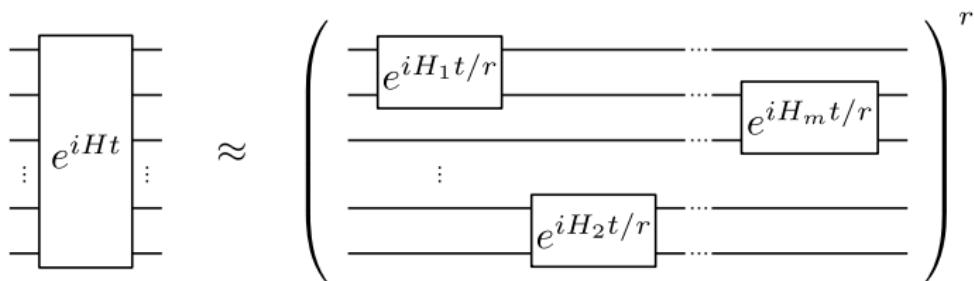


# QUANTUM ALGORITHMS 2:

## QUANTUM SIMULATION AND CHEMISTRY



**Simon Apers**  
(CNRS & IRIF, Paris)

([simonapers.github.io/mckinsey.html](http://simonapers.github.io/mckinsey.html))

## TUTORIAL 1: BASICS

quantum circuits

quantum Fourier transform

Grover search

## TUTORIAL 2: CHEMISTRY

quantum problems

quantum simulation

variational quantum algorithms

## TUTORIAL 3: OPTIMIZATION

adiabatic algorithm

HHL

quantum walks

## **QUANTUM PROBLEMS**

QUBIT ENCODING

QUANTUM SIMULATION

VARIATIONAL QUANTUM ALGORITHMS

## Quantum problems

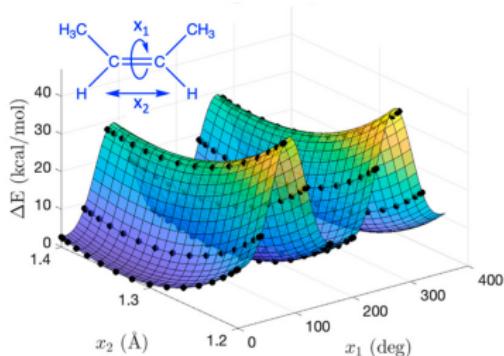
*“Nature isn’t classical, dammit, and if you want to make a simulation of Nature, you’d better make it quantum mechanical, and by golly it’s a wonderful problem because it doesn’t look so easy.”*

- R. Feynman, “Simulating physics with computers” (1981)

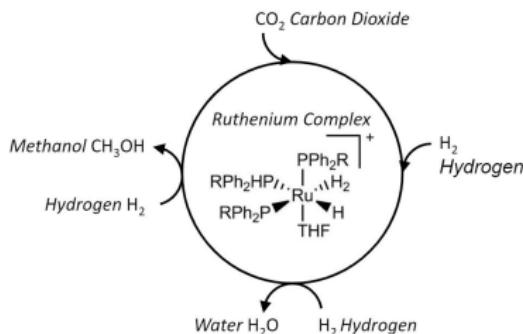


# Chemistry problems:

design chemicals, drugs,  
reaction processes (e.g., carbon fixation, batteries)



potential energy surface (2-butene)



reaction chain (carbon fixation)

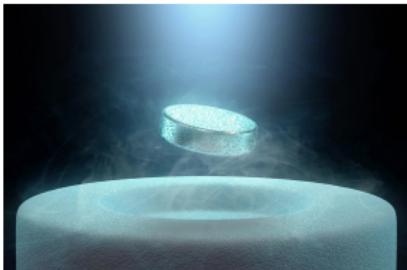
need:

ground state energy, quantum dynamics

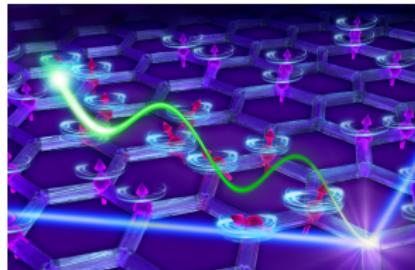
classical approaches (Hartree-Fock, DFT) often fall short

