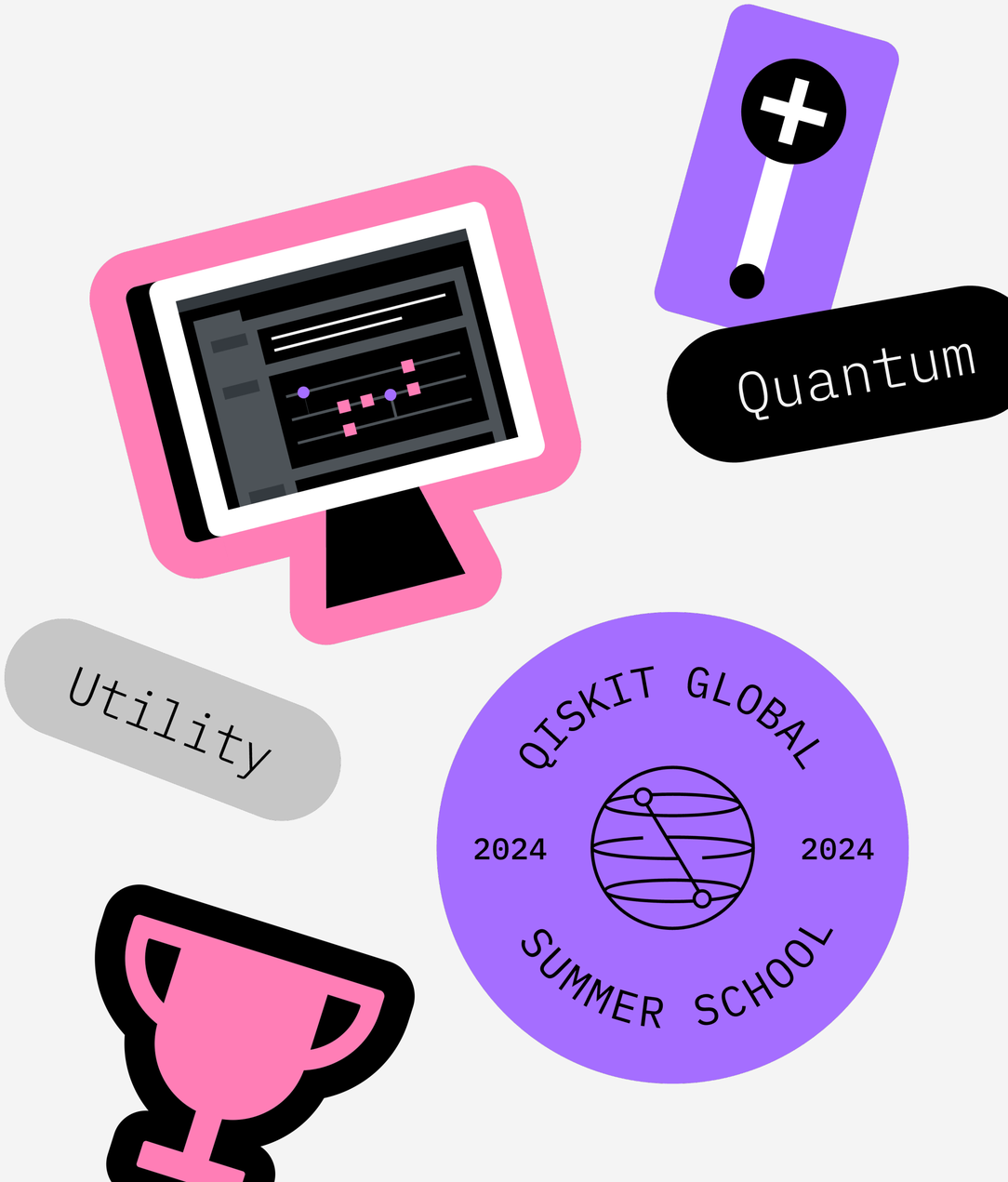
Qiskit Global Summer School 2024

Hamiltonian dynamics: applications and simulation



Mario Motta
Senior Research Staff Member
IBM

Definition of Hamiltonian dynamics

Hamiltonian dynamics

The state of an isolated quantum system evolves in time according to the Schrodinger equation

$$i\frac{d}{dt}|\phi(t)\rangle = \hat{H}(t)|\phi(t)\rangle$$

The formal solution of the Schrodinger equation is

$$|\phi(t)\rangle = \mathrm{Texp}\left(-i\int_0^t ds\hat{H}(s)\right)|\phi(0)\rangle$$

For a time-independent Hamiltonian, $|\phi(t)\rangle = e^{-it\hat{H}}|\phi(0)\rangle$.

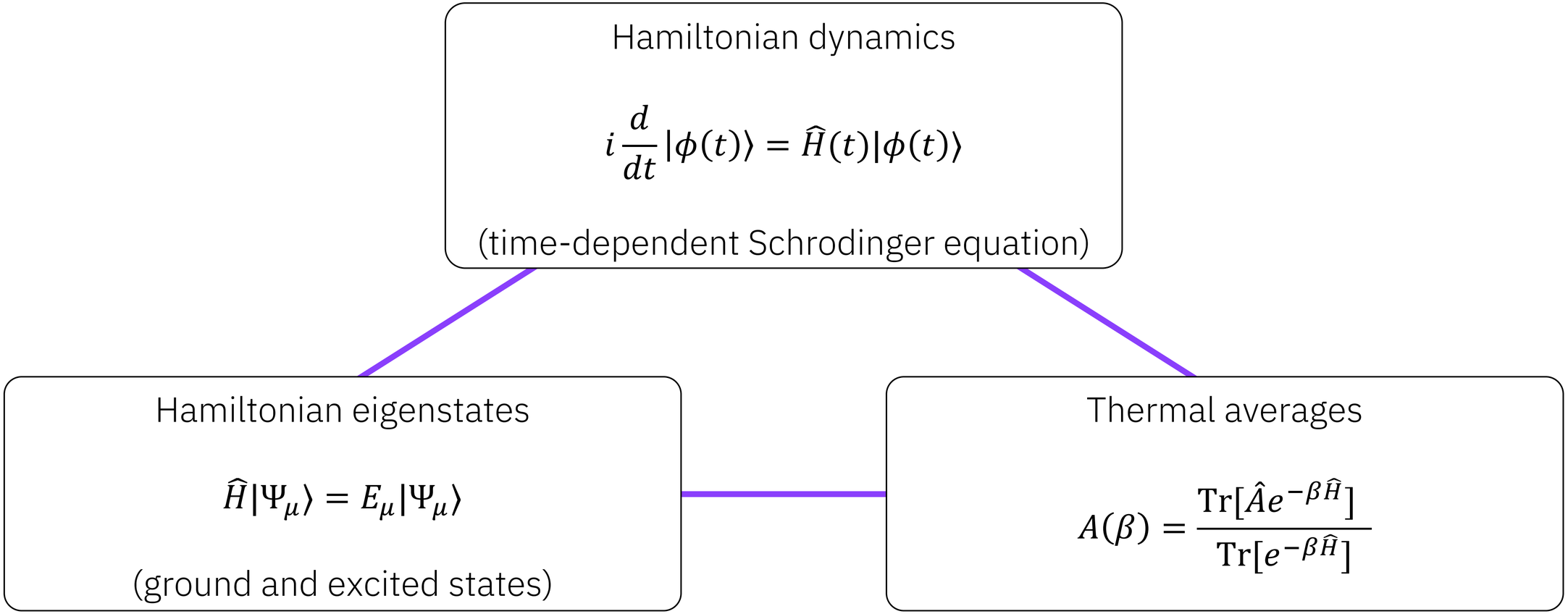
To simulate Hamiltonian dynamics on a quantum computer means:

- to map, exactly or approximately, $|\phi(t)\rangle$ on the state of a quantum computer, and

- to calculate e.g. the expectation value of an observable at time t, $A(t) = \langle\phi(t)|\hat{A}|\phi(t)\rangle$

