(t)}{dt} = -i\left[\bar{\boldsymbol{H}}, \sigma(t)\right],$$

$$\bar{\boldsymbol{H}} = I_\eta \otimes \mathbf{1} \otimes \hat{p}_s + \boldsymbol{H}(\hat{s}) = I_\eta \otimes \mathbf{1} \otimes \hat{p}_s + \hat{\eta} \otimes \boldsymbol{A}_2(\hat{s}) + I_\eta \otimes \boldsymbol{A}_1(\hat{s}),$$

$$\sigma(0) = |y_0\rangle\langle y_0| \otimes \rho_0, \qquad |y_0\rangle = \frac{\mathbf{y}_0}{\|\mathbf{y}_0\|},$$

$$\rho_0 = \iint ds ds' g(s,s') |s\rangle\langle s'|, \qquad \iint ds g(s,s) = 1,$$

where $\rho_0 = \rho_0^\dagger$ *and* ρ_0 *is also positive semidefinite.*

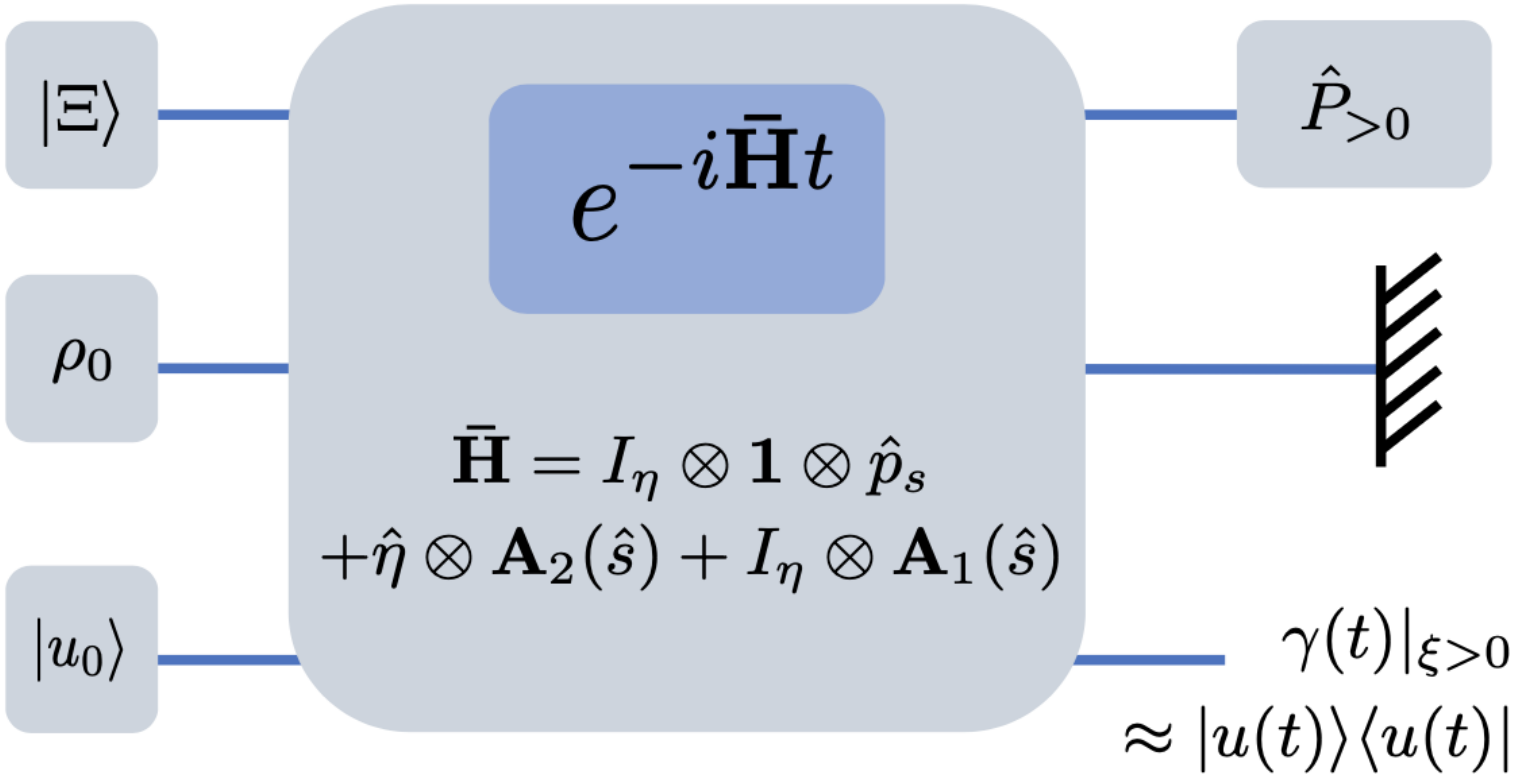
Retrieval of solution of original non-autonomous linear PDE

Theorem continued:

- **(Protocol 1): With the choice of** ρ_0 **where** $g(s,s)=\delta(s)$, **then** $|y(t)\rangle\langle y(t)| = \mathrm{Tr}_s(\sigma(t))$ **where the trace is over the** $|s\rangle$ **mode.**
- **(Protocol 2): Alternatively, with the choice of measuring** $\sigma(t)$ **in the mode** $|s=t\rangle$, **then for small**$\epsilon \ll 1$, $|y(t)\rangle\langle y(t)| \approx \frac{\mathrm{Tr}_s((I_\eta \otimes 1 \otimes \int_{s' \in [t-\epsilon, t+\epsilon]} ds'\ |s=s'\rangle\langle s=s'|)\sigma(t))}{\int_{s' \in [-\epsilon,\epsilon]} ds'\ g(s',s')}$ which approximately retrieves $|y(t)\rangle$ with success probability $\int_{s' \in [-\varepsilon,\varepsilon]} ds'\ g(s',s')$. The success probability is close to one if the density $g(s,s)$ is localized near $s \approx 0$.

Given any measurement $\hat{P}_{>0} = \int_0^\infty f(\xi)|\xi\rangle\langle\xi| \mathrm{d}\xi$, then $|u(t)\rangle$ can be retrieved from $|y(t)\rangle$ using $\hat{P}_{>0}|y(t)\rangle \propto |u(t)\rangle$ with success probability $\mathcal{O}(\int_0^\infty f(\xi)\mathrm{e}^{-\xi}\mathrm{d}\xi(\|\boldsymbol{u}(t)\|/\|\boldsymbol{u}_0\|)^2)$.

