

Lecture # 15 (2024)

Other approaches have been developed for quantum time evolution. Below I list a few without going into details:

- 1) qDrift → developed in
Campbell, Phys Rev Lett 123, 070503
(2019)

it is based on ensemble averaging of the $\xrightarrow{\text{ Trotterized}}$ time-evolution operator at each time step -

when the operator set in $H = \sum_k H_k$ is small one can typically identify an optimal ordering of the operators to min Trotter errors , but when the set is large this becomes unfeasible -

However , as discussed previously , under unbiased sampling of orderings , the mean expectation value of operators should be closer to the exact one , as the contributions from commutators statistically average to zero .

In the qDrift protocol the probability of selecting a particular time-evolution operator

$$U_k(\Delta t) = e^{-iH_k \Delta t}$$

is defined by the "weight" of H_k in the total Hamiltonian -

Let us write

$$\hat{H} = \sum_{k=1}^L H_k = \sum_{k=1}^L h_k \underbrace{\bar{H}_k}_{\hookrightarrow \text{normalized}}$$

(largest singular value = 1)

then the proba of selecting $U_k(\Delta t)$ is

$$p_k = \frac{h_k}{\Lambda} \quad \text{where} \quad \Lambda = \sum_{k=1}^L h_k$$

for each member of the ensemble (each shot) and for each time step, a classical computer is used to select $U_k(\Delta t)$ based on the proba distribution defined by the $\{p_k\}$ - This produces a sequence of N ordered U_k 's forming

$$U_{\vec{k}}(\Delta t) = \prod_{k=1}^N e^{-i \Lambda \bar{H}_{k,j} \frac{\Delta t}{N}}$$

$(\Delta t \equiv \epsilon/N \text{ here})$ where $\vec{k} = (k_1, k_2, \dots, k_N)$

see that for q. chem syst

q Drift allows for smaller gate counts
at small time than Trotter.

For large $t \rightarrow$ does worse but
there are very large times for which
gate counts $\gtrsim 10^{23}$ -

However such classical sampling techniques
lead to the same issues discussed
previously = if the fluctuations are too large
the cancellations do not occur and
the method fails.

In simulations of low-dim QFT, it
performs worse than ordering based
on random sampling (which was worse
than LO Trotter with fixed ordering).

Such algo. may however be useful
in the context of future quantum computer
with "higher-fidelity" qubits / gates.

2) Linear Combinations of Unitaries (LCU)

If the classical averaging does not perform well, why don't we try to do the averaging directly on the quantum circuit?

$$\text{ex: } H = H_1 + H_2$$

Can we build a circuit that implements

$$\frac{1}{2} [U_1(\Delta_t) U_2(\Delta_t) + U_2(\Delta_t) U_1(\Delta_t)] \\ = e^{-i(H_1+H_2)\Delta t} + \mathcal{O}(\Delta t^3)$$

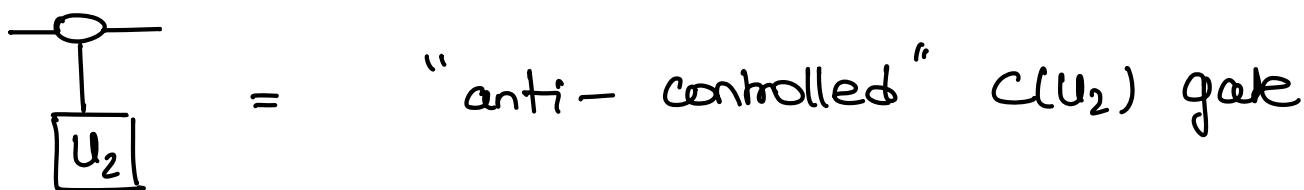
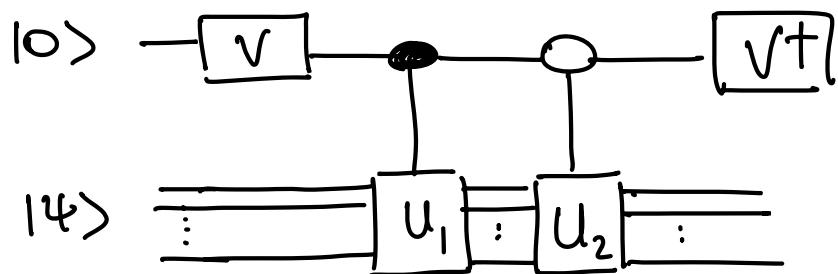
?