The central problems of quantum simulations

Hamiltonian dynamics is an important problem of quantum simulation, along with



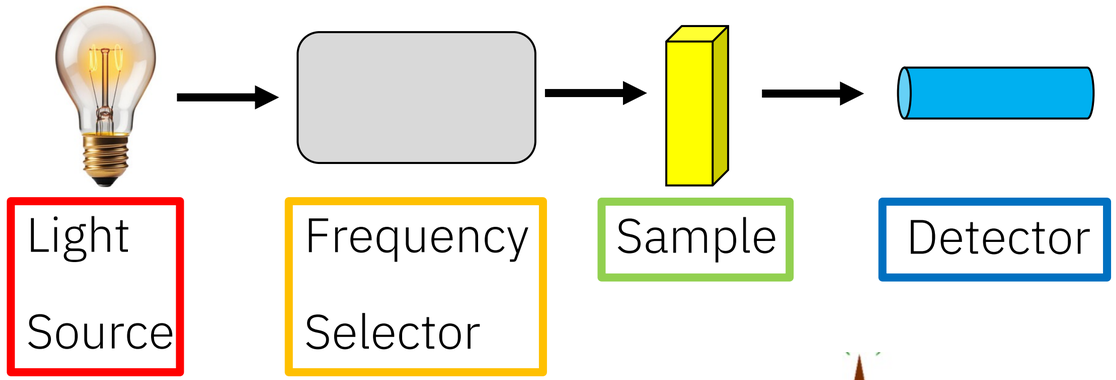
Applications of Hamiltonian dynamics

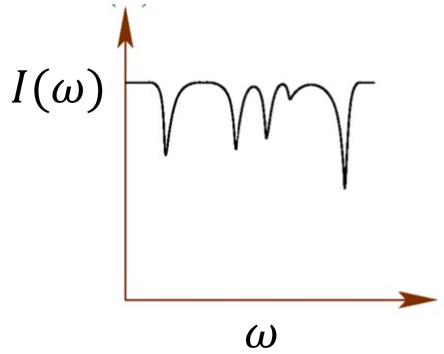
Scattering experiments

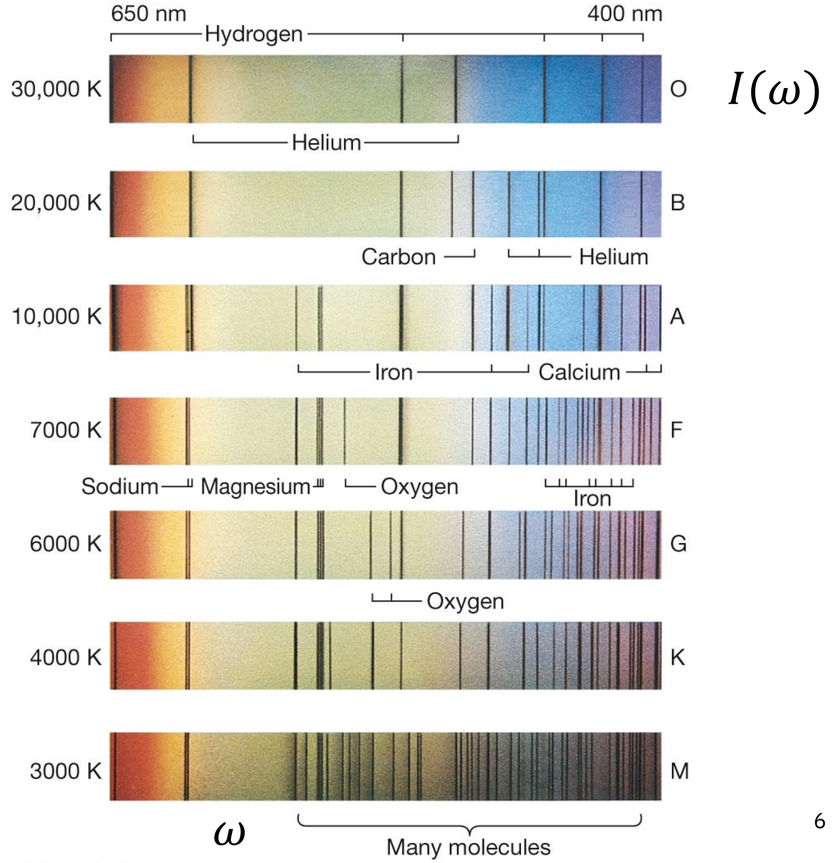
Scattering experiments are used frequently to understand the properties of materials.

Example: UV-visible absorption spectroscopy.

A sample (e.g., a gas) at equilibrium at temperature T (ground/thermal state) is impinged with monochromatic light, and the loss of intensity of light is measured as a function of frequency.







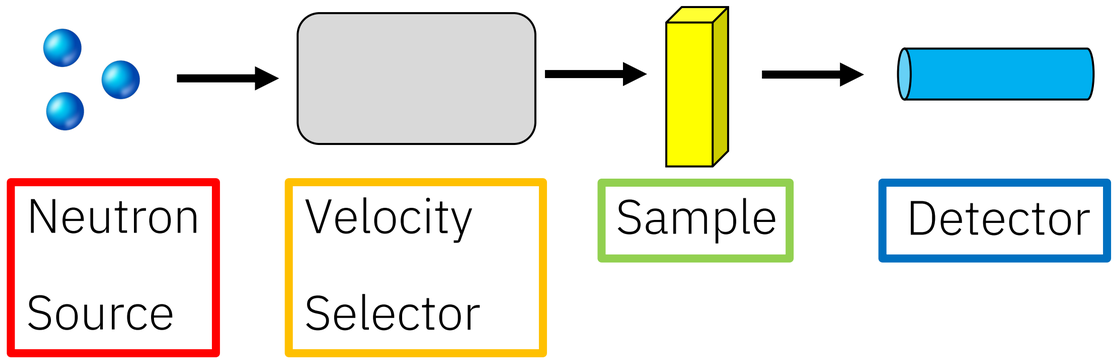
Scattering experiments

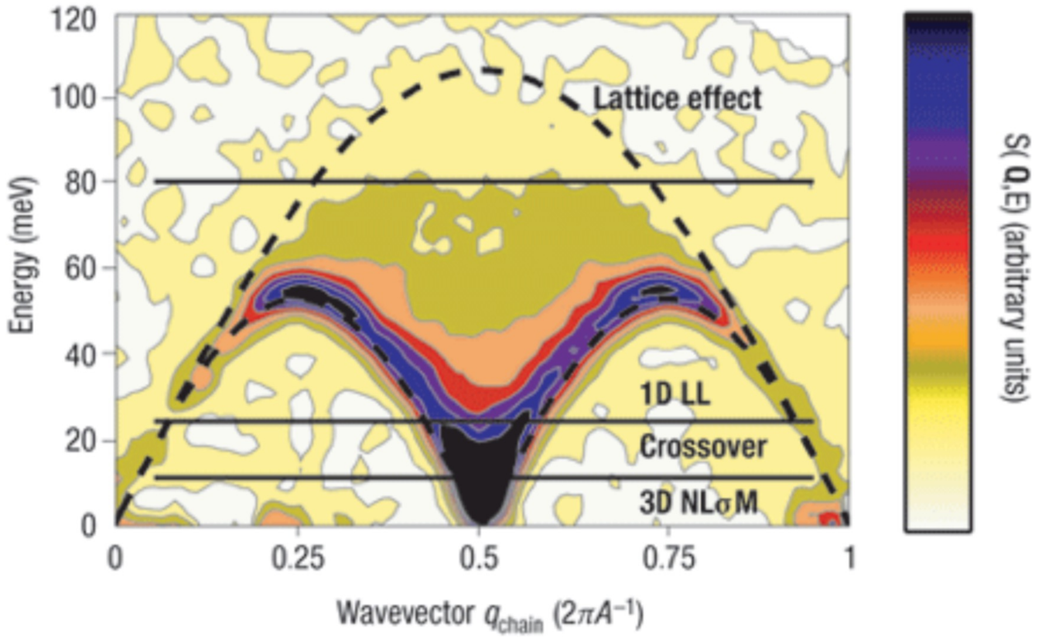
Scattering experiments are used frequently to understand the properties of materials.

Example: neutron scattering experiments.

A sample (e.g., 4-helium, a magnetic material) is impinged with neutrons at momentum $\boldsymbol{k}$, energy E,

and intensity of scattered neutrons is measured as a function of momentum $\boldsymbol{k} + \boldsymbol{q}$ and energy $E + \Delta E$.





Nature Materials, 4, 329-334, (2005)

Scattering experiments and response to perturbations

In many scattering experimental settings

1) a quantum system is prepared in the ground (or thermal equilibrium) state Ψ_0 of a Hamiltonian $\hat{H}_0$

2) a (time-dependent) perturbation $\hat{V}$ is applied.

For UV-vis spectroscopy, $\hat{V} = \boldsymbol{\varepsilon} \cdot \hat{\boldsymbol{\mu}}$ (dipole along $\boldsymbol{\varepsilon}$). For neutron scattering, $\hat{V} = \sum_{\boldsymbol{q}} V_{\boldsymbol{q}}\, e^{i\boldsymbol{q}\cdot\hat{\boldsymbol{r}}}$ (external potential).

3) The absorption of a photon with energy $\hbar\omega$ is due to an excitation $|\Psi_0\rangle \to |\Psi_\mu\rangle$ with $E_\mu - E_0 = \hbar\omega$ induced by $\hat{V}$.