Simple quantum protocol: non-unitary system



Example: 1D Fokker-Planck equation

We consider the time-dependent Fokker–Planck equation

$$\partial_t \boldsymbol{q}(t,x) = g(t)\,\nabla\cdot(x\boldsymbol{q}(t,x)) + \beta(t)\,\Delta\boldsymbol{q}(t,x) =: -\mathrm{i}\boldsymbol{A}\boldsymbol{q}(t,x),$$

which characterises the evolution of the probability density function for a time-dependent Ornstein–Uhlenbeck process $\mathrm{d}X(t) = -\nabla_x U\big(t,X(t)\big)\ \mathrm{d}t + \sqrt{2\beta(t)}\ \mathrm{d}W(t)$, where the time-dependent potential $U(t,x) = g(t)\frac{x^2}{2}$. By theorem 5, the Hamiltonian conservation part $\boldsymbol{A}_1$ and the interaction part $\boldsymbol{A}_2$ are

$$\boldsymbol{A}_1 = -g(t)\,\hat{x}\,\hat{p} + i\,\frac{g(t)}{2}\mathbf{1}, \qquad \boldsymbol{A}_2 = -\frac{g(t)}{2}\mathbf{1} + \beta(t)\,\hat{p}^2.$$

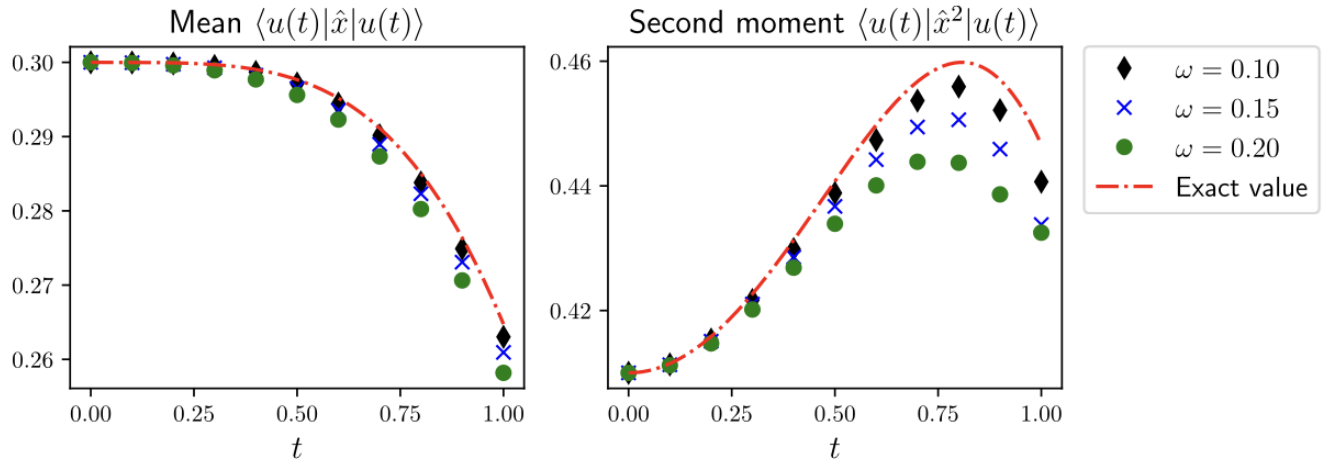
Example: 1D Fokker-Planck equation

We use the following observables $\langle q(t)|\hat{x}|q(t)\rangle$, $\langle q(t)|\hat{x}^2|q(t)\rangle$ where $|q(t)\rangle$ is the normalised quantum state of $\boldsymbol{q}(t,x)$. In total, we consider three cases where explicit solutions are available:

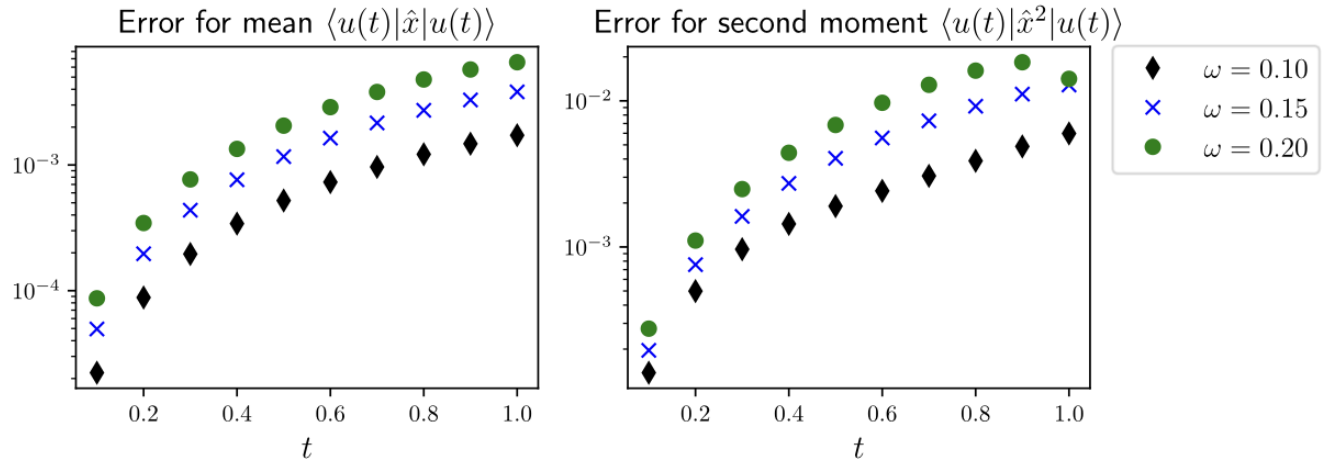
$$\begin{cases} \text{Case (1):} & g(t) = 0.5s,\ \beta(t) = 0.5s; \\ \text{Case (2):} & g(t) = 0.5s,\ \beta(t) = 0.3; \\ \text{Case (3):} & g(t) = 0.5s^3, \beta(t) = 0.3s. \end{cases}$$

In all three cases, the initial condition $\boldsymbol{q}(0,\cdot) = \mathcal{N}\left(0.3, 0.8^2\right)$. In simulation, we used the Galerkin method with parameters $N_s = 128$, $\varsigma_s = 0.2$, $N_\eta = 128$, $\varsigma_\eta = 2.0$, $N_u = 64$, $\varsigma_u = 2.0$, which amounts to using 7 qubits for time dilation, 7 qubits for Schrodingersation, 6 qubits for approximating the original Fokker–Planck equation. Notably, we will numerically demonstrate below that with a noiseless Hamiltonian simulation, we can simulate a 1D time-dependent PDE only *with a total of 20 qubits*. Such an amount of noisy qubits is already available at present.

Example: 1D Fokker-Planck equation



(a) Observables with respect to time



$$g(t) = 0.5s^3, \beta(t) = 0.3s.$$

Unifying framework for digital quantum simulation for time-dependent Hamiltonians

Messy literature for dealing with time-dependent Hamiltonians (mostly digital protocls) … is there a way of unifying them?