## Material science problems:

design of new materials,  
study of fundamental physics



superconductivity



Majorana fermions

classical theory (mean-field, band theory)  
fails for strong interactions

e.g., Mott insulators

## Quantum problems

input:

(description of) quantum system

goal:

predict properties

means:

- (a) preparation of ground state
- (b) simulation of quantum dynamics

## Quantum problems (formalized)

input:

Hamiltonian  $H$

describes energy of the quantum system

(time-independent) Schrödinger's equation:

$$H |\phi\rangle = E |\phi\rangle$$

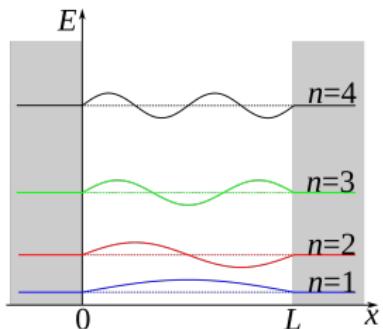
## classroom example: single quantum particle

wave function

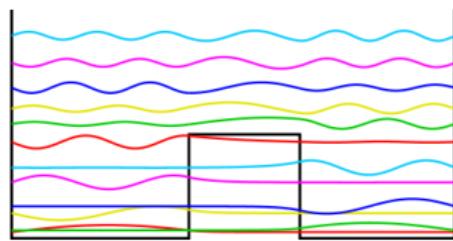
$$\psi(x), \quad x \in \mathbb{R}$$

Hamiltonian

$$H = -\frac{1}{2m} \nabla^2 + V(x)$$



particle in a box



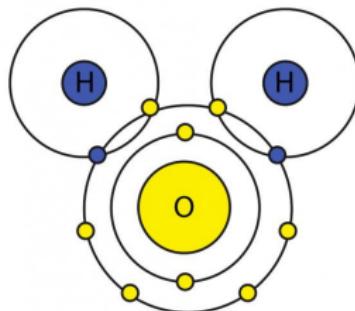
double well potential

## chemistry example: molecular Hamiltonian

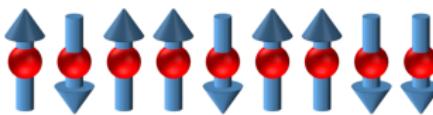
$N$ -particle wave function  $\psi(x_1, \dots, x_N)$

Hamiltonian

$$H = - \underbrace{\frac{1}{2m} \sum_i \nabla_i}_{\text{kinetic energy}} - \underbrace{\sum_{i,\ell} \frac{1}{|x_i - R_\ell|}}_{\text{electron-nucleus}} + \underbrace{\frac{1}{2} \sum_{i \neq j} \frac{1}{|x_i - x_j|}}_{\text{electron-electron}}$$



## condensed matter example: spin chain



basis state  $|z\rangle = |\uparrow\downarrow\uparrow\uparrow \dots \downarrow\rangle = |1011\dots0\rangle$

classical Ising Hamiltonian

$$H = - \sum_{\langle i,j \rangle} Z_i Z_j$$

using  $Z_i |z\rangle = (-1)^{z_i} |z\rangle$  we have

$$H |z\rangle = - \sum_{\langle i,j \rangle} Z_i Z_j |z\rangle = - \sum_{\langle i,j \rangle} (-1)^{z_i + z_j} |z\rangle = E(z) |z\rangle$$

basis states are eigenstates  
energy  $E(z)$  measures # unaligned pairs

## *quantum* Ising Hamiltonian

$$H = \underbrace{- \sum_{\langle i,j \rangle} Z_i Z_j}_{\text{magnetic interaction}} + \underbrace{\sum_i X_i}_{\text{external magnetic field}}$$

$H |z\rangle \neq E_z |z\rangle$ : basis states no longer eigenstates

**quantum eigenstates**  $|\phi\rangle = \sum_{z \in \{0,1\}^n} \alpha_z |z\rangle$

! representation on classical computer:  $2^n$  bits  
vs. representation on quantum computer:  $n$  qubits

# Quantum problems (formalized)

goal:

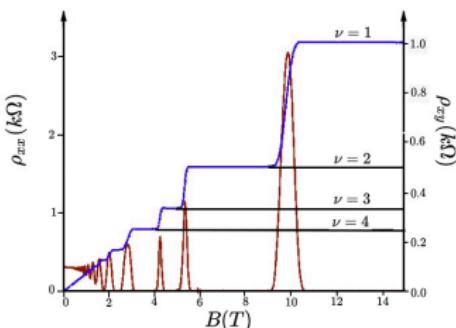
predict properties

static properties:

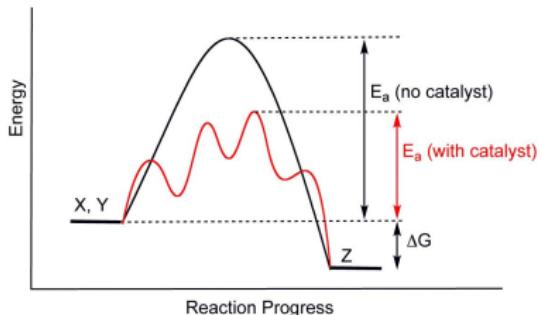
magnetization, conductivity, ground state energy

dynamic properties:

tunnelling probability, reaction rate



quantum Hall effect



chemical catalysis

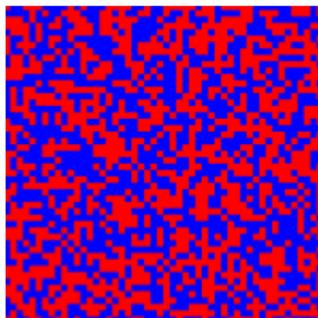
via “observables”

= Hermitian matrix  $A$ ,  
expected outcome  $\langle \phi | A | \phi \rangle$

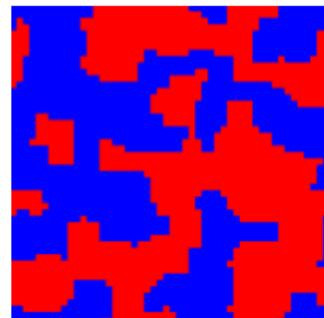
energy:  $A = H$

magnetization / correlation:  $A = Z_i Z_j$

e.g., Ising model:



high energy, low magnetization



low energy, high magnetization

## Quantum problems (formalized)

means:

(a) preparation of ground state

$$|\nu_0\rangle = \operatorname{argmin}_{|\psi\rangle} \langle\psi|H|\psi\rangle$$

maybe thermal or Gibbs state

**(b)** simulation of quantum dynamics

via (time-dependent) Schrödinger's equation

$$\frac{\partial}{\partial t} |\psi(t)\rangle = -iH |\psi(t)\rangle$$

with solution

$$|\psi(t)\rangle = e^{-iHt} |\psi(0)\rangle ,$$

where

$$e^{-iHt} = \sum_{k=0}^{\infty} \frac{1}{k!} (-iHt)^k$$

**EX:** verify this

**Can quantum computers solve all quantum problems?**  
(given “good” representation of state space and Hamiltonian)

**yes** for simulating quantum dynamics

(probably) **no** for preparing ground states

e.g., 2-local ZX Hamiltonian

$$H = \sum_i a_i Z_i + b_i X_i + \sum_{i,j} c_{i,j} Z_i X_j$$

is “QMA-complete”

## References

- **Quantum chemistry background:** McArdle, S., Endo, S., Aspuru-Guzik, A., Benjamin, S. C., & Yuan, X. (2020). Quantum computational chemistry. *Reviews of Modern Physics*, 92(1), 015003
- **Examples:** Bauer, Bravyi, Motta, & Chan (2020). Quantum algorithms for quantum chemistry and quantum materials science. *Chemical Reviews*, 120(22), 12685-12717
- **Algorithmic challenges:** Clinton, Cubitt, Flynn, Gambetta, Klassen, Montanaro, Piddock, Santos, Sheridan (2022). Towards near-term quantum simulation of materials. TQC'23, arXiv:2205.15256
- **Case study (carbon fixation):** von Burg, V., Low, G. H., Häner, T., Steiger, D. S., Reiher, M., Roetteler, M., & Troyer, M. (2021). Quantum computing enhanced computational catalysis. *Physical Review Research*, 3(3), 033055

