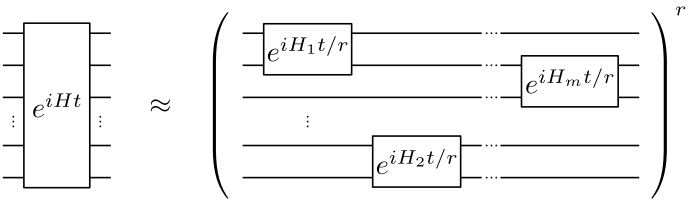
QUANTUM ALGORITHMS 2:

QUANTUM SIMULATION AND CHEMISTRY



Simon Apers
(CNRS & IRIF, Paris)

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

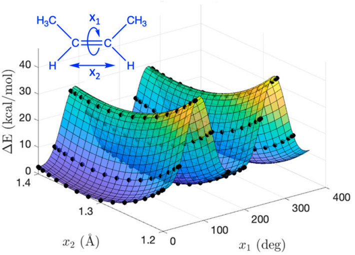
Quantum problems

"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."

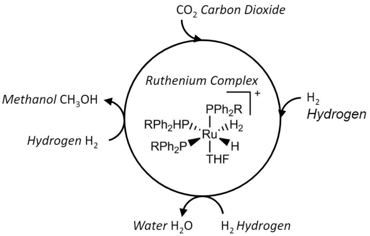
- R. Feynman, "Simulating physics with computers" (1981)

Chemistry problems:

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



potential energy surface (2-butene)



reaction chain (carbon fixation)

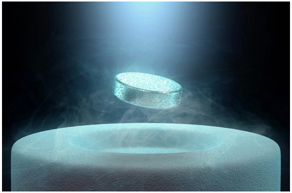
need:

ground state energy, quantum dynamics

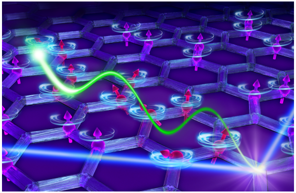
classical approaches (Hartree-Fock, DFT) often fall short

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:

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

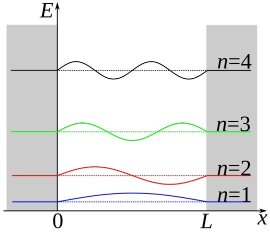
classroom example: single quantum particle

wave function

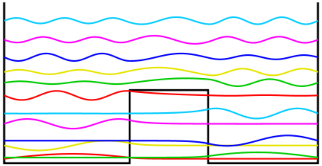
$$\psi(x),\ x \in \mathbb{R}$$

Hamiltonian

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



particle in a box



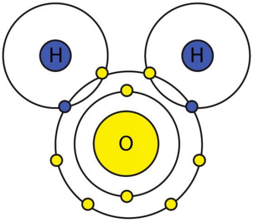
double well potential

chemistry example: molecular Hamiltonian

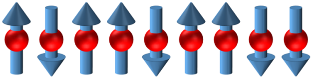
N-particle wave function $\psi(x_1, \ldots, x_N)$

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 $|z\rangle = |\uparrow\downarrow\uparrow\uparrow \ldots \downarrow\rangle = |1011\ldots 0\rangle$

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

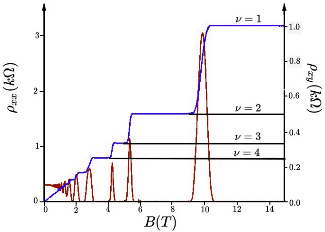
! representation on classical computer: 2^n bits
vs. representation on quantum computer: n qubits

Quantum problems (formalized)

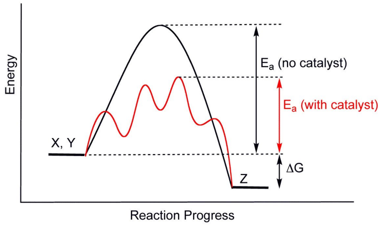
goal:
predict properties

static properties:
magnetization, conductivity, ground state energy

dynamic properties:
tunnelling probability, reaction rate



quantum Hall effect



chemical catalysis

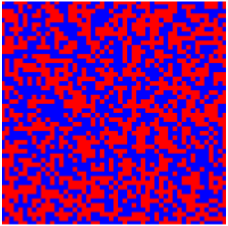
via “observables”