Product formula

- M. Suzuki, Proc. Jpn. Acad. B (1993) [Suzuki's time operator]
- Huyghebaert and D. Raedt, J. Phys. A: Math. Gen. (1990) [integral-based query]

Multi-Product Formula & qDrift

- Watkins, Wiebe, Roggero, and Lee, PRX Quantum (2024) [Discrete clock]
- Berry, Childs, Su, Wang, and Wiebe, Quantum (2020) [Continuous qDrift]

Dyson & Qubitization

- Kieferová, Scherer, and Berry, PRA (2019) [Dyson's expansion]
- Mizuta and Fujii, Quantum (2023) [Sambe's space]

Magnus expansion

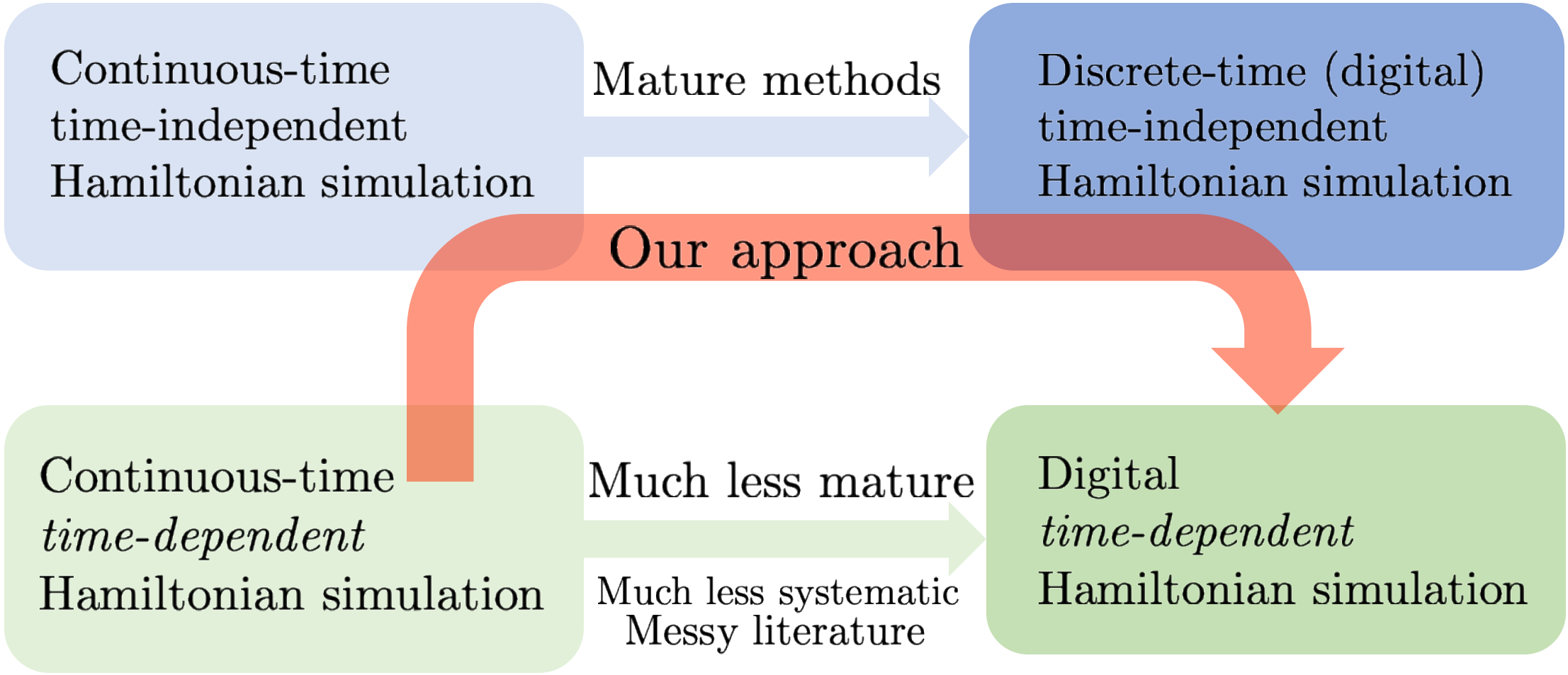
- Ikeda, Abrar, Chuang, and Sugiura, Quantum (2023)
- Casares, Zini, and Arrazola, CFQM, (2024), arXiv:2403.13889

Analogue algorithms as a starting point to identify new digital algorithms

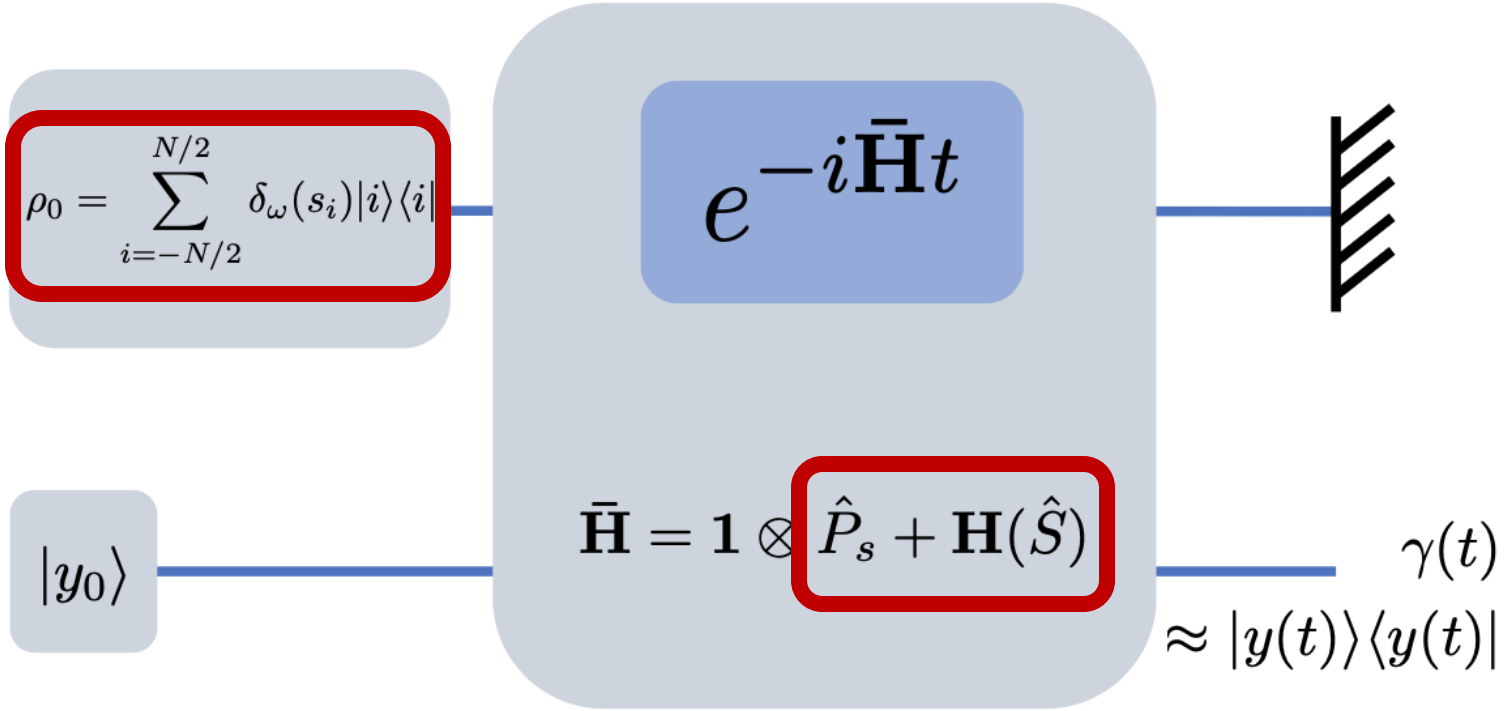
Continuous formulations are exact:

- Different numerical schemes for PDEs arise from the original *continuous formulation* of the PDE itself
- Different digital quantum algorithms for PDEs arise from the different methods of discretising the position and momentum operators in Schrodingerisation in its *continuous formulation*
- A *continuous formulation* for time-dependent Hamiltonian simulation can similarly be discretised in different ways to give different digital algorithms

Analogue algorithms as a starting point to identify new digital algorithms



Discretising the imperfect clock register



Discretising $\hat{S}$ and $\hat{P}_s$

Discretising the imperfect clock register

Sambe-Howland's clock + Different discretization for time-independent dynamics
= Quantum Algorithm for time-dependent Hamiltonian Dynamics

ω	**Discretize s**	**Algorithm**	**Remark**
$\omega \to 0$	Operator-Splitting	Product formula, MPF, qDrift	Our work
$\omega \to 0$	Taylor expansion	Taylor-LCU	Our work
$0 < \omega \ll 1$	Finite-difference	Qubitization-based; so far limited to first-order	Watkins, etc, 2024
$\omega \to \infty$	Spectral	Qubitization-based; log scale wrt error	Mizuta & Fujii, 2023

Recovering the product formula (I)

Sambe-Howland's clock: $\mathcal{U}(t+\Delta t, t)|\psi\rangle = \langle \mathbb{I}|e^{-i\overline{H}\Delta t}|t\rangle|\psi\rangle$

Example: Digitized Adiabatic Computing $H(s) = f_1(s)\ \boldsymbol{h}_1 + f_2(s)\ \boldsymbol{h}_2$

Step 1: Augmented Hamiltonian: $\overline{H} = \hat{p}_s \otimes I + f_1(\hat{s}) \otimes \boldsymbol{h}_1 + f_2(\hat{s}) \otimes \boldsymbol{h}_2$

Step 2: decompose

$$\overline{H} = A_1 + A_2 + A_3 \qquad A_1 = \hat{p}_s \otimes I \qquad A_2 = f_1(\hat{s}) \otimes \boldsymbol{h}_1 \qquad A_3 = f_2(\hat{s}) \otimes \boldsymbol{h}_2$$

Step 3: Apply time-independent product formula for $e^{-i\overline{H}\Delta t}$,

$$e^{-i\overline{H}\Delta t} \approx e^{-iA_1\Delta t} e^{-iA_2\Delta t} e^{-iA_3\Delta t}$$

$$\implies \mathcal{U}(t+\Delta t, t)|\psi\rangle \approx e^{-if_1(t)\boldsymbol{h}_1\Delta t} e^{-if_2(t)\boldsymbol{h}_2\Delta t}\,|\psi\rangle$$

(we get a time-dependent alg!)

Recovering the product formula (I)

For the general results, we can use L local operators (beyond $L = 2$ herein)

- For symmetric q cycled time-independent product formula with order n

$$\overline{H} = A_1 + A_2 + A_3 \qquad A_1 = \hat{p}_s \otimes I \qquad A_2 = f_1(\hat{s}) \otimes \boldsymbol{h}_1 \qquad A_3 = f_2(\hat{s}) \otimes \boldsymbol{h}_2$$

Recover the Suzuki's formula

[Suzuki, Proc. Jpn. Acad. B (1993)]

- For symmetric q cycled time-independent product formula with order n

$$\overline{H} = A_1 + A_2 + A_3 \qquad A_1 = f_1(\hat{s}) \otimes \boldsymbol{h}_1 \qquad A_2 = \hat{p}_s \otimes I \qquad A_3 = f_2(\hat{s}) \otimes \boldsymbol{h}_2$$

This case always ends up with a time-dependent scheme using the same number of matrix exponential (quantum gates) as the time-independent case.

Answers how to construct the minimum gate time-dependent product formula from

[Ikeda, Abrar, Chuang, and Sugiura, Quantum (2023)]

Recovering the product formula (II)

Example: Digitized Adiabatic Computing $H(s) = f_1(s)\ \boldsymbol{h}_1 + f_2(s)\ \boldsymbol{h}_2$

Step 1: Augmented Hamiltonian: $\overline{H} = \hat{p}_s \otimes I + f_1(\hat{s}) \otimes \boldsymbol{h}_1 + f_2(\hat{s}) \otimes \boldsymbol{h}_2$

Step 2: decompose

$$\overline{H} = A_1 + A_2 + A_3$$
$$A_1 = f_1(\hat{s}) \otimes \boldsymbol{h}_1 + \hat{p}_s \otimes \boldsymbol{I} \qquad A_2 = -\hat{p}_s \otimes \boldsymbol{I} \qquad A_3 = f_2(\hat{s}) \otimes \boldsymbol{h}_2 + \hat{p}_s \otimes \boldsymbol{I}$$

Step 3: Apply time-independent product formula for $e^{-i\overline{H}\Delta t}$, e.g., Strang-splitting, one obtains

$$e_{\mathcal{T}}^{-i\left(\int_{t+\frac{\Delta t}{2}}^{t+\Delta t} f_1(s)\mathrm{d}s\right)\boldsymbol{h}_1}\ e_{\mathcal{T}}^{-i\left(\int_{t}^{t+\Delta t} f_2(s)\mathrm{d}s\right)\boldsymbol{h}_2}\ e_{\mathcal{T}}^{-i\left(\int_{t}^{t+\frac{\Delta t}{2}} f_1(s)\mathrm{d}s\right)\boldsymbol{h}_1}$$

This recovers the formula in [Huyghebaert and D. Raedt, J. Phys. A: Math. Gen. (1990)]

Recovering the product formula (II)

It was discussed as unknown how to achieve high-order time-dependent product formula using gates like $\exp\left\{-i\int_s^t f_k(r)\mathrm{d}r\boldsymbol{h}_k\right\}$

[Ikeda, Abrar, Chuang, and Sugiura, Quantum (2023)]