QUANTUM PROBLEMS

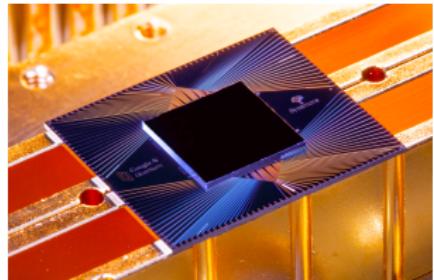
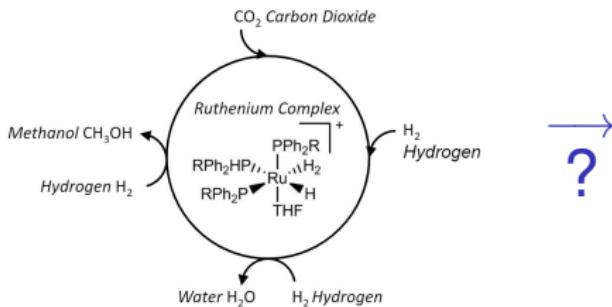
**QUBIT ENCODING**

QUANTUM SIMULATION

VARIATIONAL QUANTUM ALGORITHMS

## Qubit encoding:

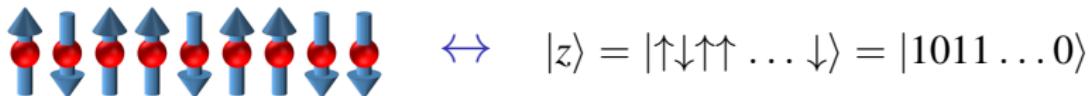
mapping physical system to qubit Hamiltonian



## Example 1: quantum Ising model

$$H = a \sum_{\langle i,j \rangle} Z_i Z_j + b \sum_i X_i$$

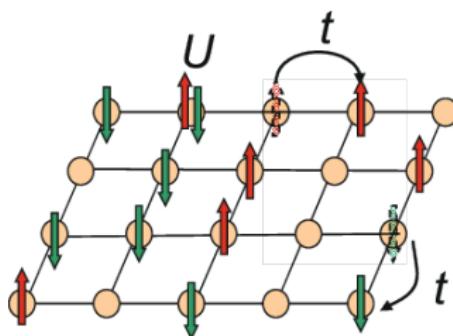
1-to-1 correspondence between spins and qubits



## Quantum encoding 2: Fermi-Hubbard model

fermions hopping on lattice

$$H = t \sum_{\langle i,j \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$



Jordan-Wigner transformation maps fermions to qubits

## Quantum encoding 3:

“molecular Hamiltonian”

$$H = - \sum_i \nabla_i - \sum_\ell \nabla_\ell - \sum_{i,\ell} \frac{1}{|x_i - R_\ell|} + \sum_{i \neq j} \frac{1}{|x_i - x_j|} + \sum_{k \neq \ell} \frac{1}{|R_k - R_\ell|}$$

↓ (Born-Oppenheimer approximation)

“electronic Hamiltonian”  $H = - \sum_i \nabla_i - \sum_{i,\ell} \frac{1}{|x_i - R_\ell|} + \sum_{i \neq j} \frac{1}{|x_i - x_j|}$

↓ (orbitals + second quantization)

“fermionic Hamiltonian”  $H = \sum_{\langle i,j,k,\ell \rangle} a_{ijkl} c_i^\dagger c_j^\dagger c_k c_\ell$

↓ (Jordan-Wigner)

“qubit Hamiltonian”  $H = \sum_i a_i Z_i + b_i X_i + \sum_{i,j} c_{i,j} Z_i X_j$

QUANTUM PROBLEMS

QUBIT ENCODING

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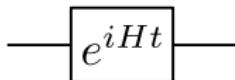
**Quantum simulation:**  
or “quantum numerical methods”

input: qubit Hamiltonian

$$H = \sum_{\ell} H_{\ell}$$

assumption:  
 $H_{\ell}$ 's are  $k$ -local

goal:  
Hamiltonian simulation



by assumption: individual terms  $H_\ell$  easy to simulate

$$\text{---} \boxed{e^{iH_\ell t}} \text{---}$$

e.g., Ising model: terms  $H_\ell = Z_i Z_j$

**EX:** define

$$e^{-i\theta Z} \equiv \begin{bmatrix} e^{-i\theta} & 0 \\ 0 & e^{i\theta} \end{bmatrix} \equiv -[R_z(\theta)]$$

