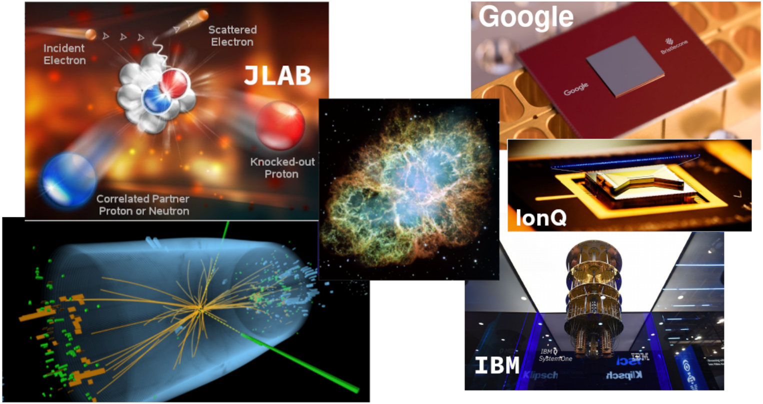
Quantum Simulation for Nuclear and Neutrino Physics

Alessandro Roggero



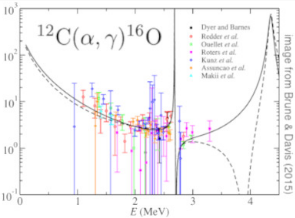
MPA Summer School

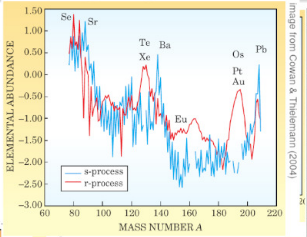
Chiemsee – 10-15 Sep, 2023

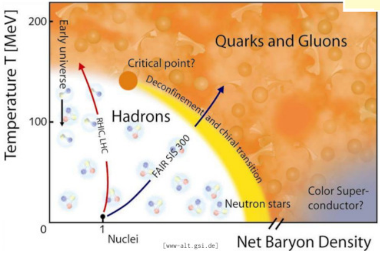
Trento Institute for
Fundamental Physics
and Applications

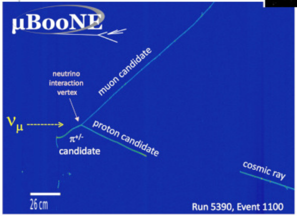
Plan for these lectures

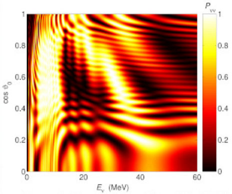
Quantum Simulation for Nuclear Physics	Quantum Simulation for Neutrino Physics





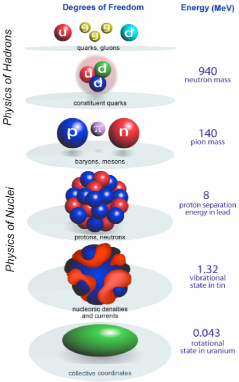






Duan, Fuller, Carlson, Qian PRL(2006)

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

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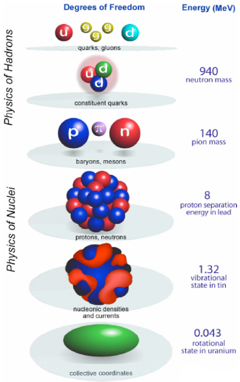

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Two main goals:

- 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

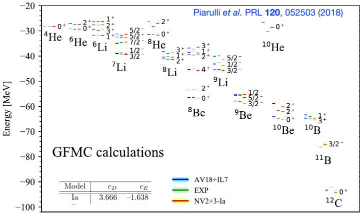
$$H = \sum_i \frac{p^2}{2m} + \frac{1}{2}\sum_{i,j} V_{ij} + \frac{1}{6}\sum_{i,j,k} W_{ijk} + \cdots$$

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)



What is a Quantum Computer?

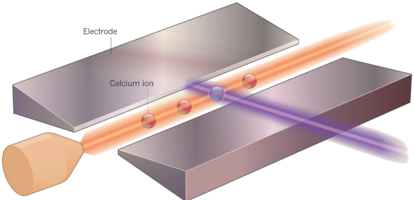


figure from E.Zohar

A Quantum Computer is a controllable quantum many-body system that allows to enact unitary transformations on an initial state ρ_0

$$\rho_0 \rightarrow U\rho_0 U^\dagger$$

n degrees of freedom so $\rho \in \mathcal{H}^{\otimes n}$

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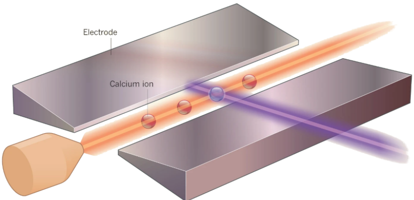

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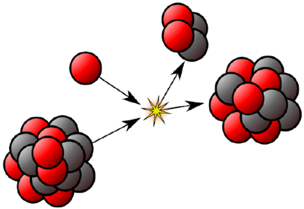
In a Quantum Simulation we want to use this freedom to describe the time-evolution of a closed system

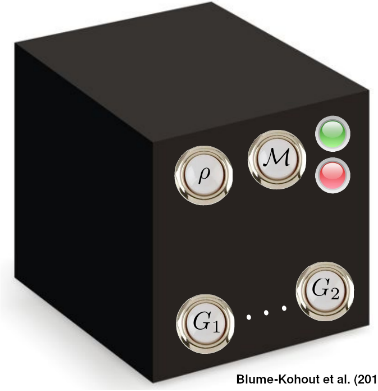
$$\rho(t) \rightarrow U(t)\rho_0 U(t)^\dagger$$

described by some Hamiltonian

$$U(t) = \exp\left(itH\right) \; .$$



Black box model for a quantum computer

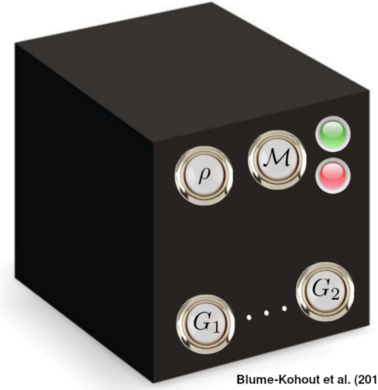


Blume-Kohout et al. (2013)

Box contains n qubits (2-level sys.) together with a set of buttons

- initial state preparation ρ
- projective measurement $\mathcal{M}$
- quantum operations G_k

Black box model for a quantum computer



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We can build a **universal** black box with only a **finite number** of buttons

