Nuclear structure (and reactions) with Quantum Computers - I

Alessandro Roggero

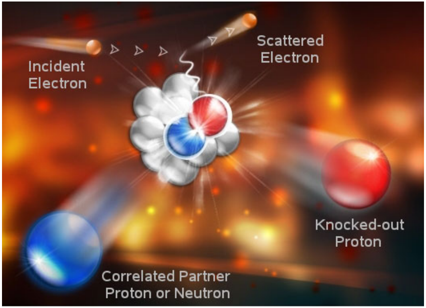


figure credit: JLAB collab.

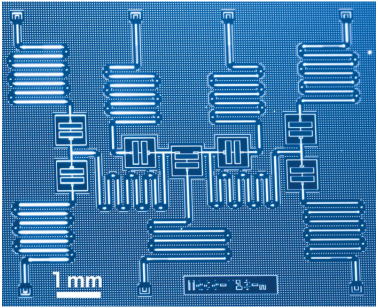
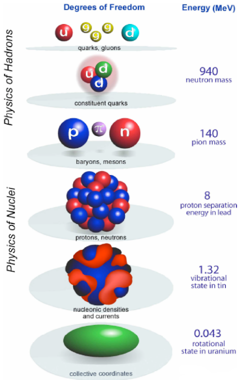


figure credit: IBM

QC and QIS for NP

JLAB – 17 March, 2020

Introduction: the nuclear many-body problem



Bertsch, Dean, Nazarewicz (2007)

$$\mathcal{L}_{QCD} = \sum_f \overline{\Psi}_f \left(i\gamma^\mu D_\mu - m_f \right) \Psi_f - \frac{1}{4} G^a_{\mu\nu} G^{\mu\nu}_a$$

- in **principle** can derive everything from here

Effective theory for nuclear systems

$$H = \sum_i \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i,j} V_{ij} + \frac{1}{6} \sum_{i,j,k} W_{ijk} + \cdots$$

- easier to deal with than the QCD lagragian
- describes correctly low energy physics
- non-perturbative $\rightarrow$ still very challenging

Two main goals:

- energy spectrum (eigenvalues)
- scattering cross sections/response to external probes (eigenvectors)

Why is this difficult?

GOAL: compute the ground state energy with error at most ϵ

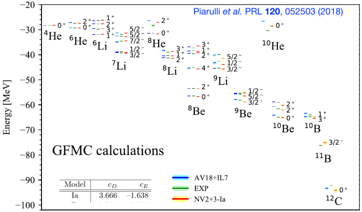
$$H = \sum_i \frac{p^2}{2m} + \frac{1}{2}\sum_{i,j} V_{ij} + \frac{1}{6}\sum_{i,j,k} W_{ijk} + \cdots$$

PROBLEM: large dimension of the Hilbert space $N = dim(\mathcal{H}) > 4^A$

Classical computational cost

- Full diagonalization: $O(N^3)$
- sparse Lanczos*: $O\left(dN\frac{\log(N)}{\sqrt{\epsilon}}\right)$
- MC no sign prob.: $O\left(\frac{\log(N)^\alpha}{\epsilon^2}\right)$
- MC with sign prob.: $O\left(\frac{N^\beta}{\epsilon^2}\right)$

*see eg. Kuczynski & Wozniakowski (1989)



Why quantum computing?