The problem is that a sum of unitaries is not a priori unitary itself, and thus cannot be directly implemented on a quantum computer.

However, it can be implemented if the system is embedded into a larger system and the transformation corresponds to unitaries in the larger system (and measurements are performed on the extra qubits and not on the (sub) system of interest).

This relates to the theory of open quantum systems that we will study in a few weeks.

The idea is the following. Consider the circuit:



applies U_2 to target if control qubit is in state $|0\rangle$, nothing otherwise.

V is a one qubit unitary

$$V = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad \text{with} \quad \begin{cases} c = -e^{i\varphi} b^* \\ d = e^{i\varphi} a^* \\ |a|^2 + |b|^2 = 1 \end{cases}$$

$$\Rightarrow \begin{cases} V|0\rangle = a|0\rangle + c|1\rangle \\ V|1\rangle = b|0\rangle + d|1\rangle \end{cases}$$

$$V^\dagger = \begin{pmatrix} a^* & c^* \\ b^* & d^* \end{pmatrix} \Rightarrow \begin{cases} V^\dagger|0\rangle = a^*|0\rangle + b^*|1\rangle \\ V^\dagger|1\rangle = c^*|0\rangle + d^*|1\rangle \end{cases}$$

The circuit acts as following :

$$|1\rangle \otimes |0\rangle \mapsto |1\rangle \otimes V|0\rangle$$

$$= |1\rangle \otimes [a|0\rangle + c|1\rangle]$$

$$\mapsto \{a|1\rangle|0\rangle + c|1\rangle|1\rangle\}$$

$$\mapsto \{a|1\rangle|0\rangle + c|1\rangle|1\rangle\}$$

$$\mapsto \{a|1\rangle(a^*|0\rangle + b^*|1\rangle) + c|1\rangle(c^*|0\rangle + d^*|1\rangle)\}$$

$$= \{(|a|^2|1\rangle|0\rangle + |c|^2|1\rangle|1\rangle)|0\rangle$$

$$+ (ab^*|1\rangle|0\rangle + cd^*|1\rangle|1\rangle)|1\rangle\}.$$

Now if we measure the ancilla (extra) qubit and keep only members of the measurement ensemble that measure $|0\rangle$, the state of the full system has collapsed to:

$$(|\alpha|^2 |U_2|4\rangle + |\beta|^2 |U_1|4\rangle) \otimes |0\rangle$$

Here we are interested in $|\alpha|^2 = |\beta|^2 = 1/2$

\rightarrow choose $a = c = 1/\sqrt{2}$ and \sqrt{r} real

$$\begin{aligned} \Rightarrow r &= \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \\ &= \frac{1}{\sqrt{2}} (\mathbb{I} - iY) \\ &= \cos\left(\frac{\pi}{4}\right) \mathbb{I} - i \sin\left(\frac{\pi}{4}\right) Y \\ &= e^{-i \frac{\pi}{4} Y} \\ &= \text{rotation of angle } \frac{\pi}{2} \text{ around the } y \text{ axis.} \end{aligned}$$

This procedure can be generalized to linear combinations of multiple unitaries controlled by multiple ancilla qubits.