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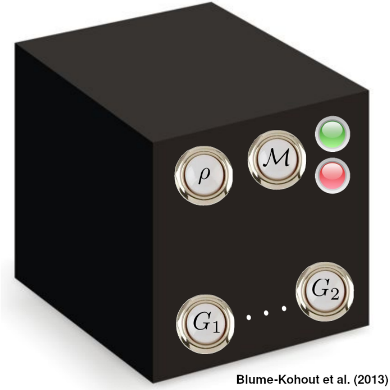

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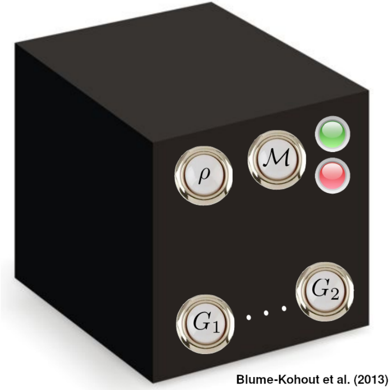

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$$|\Psi(0)\rangle \rightarrow |\Psi(t)\rangle = e^{-iHt}|\Psi(0)\rangle$$

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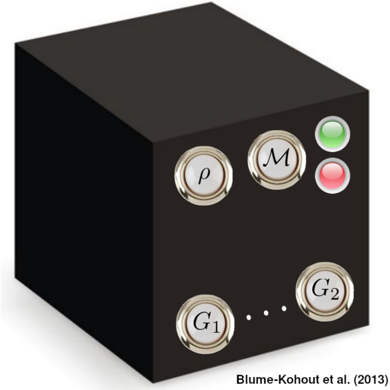

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2. map physical states to bb states

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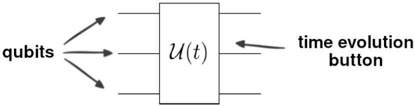

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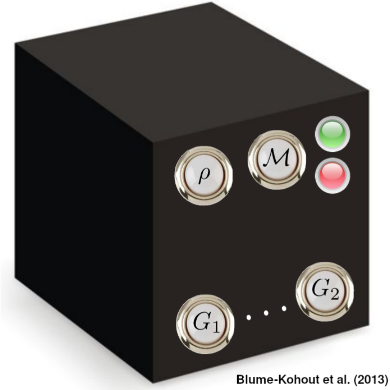

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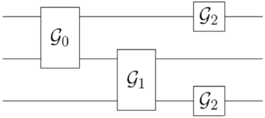
1. discretize the physical problem
2. map physical states to bb states
3. push correct button sequence

$$|\Psi(0)\rangle \rightarrow |\Psi(t)\rangle = e^{-iHt}|\Psi(0)\rangle$$



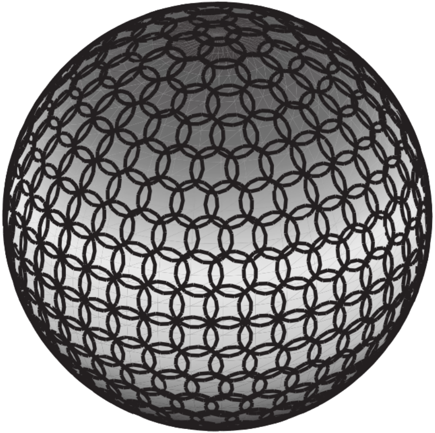
Can we always do this?

image from Nielsen&Chuang

Any unitary operation can be thought as the time evolution operator for some (Hermitian) Hamiltonian

$$U \quad \leftrightarrow \quad e^{iH}$$

A simple counting argument shows that for a fixed choice of universal buttons (quantum gates) there are unitary operations on n qubits which will require $O(2^n)$ operations



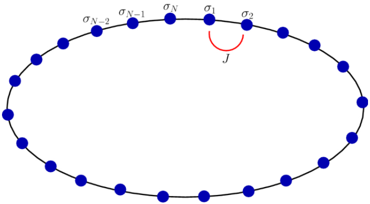
We can find Hamiltonians whose time evolution cannot be simulated **efficiently**

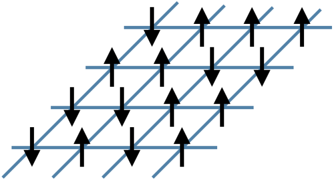
Efficient Hamiltonian Simulation

Hamiltonians encountered in physics have usually structure, like locality

$$H_{Ising}^{1D} = J \sum_{i=1}^{N} Z_i Z_{i+1} + h \sum_{i=1}^{N} X_i$$

$$H_{Heis}^{1D} = J \sum_{i=1}^{N} \vec{\sigma}_i \cdot \vec{\sigma}_{i+1}$$





$$H_{Ising}^{2D} = J \sum_{\langle i,j \rangle} Z_i Z_j + h \sum_{i} X_i$$

$$H_{Heis}^{2D} = J \sum_{\langle i,j \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j$$

All these situations are examples of 2-local spin Hamiltonians

Qubit mapping for nuclear Hamiltonians

PROBLEM: Nuclear Physics is not a spin model! What about fermions?

$$\hat{H} = \sum_i \frac{\hat{p}_i^2}{2m} + \frac{1}{2}\sum_{i,j} \hat{V}_{ij} + \frac{1}{6}\sum_{i,j,k} \hat{W}_{ijk} + \cdots$$

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- first discretize the problem by describing it using a set of M orbitals and build many-body states in occupation number basis (Fock space)

$$\hat{H} = \sum_{ij} K_{ij}\hat{a}_i^\dagger \hat{a}_j + \sum_{ijkl} V_{ijkl}\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l + \sum_{ijklmn} W_{ijklmn}\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k^\dagger \hat{a}_l \hat{a}_m \hat{a}_n + \cdots$$

with $\{\hat{a}_i, \hat{a}_j^\dagger\} = \delta_{ij}$ and $\{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = \{\hat{a}_i, \hat{a}_j\} = 0.$

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- the Hilbert space has dimension 2^M and could be fitted into M qubits
- need a correct map for the creation/annihilation operators there

Fermion to spin mapping: Jordan Wigner transformation

The fermionic Fock space with M modes can be mapped into the Hilbert space of M spins using the following identification

$$\left.\begin{aligned} a_k &= \left(\prod_{j=0}^{k-1} -Z_j\right)\frac{X_k+iY_k}{2} \\ a_k^\dagger &= \left(\prod_{j=0}^{k-1} -Z_j\right)\frac{X_k-iY_k}{2} \end{aligned}\right\} \quad \Rightarrow \quad \{a_j, a_k^\dagger\} = \delta_{j,k}$$

- occupation encoded into value of spin projection, $\sigma_k^\pm = \frac{X_k \pm iY_k}{2}$

$$|vac\rangle = |\uparrow\uparrow\uparrow\uparrow\rangle \quad a_2^\dagger |vac\rangle = |\uparrow\uparrow\downarrow\uparrow\rangle \quad a_2^\dagger |\uparrow\uparrow\downarrow\uparrow\rangle = 0$$

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- fermionic phase encoded into the string of Pauli Z operators

$$\begin{aligned} a_2^\dagger a_1^\dagger|vac\rangle &= \left(Z_0 Z_1 \sigma_2^-\right)\left(-Z_0\sigma_1^-\right)|vac\rangle \\ &= -\sigma_2^- Z_1 \sigma_1^-\,|vac\rangle \\ &= \sigma_2^-\sigma_1^- Z_1\,|vac\rangle = \sigma_1^- Z_1 \sigma_2^-\,|vac\rangle = -a_1^\dagger a_2^\dagger|vac\rangle \end{aligned}$$

since $\{\sigma_k^\pm, Z_k\} = 0$ and operators commute when acting on $i \neq k$.