show that

$$-[X] \equiv -[H] - [Z] - [H]$$

and

$$e^{-i\theta X} \equiv -[H] - [R_z(\theta)] - [H]$$

unfortunately,

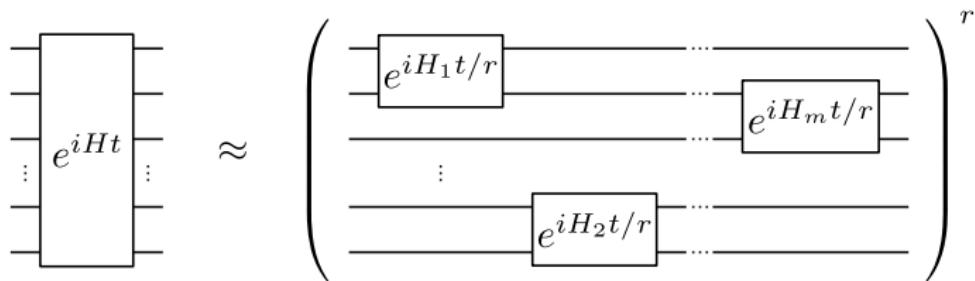
$$e^{iHt} = e^{i(\sum_{\ell} H_{\ell})t} \neq \prod_{\ell} e^{iH_{\ell}t}$$

$$-\boxed{e^{iHt}}- \neq -\boxed{e^{iH_1t}}- \cdots -\boxed{e^{iH_mt}}-$$

due to **non-commutativity**:  $AB \neq BA$

main technique: **Trotterization**

$$\begin{aligned} e^{iHt} &= \lim_{r \rightarrow \infty} \left( e^{iH_1 t/r} e^{iH_2 t/r} \dots e^{iH_m t/r} \right)^r \\ &= \left( e^{iH_1 t/r} e^{iH_2 t/r} \dots e^{iH_m t/r} \right)^r + O(t^2/r) \end{aligned}$$



## EX: Lie-Trotter formula

consider  $A, B$  Hermitian and  $\|A\|, \|B\| \leq 1$

for  $0 < \delta < 1$ , show that

$$e^{(A+B)\delta} = e^{A\delta} e^{B\delta} + O(\delta^2)$$

$$\begin{array}{c} \text{---} \\ \text{---} \\ \vdots \\ \text{---} \\ e^{iHt} \\ \vdots \\ \text{---} \end{array} = \left( \begin{array}{c} \text{---} \\ \boxed{e^{iH_1 t/r}} \\ \text{---} \\ \vdots \\ \text{---} \\ \boxed{e^{iH_m t/r}} \\ \text{---} \\ \vdots \\ \text{---} \end{array} \right)^r + O(t^2/r)$$

Trotter complexity:

error is  $\varepsilon$ -small if we pick

$$r \sim t^2/\varepsilon$$

higher ( $k$ -th) order formulas:

$$r \sim t^{1+1/k}/\varepsilon^{1/k}$$

## Quantum simulation: recent developments

“optimal” Hamiltonian simulation in time

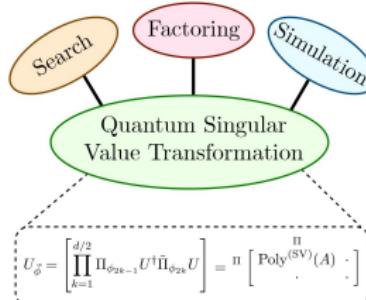
$$t + \log(1/\varepsilon)$$

interesting challenges:

- time-dependent Hamiltonians (e.g., annealing)
  - better understanding of Trotterization

Hamiltonian simulation = driving force in quantum algorithms

led to “quantum singular value transformation”  
= grand unification of quantum algorithms



QUANTUM PROBLEMS  
QUBIT ENCODING  
QUANTUM SIMULATION  
**VARIATIONAL QUANTUM ALGORITHMS**

## variational principle

ground state energy

$$\lambda_0 = \min_{|\psi\rangle} \langle\psi|H|\psi\rangle$$

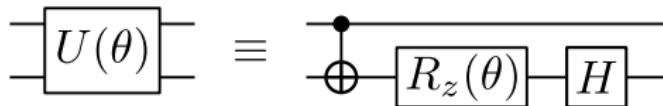
ground state

$$|\nu_0\rangle = \operatorname{argmin}_{|\psi\rangle} \langle\psi|H|\psi\rangle$$