Using Sambe-Howland's clock,

- if we choose any time-independent product formula,
- if we choose decomposition

$$\overline{H} = A_1 + A_2 + A_3$$
$$A_1 = f_1(\hat{s}) \otimes \boldsymbol{h}_1 + \hat{p}_s \otimes \boldsymbol{I} \qquad A_2 = -\hat{p}_s \otimes \boldsymbol{I} \qquad A_3 = f_2(\hat{s}) \otimes \boldsymbol{h}_2 + \hat{p}_s \otimes \boldsymbol{I}$$

then we get a time-dependent scheme with the above form

This answers their open question

Recovering the multi-product formula

Time-independent case: $e^{-iH\Delta t} = \sum_{j=1}^{M} \alpha_j \left(U_2(\frac{\Delta t}{k_j}) \right)^{k_j} + \mathcal{O}(\Delta t)^{2m+1}$ where

$$\begin{bmatrix} 1 & 1 & \cdots & 1 \\ k_1^{-2} & k_2^{-2} & \cdots & k_M^{-2} \\ \vdots & \vdots & \vdots & \vdots \\ k_1^{-2(m-1)} & k_2^{-2(m-1)} & \cdots & k_M^{-2(m-1)} \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_M \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

Time-dependent case: $e^{-i\overline{H}\Delta t} = \sum_{j=1}^{M} \alpha_j \left(\overline{U}_2(\frac{\Delta t}{k_j}) \right)^{k_j} + \mathcal{O}(\Delta t)^{2m+1}$

By simplifying its effect on the state $|t\rangle_s |\psi\rangle$, one gets time-dependent MPF

Recovering qDrift

Time-independent case: suppose Hamiltonian $H = \int \mathrm{d}\omega \; \lambda(\omega) H_\omega$

$$\text{(qDrift)} \qquad \underbrace{e^{-i\Delta t H} \; \rho \; e^{i\Delta t H}}_{\text{target}} \approx \underbrace{\int \mathrm{d}\omega \; \lambda(\omega) e^{-i\Delta t H_\omega} \rho e^{i\Delta t H_\omega}}_{\text{average of local evolution}}$$

[Campbell, PRL, 2019]

- Use $\overline{H} = \sum_k \lambda_k \big(\hat{p}_s \otimes I + \frac{1}{\lambda_k} H_k(\hat{s})\big)$

$$\implies \mathcal{U}(t+\Delta t, t) \rho \mathcal{U}(t+\Delta t, t)^\dagger \approx \sum_k \lambda_k U_k \rho U_k^\dagger, \quad U_k = \exp_{\mathcal{T}} \Big(-i \int_t^{t+\Delta t} \frac{H_k(s)}{\lambda_k} \mathrm{d}s \Big)$$

- Use $\overline{H} = \sum_k \int_0^1 \mathrm{d}r \; \mu(k,r) \big(\hat{p}_s \otimes I + \frac{1}{\mu(k,r)} H_k(\hat{s})\big)$

$\implies$ it recovers "continuous qDrift"

[Berry, Childs, Su, Wang, and Wiebe, Quantum (2020)]

Discovering higher performance time-dependent Hamiltonian simulation methods

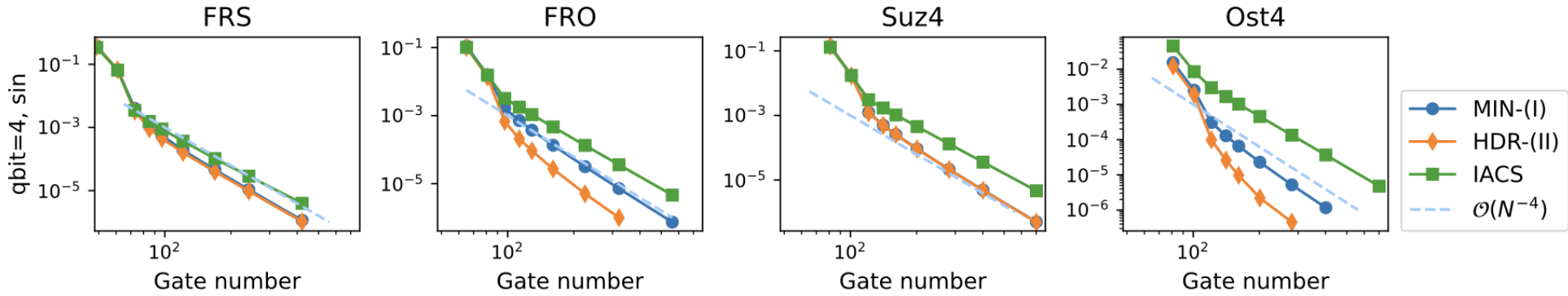
Adiabatic Google's PageRank

$$H(t) = T(1 - f(t))\boldsymbol{h}_1 + Tf(t)\boldsymbol{h}_2$$

$$\boldsymbol{h}_1 = I - |+\rangle^{\otimes n}\langle +|^{\otimes n}, \qquad \boldsymbol{h}_2 = (I - G)^\dagger (I - G), \qquad G = 0.85P^T + 0.15E$$

$$f(t) = \sin\left(\tfrac{\pi}{2}t\right), \qquad T = 40$$

Averaged error (trace distance)



- IACS refers to a Magnus-motivated scheme from [Ikeda, Abrar, Chuang, and Sugiura, Quantum (2023)]
- HDR-(II) is our newly developed family of higher-order scheme

Summary of recovering old and discovering new schemes

Sambe-Howland's Clock with Product Formula $\overline{H} = A_1 + A_2 + A_3$

Ordered Decomposition	Time-independent	Time-dependent	Gate (general)	Gate (DAS)
$A_1 = \hat{p}_s \otimes \mathbf{I}$ $A_2 = H_1(\hat{s})$ $A_3 = H_2(\hat{s})$	Suzuki [6]	Suzuki [21]	$2\Lambda q - q$	$2\Lambda q - 2q + 1$
	any product formula with q-cycles	Theorem 6	$2\Lambda q - q$	$2\Lambda q - 2q + 1$
$A_1 = H_1(\hat{s})$ $A_2 = \hat{p}_s \otimes \mathbf{I}$ $A_3 = H_2(\hat{s})$	any product formula with q-cycles	Theorem 6	$2\Lambda q - 2q + 1$	$2\Lambda q - 2q + 1$
$A_1 = \hat{p}_s \otimes \mathbf{I} + H_1(\hat{s})$ $A_2 = -\hat{p}_s \otimes \mathbf{I}$ $A_3 = \hat{p}_s \otimes \mathbf{I} + H_2(\hat{s})$	first-order Trotter	Huyghebaert, De Raedt [20]	Λ	Λ
	Strang splitting ($q = 1$)	Huyghebaert, De Raedt [20]	$2\Lambda - 1$	$2\Lambda - 1$
	any product formula with q-cycles	Theorem 8	$2\Lambda q - 2q + 1$	$2\Lambda q - 2q + 1$