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- works great for 1D local models, otherwise many Z terms

$$a_8^\dagger a_1 = -\sigma_8^- Z_7 Z_6 Z_5 Z_4 Z_3 Z_2 Z_1 \sigma_1^+$$

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Many other mappings available

- Bravy-Kitaev
- auxiliary fermions
- BK-Superfast
- LDPC codes

Bravyi & Kitaev (2000) , Verstraete & Cirac (2005), Havlicek et al. (2017), Steudtner & Wehner (2017)

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
- Manipulate state, e.g. evolve under unitary time evolution
- Measure properties of final state

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- Discretize physical problem on finite Hilbert space
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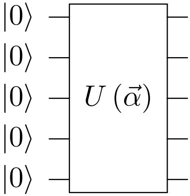
- Manipulate state, e.g. evolve under unitary time evolution
- Measure properties of final state

- many options for preparing low energy states with a given encoding

Variational State Preparation

Exploit variational principle for the energy to find some reasonable parametrization for the ground-state

$$E(\vec{\alpha}) = \langle \Psi(\vec{\alpha}) | H | \Psi(\vec{\alpha}) \rangle \geq E_0$$



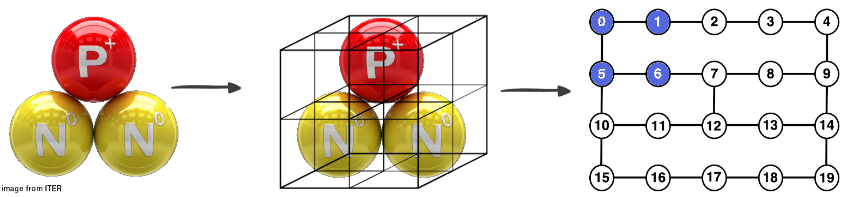
see e.g. J.McClean, J. Romero, et.al. (2016), M. Cerezo, A. Arrasmith, R. Babbush, et al. (2021)

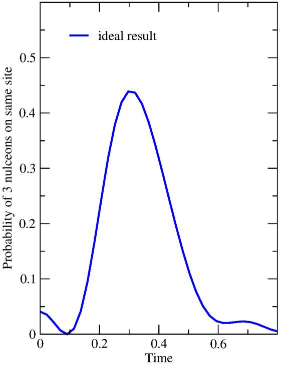
First programmable quantum devices are here

some figures from M.Savage

Real time dynamics on current generation devices

AR, Li, Carlson, Gupta, Perdue PRD(2020)





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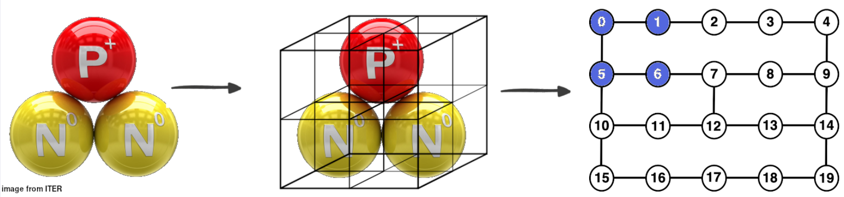
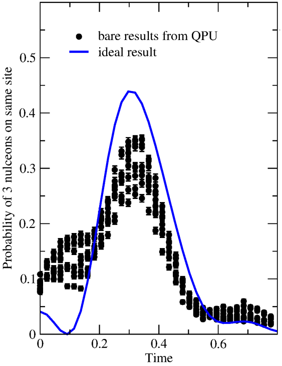
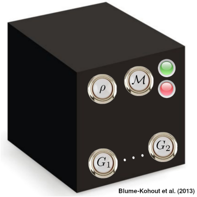




Error sources

- decoherence (environment)
- imperfect calibration



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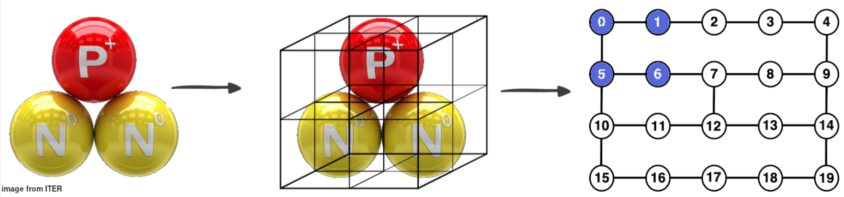
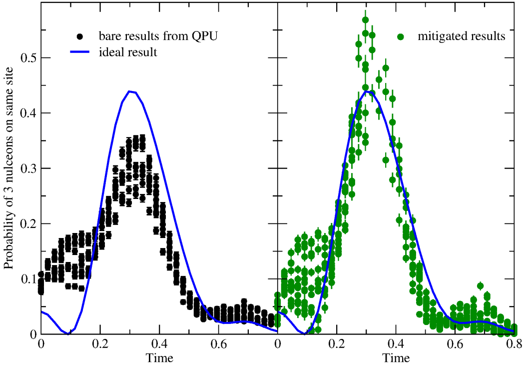
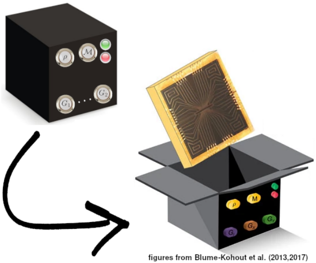




- Error mitigation is crucial



figures from Blume-Kohout et al. (2013,2017)