According to Fermi's golden rule, the absorption is described by

$$A(\omega) \propto \sum_\mu p_{0\to\mu}\,\delta(E_\mu - E_0 - \hbar\omega) = \sum_\mu \left|\langle\Psi_\mu|\hat{V}|\Psi_0\rangle\right|^2 \delta(E_\mu - E_0 - \hbar\omega) = \int dt\, \frac{e^{it\omega}}{2\pi}\, \langle\Psi_0|e^{it\hat{H}_0}\hat{V}e^{-it\hat{H}_0}\hat{V}|\Psi_0\rangle$$

response function

Response functions are a fundamental aspect of physics:

they link experimental observations and the underlying many-body quantum mechanics.

Fetter & Walecka, "Quantum Theory of Many-Particle Systems", Dover

Response to (strong) external fields

Fermi's golden rule is a "linear response approximation" to the more general setup where:

1) A system is prepared at equilibrium in the ground state Ψ_0 of a Hamiltonian $\hat{H}_0$

2) A (time-dependent) perturbation is applied, and the system evolves in time with

$$i\frac{d}{dt}|\phi(t)\rangle = \left(\hat{H}_0 + \hat{V}(t)\right)|\phi(t)\rangle$$

3) A time-dependent expectation value is measured, $A(t) = \langle\phi(t)|\hat{A}|\phi(t)\rangle$. Linear response corresponds to

$$e^{-it(\hat{H}_0+\hat{V})} \simeq e^{-it\hat{H}_0}\left[1 - i\int_0^t ds\,\hat{V}_I(s)\right], \hat{V}_I(s) = \mathrm{e}^{is\hat{H}_0}\hat{V}(t)\mathrm{e}^{-is\hat{H}_0} \rightarrow A(t) \simeq A(0) + \int_0^t ds\,\langle\Psi_0|\left[i\hat{V}_I(s), \hat{A}_I(t)\right]|\Psi_0\rangle$$

This is also the setup of quantum quenching experiments(1) used to study aspect of non-equilibrium physics (e.g., thermalization and universal aspects of critical dynamics).

(1) quench = a process where a parameter of a many-body Hamiltonian is changed in time, taking the system from a stationary state into a complicated time-dependent state

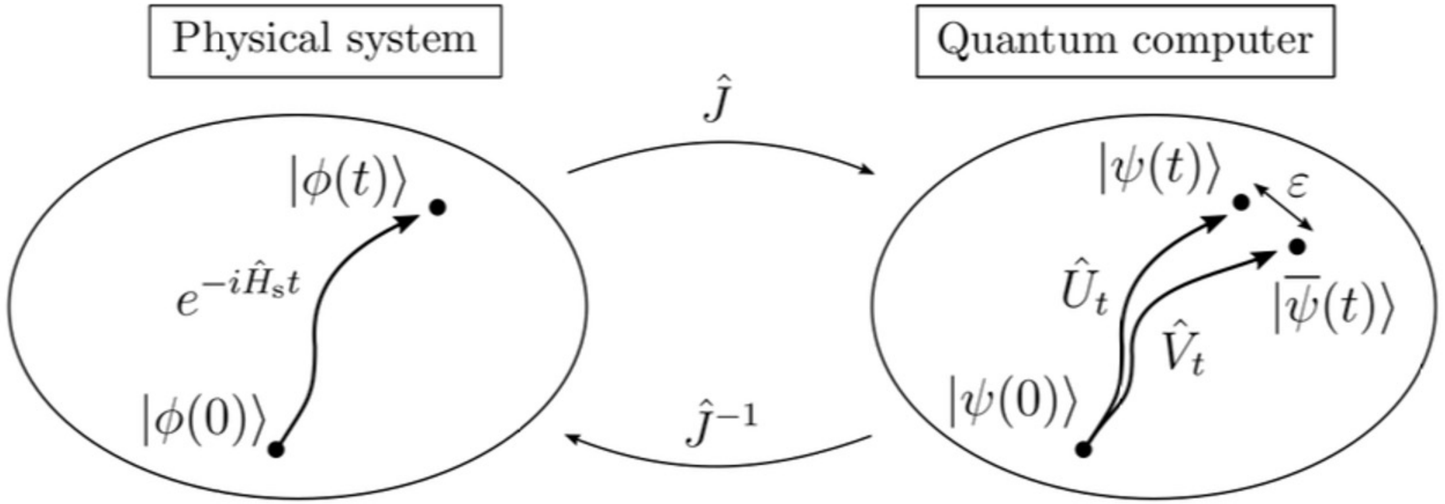
Simulation of Hamiltonian dynamics

Quantum simulation of Hamiltonian dynamics

See K. Sung's lecture

A function J can be used to transform the wavefunctions/operators of a quantum system into the wavefunctions/operators of a quantum device.

The simulation of the time evolution $|\phi(0)\rangle \rightarrow |\phi(t)\rangle$ is performed by a quantum circuit $\hat{V}_t$ that approximates the time-evolution operator $\hat{U}_t = e^{-itH}$ with accuracy ε.



The simulation is efficient if the number of elementary gates in the circuit $\hat{V}_t$ scales at most polynomially with respect to the number of qubits n, the desired precision $1/\varepsilon$, and the evolution time t.

A. M. Childs, "Quantum Information Processing in Continuous Time"

Example 1: a single Pauli operator

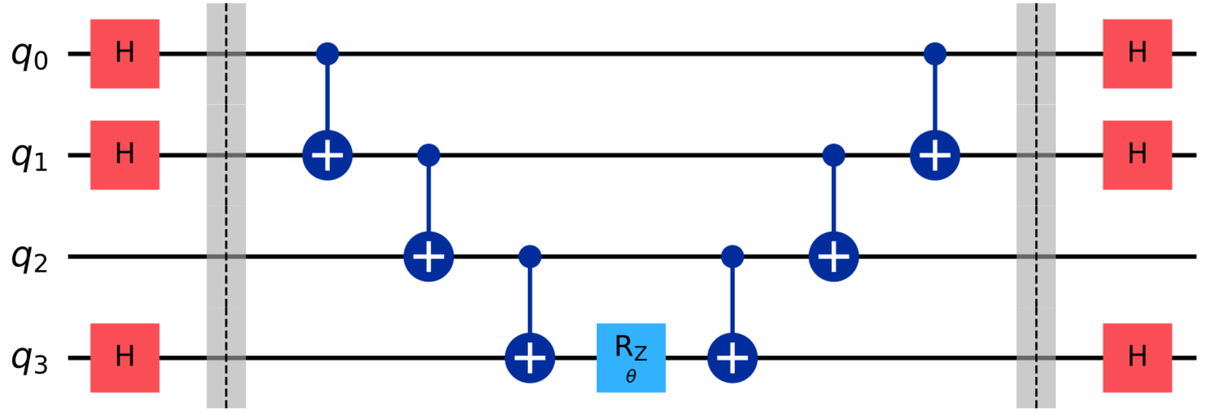
For a single n-qubit Pauli operator, e.g. $\hat{H} = cXZXX = \gamma P$,

the exponential e^{-itP} can be computed efficiently and exactly.

1) Transform the Pauli operator into a tensor product of Z operators using $X = HZH$, $Y = (HS)Z(HS)^+$

$$P = X \otimes Z \otimes X \otimes X = (H \otimes I \otimes H \otimes H)(Z \otimes Z \otimes Z \otimes Z)(H \otimes I \otimes H \otimes H)^+$$

2) Implement $e^{-it\gamma Z \ldots Z}$ with $2(n-1)$ CNOT gates and 1 Z rotation by an angle $\theta = 2t\gamma$



Exact implementation with $O(n)$ elementary gates for a generic time t.

Example 2: a one-body fermionic operator

For a 1-body Fermionic operator $\hat{H} = \sum_{pr,\sigma} h_{pr}\, \hat{a}^{+}_{p\sigma}\, \hat{a}_{r\sigma}$ acting on M spatial orbitals,

the exponential $e^{-it\hat{H}}$ can be computed efficiently and exactly.