If one wants to implement

$$\hat{O} = \sum_{k=0}^{M-1} \alpha_k U_k$$

one needs to first prepare the state of the ancilla qubits with V acting as

$$V |0\rangle = \underbrace{\sum_{k=0}^{M-1} \sqrt{\frac{|\alpha_k|}{\lambda}}}_{|00\dots 0\rangle} |k\rangle$$

$$\text{where } \lambda = \sum_{k=0}^{M-1} |\alpha_k|$$

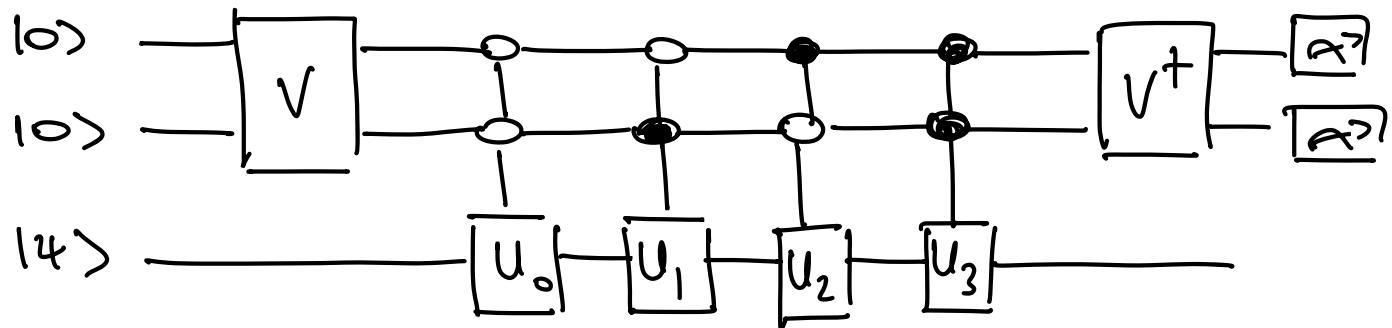
Then comes the "selection" operator W_{sel} composed of multiple - controlled and anti controlled gates, acting as

$$W_{\text{sel}} |0\rangle |k\rangle = U_k |0\rangle |k\rangle$$

Finally we undo the preparation step by applying V^\dagger to the ancilla qubits and we measure them, keeping only states of the full system corresponding to ancilla outcome $|0\rangle = |0\dots 0\rangle$.

Example circuit to implement

$$\hat{O} = \sum_{k=0}^3 \alpha_k U_k$$



we will see how to construct circuits for the state preparation step (V).

This LCU method has been proposed by Childs & Wiebe in Quantum Info and Computation Vol 12, 0901 (2012).

It has many possible applications beyond time-evolution.

While this method offers a nice way to eliminate Trotter errors from the commutator without classical sign problems, we see that the number of gates and ancilla qubits grows quickly.

3) Truncated Taylor series of the time evolution operator

$$\begin{aligned} U(t) &= e^{-iHt} \\ &= I - iHt + \frac{(iHt)^2}{2!} + \dots \\ &= I - i \sum_{k=1}^L H_k t - \frac{1}{2} \left(\sum_k H_k \right)^2 t^2 + \dots \end{aligned}$$

Ref: Berry, Childs, Cleve, Khozai, Somma
Phys. Rev. Lett 114, 090502 (2015)

4) Fast-Forwarding

see e.g. • Atia et al, Nat Commun 8 1572
... (2017)

• Cirstoiu et al.

Nature, npj quantum info 6, 82
(2020)

The idea is to diagonalize the time evolution operator for one time step:

$$U(\Delta t) = e^{-iH\Delta t} = W D W^+ \\ \Rightarrow U(t) = W D^{N_S} W^+ \quad (t = \Delta t \times N_S)$$

This is useful if the diagonalization can be done efficiently

(e.g. systems with high degrees of symmetries, when H_{ami} is block diag ...)

In that case the # of gates for the time evolution is sublinear in t .

(versus $\sim t^2$ in LO Trotter).

③ Estimating energy eigenvalues and preparing energy eigenstates.