Quick introduction to quantum gates

single-qubit gates

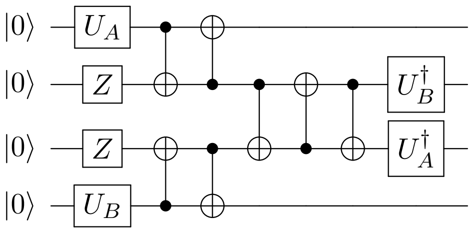
$$-\boxed{R_{\hat{n}}(\theta)}- = \exp\left(i\theta\frac{\hat{n}\cdot\vec{\sigma}}{2}\right)$$

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

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

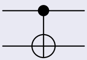
$$\sigma_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = -\boxed{Z}-$$

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



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 introduction to quantum gates

single-qubit gates

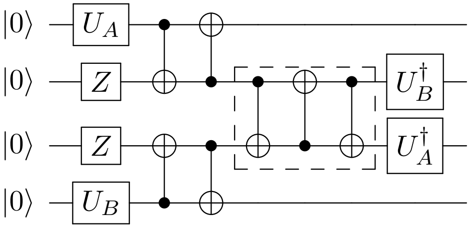
$$\boxed{R_{\hat{n}}(\theta)} = \exp\left(i\theta\frac{\hat{n}\cdot\vec{\sigma}}{2}\right)$$

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

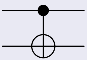
$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \boxed{Y}$$

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

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



two-qubit entangling gate

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

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

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Quick introduction to quantum gates II

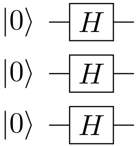
Hadamard Gate

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

- rotates between Z and X basis

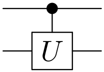
$$\left.\begin{aligned} H|0\rangle &= |+\rangle \\ H|1\rangle &= |-\rangle \end{aligned}\right\} \qquad X|\pm\rangle = \pm|\pm\rangle$$

- generates uniform superposition



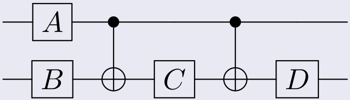
$$H^{\otimes 3}|0\rangle = \frac{1}{\sqrt{2^3}}\sum_{k=0}^{2^3-1}|k\rangle$$

Generic controlled unitary

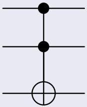


$$= \begin{pmatrix}\mathbb{1} & 0\\ 0 & U\end{pmatrix}$$

Single qubit U — Barenco et al. (1995)



Controlled CNOT: Toffoli

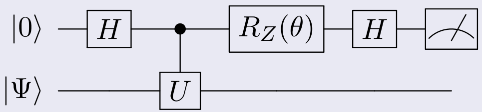


$= [$6 CNOT + 9 single qubit$]*$

* see eg. Nielsen & Chuang

Measuring an observable: 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. $|\Phi_3\rangle = \frac{|0\rangle\otimes(\mathbb{1}+U)|\Psi\rangle}{2} + \frac{|1\rangle\otimes(\mathbb{1}-U)|\Psi\rangle}{2}$

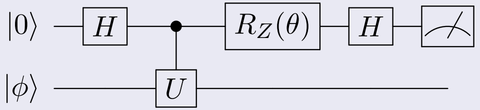
Result of ancilla measurement

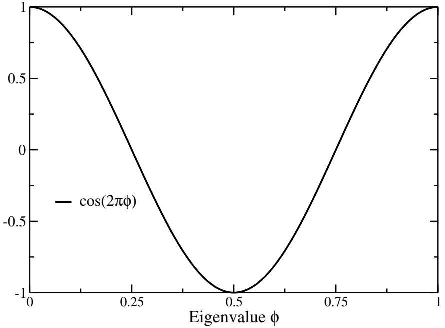
$$\langle Z\rangle_a = \frac{\langle\Psi|\left(U + U^\dagger\right)|\Psi\rangle}{2} = \mathcal{R}\langle\Psi|U|\Psi\rangle$$

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

EXAMPLE: 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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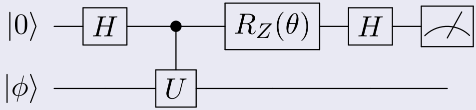

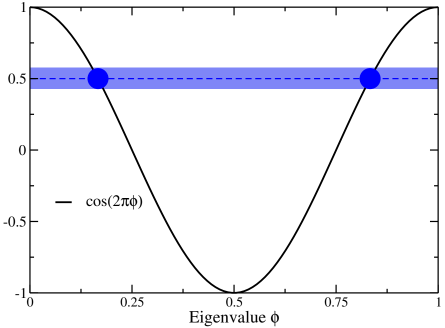

- for $\theta = 0$: $\langle Z \rangle_a = cos(2\pi\phi)$
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$$Var[Z_a] \sim \frac{1}{M}$$

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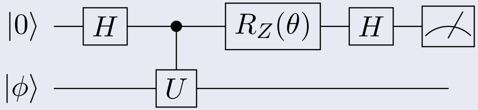

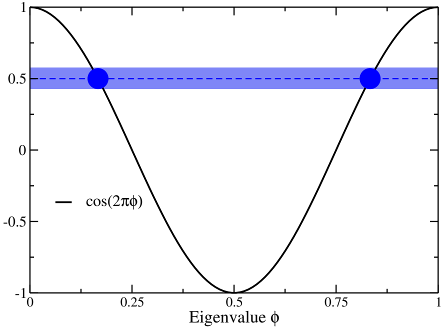

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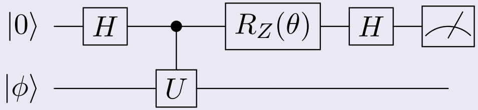

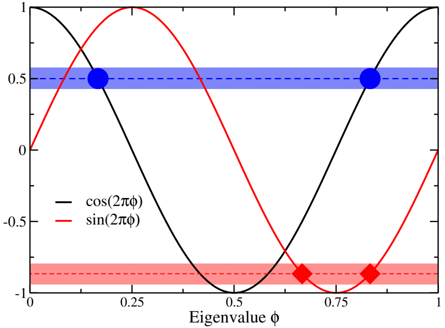

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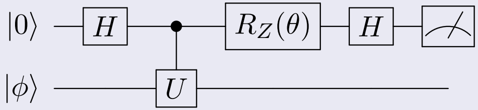

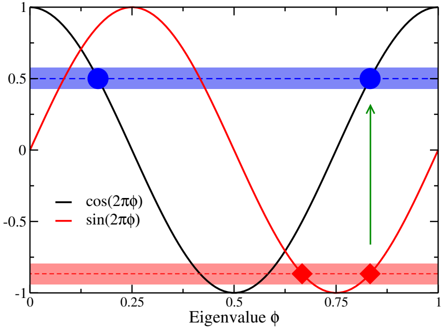

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Quantum phase estimation in one slide