"Gate (general)" means the number of gates for one-step approximation without any assumption on original Hamiltonian, whereas "Gate (DAS)" means the number of gates for digital adiabatic simulation where $H_k(s) = f_k(s)\boldsymbol{h}_k$. We assume that time-independent decomposition has q-cycles as in

$$e^{(A+B)\Delta t} = e^{Aa_1\Delta t} e^{Bb_1\Delta t} \cdots e^{Bb_q\Delta t} e^{Aa_{q+1}\Delta t} + \mathcal{O}\left(\Delta t^{n+1}\right)$$

Summary of recovering old and discovering new schemes

Sambe-Howland's Clock with Multi-Product Formula $\overline{H} = A_1 + A_2 + A_3$

Ordered Decomposition	Base	Time-independent MPF	Time-dependent MPF
$A_1 = \hat{p}_s \otimes \mathbf{I}$ $A_2 = H_1(\hat{s})$ $A_3 = H_2(\hat{s})$	Strang splitting	[9]	Theorem 9 (using continuous-clock) (Conjectured in [23] using discrete clock) (cf. [49] using Suzuki's time operator)
$A_1 = \hat{p}_s \otimes \mathbf{I} + H_1(\hat{s})$ $A_2 = -\hat{p}_s \otimes \mathbf{I}$ $A_3 = \hat{p}_s \otimes \mathbf{I} + H_2(\hat{s})$			see Theorem 10

Summary of recovering old and discovering new schemes

Sambe-Howland's Clock with qDrift $\overline{H} = \sum_{k=1}^{\Lambda} \int_0^1 \mathrm{d}r\, \mu(k,r) \left(\hat{p}_s \otimes \mathrm{I} + \frac{H_k(\hat{s})}{\mu(k,r)} \right)$

where μ is any probability measure for $(k,r) \in \{1,2,\cdots,\Lambda\} \times [0,1]$

Measures	Time-independent qDrift	Time-dependent qDrift	Error Scaling	Notes
$\mu(k,r) = \mu_k$ is independent of r	[14]	see (35)	see Lemma 12	/
general measure μ		see (37)	see Lemma 13	recover "continuous qDrift" [26]; see Lemma 14

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

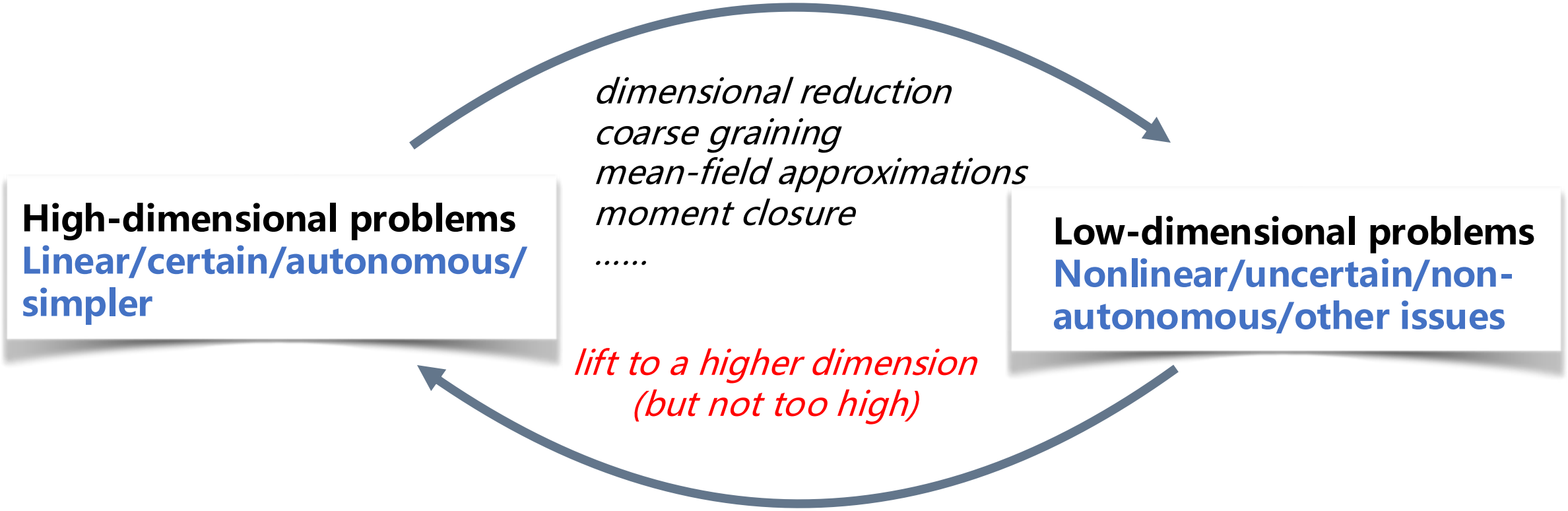
4. Linear non-autonomous systems become linear autonomous

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

Reference list for Part II: Non-autonomous PDEs

Non-autonomous PDEs:

- *Quantum simulation for time-dependent Hamiltonians -- with applications to non-autonomous ordinary and partial differential equations*, Yu Cao, Shi Jin and Nana Liu*, arXiv: 2312.02817, Journal of Physics A, Vol 58, 155304, 2005

- *A unifying framework for quantum simulation algorithms for time-dependent Hamiltonian dynamics*, Yu Cao*, Shi Jin and Nana Liu*, arXiv: 2411.03180, 2024

Overview of summer lectures on Schrodingerisation

PART II: Special topics

- **Nonlinear ODEs and PDEs**
- **Uncertain ODEs/PDEs**
- **Non-autonomous mapped to autonomous PDEs**
- **Application to linear algebra, ground state and thermal state preparation**

Quantum simulation of partial differential equations via Schrodingerisation

PART II: Special topics
Linear algebra, ground state and thermal state preparation

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Shanghai Jiao Tong University

CEMRACS 15-19 Jul 2025

Overview of summer lectures on Schrodingerisation

PART II: Special topics

- **Nonlinear ODEs and PDEs**
- **Uncertain and stochastic ODEs/PDEs**
- **Non-autonomous mapped to autonomous PDEs**
- **Application to linear algebra, ground state and thermal state preparation**

II. Linear algebra, ground state and thermal state preparation

``Turning iterative solvers into ODEs"

Based on:
"Quantum simulation of discrete linear dynamical systems and simple iterative methods in linear algebra via Schrodingerisation," (arXiv:2304.02865), Proceedings of the Royal Society A, 2024, Shi Jin and Nana Liu*

"Quantum simulation of partial differential equations via Schrodingerisation", Physical Review Letters (arXiv: 2212.13969), Shi Jin, Nana Liu, Yue Yu

Linear systems of equations

- Classical methods -

Iterative algorithms: e.g. Jacobi method $\tilde{O}(s_A D N_t)$

Other algorithms: e.g. Classical Gaussian elimination $\tilde{\mathcal{O}}(\mathrm{poly}(D))$