We saw that a QC can efficiently simulate the time-evolution of a quantum system with a local Hamiltonian (it can solve the time-dep. Schrödinger eq.) -

Another topic of interest for physicists and chemists is the time-independent Schrödinger eq., that is, compute the energy eigenvalues of a Hamiltonian H -
 (time-indep.)

$$\boxed{H|\psi_\alpha\rangle = E_\alpha|\psi_\alpha\rangle}$$

- Classically:

The "brute force" approach is to diagonalize the Hamiltonian matrix

$$|\psi_\alpha\rangle = \sum_{x=0}^{2^n-1} a_x^{(\alpha)} |x\rangle$$

$$H = \begin{pmatrix} \langle \alpha | H | \alpha' \rangle \end{pmatrix} = \begin{pmatrix} \langle 0|H|0\rangle & \cdots & \langle 0|H|2^n-1\rangle \\ \langle 1|H|0\rangle & \cdots & \vdots \\ \vdots & \ddots & \vdots \\ \langle 2^n-1|H|2^n-1\rangle & & \end{pmatrix}$$

$$\Rightarrow \left\{ a_{\alpha}^{(2)} \right\}$$

Typically this can only be done for small systems -

If one has more than a few particles, one has to resort to drastic approximations.

Tools: There may be some cases where eigenstates can be found efficiently:

- * If H is sparse and has a simple structure, it may be easy.
- * Sometimes, it is possible to express H in a certain basis $\{| \Phi_i \rangle\}$ such that all off-diagonal terms of the matrix are negative:

$$\langle \phi_i | H | \phi_j \rangle = \underbrace{\epsilon_i}_{\text{diagonal part}} \delta_{ij} - \underbrace{h_{ij}}_{\text{nn diagonal part.}}$$

with $h_{ij} \geq 0$

in that case the ground state of H
 (eigenstate $|4_0\rangle$ with lowest eigenvalue)
 can be expressed as :

$$|4_0\rangle = \sum_{i=0}^{2^n-1} A_i^{(0)} |\phi_i\rangle$$

with $A_i \geq 0, \forall i$.

because $|4_0\rangle$ (being the gs) maximizes

$$\langle 4_0 | h | 4_0 \rangle = \sum_{ij} A_i^{(0)*} A_j^{(0)} h_{ij}.$$

\Rightarrow optimal to choose $A_i^{(0)*} A_j^{(0)} \geq 0$
 $\forall i, j$.

In that case (when $A_i \geq 0, \forall i$), there
 are Monte Carlo sampling algo
 that can find the A_i 's efficiently
 (and accurately).

But if the b_{ij} are not all ≥ 0 ,
the sampling algorithms may not work
well because there can be delicate
cancellations btw positive & negative
terms contributing to $\langle \Psi_0 | h | \Psi_0 \rangle$
→ this is another case of
the so-called "sign problem".

* if the entanglement or magic of the system
scale in a particular way (see later)

but in general efficient classical
algorithms are not known -

→ Can quantum computers also bring an advantage to this problem?
 One possibility is to use the quantum phase estimation algorithm (QPE).

How?