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

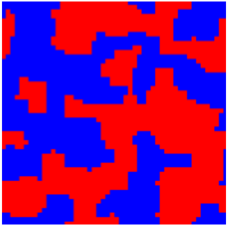
energy: $A = H$

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

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

maybe thermal or Gibbs state

(b) simulation of quantum dynamics

via (time-dependent) Schrödinger's equation

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

with solution

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

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

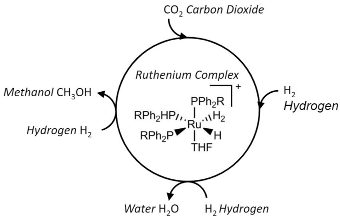
Qubit encoding

Quantum simulation

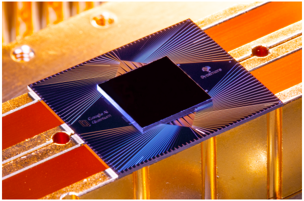
Variational quantum algorithms

Qubit encoding:

mapping physical system to qubit Hamiltonian



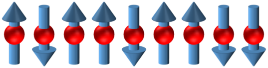
$\xrightarrow{\quad}$
?



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

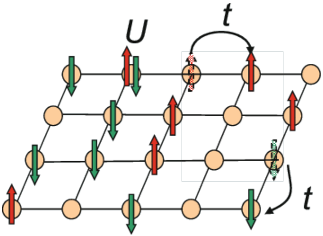


$$\leftrightarrow \quad |z\rangle = |{\uparrow\downarrow\uparrow\uparrow} \ldots \downarrow\rangle = |1011\ldots0\rangle$$

Quantum encoding 2: Fermi-Hubbard model

fermions hopping on lattice

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



Jordan-Wigner transformation maps fermions to qubits

Quantum encoding 3:

"molecular Hamiltonian"

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

$\downarrow$ (Born-Oppenheimer approximation)

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

$\downarrow$ (orbitals + second quantization)

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

$\downarrow$ (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

QUANTUM SIMULATION

VARIATIONAL QUANTUM ALGORITHMS

Quantum simulation:

or “quantum numerical methods”

input: qubit Hamiltonian

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

assumption:

H_ℓ’s are k-local

goal:

Hamiltonian simulation

$$-\boxed{e^{iHt}}-$$

by assumption: individual terms H_ℓ easy to simulate

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

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

EX: define

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

show that

$$-\boxed{X}- \equiv -\boxed{H}-\boxed{Z}-\boxed{H}-$$

and

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

unfortunately,

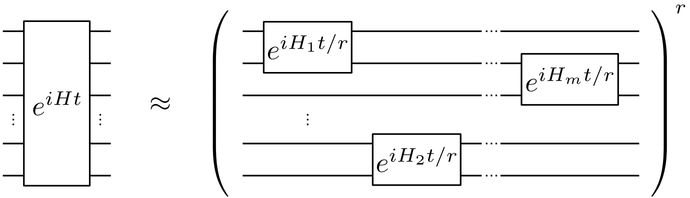
$$e^{iHt} = e^{i\left(\sum_\ell H_\ell\right)t} \neq \prod_\ell e^{iH_\ell t}$$

$$-\boxed{e^{iHt}}- \;\neq\; -\boxed{e^{iH_1 t}}- \cdots -\boxed{e^{iH_m t}}-$$

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

main technique: **Trotterization**

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

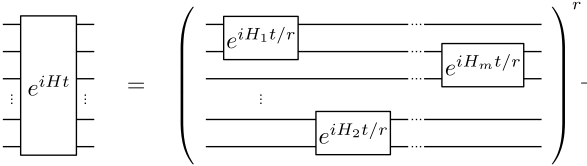


EX: Lie-Trotter formula

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

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

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



$+ O(t^2/r)$

Trotter complexity:

error is ε-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

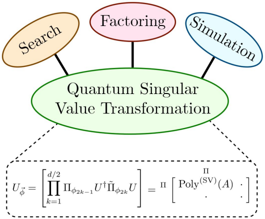
“optimal” Hamiltonian simulation in time