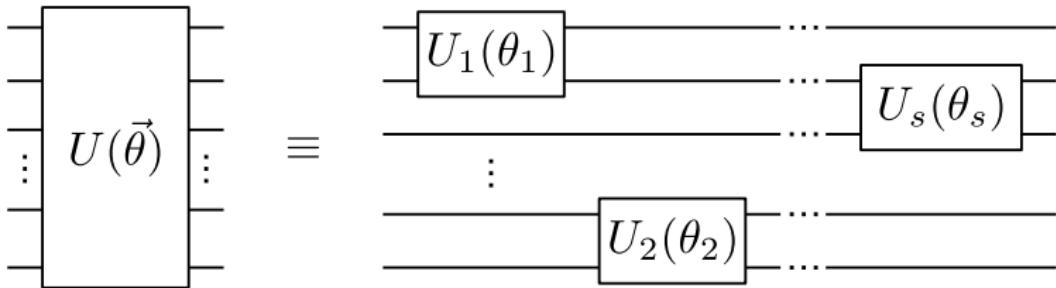
→ optimization problem!

## variational quantum algorithms

parameterized quantum gate (example)



parameterized quantum circuit



let

$$|\psi(\vec{\theta})\rangle = U(\vec{\theta}) |0\rangle$$

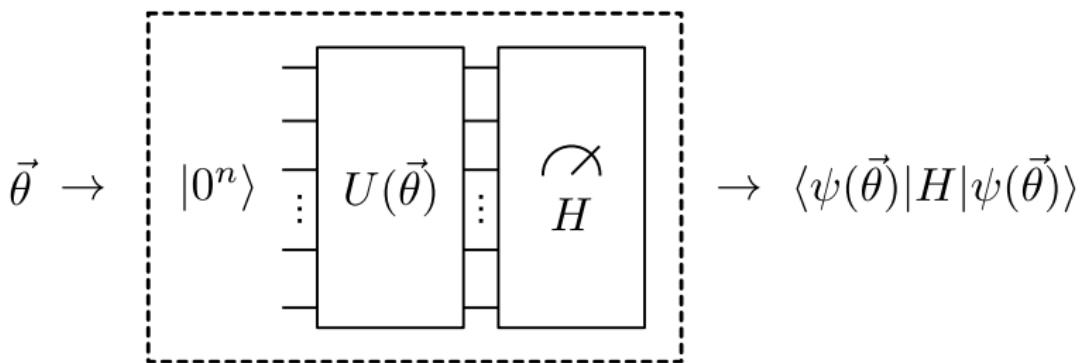
and rephrase

$$\min_{|\psi\rangle} \langle\psi|H|\psi\rangle$$

as

$$\min_{\vec{\theta}} \langle\psi(\vec{\theta})|H|\psi(\vec{\theta})\rangle$$

optimization over parameters  $\vec{\theta}$



considerations:

- choice parameterized circuit  $U(\vec{\theta})$ 
  - tuning of parameters  $\theta$
  - energy measurement

**choice parameterized circuit  $U(\vec{\theta})$**

different ansätze

e.g., “Hamiltonian variational ansatz”  
inspired by adiabatic algorithm

care about expressibility, symmetry preservation

**tuning of  $\vec{\theta}$ :**

classical optimization problem  
(= “hybrid” quantum algorithm)

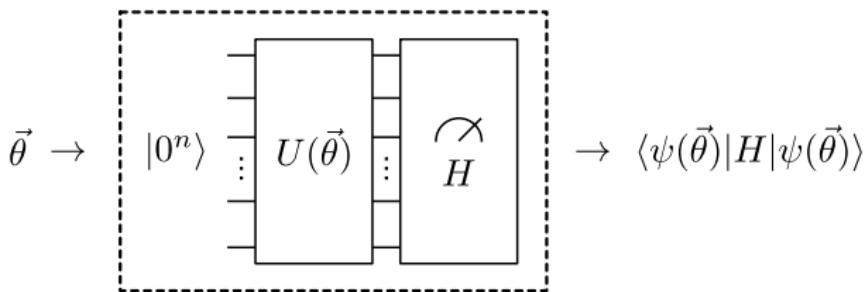
mostly heuristic art  
seems to work well