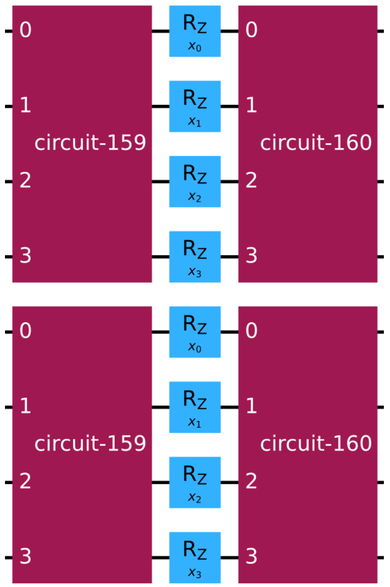
1) A 1-body Fermionic operator can be diagonalized by an orbital rotation (Bogoliubov transformation)

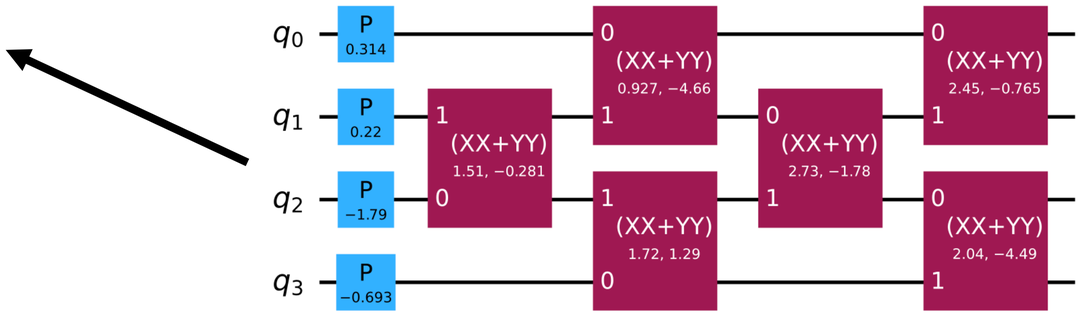
$$\hat{H} = W_\kappa^{+} \hat{D} W_\kappa \qquad \hat{D} = \sum_{p\sigma} \varepsilon_p\, \hat{a}^{+}_{p\sigma}\, \hat{a}_{p\sigma}$$

2) An orbital rotation can be implemented with a circuit of $2M$ Z rotations and $M(M-1)$ $XX+YY$ gates

3) Implement $e^{-it\hat{D}}$ with $2M$ Z rotations of angles $x_p = 2t\varepsilon_p$

Exact implementation with $O(M^2)$ elementary gates for a generic time t.





J. Zhang et al, Phys. Rev. Appl 9, 044036 (2018)
See K. Sung's lecture and ffsim's OrbitalRotationJW

Product formulae

If a Hamiltonian has the form $\hat{H} = \sum_i \hat{H}_i$ and each term $\hat{H}_i$ can be simulated efficiently,

then also $\hat{H}$ can be simulated efficiently.

Product formulae are a class of formulae that approximate $e^{-it\hat{H}}$ using products of the operators $e^{-i\gamma\hat{H}_i}$

General observations:

1) The first ingredient of product formulae is to break the time $[0, t]$ into n_s steps of duration $\Delta t = \frac{t}{n_s}$.

2) The time-evolution operator for a single step is approximated with an error scaling as Δt^k for some $k \geq 2$.

3) The error of product formulae decreases to 0 when the number of step increases

A. M. Childs et al, Physical Review X 11, 011020 (2021)

Product formulae –primitive approximation

The ”primitive approximation” is simply

$$\hat{U}_{\Delta t} = e^{-i\,\Delta t\hat{H}} \simeq e^{-i\Delta t\hat{H}_L} \ldots e^{-i\Delta t\hat{H}_1} = \hat{V}_{\Delta t}$$

The two operators differ at 2nd order in Δt:

$$\hat{U}_{\Delta t} = e^{-i\,\Delta t\hat{H}} = 1 + (-i\Delta t)\sum_i \hat{H}_i + \frac{(-i\Delta t)^2}{2}\sum_{ij} \hat{H}_i\hat{H}_j + \cdots$$

$$\hat{V}_{\Delta t} = e^{-i\Delta t\hat{H}_L} \ldots e^{-i\Delta t\hat{H}_1} = 1 + (-i\Delta t)\sum_i \hat{H}_i + \frac{(-i\Delta t)^2}{2}\sum_i \hat{H}_i^2 + \frac{(-i\Delta t)^2}{2}\sum_{i<j} 2\hat{H}_i\hat{H}_j + \cdots$$

$$\left|\left|\hat{U}_{\Delta t} - \hat{V}_{\Delta t}\right|\right| = \left|\left|\frac{(-i\Delta t)^2}{2}\sum_{i<j}[\hat{H}_i, \hat{H}_j]\right|\right| + \cdots \simeq C\Delta t^2$$

Simulation for time t with accuracy $\boldsymbol{\varepsilon}$ requires $\boldsymbol{n_s = O(Ct^2/\varepsilon)}$ steps.

Simulation is efficient provided L and C grow polynomially with system size.

A. M. Childs et al, Physical Review X 11, 011020 (2021)

Product formulae –second-order Suzuki formula

The ”2nd order Suzuki approximation” is

$$\hat{U}_{\Delta t} = e^{-i\,\Delta t\hat{H}} \simeq e^{-\frac{i\Delta t\hat{H}_1}{2}} \ldots e^{-\frac{i\Delta t\hat{H}_L}{2}} e^{-\frac{i\Delta t\hat{H}_L}{2}} \ldots e^{-\frac{i\Delta t\hat{H}_1}{2}} = \hat{V}^{(2)}{}_{\Delta t}$$

The two operators differ at 3rd order in Δt:

$$\left|\left|\hat{U}_{\Delta t} - \hat{V}^{(2)}{}_{\Delta t}\right|\right| = \tilde{C}\Delta t^3 + \cdots$$

Primitive: $e^{-i\Delta t\hat{H}_1}$ $e^{-i\Delta t\hat{H}_2}$ $e^{-i\Delta t\hat{H}_3}$ $e^{-i\Delta t\hat{H}_4}$ $e^{-i\Delta t\hat{H}_5}$ $e^{-i\Delta t\hat{H}_6}$

Suzuki: $e^{-\frac{i\Delta t\hat{H}_1}{2}}$ $e^{-\frac{i\Delta t\hat{H}_2}{2}}$ $e^{-\frac{i\Delta t\hat{H}_3}{2}}$ $e^{-\frac{i\Delta t\hat{H}_4}{2}}$ $e^{-\frac{i\Delta t\hat{H}_5}{2}}$ $e^{-\frac{i\Delta t\hat{H}_6}{2}}$ $e^{-\frac{i\Delta t\hat{H}_6}{2}}$ $e^{-\frac{i\Delta t\hat{H}_5}{2}}$ $e^{-\frac{i\Delta t\hat{H}_4}{2}}$ $e^{-\frac{i\Delta t\hat{H}_3}{2}}$ $e^{-\frac{i\Delta t\hat{H}_2}{2}}$ $e^{-\frac{i\Delta t\hat{H}_1}{2}}$

Simulation for time t with accuracy $\boldsymbol{\varepsilon}$ requires $\boldsymbol{n_s = O(\tilde{C}^{1/2} t^{3/2}/\varepsilon^{1/2})}$ steps.

Simulation is efficient provided L and $\tilde{C}$ grows polynomially with system size.

Example 1: linear combinations of Pauli operators

Product formulae apply to linear combinations of Pauli operators.

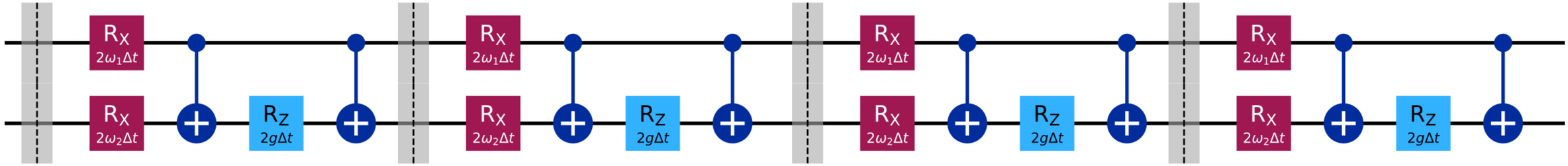
For example, consider a 2-site Ising Hamiltonian

$$\hat{H} = \omega_1 I \otimes X_1 + \omega_2 X_2 \otimes I + g Z_2 \otimes Z_1$$

Its dynamics can be simulated with a primitive approximation,

$$\hat{V}(\Delta t) = e^{-ig\Delta t(Z_2 \otimes Z_1)} e^{-i\omega_1 \Delta t X_1} e^{-i\omega_2 \Delta t X_2} = c\text{NOT}\,(R_z(2g\Delta t) \otimes I)\, c\text{NOT}\,(R_x(2\omega_2\Delta t) \otimes R_x(2\omega_1\Delta t))$$

leading to the circuit



Example 2: the electronic structure Hamiltonian

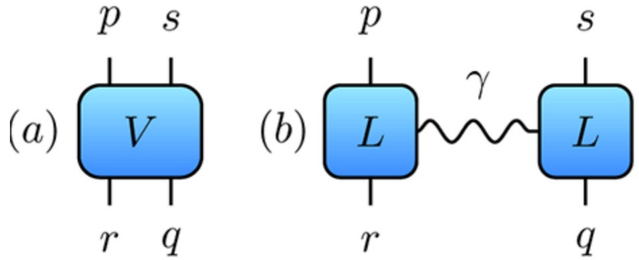
The Hamiltonians of electrons in a molecule is

$$\hat{H} = \sum_{pr,\sigma} h_{pr}\, \hat{a}^{+}_{p\sigma}\, \hat{a}_{r\sigma} + \sum_{prqs,\sigma\tau} \frac{(pr|qs)}{2}\, \hat{a}^{+}_{p\sigma} \hat{a}^{+}_{q\tau} \hat{a}_{s\tau} \hat{a}_{r\sigma}$$