GOAL: compute eigenvalue ϕ with error δ using exact eigenvector $|\phi\rangle$

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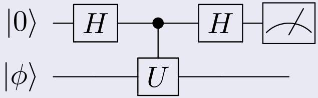

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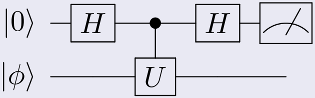
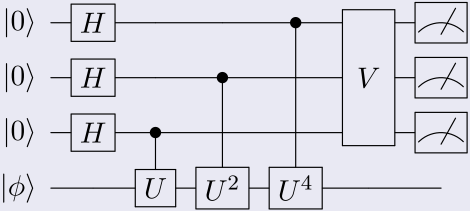


- Quantum Phase Estimation (QPE) uses $O(1/\delta)$ controlled-U operations, $O(\log(1/\delta))$ ancilla qubits and only $O(1)$ experiments



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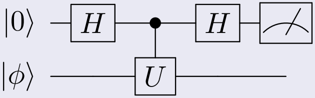

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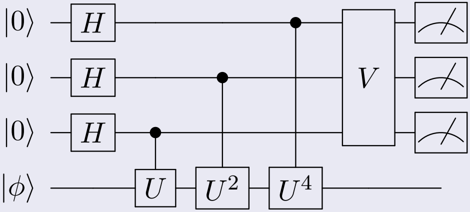
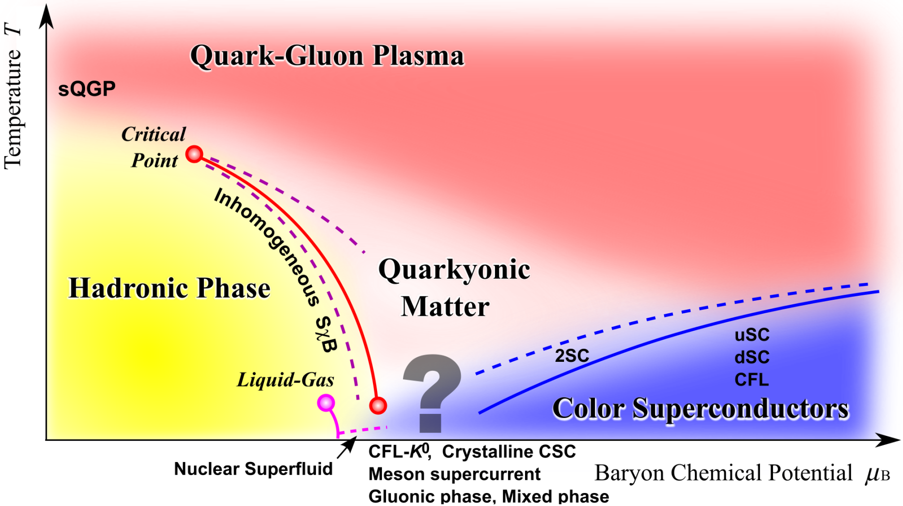


BONUS: works even if $|\phi\rangle \to \alpha|\phi\rangle + \beta|\xi\rangle$ with $O(1/\alpha^2)$ experiments

The QCD phase diagram

figure from Fukushima & Hatsuda (2011)



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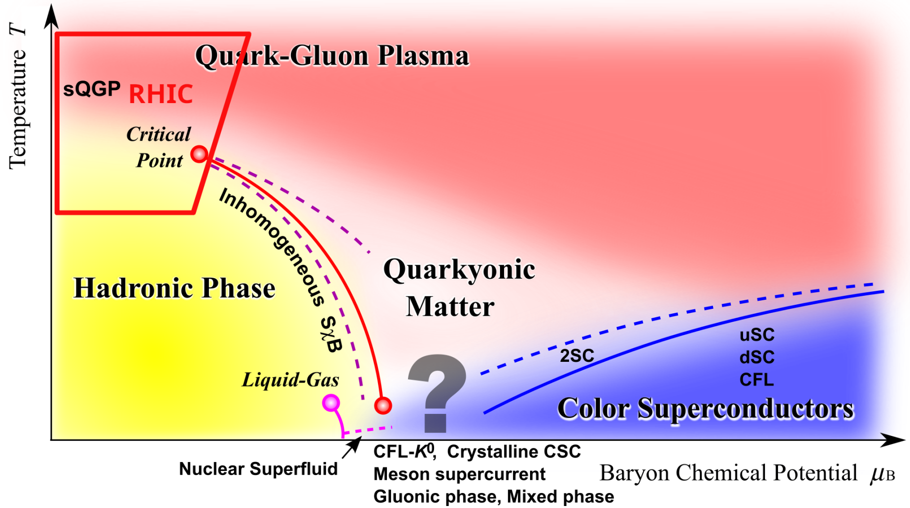

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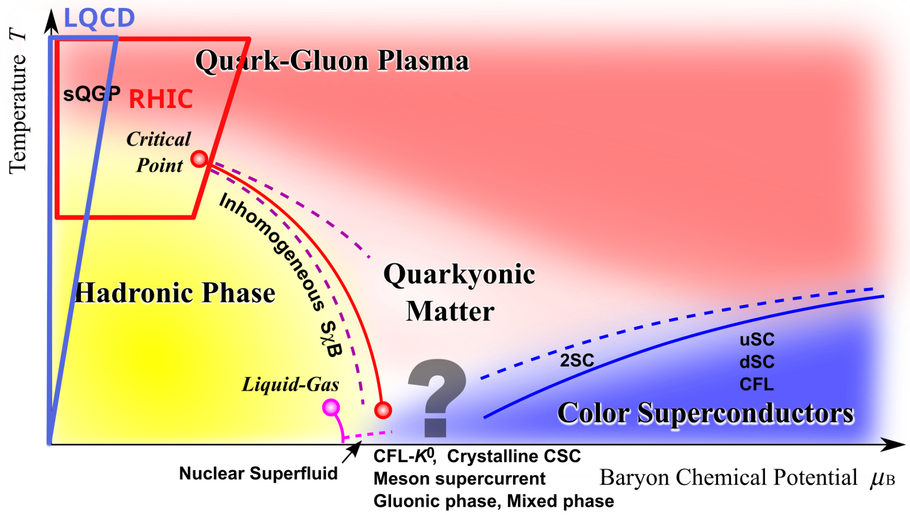