GOAL: compute the ground state energy with error at most ϵ

$$H = \sum_i \frac{p^2}{2m} + \frac{1}{2}\sum_{i,j} V_{ij} + \frac{1}{6}\sum_{i,j,k} W_{ijk} + \cdots$$

Quantum Phase Estimation (QPE)

Time evolution is cheap

- many Hamiltonians such that

$$|\Psi(t+\tau)\rangle = \exp\left(i\tau H\right)|\Psi(t)\rangle$$

  costs only $O\left(\tau \log(N)^\alpha\right)$

- QPE uses this to solve our goal in $O\left(\frac{\log(N)^\gamma}{\epsilon^\kappa}\right)$ for $1 \leq \kappa \leq 3$

IMPORTANT REMARKS:

1. many repetitions required, need stable quantum processor for only $O\left(\frac{\log(N)^\gamma}{\epsilon}\right)$ operations
2. this is not always possible*
3. if it is, dynamics is as easy/complicated as static

* see eg. Childs&Kothari(2009)

Plan for the next 4 lectures

General scheme for many-body quantum simulations

- Discretize physical problem on finite Hilbert space
- Encode discrete problem into spin problem
- Prepare an encoded low energy state
- Measure it's properties

Lecture 1

- introduction
- measurements

Lecture 2

- Quantum Phase Estimation
- simple time evolution

Lecture 3

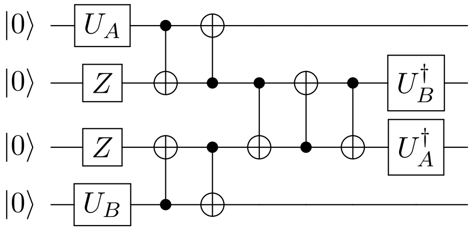
- scattering cross sections
- exclusive processes

Lecture 4

- efficient time evolution
- Qubitization

Quick recap on quantum gates

see DL lectures



single-qubit gates

$$-\boxed{R_{\hat{n}}(\theta)}- = \exp\left(i\theta\frac{\hat{n}\cdot\vec{\sigma}}{2}\right)$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = -\boxed{X}-$$

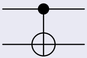
$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = -\boxed{Y}-$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = -\boxed{Z}-$$

$$S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} = -\boxed{S}-$$

two-qubit entangling gate

CNOT =



$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

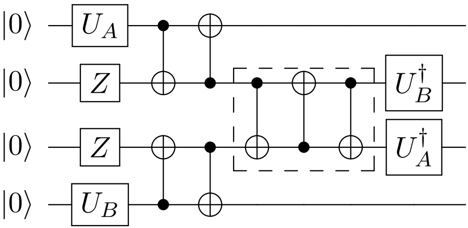
$$|\Phi_0\rangle = a\,|00\rangle + b\,|01\rangle + c\,|10\rangle + d\,|11\rangle$$

$$|\Phi_1\rangle = a\,|00\rangle + b\,|01\rangle + c\,|11\rangle + d\,|10\rangle$$

EXERCISE: show that $\forall U_A, U_B$ the output of the circuit above is $|0000\rangle$

Quick recap on quantum gates

see DL lectures



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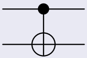
CNOT =  = $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$

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Quick recap on quantum gates II

see DL lectures

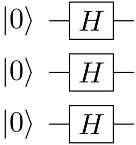
Hadamard Gate

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$$

- rotates between Z and X basis

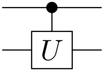
$$\left.\begin{aligned}H|0\rangle &= |+\rangle\\ H|1\rangle &= |-\rangle\end{aligned}\right\} \qquad X|\pm\rangle = \pm|\pm\rangle$$

- generates uniform superposition



$$H^{\otimes 3}|0\rangle = \frac{1}{\sqrt{2^3}}\sum_{k=0}^{2^3-1}|k\rangle$$

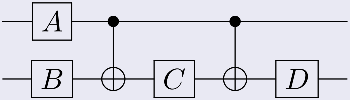
Generic controlled unitary



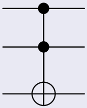
$$= \begin{pmatrix}\mathbb{1} & 0\\ 0 & U\end{pmatrix}$$

Single qubit U

Barenco et al. (1995)