See K. Sung's lecture

The 2-body operator (a) can be written using a low-rank decomposition (b)

$$(pr|qs) \simeq \sum_{\gamma=1}^{N_\gamma} L^{\gamma}_{pr} L^{\gamma}_{qs} \qquad , \qquad N_\gamma = O(M)$$



As a 1-body operator plus $O(M)$ squares of one-body operators

$$\hat{H} = \hat{J}_1 + \sum_{\gamma} \hat{L}^2_{\gamma} \qquad \hat{J}_1 = \sum_{pr,\sigma} \left(h_{pr} - \frac{(pq|qr)}{2} \right) \hat{a}^{+}_{p\sigma}\, \hat{a}_{r\sigma} \qquad \hat{L}_{\gamma} = \sum_{pr,\sigma} L^{\gamma}_{pr}\, \hat{a}^{+}_{p\sigma}\, \hat{a}_{r\sigma}$$

W. Purwanto, H. Krakauer, Y. Virgus, and S. Zhang, J. Chem. Phys. 135, 164105 (2011)
MM et al, npj Quantum Inf 7, 83 (2021)
W. Huggins et al, npj Quantum Information 7, 23 (2021)

Example 2: the electronic structure Hamiltonian

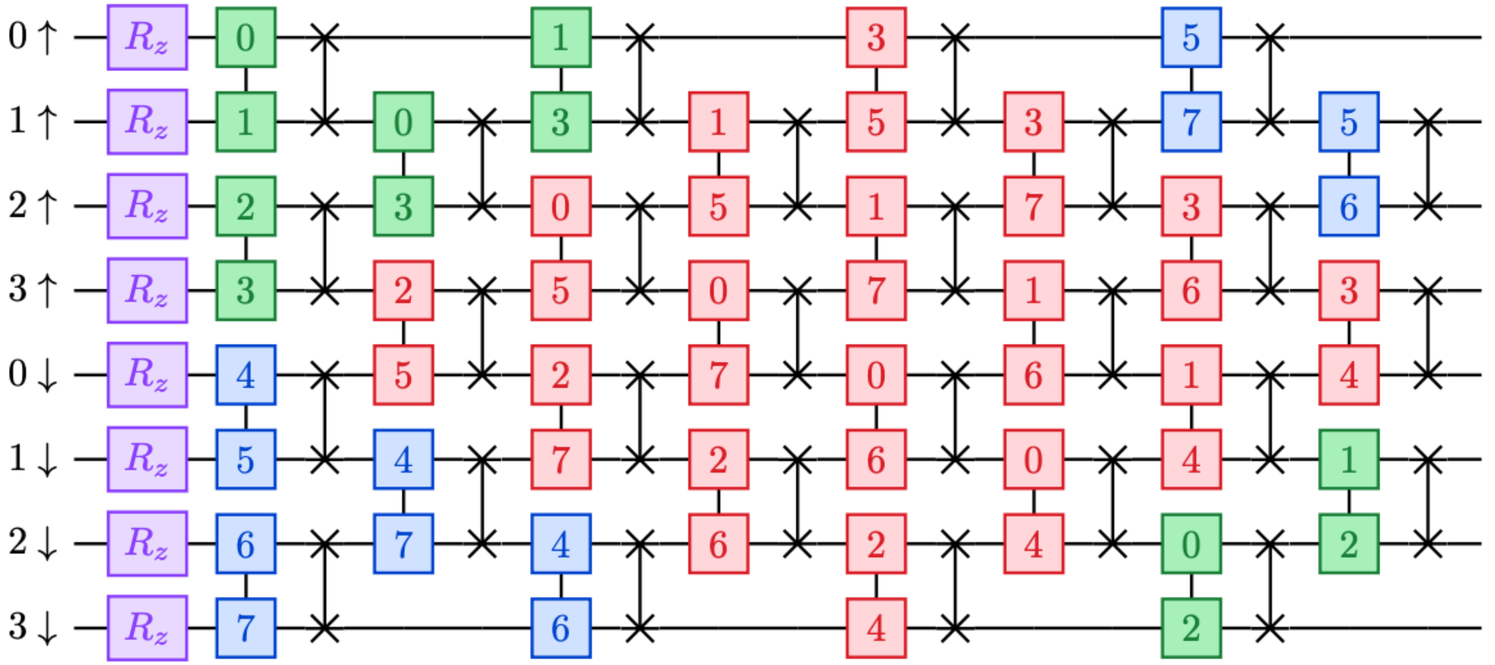
The representation

$$\hat{H} = \hat{J}_1 + \sum_\gamma \hat{L}_\gamma^2 = W_{\kappa_0}^+ D_0 W_{\kappa_0} + \sum_\gamma W_{\kappa_\gamma}^+ D_\gamma^2 W_{\kappa_\gamma} \; \hat{D}_0 = \sum_{p\sigma} \zeta_p \; \hat{a}_{p\sigma}^+ \hat{a}_{p\sigma} \hat{D}_\gamma = \sum_{p\sigma} \lambda_p^\gamma \; \hat{a}_{p\sigma}^+ \hat{a}_{p\sigma}$$

Is the starting point for a primitive approximation requiring $O(M^3)$ gates and depth $O(M^2)$ per Trotter step.

The cost is dominated by $e^{-it\hat{D}_\gamma^2}$, which consists of $O(M^2)$ ZZ rotations and has depth $O(M)$.

Below is an example, compiled with a SWAP network (assuming qubits have linear connectivity).



MM et al "Subspace methods for electronic structure simulations on quantum computers." *Elec. Struct. 6*, 013001 (2024)

Advanced methods

Cost of primitive product formula: $n_s = O(Ct^2/\varepsilon)$

Cost of 2nd order Suzuki product formula: $n_s = O(\tilde{C}^{1/2}t^{3/2}/\varepsilon^{1/2})$

Cost is always higher than $\boldsymbol{O(t)}$.

No-fast-forwarding theorem: for a generic Hamiltonian, cost always higher than $O(t)$. Can $\boldsymbol{O(t)}$ be achieved?

D. W. Berry et al, Comm. Math. Phys 270, 359-371 (2007)
A. M. Childs and R. Kothari, Quantum Inf. Comput, 10 (2009)

- Approximation of $e^{-i\,\Delta t\hat{H}}$ by a truncated Taylor series: $O(\tau\,\ln(\tau/\varepsilon)/\ln(\ln(\tau/\varepsilon)))$, $\tau = \left|\left|\hat{H}\right|\right|_1 t$

- Approximation of $e^{-i\,\Delta t\hat{H}}$ by a truncated Jacobi-Anger series: $O(\tau + \ln(1/\varepsilon))$, $\tau = \left|\left|\hat{H}\right|\right|_1 t$

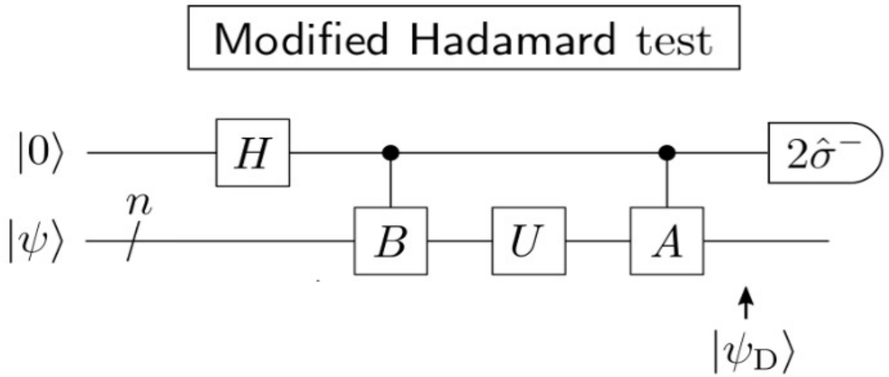
D. W. Berry et al, Phys. Rev. Lett, 114, 090502 (2015)
G. H. Low and I. L. Chuang, Quantum 3, 163 (2019)

Measurement of response functions

Computing response functions is not straightforward (they are not normal expectation values).

Computing response functions requires:

1) ground-state preparation $|\psi\rangle$
2) time evolution U
3) a “modified Hadamard test” circuit (for A, B unitary operators)



$$\langle\psi_D|2\hat{\sigma}^- \otimes \mathbb{1}|\psi_D\rangle = \langle\psi|\hat{U}^\dagger \hat{A}\hat{U}\hat{B}|\psi\rangle.$$

R. Somma, G. Ortiz, E. Knill, and J. Gubernatis, Int. J. Theor. Phys 1, 189–206 (2003)

Techniques to economize the computation of response functions are intensely researched.