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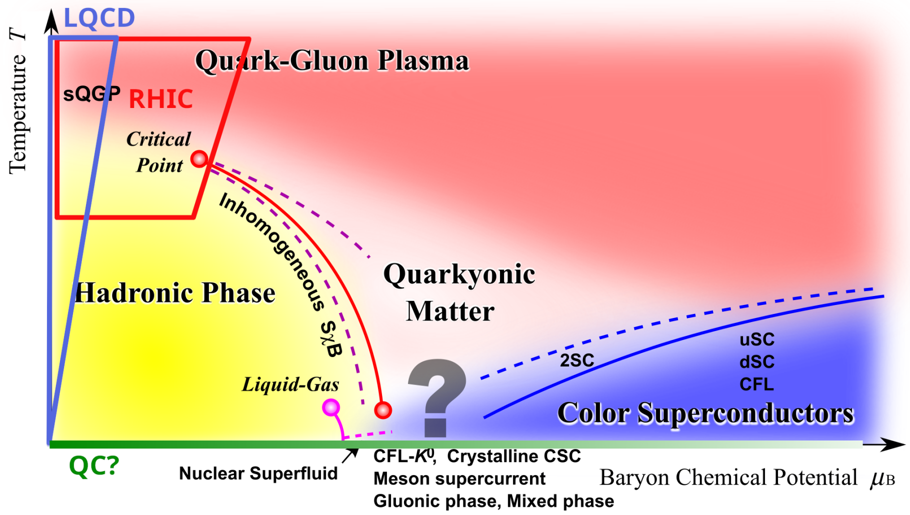
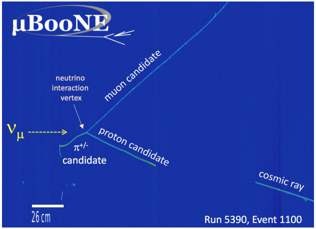


Exclusive cross sections in neutrino oscillation experiments



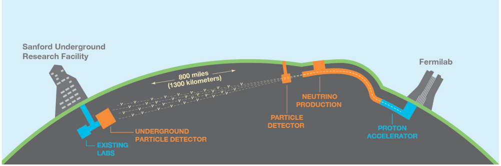
Goals for ν oscillation exp.

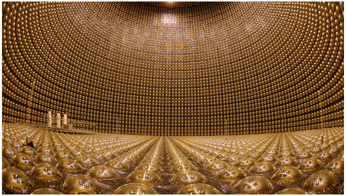
- neutrino masses
- accurate mixing angles
- CP violating phase

$$P(\nu_\alpha \rightarrow \nu_\alpha) = 1 - sin^2(2\theta)sin^2\left(\frac{\Delta m^2 L}{4E_\nu}\right)$$

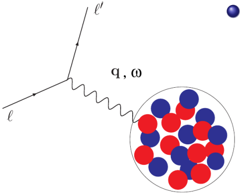
- need to use measured reaction products to constrain E_ν of the event

DUNE, MiniBooNE, T2K, Minerνa, NOνA,. . .





Inclusive cross section and the response function

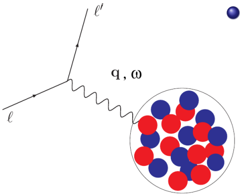


- xsection completely determined by response function

$$R_O(\omega) = \sum_f \left| \langle f | \hat{O} | \Psi_0 \rangle \right|^2 \delta\left(\omega - E_f + E_0\right)$$

  - excitation operator $\hat{O}$ specifies the vertex

Inclusive cross section and the response function



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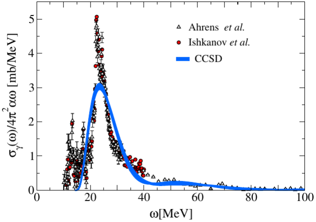
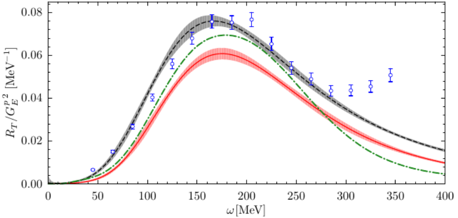
Extremely challenging classically for strongly correlated quantum systems

- dipole response of ^{16}O



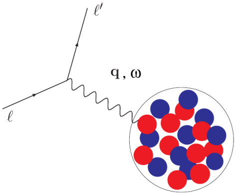
Bacca et al. (2013) LIT+CC

- quasi-elastic EM response of ^{12}C



Lovato et al. (2016) GFMC

Towards exclusive scattering using quantum computing

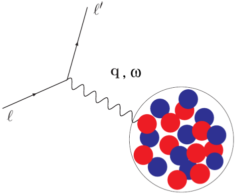


- response $R(\omega) \Leftrightarrow$ probability for events at fixed ω
- exclusive x-sec $\rightarrow$ events with specific final states

IDEA: prepare the following state on QC

$$|\Phi\rangle = \sum_\omega \sqrt{R(\omega)}\, |\omega\rangle \otimes |\psi_\omega\rangle$$

Towards exclusive scattering using quantum computing



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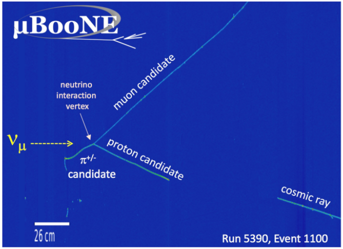
$$|\Phi\rangle = \sum_\omega \sqrt{R(\omega)}\,|\omega\rangle \otimes |\psi_\omega\rangle$$

- measurement of first register returns ω with probability $R(\omega)$
- after measurement, the second register contains final states at ω!

Blume-Kohout et al. (2013)



AR & Carlson PRC(2019)

Prospects of impact of QC on Nuclear Physics

AR, Li, Carlson, Gupta, Perdue PRD(2020)

Cost estimates for realistic response in medium mass nuclei

We need ≈ 4000 qubits and push the gate buttons $\approx 10^6 - 10^8$ times

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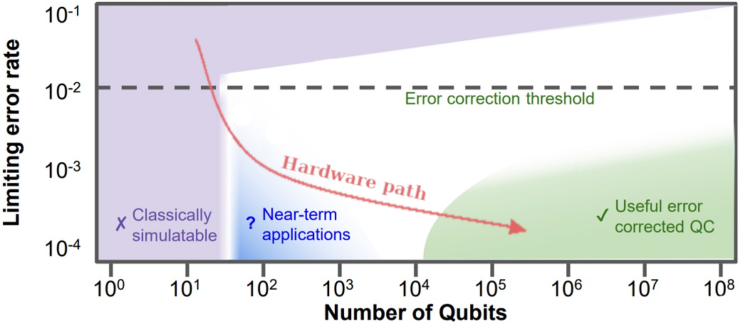