## energy estimation:

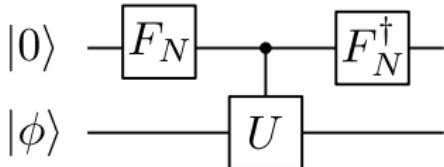
given: (encoding of) Hamiltonian  $H$ , state  $|\phi\rangle$

goal: estimate energy

$$\langle \phi | H | \phi \rangle$$



## solution 1: quantum phase estimation



**lemma:** given  $|\phi\rangle$  such that  $U|\phi\rangle = e^{i2\pi\theta}|\phi\rangle$ , can estimate  $\theta$  to precision  $\varepsilon$  with  $O(1/\varepsilon)$  calls to  $U$ .

→ set  $U = e^{iH}$  using Hamiltonian simulation

## solution 2: expanding Hamiltonian

$$H = \sum_{\ell} H_{\ell}$$

$$\langle \psi | H | \psi \rangle = \sum_{\ell} \langle \psi | H_{\ell} | \psi \rangle$$

↓

suffices to estimate  $\langle \psi | H_{\ell} | \psi \rangle$  for all  $\ell \in [m]$

# terms  $m$  often bounded

e.g., pairwise interactions  $\rightarrow m \in O(n^2)$

## EX:

measuring  $\langle \psi | Z | \psi \rangle$ :

recall the 1-qubit measurement

$$|\psi\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle \xrightarrow{\text{ } \square \text{ }} \begin{array}{l} |0\rangle \text{ with probability } |\alpha_0|^2 \\ |1\rangle \text{ with probability } |\alpha_1|^2 \end{array}$$

show that  $\langle \psi | Z | \psi \rangle = 2|\alpha_0|^2 - 1$

measuring  $\langle \psi | X | \psi \rangle$ :

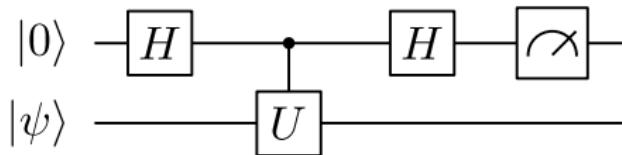
show that

$$|\psi\rangle \xrightarrow{\text{ } \square \text{ } H \text{ } \square \text{ }} \begin{array}{l} |0\rangle \text{ with probability } \frac{1}{2}|\alpha_0 + \alpha_1|^2 \\ |1\rangle \text{ with probability } \frac{1}{2}|\alpha_0 - \alpha_1|^2 \end{array}$$

and  $\langle \psi | X | \psi \rangle = |\alpha_0 + \alpha_1|^2 - 1$

## EX: unitary Hamiltonian

consider  $U$  that is both unitary ( $U^\dagger U = I$ ) and Hermitian ( $U = U^\dagger$ )



show that this circuit outputs “0” with probability

$$\frac{1 + \langle \psi | U | \psi \rangle}{2}$$

## Figure references

PES: Kwon, Hyuk-Yong, et al. "Interpolation methods for molecular potential energy surface construction." *The Journal of Physical Chemistry A* 125.45 (2021): 9725-9735.

Carbon fixation: <https://www.microsoft.com/en-us/research/blog/state-of-the-art-algorithm-accelerates-path-for-quantum-computers-to-address-climate-change/>

H<sub>2</sub>O molecule: <https://www.e-education.psu.edu/earth111/node/838>

spin chain: <https://labsites.rochester.edu/nicholgroup/research/>

Hall effect: [https://en.wikipedia.org/wiki/Quantum\\_Hall\\_effect](https://en.wikipedia.org/wiki/Quantum_Hall_effect)

catalyst: <https://www.thoughtco.com/definition-of-catalyst-604402>

Ising model: <https://rf.mokslasplius.lt/isng-model/>

Hubbard model: [https://en.wikipedia.org/wiki/Hubbard\\_model](https://en.wikipedia.org/wiki/Hubbard_model)