K. Mitarai and K. Fujii, Phys. Rev. Res 1, 013006 (2019)
E. Kokcu et al, arXiv:2302.10219 (2023)
C. Cortes and S. Gray, Phys. Rev. A 105, 022417 (2022)

BQP-completeness Hamiltonian dynamics

The BQP complexity class

BQP = bounded-error quantum polynomial time.

The class of “decision problems” that a quantum computer can solve

with polynomial resources and high probability.

A. Kitaev, A. Shen, and M. N. Vyalyi, “Classical and Quantum Computation”, AMS

For many Hamiltonians, dynamics can be simulated with polynomial resources and a small error rate: problem in BQP!

Conversely, every problem in BQP can be formulated in terms of Hamiltonian dynamics (completeness).

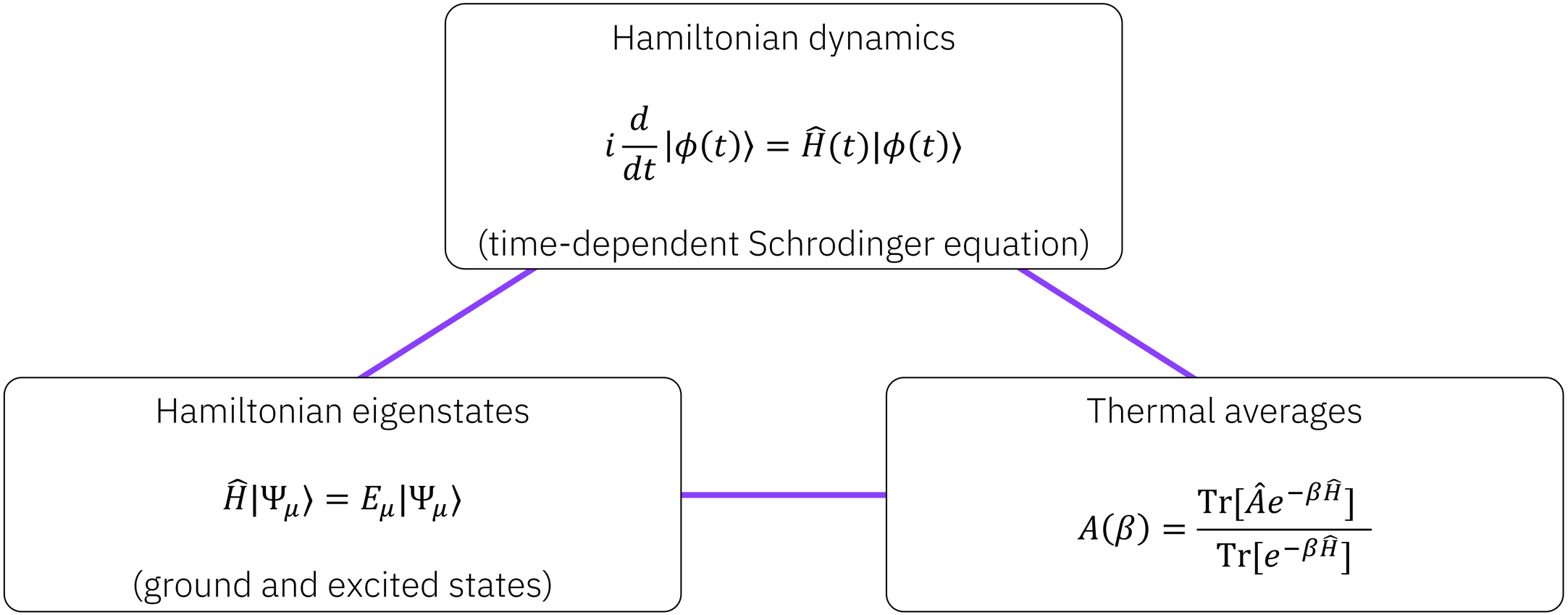
This results was obtained by R. P. Feynman in his seminal 1980s papers.

R. P. Feynman, “Quantum mechanical computers,” Opt. news, 11, 11-20 (1985)
R. P. Feynman, “Simulating physics with computers” Int J Theor Phys 21, 467–488 (1982)

Hamiltonian dynamics and Hamiltonian eigenstates

Hamiltonian dynamics as a quantum subroutine

Hamiltonian dynamics can serve as a subroutine in quantum algorithms for eigenstate approximation.



The QMA complexity class

BQP = bounded-error quantum polynomial time.

Decision problems that a quantum computer can solve with polynomial resources and high probability.

Hamiltonian dynamics is BQP-complete.

QMA = Quantum Merlin-Arthur

Decision problems whose solution can be verified (though not produced) with polynomial resources.

For many Hamiltonians, the eigenstate problem is in QMA: a hard problem for quantum computers.

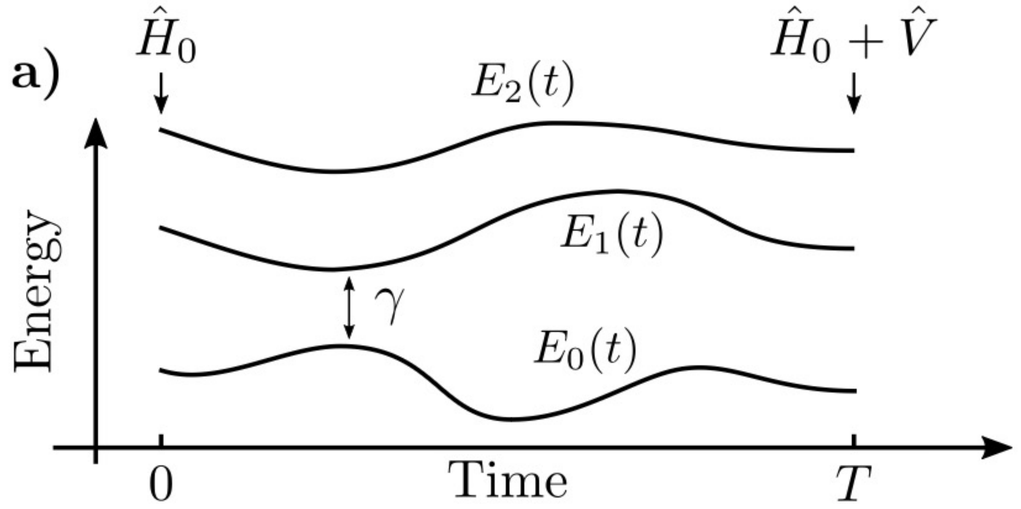
J. Kempe, A. Kitaev, and O. Regev SIAM J. Comput 35, 1070 (2006)

A. Kitaev, A. Shen, and M. N. Vyalyi, "Classical and Quantum Computation", AMS

Adiabatic state preparation

Given a Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$ where $\hat{H}_0$ has known and efficiently preparable ground state, the goal is to prepare the ground state of $\hat{H}$.

ASP This method is based on the adiabatic theorem of quantum mechanics:
if a system is prepared in the ground state of a Hamiltonian, and the Hamiltonian changes slowly, the system remains in the instantaneous ground state under certain conditions.



E. Farhi et al, Science 292, 472-475 (2001)

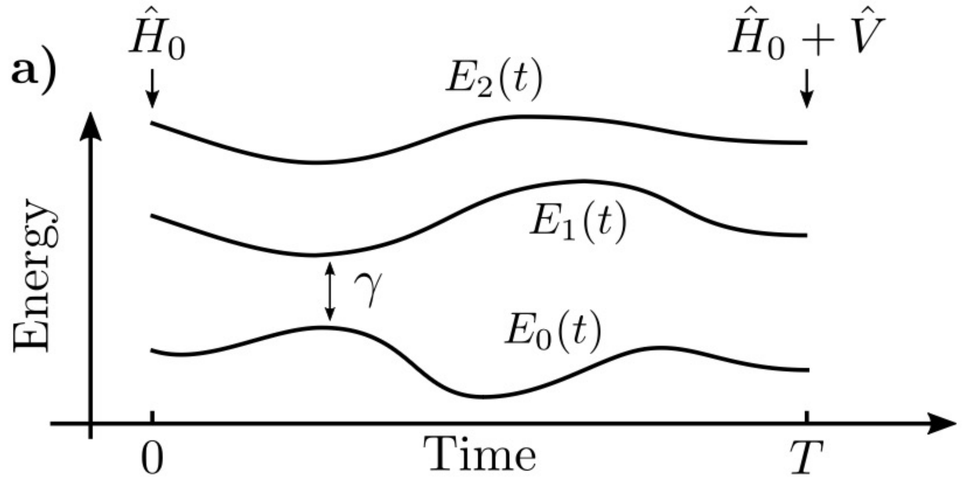
Adiabatic state preparation

More precisely, the solution of the time-dependent Schrodinger equation

$$i\frac{d}{dt}|\phi(t)\rangle = \hat{H}(t/T)|\phi(t)\rangle \qquad t \leq T \qquad \hat{H}(s) = \hat{H}_0 + s\hat{V}$$