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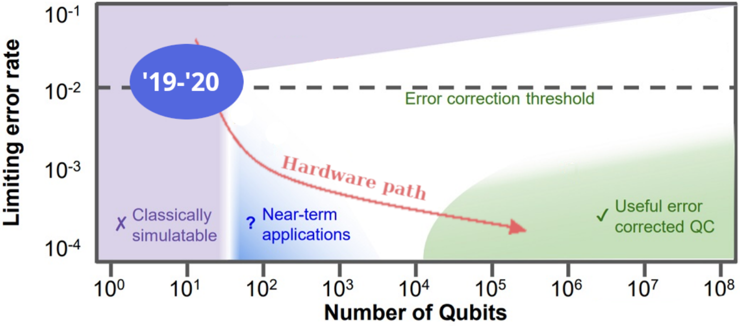

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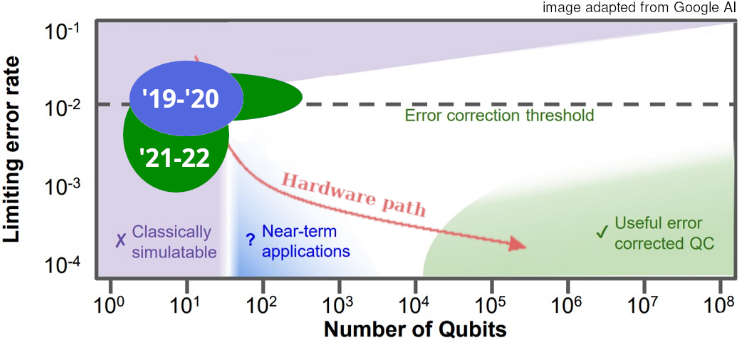

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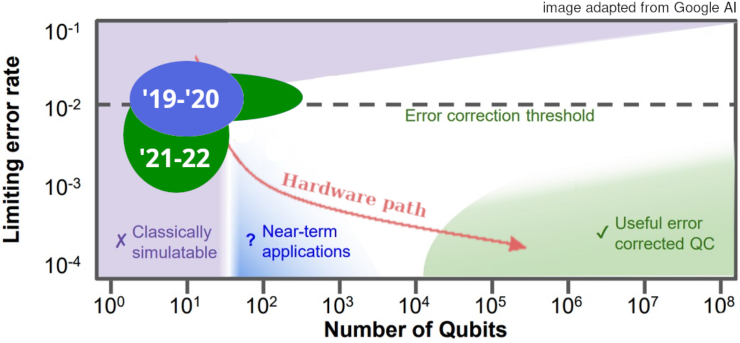


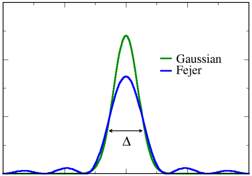
- Still possible to optimize further (other encodings need ≈ 500 qubits)
- Insights for classical methods could come before we have a large QC!

Nuclear dynamics with quantum (inspired) computing?

We can prepare the following state

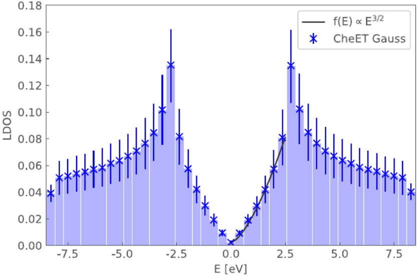
$$|\Phi_\Delta\rangle = \sum_\omega \sqrt{R_\Delta(\omega)}\,|\omega\rangle \otimes |\psi_\omega\rangle$$

with R_Δ is an integral transform of the response with energy resolution Δ

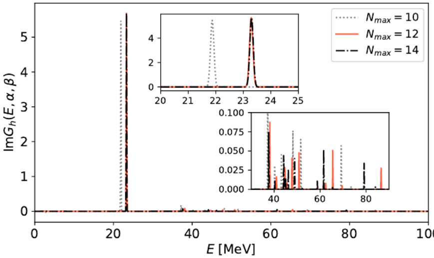


AR & Carlson PRC(2019), **AR** PRA(2020)

- Gaussian approach uses the fact that Chebyshev polynomials can be evaluated efficiently on quantum computers (Berry, Childs, Low, Chuang, . . .)



Sobczyk, **AR** PRE(2022)



Sobczyk, Bacca, Hagen, Papenbrock (2022)

Summary & Conclusions

- Advances in theory and computing are opening the way to ab-initio calculation of equilibrium properties in the medium-mass region
- New ideas are needed to study nuclear dynamics in large open-shell nuclei, out-of-equilibrium processes and QCD at finite μ
- Quantum Computing has the potential to bridge this gap and increasingly better experimental test-beds are being built
- Error mitigation techniques will be critical to make the best use of these noisy near-term devices
- Early impact of QC on nuclear physics might come as insights into classical many-body methods and the role of entanglement

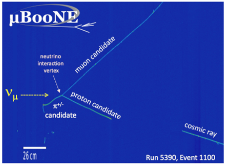


image from Brune & Davis (2015)

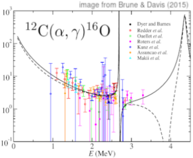
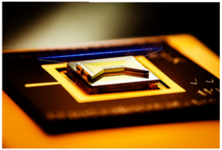
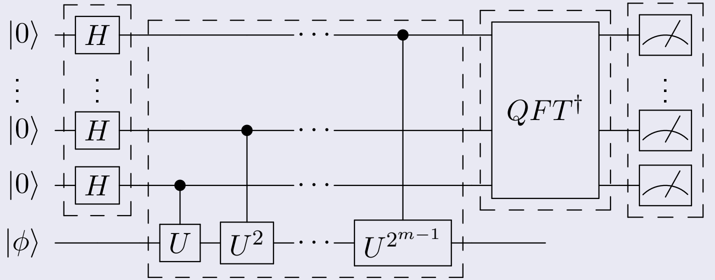


image from Chandra collab.



Filling in the details for QPE

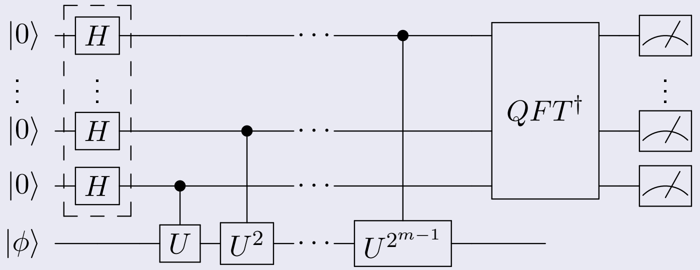
Abrams & Lloyd (1999)



The QPE algorithm has 4 main stages

1. prepare m ancilla in uniform superposition of basis states
2. apply controlled phases using U^k with $k = 2^0, 2^1, \ldots, 2^{m-1}$
3. perform (inverse) Fourier transorm on ancilla register
4. measure the ancilla register