Controlled CNOT: Toffoli



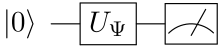
= [6 CNOT + 9 single qubit]∗

* see eg. Nielsen & Chuang

Measuring an observable: single qubit case

Computational basis is eigenbasis of Z so that, if $|\Psi\rangle = U_\Psi |0\rangle$, we have

$$\langle\Psi|Z|\Psi\rangle = |\langle 0|\Psi\rangle|^2 - |\langle 1|\Psi\rangle|^2 \equiv$$



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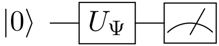

We now need to repeat calculation M times to estimate the probabilities

$$P(0) = |\langle 0|\Psi\rangle|^2 \sim \frac{\sum_k \delta_{s_k,0}}{M} \qquad Var\left[P(0)\right] \sim \frac{v_0}{M} \longrightarrow 0\ .$$

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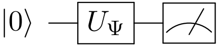

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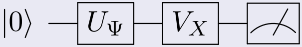
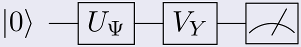
Other expectation values accessible by basis transformation

$X = V_X Z V_X^\dagger$



$Y = V_Y Z V_Y^\dagger$



- for X we can use $X = V_X Z V_X^\dagger$ where V_X is the Hadamard

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

- for Y we can use $Y = SXS^\dagger$ so that $V_Y = SV_X = SH$

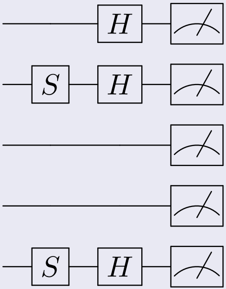
Measuring an observable: the Pauli group

Given a state $|\Psi\rangle$ defined over n qubits and an encoded operator

$$O = \sum_{k=1}^{N_K} c_k P_k \quad P_k \in \{(\mathbb{1}, X, Y, Z)^{\otimes n}\}$$

we want to measure the expectation value $\langle\Psi|O|\Psi\rangle$ [McClean et al. (2014)].

Example: $X_0 Y_1 Z_2 Z_3 Y_4$



- $\forall k$ perform M experiments to get $\langle P_k\rangle$ with

$$Var[P_k] \sim \frac{\langle P_k^2\rangle - \langle P_k\rangle^2}{M} = \frac{1-\langle P_k\rangle^2}{M}$$

- we can now evaluate $\langle O\rangle$ with variance

$$Var[O] = \sum_{k=1}^{N_K} |c_k|^2 Var[P_k]$$

$\Rightarrow$ total error $\propto \sqrt{N_K/M}$.

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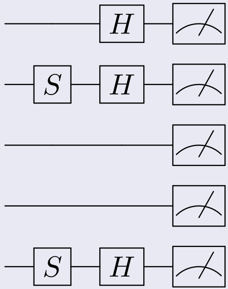
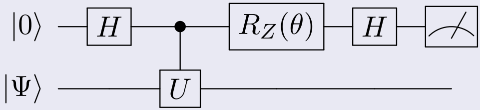


- naive estimator has total error $\propto \sqrt{N_K/M}$
- we can measure multiple terms together!

$$X_0 Y_1 Z_2 Z_3 Y_4 \begin{cases} X_0 Y_1 \mathbb{1}_2 Z_3 Y_4 \\ X_0 Y_1 \mathbb{1}_2 \mathbb{1}_3 Y_4 \\ \dots \\ \mathbb{1}_0 Y_1 \mathbb{1}_2 \mathbb{1}_3 \mathbb{1}_4 \\ X_0 X_1 Z_2 Z_3 X_4 \\ \dots \end{cases} \Rightarrow \epsilon_{tot} \propto \sqrt{\frac{N_G}{M}}$$

refs: 1907.03358,1907.07859,1907.09040,1907.13117,1908.06942,...