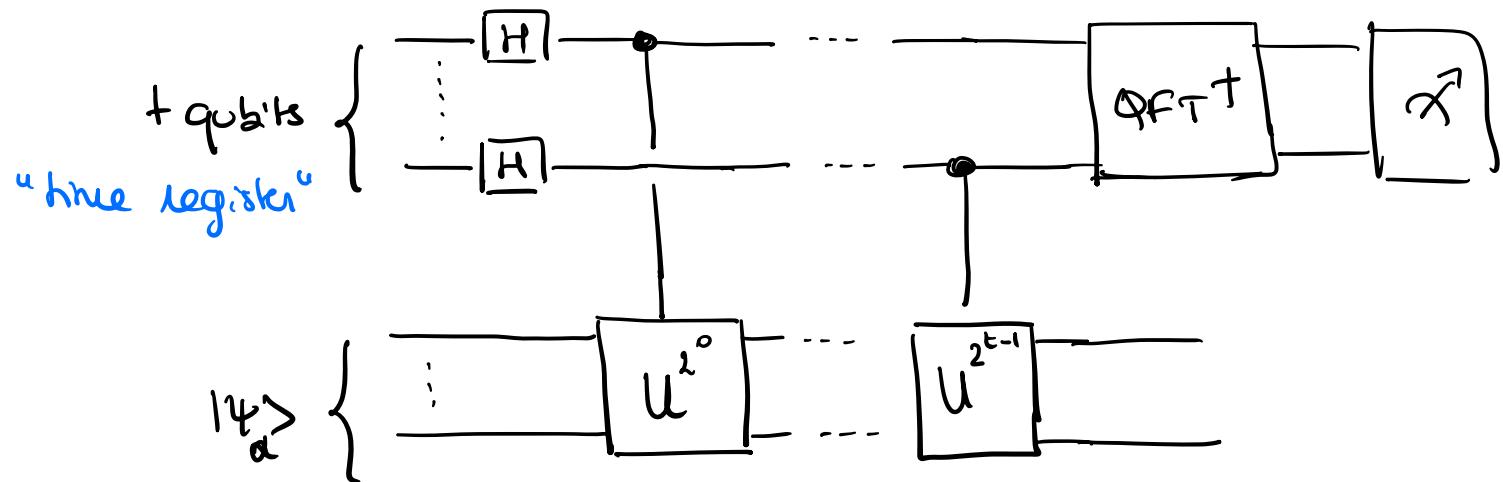
We want eigenvalues of H but H is Hermitian, not unitary, and QPE can only estimate eigenvalues of unitary operators U .

→ take $\hat{U} = e^{-iH}$

where T
is some value
of time (fixed)

U has eigenvalues $e^{-iE_\alpha T}$ where E_α are eigenvalues of H .

The following QPE circuit



will estimate $\Theta_\alpha = F_\alpha \frac{T}{2\pi}$ up to m -bits

of accuracy where $t = m + \log \left(2 + \frac{1}{2\epsilon} \right)$
 $(\epsilon = \text{proba of failure})$

$$e^{-iH(T2^j)}$$

$\Downarrow 2^j$

($t=m$ if Θ can be rep with t bits
 and no failure).

Performing U with $2^j = (2^0, 2^1, \dots, 2^{t-1})$

is like simulating the time evolution
 governed by H for various times

$$G = T \times 2^0, T \times 2^1, \dots, T \times 2^{t-1}$$

(which we can do efficiently if H is local).

Reminder :

if start with $|4_\alpha\rangle$ in the bottom -

The state of the top (time) register is

$$\frac{1}{2^{t/2}} \sum_{y=0}^{2^t-1} e^{(2\pi i) y \Theta_\alpha} |y\rangle \quad \text{before the QFT}^\dagger$$

$$\text{and } \frac{1}{2^t} \sum_{x,y} e^{(2\pi i) y (\Theta_\alpha - \frac{x}{2^t})} |\alpha\rangle \quad \text{after the QFT}^\dagger$$

\Rightarrow if we measure in the computational basis

we get outcome $|\alpha\rangle$ with proba

$$p(\alpha) = \left| \frac{1}{2^t} \sum_y e^{(2\pi i)y(\Theta_\alpha - \frac{\alpha}{2^t})} \right|^2$$

which is peaked for $\Theta_\alpha - \frac{\alpha}{2^t} = 0$

- exactly if Θ_α can be rep exactly with t bits. $\rightarrow p(\alpha = 2^t \Theta_\alpha) = 1$.

- otherwise obtain m-bit approx to Θ_α with $t = m + \log(2 + \gamma/2\epsilon)$

$$p(\alpha = 2^t \Theta_\alpha) \geq 1 - \epsilon$$

Once we have $\Theta_\alpha = \frac{2\pi}{T} E_\alpha$ (to certain accuracy) $\Rightarrow E_\alpha$

Now in practice one can only prepare some superposition of eigenstates of $U = e^{-iH\tau}$