Starting from the ground state of $\hat{H}_0$ converges to the ground state of $\hat{H}_0 + \hat{V}$ for increasing T...
provided the Hamiltonian remains gapped.

$$\left\| |\phi(T)\rangle - |\Psi_0\rangle \right\| \leq \frac{1}{T}\left[\frac{\left\|\hat{V}\right\|}{\gamma^2(T)} + \frac{\left\|\hat{V}\right\|}{\gamma^2(0)} + \int_0^1 ds\ \frac{5\left\|\hat{V}\right\|^2}{\gamma^3(s)}\right]$$



Adiabatic state preparation

The time-dependent Schrodinger equation

$$i\frac{d}{dt}|\phi(t)\rangle = \hat{H}(t/T)|\phi(t)\rangle \qquad t \leq T \qquad \hat{H}(s) = \hat{H}_0 + s\hat{V}$$

can be simulated, for example, with a primitive product formula

$$|\phi(T)\rangle \simeq e^{-i\Delta t\hat{H}_0}e^{-i\Delta t s_{n_s-1}\hat{V}} \ldots e^{-i\Delta t\hat{H}_0}e^{-i\Delta t s_0\hat{V}}|\phi(0)\rangle$$

$$s_k = \frac{k}{n_s}, \qquad k = 0 \ldots n_s$$

The simulation of Hamiltonian dynamics is used in ASP as a subroutine to approximate ground states!

The ASP circuits, even for situations where T is finite, may be very deep. How to improve?

Quantum approximate optimization algorithm

QAOA is very similar to ASP, except the coefficients in

$$|\phi(T)\rangle \simeq e^{-i\Delta t\hat{H}_0}e^{-i\Delta t s_{n_s-1}\hat{V}} \dots e^{-i\Delta t\hat{H}_0}e^{-i\Delta t s_0\hat{V}}|\phi(0)\rangle$$

are replaced with free parameters

$$|\phi(\gamma,\beta)\rangle \simeq e^{-i\beta_{n_s-1}\hat{H}_0}e^{-i\gamma_{n_s-1}\hat{V}} \dots e^{-i\beta_0\hat{H}_0}e^{-i\gamma_0\hat{V}}|\phi(0)\rangle$$

The energy $\mathrm{E}(\gamma,\beta) = \langle\phi(\gamma,\beta)|\hat{H}|\phi(\gamma,\beta)\rangle$

1) must be optimized with respect to the parameters (γ,β)
2) is always an upper bound to the ground-state energy of $\hat{H}$
3) The lowest energy $\mathrm{E_n} = \min_{\gamma,\beta} E(\gamma,\beta)$ decreases monotonically with n_s

a) n_s can be decreased/increased based on the error rates of the quantum device.
b) Hamiltonian dynamics is used within QAOA as a subroutine to define a variational ansatz.

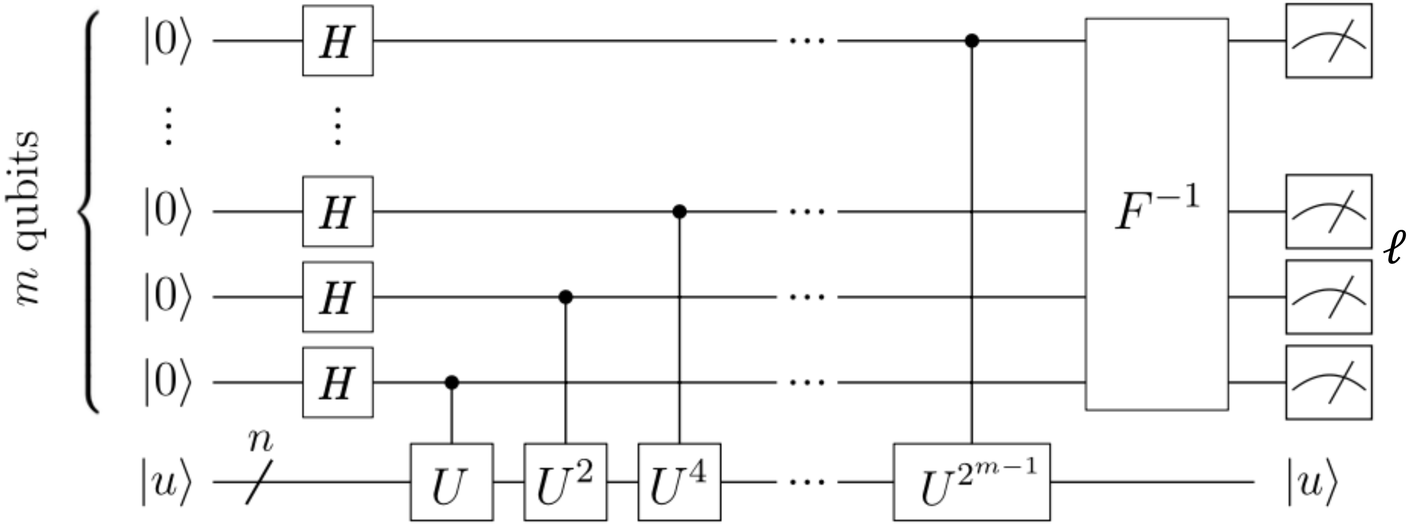
E. Farhi, J. Goldstone, and S.Gutmann, "A quantum approximate optimization algorithm", arXiv:1411.4028 (2014)

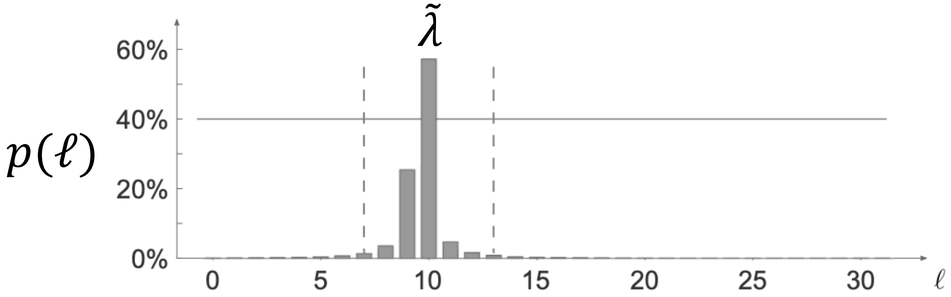
Quantum phase estimation

QPE: a technique to measure the eigenvalues of $e^{-th\hat{H}}$ (or an approximation thereof) and to prepare (probabilistically) its eigenstates.

Given A set of n qubits prepared in an eigenvector $|u\rangle$ of a unitary operator $\hat{U}$.
Assumption: The controlled gates $c\hat{U}^{2^j}$ can be implemented efficiently.
Goal: Find the eigenvalue $u = e^{i2\pi\lambda}$ associated with $|u\rangle$.

Setup: m auxiliary qubits, controlled powers of U, inverse Fourier transform, measurement of $\ell \in \{0 \dots 2^m - 1\}$.





$$\lambda = \frac{\tilde{\lambda}}{2^m} + \delta$$

$$p(\tilde{\lambda}) = \frac{1}{2^{2m}} \frac{\sin^2(\pi\delta 2^m)}{\sin^2(\pi\delta)} > \frac{4}{\pi^2} > 0.4$$

https://github.com/qiskit-community/qiskit-textbook/blob/main/content/ch-algorithms/quantum-phase-estimation.ipynb

Quantum phase estimation

Eigenstates of $\widehat{U}$ are generally not available.
In general, the input state of QPE is a superposition $|\psi\rangle = \sum_u c_u |u\rangle$ of eigenstates.