Measuring an observable: Hadamard test



Kitaev (1995)

When $\theta = 0$ we have:

1. $|\Phi_0\rangle = |0\rangle \otimes |\Psi\rangle$
2. $|\Phi_1\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes |\Psi\rangle$
3. $|\Phi_2\rangle = \frac{|0\rangle \otimes |\Psi\rangle}{\sqrt{2}} + \frac{|1\rangle \otimes U|\Psi\rangle}{\sqrt{2}}$
4. $|\Phi_3\rangle = \frac{|0\rangle \otimes (\mathbb{1}+U)|\Psi\rangle}{2} + \frac{|1\rangle \otimes (\mathbb{1}-U)|\Psi\rangle}{2}$

Result of ancilla measurement

$$\langle Z\rangle_a = \frac{\langle\Psi|\left(U + U^\dagger\right)|\Psi\rangle}{2} = \mathcal{R}\langle\Psi|U|\Psi\rangle$$

EXERCISE: find the proper angle θ needed to measure the imaginary part

EXAMPLE 1: the SWAP test

- State Tomography: reconstruction of state $|\Psi\rangle$ costs $O(N)$ samples
- State Overlap: we can compute $|\langle\Psi|\Phi\rangle|^2$ using only $O(\log(N))$ gates

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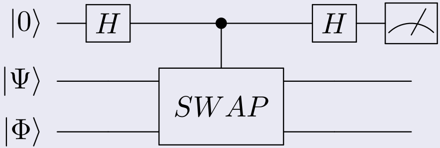
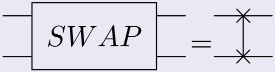


Buhrman, Cleve, Watrous & de Wolf (2001)

$$\Rightarrow \langle Z\rangle_a = |\langle\Psi|\Phi\rangle|^2$$

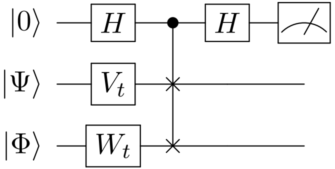
The SWAP gate

SWAP $|\Psi\rangle \otimes |\Phi\rangle = |\Phi\rangle \otimes |\Psi\rangle$



2 qubits $\Rightarrow \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$

Why should we care?

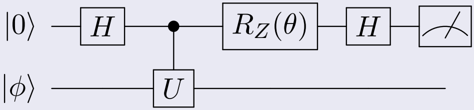


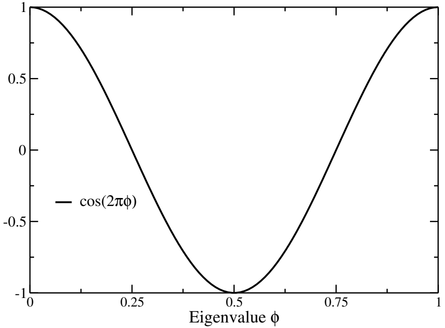
$$\Rightarrow M(\Psi \leftrightarrow \Phi) = \left|\langle\Psi|V_t^\dagger W_t|\Phi\rangle\right|^2$$

Efficient transition matrix element!

EXAMPLE 2: eigenvalue estimation

Take a unitary U and an eigenvector $|\phi\rangle$ so that: $U|\phi\rangle = e^{i2\pi\phi}|\phi\rangle$





- for $\theta = 0$: $\langle Z \rangle_a = cos(2\pi\phi)$

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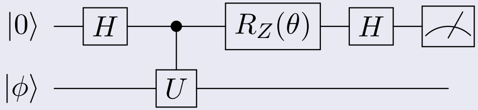

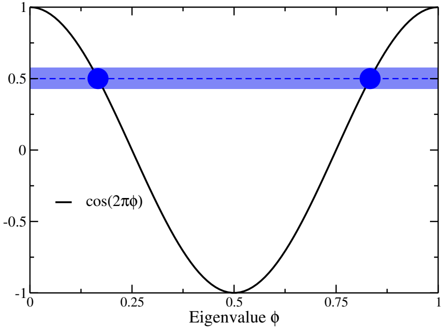

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- error δ with $M \propto 1/\delta^2$ samples:

$$Var[Z_a] \sim \frac{1}{M}$$

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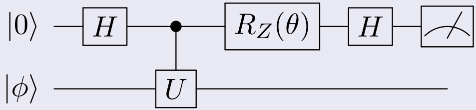