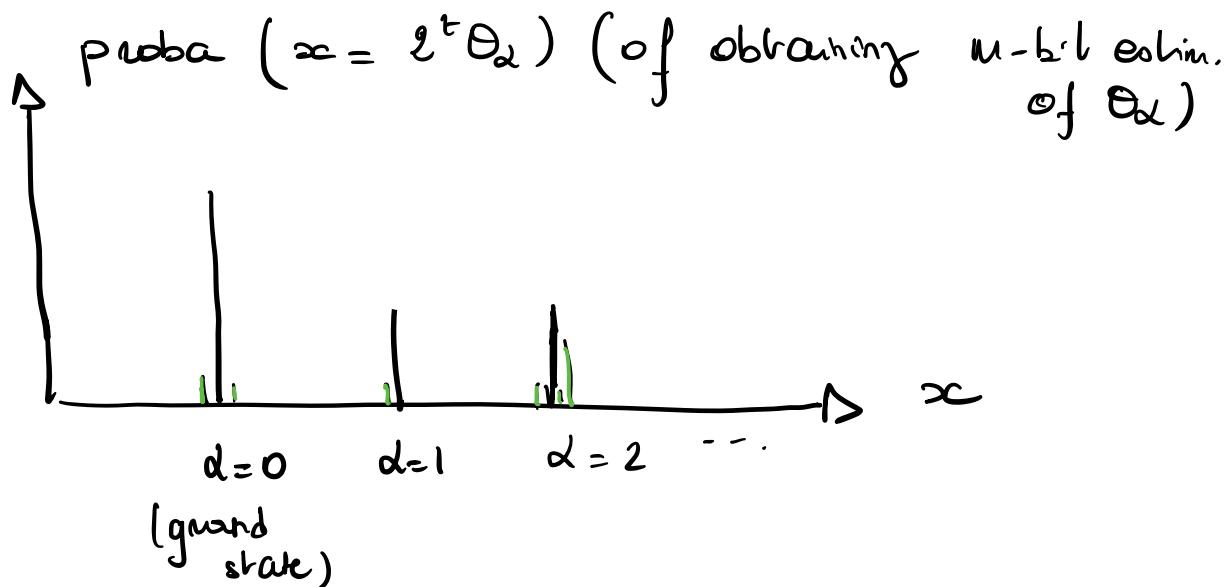
$$|\Phi\rangle = \sum_d c_d |Y_d\rangle$$

→ we will obtain an m-bit estimate

$$\text{of } \Theta_d = \frac{E_d \cdot T}{2\pi} \text{ with proba of success}$$

$$|c_d|^2 \times (1 - \epsilon)$$

⇒ if we prepare the syst in $|\Phi\rangle$ and repeat the computation many times we will obtain some proba distrib's:



- The location of each main peak provides an estimate of the energy eigenvalues:

$$\theta_\alpha = \frac{E_\alpha \cdot T}{\lambda \pi} \quad \alpha = 0, 1, 2, \dots$$

- The height of each peak is

$$|c_\alpha|^2 [1 - \epsilon]$$

and thus can provide an estimate of
 $c_\alpha = \text{overlap } |\langle \psi_\alpha | \Phi \rangle|$ btw the
 prepared state and the eigenstate
 $|\psi_\alpha\rangle$.

→ How costly is this procedure?

We saw previously that the circuit simulating time evolution of an n -qubit system, governed by geometrically local H , over time \mathcal{G} , with accuracy δ , requires

$$\mathcal{O}((n\mathcal{G})^2 \times \frac{h^2}{\delta}) \times \mathcal{O}(\text{poly log } (n\mathcal{G})^2 \frac{h^2}{\delta^2})$$

$$= \mathbb{O}((n\mathcal{G})^2 \frac{h^2}{\delta}) \quad (\text{LO Trotter})$$

gates from some approx. universal gate set

Here we require accuracy of 2^{-m} for QPE →

it is sufficient to achieve an error

$\delta = 2^{-m}$ for evolution over the longest time $\mathcal{G} = T \times 2^{t-1}$

$$\Rightarrow \text{circuit size} = \mathbb{O}\left[n^2 (2^{t-1})^2 2^m h^2 T^2\right]$$

$$\text{Since } t = m + \log(2 + \frac{1}{2\epsilon}) \sim m$$

the circuit size is

$$\Theta\left(n^2 2^{3m} \underbrace{(h^2 T^2)}_{\text{cost}}\right)$$

- if the accuracy 2^{-m} is fixed, this is polynomial in n
- we can also require a stronger condition:
if we want the accuracy 2^{-m} to scale
as the inverse of some power of our system
size :

$$2^{-m} \sim n^{-c} \quad (c)$$

\Rightarrow This will require a circuit size

$$\Theta\left(n^{2+3c} \times h^2 T^2\right)$$

which is also polynomial in n .