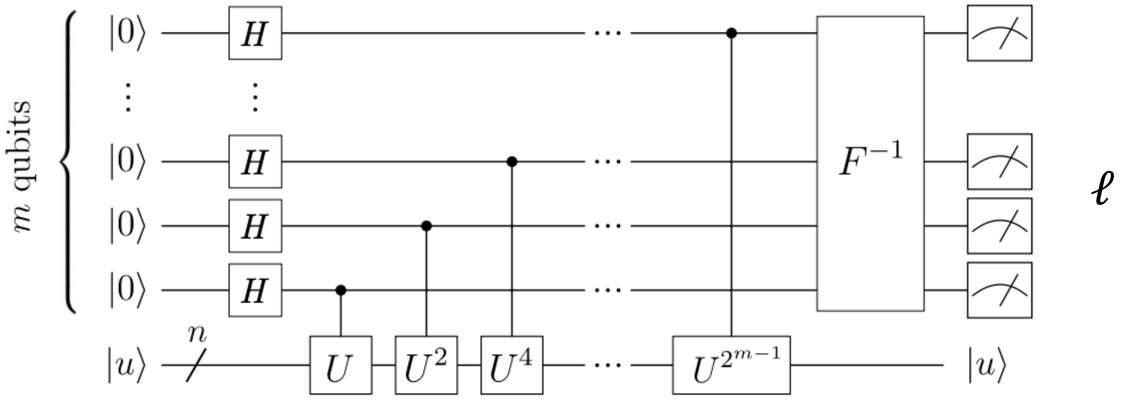
The probability distribution for ℓ features multiple peaks, at $\ell \simeq \tilde{\lambda}_u$ with $u = e^{i2\pi\lambda_u}$ and $\lambda_u = \frac{\tilde{\lambda}_u}{2^m} + \delta_u$.
The probability to obtain $\tilde{\lambda}_u$ for a given u is bounded by

$$p(\tilde{\lambda}_u) \geq |c_u|^2 p(\tilde{\lambda}_u|u) > 0.4\,|c_u|^2$$

With probability proportional to $|c_u|^2$ -- high is $|\psi\rangle$ is close to an eigenstate $|u\rangle$ -- the integer $\tilde{\lambda}_u$ is measured, and the qubits collapse into an approximation to the eigenstate $|u\rangle$.

When $\widehat{U} = e^{-th\hat{H}}$, QPE can be used to prepare Hamiltonian eigenstates and measure Hamiltonian eigenvalues.

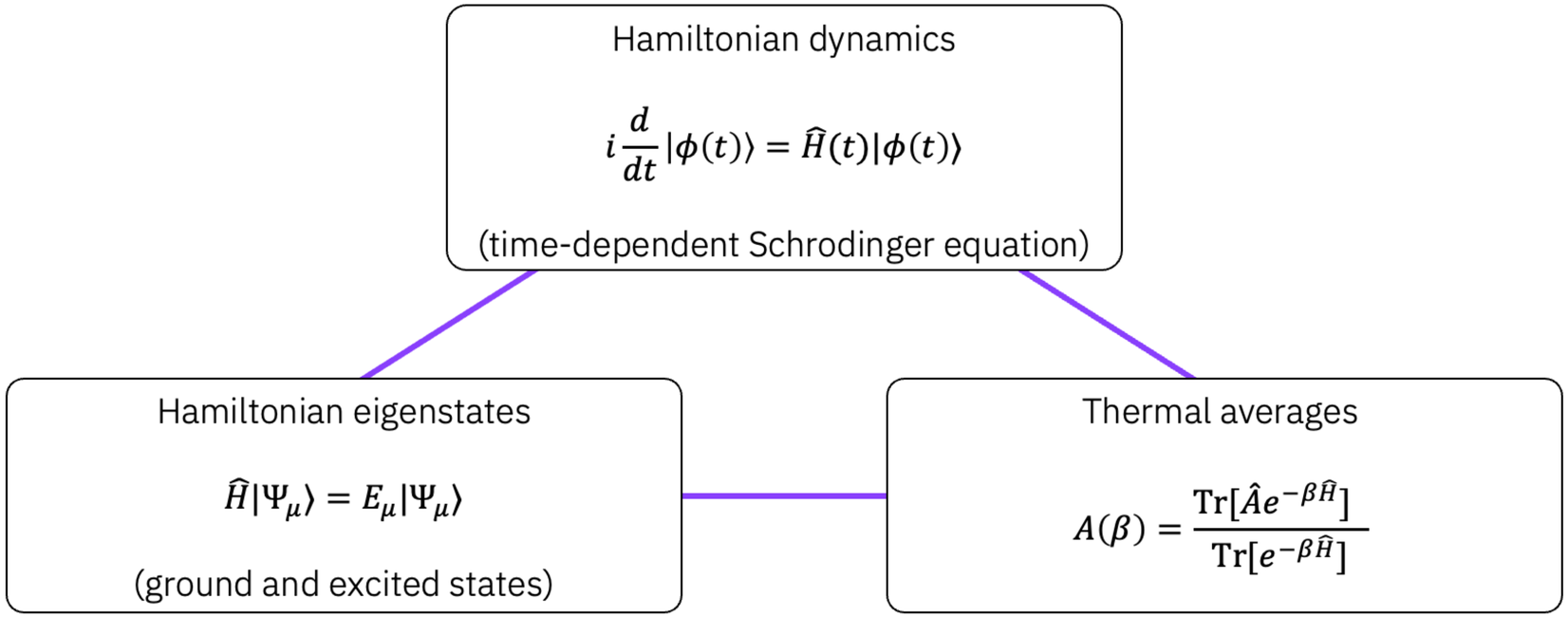
Obtaining a desired eigenpair is likely if QPE has an input state that is close to an eigenstate of $\widehat{U} = e^{-th\hat{H}}$.



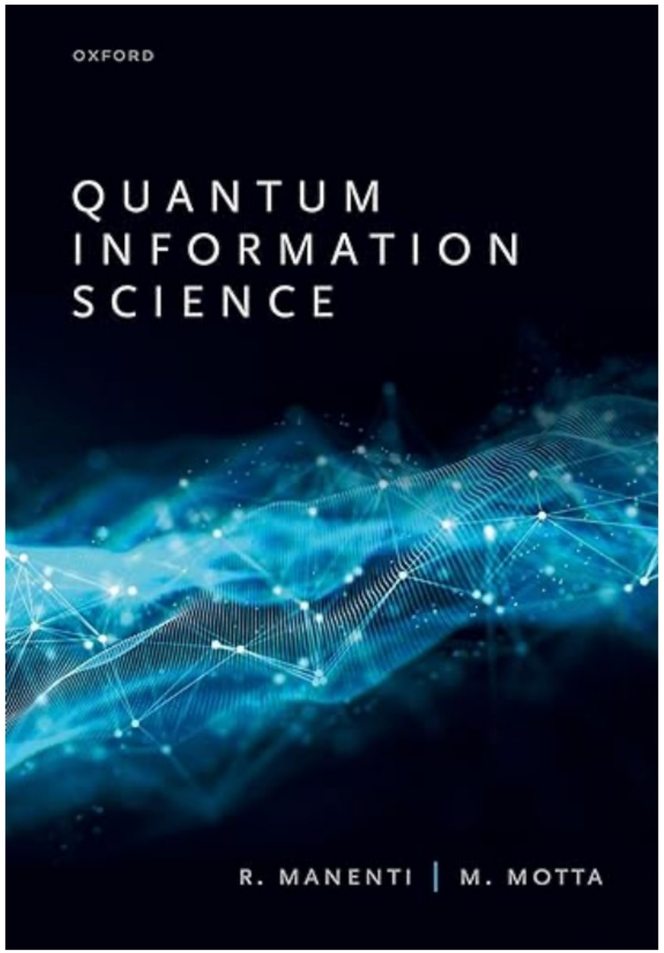
Summary

Hamiltonian dynamics

1) is useful to interpret (and predict) the outcomes of e.g., scattering experiments and quantum quenches
2) is a natural application for quantum computers (BQP-completeness)
3) is a very useful subroutine in algorithms for Hamiltonian eigenstates (ASP, QAOA, QPE, …)



Additional References



Quantum simulation

I. M. Georgescu, S. Ashhab, and Franco Nori
Rev. Mod. Phys. **86**, 153 – Published 10 March 2014

Quantum Algorithms for Quantum Chemistry and Quantum Materials Science

Bela Bauer*, Sergey Bravyi*, Mario Motta*, and Garnet Kin-Lic Chan*

Cite this: *Chem. Rev.* 2020, 120, 22, 12685–12717 Article Views | Altmetric | Citations | SI

Quantum Chemistry in the Age of Quantum Computing

Yudong Cao, Jonathan Romero, Jonathan P. Olson, Matthias Degroote, Peter D. Johnson, Mária Kieferová, Ian D. Kivlichan, Tim Menke, Borja Peropadre, Nicolas P. D. Sawaya, Sukin Sim, Libor Veis, and Alán Aspuru-Guzik*

Cite this: *Chem. Rev.* 2019, 119, 19, 10856–10915 Article Views | Altmetric | Citations | Share | Add to | Export

Variational quantum algorithms

M. Cerezo, Andrew Arrasmith, Ryan Babbush, Simon C. Benjamin, Suguru Endo, Keisuke Fujii, Jarrod R. McClean, Kosuke Mitarai, Xiao Yuan, Lukasz Cincio & Patrick J. Coles

Nature Reviews Physics **3**, 625–644 (2021) | Cite this article

WIREs COMPUTATIONAL MOLECULAR SCIENCE

Advanced Review

Emerging quantum computing algorithms for quantum chemistry

Mario Motta, Julia E. Rice