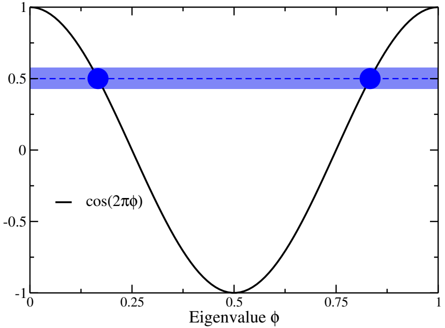

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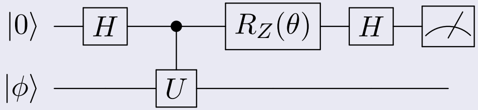

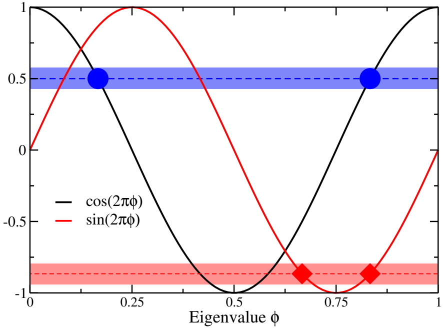

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- for $\theta = \theta_{ex}$: $\langle Z\rangle_a = sin(2\pi\phi)$

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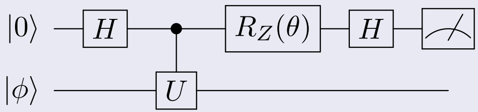

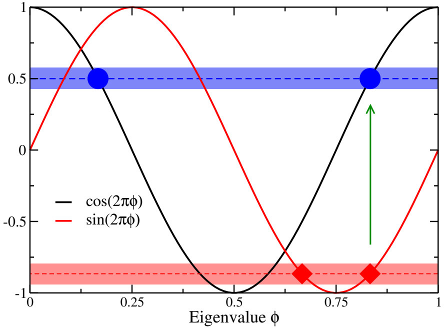

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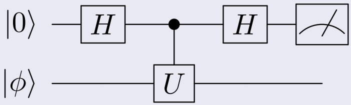
EXAMPLE 3: Can we apply a non-unitary operation?

YES, but only with some probability

- this can be useful for example if the transition matrix element we considered before is genereated by a non unitary operator



$$\Rightarrow \quad |0\rangle \otimes \frac{\mathbb{1}+U}{2}|\phi\rangle + |1\rangle \otimes \frac{\mathbb{1}-U}{2}|\phi\rangle$$

- we will measure $|0\rangle$ with $P_0 = \frac{1}{2}\left(1 + \mathcal{R}\langle\phi|U|\phi\rangle\right) \Rightarrow |\phi_0\rangle = \frac{\mathbb{1}+U}{2\sqrt{P_0}}|\phi\rangle$

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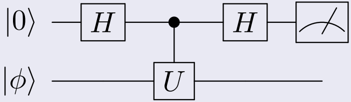

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- we will measure $|0\rangle$ with $P_0 = \frac{1}{2}\left(1 + \mathcal{R}\langle\phi|U|\phi\rangle\right) \Rightarrow |\phi_0\rangle = \frac{\mathbb{1}+U}{2\sqrt{P_0}}|\phi\rangle$

Concrete example: projection operators

If we take U to be the reflection around $|\psi\rangle$, like $U = (2|\psi\rangle\langle\psi| - \mathbb{1})$, we find

$$P_0 = |\langle\phi|\psi\rangle|^2 \quad \Rightarrow \quad |\phi_0\rangle = \frac{|\psi\rangle\langle\psi|}{\sqrt{P_0}}|\phi\rangle = |\psi\rangle$$