\Rightarrow The resources we need to estimate the energy scale polynomially in system size n .

However, there is a catch:

if we want to estimate an energy eigenvalue E_α to accuracy $2^{-m} \sim n^{-c}$
 $= O\left(\frac{1}{\text{poly}(n)}\right)$ in time which is $O(\text{poly}(n))$,

the initial (prepared) state $|\Phi\rangle$ must have an overlap with $|\Psi_\alpha\rangle$ which is at least $\frac{1}{\text{poly}(n)}$:

$$|c_\alpha|^2 = |\langle \Psi_\alpha | \Phi \rangle|^2 > \frac{1}{\text{poly}(n)}$$

(Because the proba of success $\leq |c_\alpha|^2$)

If that is the case \rightarrow can get a good estimate of E_α in polynomial number of trials.
And, as a bonus, we also obtain $c_\alpha = \langle \Psi_\alpha | \Phi \rangle$, which gives info on the wave function (the state $|\Psi_\alpha\rangle$ itself).

But usually preparing a state $|\tilde{\Phi}\rangle$ with overlap $|c_\alpha|^2 > \frac{1}{\text{poly}(n)}$ is difficult:

if one considers a randomly-prepared n-qubit state

$|c_\alpha|^2$ is typically exponentially small

$$\text{i.e. } |c_\alpha|^2 \sim \frac{1}{\text{exp}(n)}$$

\Rightarrow in that case we would need an expo. number of trials, i.e. exponentially long time to estimate E_α .

\Rightarrow is there a way to prepare a state $|\tilde{\Phi}\rangle$ which has a better overlap with an eigenstate $|\psi_\alpha\rangle$?

Yes, if we are looking for the ground state $|\psi_0\rangle$, there is a general procedure for constructing a state with significant overlap with $|\psi_0\rangle$, which works sometimes (but not always) -

This procedure involves the quantum adiabatic theorem and is the following:

We start with a Hamiltonian H_{easy} whose ground state is easy to find classically and thus can be easily prepared. (at least to good approx)

Then we simulate Schrödinger evolution governed by a time-dependent Hamiltonian such that

$$\begin{cases} H(0) = H_{\text{easy}} \\ H(\tau_{\max}) = H_{\text{hard}} \end{cases}$$

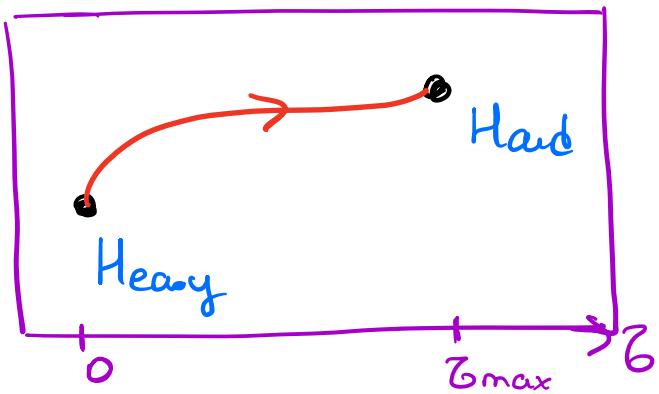
↳ the Hamiltonian whose gs we want to compute