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

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

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VARIATIONAL QUANTUM ALGORITHMS

variational principle

ground state energy

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

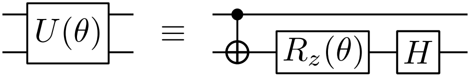
ground state

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

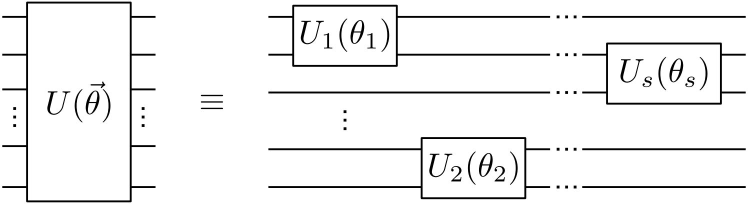
$\rightarrow$ optimization problem!

variational quantum algorithms

parameterized quantum gate (example)



parameterized quantum circuit



let

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

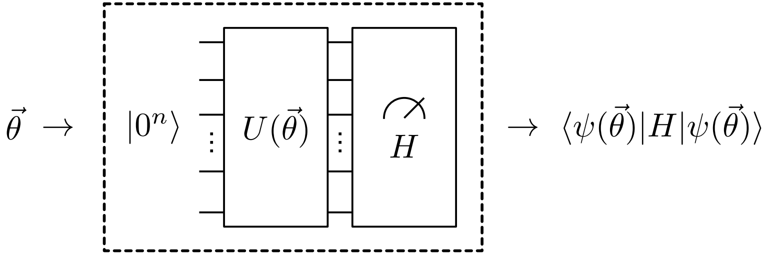
and rephrase

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

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 θ

– 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)

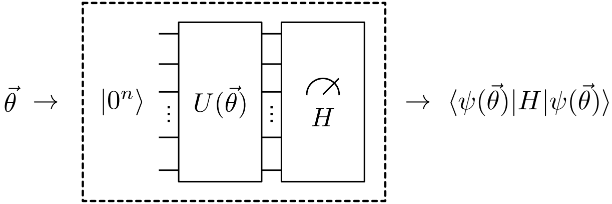
mostly heuristic art
seems to work well

energy estimation:

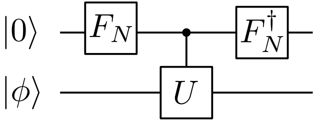
given: (encoding of) Hamiltonian H, state $|\phi\rangle$

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 θ to precision ε with $O(1/\varepsilon)$ calls to U.

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

solution 2: expanding Hamiltonian

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

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

$$\downarrow$$

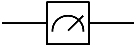
suffices to estimate $\langle\psi|H_\ell|\psi\rangle$ for all $\ell \in [m]$

$\#$ 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

$|\psi\rangle = \alpha_0\,|0\rangle + \alpha_1\,|1\rangle$ 

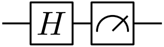
$|0\rangle$ with probability $|\alpha_0|^2$

$|1\rangle$ with probability $|\alpha_1|^2$

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

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

show that

$|\psi\rangle$ 

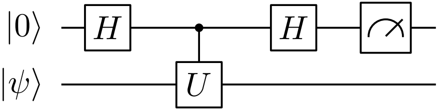
$|0\rangle$ with probability $\frac{1}{2}|\alpha_0 + \alpha_1|^2$

$|1\rangle$ with probability $\frac{1}{2}|\alpha_0 - \alpha_1|^2$

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/

H2O 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

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

Ising model: https://rf.mokslasplius.lt/ising-model/

Hubbard model: https://en.wikipedia.org/wiki/Hubbard_model