- Most well-known early quantum example -

Harrow, Hassidim and Lloyd HHL (2009):

$$\text{Want to prepare } |y\rangle \propto A^{-1}|b\rangle$$

$$\tilde{\mathcal{O}}(s_A \kappa_A^2/\epsilon)$$

κ_A: condition number

Sparse

Well-conditioned

Application of Schrodingerisation to linear algebra

Solve linear algebra problems iteratively:

$$y_{k+1} = Gy_k + g, \quad k \in \mathbb{Z}^+ \cup \{0\}$$

where $y_k, g \in \mathbb{R}^d$ and G is a $d \times d$ matrix. Here, k labels the time step in the iterative approach

Define: $x_k = (y_k, 1)^T$

$$x_{k+1} = Cx_k, \quad C = \begin{pmatrix} G & g \\ \mathbf{0}^T & 1 \end{pmatrix},$$

where C is a $(d+1) \times (d+1)$ matrix and $\mathbf{0}^T = (0, \ldots, 0)$ is d-dimensional. We can rewrite this in the form

$$x_{k+1} - x_k = \begin{pmatrix} y_{k+1} - y_k \\ 0 \end{pmatrix} = (C - I)x_k.$$

arXiv:2304.02865

Application of Schrodingerisation to linear algebra

$$x_{k+1} - x_k = \begin{pmatrix} y_{k+1} - y_k \\ 0 \end{pmatrix} = (C - I)x_k.$$

From this form, it is simple to see, for instance, that the iterative method converges or reaches its steady state when $y_{k+1} \approx y_k$, i.e.

$$y_{k+1} - y_k = (G - I)y_k + g \to 0,$$

which coincides with identifying the ground state of $C - I$. Since

$$x_{k+1} - x_k = (C - I)x_k = (C - I)C^k x_0 = C^k(Cx_0 - x_0) = C^k(x_1 - x_0),$$

then

$$||x_{k+1} - x_k|| \leq ||C||^k ||x_1 - x_0||.$$

When the spectral radius of C is $r(C) = r(G) < 1$, then $||C|| < 1$ for any subordinate norm $||\cdot||$, so the convergence rate $||C||^k$ for the state x is exponential with time step k

Application of Schrodingerisation to linear algebra

Solve linear algebra problems iteratively:

$$y_{k+1} = Gy_k + g, \qquad k \in \mathbb{Z}^+ \cup \{0\}$$

$$x_{k+1} - x_k = \begin{pmatrix} y_{k+1} - y_k \\ 0 \end{pmatrix} = (C - I)x_k. \qquad C = \begin{pmatrix} G & g \\ \mathbf{0}^T & 1 \end{pmatrix}$$

$C - I$ negative eigenvalues

$$\frac{dx}{dt} = (C - I)x, \qquad x(t = 0) = x_0.$$

Iterative systems are discrete-time limits of dynamical systems…
Now we can simulate dynamical systems with quantum simulation!

Quantum linear systems of equations

- Quantum Jacobi method

A is $D \times D$ matrix

Want to prepare $|y\rangle \propto A^{-1}|b\rangle$

$A = \Lambda + M$, M completely off-diagonal

$$y_{k+1} = Gy_k + g, \qquad G = -\Lambda^{-1}M, \quad g = \Lambda^{-1}b.$$

$$y_{k+1} = y_k \text{ when } Ay = b$$

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -Hx, \quad x(0) = x_0,$$

where $H = -(C - I) = H^\dagger$, which implies the scenario $G = G^\dagger$ and $g = 0$

Apply Schrödingerisation

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

Quantum linear systems of equations: analog simulation

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -Hx, \quad x(0) = x_0,$$

where $H = -(C - I) = H^\dagger$, which implies the scenario $G = G^\dagger$ and $g = 0$

$$|\tilde{w}(t)\rangle_{\text{CV-DV}} = \exp(-iH_{\text{CV-DV}}t)|\tilde{w}(0)\rangle_{\text{CV-DV}}.$$

$$H_{CV-DV} = H \otimes \hat{\eta}$$

Quantum linear systems of equations: analog simulation

Initial state:

$$|x_0\rangle = \frac{1}{||x_0||}\sum_{i=0}^{d}(x_0)_i|i\rangle = \frac{1}{||x_0||}\sum_{j=0}^{d}\alpha_j|E_j\rangle, \quad \alpha_j \in \mathbb{C}.$$

Since H is Hermitian, it has orthonormal eigenvectors $\{|E_j\rangle\}_{j=0}^{d}$ with corresponding eigenvalues $\{E_j\}_{j=0}^{d}$, where $E_0 < \cdots < E_d$. The normalization of the state is defined as $||\cdot||^2 = \sum_{i=0}^{d}|(\cdot)_i|^2$. Then

$$|x(t)\rangle = \frac{||x_0||}{||x(t)||}\,\mathrm{e}^{-Ht}|x_0\rangle = \frac{1}{||x(t)||}\sum_{j=0}^{d}\alpha_j\,\mathrm{e}^{-E_jt}|E_j\rangle.$$

Quantum linear systems of equations: analog simulation

We can write

$$||x(t)||^2 = ||\mathrm{e}^{-Ht}x_0||^2 = \left\| \sum_{j=0}^{d} \alpha_j \, \mathrm{e}^{-E_j t} |E_j\rangle \right\|^2 = \sum_{j=0}^{d} |\alpha_j|^2 \, \mathrm{e}^{-2E_j t}$$

$$= \mathrm{e}^{-2E_0 t}(|\alpha_0|^2 + |\alpha_1|^2 \, \mathrm{e}^{-2t\Delta_C} + L),$$

where the spectral gap is $\Delta_C = E_1 - E_0 > 0$ and $L = \sum_{k=2}^{d} |\alpha_k|^2 \exp(-2t(E_k - E_0))$. To determine how long it takes to evolve such a quantum system, we say $t = t_f$ when the fidelity between $|x(t)\rangle$ and the true ground state $|x_g\rangle = |E_0\rangle$ of H is greater or equal to $1 - \delta$, $\delta \geq 0$, i.e.

$$\mathcal{F}(|E_0\rangle, |x(t_f)\rangle) = |\langle x(t_f)|E_0\rangle|^2 = \frac{|\alpha_0|^2 \, \mathrm{e}^{-2E_0 t_f}}{||x(t_f)||^2} \geq 1 - \delta.$$

Quantum linear systems of equations: analog simulation

Hybrid DV-CV quantum simulation $H_{DV} \otimes \hat{\eta}$

$$t_f \geq \frac{1}{2\Delta_C} \ln\left(\frac{|\alpha_1|^2(1-\delta)}{|\alpha_0|^2\delta}\left(\frac{1}{1-L(1-\delta)/(|\alpha_0|^2\delta)}\right)\right)$$