For example we can choose:

$$H(\tau) = \left(1 - \frac{\tau}{\tau_{\max}}\right) H_{\text{easy}} + \frac{\tau}{\tau_{\max}} H_{\text{hard}}$$

which evolves from H_{easy} to H_{hard} as

$$\tau = 0 \rightarrow \tau_{\max}.$$



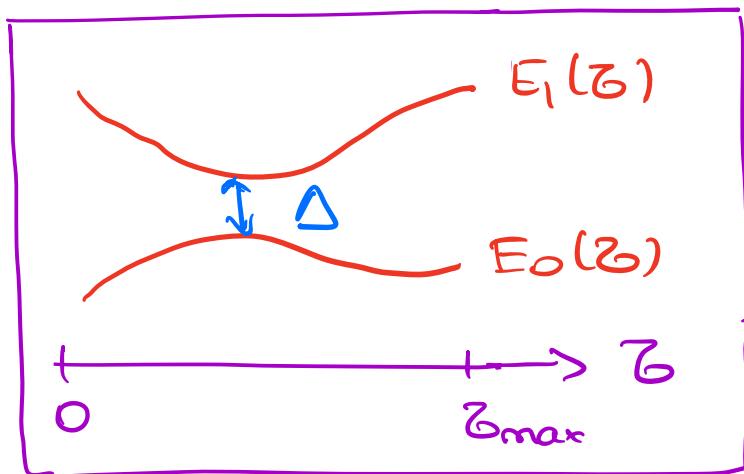
Now the quantum adiabatic theorem says that if we prepare $|\Psi(0)\rangle$ = ground state of Heavy (or a state having large overlap with gs of Heavy), then, if τ_{\max} is long enough, i.e. if $H(\tau)$ evolves sufficiently slowly, $|\Psi(\tau_{\max})\rangle$ coincides with the gs of H_{hard} (or a good approx of it).

→ how slow is "sufficiently" slow?

Let $E_0(\tau)$ be the energy of $\xrightarrow{\text{the gs of}} H(\tau)$ and let $E_1(\tau)$ be the energy of the first excited state of $H(\tau)$.

$$\text{We now define } \Delta = \min_{\zeta \in [0, \zeta_{\max}]} [E_1(\zeta) - E_0(\zeta)]$$

= minimum energy gap btw the ground and first excited state over the evolution.



The adiabatic thm says that

$$z_{\max} > \frac{A}{\Delta^c} \quad \text{where } A, c = \text{const independent of \# of qubits } n.$$

is sufficiently slow.

Therefore we have a complete polynomial algorithm for computing the g.s. energy of a local Hamiltonian to polynomial accuracy ($\frac{1}{\text{poly}(n)}$) in polynomial time if Δ no smaller than:

$$\Delta = \frac{1}{\text{poly}(n)}$$

Otherwise would need to evolve for exponential time.
↳ (Δ exp small)

Unfortunately, it seems that there are cases where energy gap is exp small & thus the gs cannot be efficiently computed even with a QC.

On the other hand it is reasonable to be hopeful that this procedure works for interesting cases - For instance chemists who want to compute gs energy of electronic systems (molecules with nuclei at fixed positions) claim (without proof) that one can adiabatically evolve from the Hartree-Fock

Hamiltonian (non interacting) to the
↳ can be solved classically

full interacting Hamiltonian, and that the gap remains larger than some constant.

There may also be a similar property in nuclei (systems of interacting p & n).

→ if that is true, QC would be a powerful tool for many interesting physics pb.

Recap so far we saw that

* Classically :

- time evolution \notin BPP (however \in PSPACE)
 - Ham: eigenstates preparation \notin BPP, \notin PSPACE
- \Rightarrow exponential time is always required.
(for large systems)

* Quantumly :

- time evolution \in BQP
(demonstrated with Trotter
original proof: Lloyd, Science 273 1073 (1996))
- Ham: eigenstates \notin BQP
(is QMA-complete)
proof: Kemper, SIAM journal of computing
35, 1070 (2006)

\Rightarrow in general

preparing eigenstates of a (c-local)
Hamiltonian requires exponential
time even on a QC

but as discussed previously the
Ham's of physically interesting systems
are not the general case -

They present particular symmetries, entanglement
patterns ... that hopefully can make
state prep. also efficient with a QC ...