When L is small (relative to $|\alpha_0|^2$), we mean $L \ll \delta|\alpha_0|^2/(1-\delta)$ and $\delta \ll 1$, we have $t_f \gtrsim (1/(2\Delta_C))\ln(|\alpha_1|^2/(\delta|\alpha_0|^2))$. For larger L, we simply include more terms in L to find t_f. If the first two eigenstates $|E_0\rangle$ and $|E_1\rangle$ dominate so that $|\alpha_1|^2 \approx 1 - |\alpha_0|^2$ then

$$t_f \gtrsim \frac{1}{2\Delta_C} \ln\left(\frac{1}{\delta}\left(\frac{1}{|\alpha_0|^2} - 1\right)\right).$$

Quantum linear systems of equations: digital simulation

Cost in digital quantum simulation to get steady-state solution:

$$\tilde{\mathcal{O}}\left(\frac{s_A \|\Lambda^{-1} M\|_{max}}{\epsilon |\alpha_0| \Delta_C}\right)$$

s_A: sparsity of A

$\|\cdot\|_{max}$: max entry

Δ_C: spectral gap

Application to ground state preparation: analog algorithm

Start with state: $$|u(0)\rangle = \sum_{j=0}^{D-1} \alpha_j |E_j\rangle, \quad \alpha_j \in \mathbb{C}$$

Evolve: $$|u(t)\rangle = \frac{e^{-\boldsymbol{H}t}}{\|u(t)\|}|u(0)\rangle = \frac{1}{\|u(t)\|)} \sum_{j=0}^{D-1} \alpha_j e^{-E_j t}|E_j\rangle$$

Long time limit: $|u(t)\rangle \to |E_0\rangle$ Ground state of $\mathbf{H}$

$$t_f \gtrsim \frac{1}{\Delta} \ln\left(\frac{1}{\delta}\left(\frac{1}{|\alpha_0|^2} - 1\right)\right) \qquad \Delta = E_1 - E_0$$

Application to ground state preparation: digital algorithm

Start with state: $$|u(0)\rangle = \sum_{j=0}^{D-1} \alpha_j |E_j\rangle, \quad \alpha_j \in \mathbb{C}$$

Evolve: $$|u(t)\rangle = \frac{e^{-\boldsymbol{H}t}}{\|u(t)\|}|u(0)\rangle = \frac{1}{\|u(t)\|)} \sum_{j=0}^{D-1} \alpha_j e^{-E_j t}|E_j\rangle$$

Long time limit: $|u(t)\rangle \to |E_0\rangle$ Ground state of $\mathbf{H}$

$$\tilde{\mathcal{O}}\left(\frac{s\|\mathbf{H}\|_{max}}{|\alpha_0|\Delta\epsilon}\right) \qquad \Delta = E_1 - E_0$$

Application to thermal state preparation: digital algorithm

Start with state: $|u(0)\rangle \propto \sum_k |E_k E_k\rangle$

Evolve: $\rho_{Gibbs} = \mathrm{Tr}_1(|u(t = 1/(2T))\rangle\langle u(t = 1/(2T))|)$

$$\rho_{Gibbs} = \sum_k e^{-E_k/T} |E_k\rangle\langle E_k|$$

Let Schrodingerisation perform this evolution

$$\tilde{\mathcal{O}}\left(s\|\mathbf{H}\|_{max}\frac{1}{T\epsilon}\sqrt{\frac{D}{Z}}\right)$$

Partition function Z

Maximum eigenvector and eigenvalue: analog algorithm

- Quantum power method

$$1 > \lambda_1 > \lambda_2 > \ldots > \lambda_d$$

Prepare maximum eigenvector of C

$$x_0 = \sum_{i=1}^{d} \gamma_i c_i$$

$$x_k = C x_{k-1} = C^k x_0.$$

$$\lambda_1 \approx \frac{x_K^T x_{K+1}}{x_K^T x_K} = \frac{x_K^T C x_K^T}{x_K^T x_K}$$

Quantum simulation via hybrid Hamiltonian $H = C \otimes \hat{\eta}$

$$t_{max} \gtrsim \frac{1}{2\tilde{\Delta}_C} \ln\left(\frac{2\mathrm{Tr}(C^\dagger C)}{\epsilon^2}\left(\frac{1}{|\gamma_1|^2} - 1\right)\right)$$

Maximum eigenvector and eigenvalue: digital algorithm

- Quantum power method

$$1 > \lambda_1 > \lambda_2 > \ldots > \lambda_d$$

Prepare maximum eigenvector of C

$$x_0 = \sum_{i=1}^{d} \gamma_i c_i$$

$$x_k = C x_{k-1} = C^k x_0.$$

$$\lambda_1 \approx \frac{x_K^T x_{K+1}}{x_K^T x_K} = \frac{x_K^T C x_K^T}{x_K^T x_K}$$

Cost in digital quantum simulation to get max eigenvector:

$$\tilde{\mathcal{O}}\left(\frac{s_C \|C\|_{max}}{\epsilon |\gamma_1| \Delta_C}\right)$$

Max eigenvalue: extra $\mathcal{O}(1/\epsilon^2)$

NOTE: All previous algorithms can have up to exponential improvement in error epsilon using modified ancilla initial state

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

Digital quantum algorithm:

	Queries to A	Queries to $\boldsymbol{u}_0$
Time-dependent $A(t)$	$\widetilde{\mathcal{O}}(\frac{\|\boldsymbol{u}_0\|}{\|\boldsymbol{u}(T)\|}\alpha_A T(\log\frac{1}{\varepsilon})^2)$	$\mathcal{O}(\frac{\|\boldsymbol{u}_0\|}{\|\boldsymbol{u}(T)\|})$
Time-independent A	$\widetilde{\mathcal{O}}(\frac{\|\boldsymbol{u}_0\|}{\|\boldsymbol{u}(T)\|}\alpha_A T\log\frac{1}{\varepsilon})$	$\mathcal{O}(\frac{\|\boldsymbol{u}_0\|}{\|\boldsymbol{u}(T)\|})$

Reference list for Part II: Linear algebra, ground state and thermal state preparation

Linear algebra, ground state and thermal state preparation

- *Quantum simulation of discrete linear dynamical systems and simple iterative methods in linear algebra via Schrodingerisation*, Shi Jin, Nana Liu*, arXiv: 2304.02865, Proceedings of the Royal Society A, Vol 480, 20230370, 2024

- *Quantum preconditioning method for linear systems problems via Schrodingerisation*, Shi Jin*, Nana Liu* and Chuwen Ma*, Yue Yu*, arXiv: 2505.06866, 2025

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

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

Overview of summer lectures on Schrodingerisation

PART II: Special topics

- **Nonlinear ODEs and PDEs**
- **Uncertain ODEs/PDEs**
- **Non-autonomous mapped to autonomous PDEs**
- **Application to linear algebra, ground state and thermal state preparation**