Filling in the details: state preparation

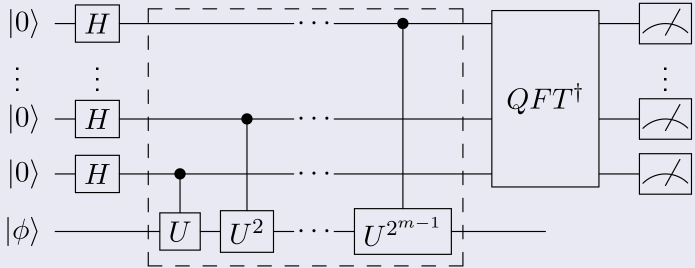


1. prepare m ancilla in uniform superposition of basis states

$$|\Phi_1\rangle = H^{\otimes m}|0\rangle_m = \left(\frac{|0\rangle+|1\rangle}{\sqrt{2}}\right)\otimes\left(\frac{|0\rangle+|1\rangle}{\sqrt{2}}\right)\otimes\cdots\otimes\left(\frac{|0\rangle+|1\rangle}{\sqrt{2}}\right)$$
$$= \frac{1}{\sqrt{2^m}}\sum_{k=0}^{2^m-1}|k\rangle$$

BINARY REPRESENTATION: use $|3\rangle$ to indicate $|00011\rangle$

Filling in the details: phase kickback



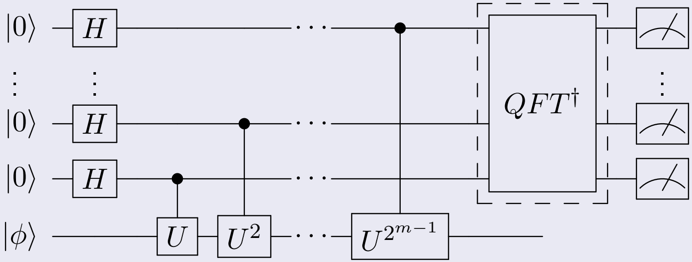
The state $|\phi\rangle$ is an eigenstate of U with $U|\phi\rangle = \exp(i2\pi\phi)|\phi\rangle$

2. each c-U^k applies a phase $\exp(i2\pi k\phi)$ to the $|1\rangle$ state of the ancilla

$$|\Phi_2\rangle = \left(\frac{|0\rangle + e^{i2\pi\phi}|1\rangle}{\sqrt{2}} \otimes \frac{|0\rangle + e^{i4\pi\phi}|1\rangle}{\sqrt{2}} \otimes \cdots \otimes \frac{|0\rangle + e^{i2^{m-1}\pi\phi}|1\rangle}{\sqrt{2}}\right) \otimes |\phi\rangle$$

$$= \frac{1}{\sqrt{2^m}} \sum_{k=0}^{2^m-1} \exp\left(i2\pi\phi k\right)|k\rangle \otimes |\phi\rangle$$

Filling in the details: inverse QFT

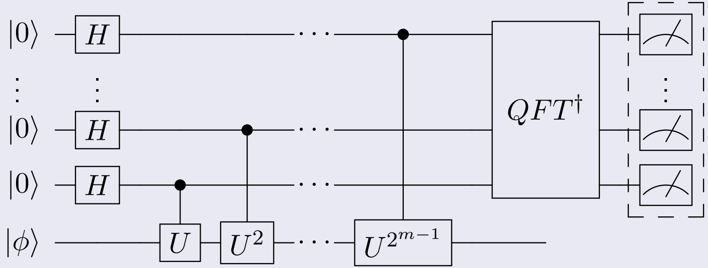


Recall that: $QFT^\dagger |k\rangle = \frac{1}{\sqrt{2^m}} \sum_{q=0}^{2^m-1} \exp\left(-i\frac{2\pi}{2^m}qk\right)|q\rangle$

3. after an inverse QFT the final state is

$$|\Phi_3\rangle = QFT^\dagger |\Phi_2\rangle = \frac{1}{2^m}\sum_{k=0}^{2^m-1}\sum_{q=0}^{2^m-1} \exp\left(i2\pi k\left(\phi - \frac{q}{2^m}\right)\right)|q\rangle \otimes |\phi\rangle$$

Filling in the details: final measurement



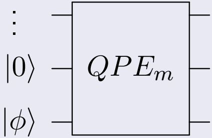
$$|\Phi_3\rangle = \sum_{q=0}^{2^m-1}\left(\frac{1}{2^m}\sum_{k=0}^{2^m-1}\exp\left(i\frac{2\pi k}{2^m}\left(2^m\phi - q\right)\right)\right)|q\rangle\otimes|\phi\rangle$$

4. if phase ϕ is a m-bit number we can find $0 \leq p < 2^m$ s.t. $2^m\phi = p$

$$|\Phi_3\rangle = \sum_{q=0}^{2^m-1}\delta_{q,p}\,|q\rangle\otimes|\phi\rangle = |p\rangle\otimes|\phi\rangle$$

$\Rightarrow$ exact solution with only 1 measurement!

Final measurement: generic phase

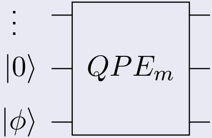


$$|\,\Phi_3\rangle = \sum_{q=0}^{2^m-1}\left(\frac{1}{2^m}\sum_{k=0}^{2^m-1} e^{i\frac{2\pi k}{2^m}(2^m\phi - q)}\right)|q\rangle \otimes |\phi\rangle$$

- when $2^m\phi$ is not an integer we can sum the term in parenthesis as

$$\sum_{k=0}^{2^m-1} e^{ixk} = \frac{1-e^{i2^m x}}{1-e^{ix}} = \exp\left(i\frac{x}{2}(2^m-1)\right)\frac{\sin\left(2^m x/2\right)}{\sin\left(x/2\right)}$$

Final measurement: generic phase



$$| \Phi_3\rangle = \sum_{q=0}^{2^m-1} \left(\frac{1}{2^m} \sum_{k=0}^{2^m-1} e^{i\frac{2\pi k}{2^m}(2^m\phi - q)} \right) |q\rangle \otimes |\phi\rangle$$

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- we will measure the ancilla register in $|q\rangle$ with probability

$$P(q) = \frac{1}{M^2}\frac{\sin^2\left(M\pi(\phi - q/M)\right)}{\sin^2\left(\pi(\phi - q/M)\right)}$$

where we have defined $M = 2^m$

Final measurement: generic phase example

example taken from A. Childs lecture notes (2011)

$$P(q) = \frac{1}{M^2} \frac{\sin^2\left(M\pi(\phi - q/M)\right)}{\sin^2\left(\pi(\phi - q/M)\right)}$$

EXERCISE: show that if $r = \lceil M\phi \rfloor$ then $P(r) \geq 4/\pi^2 \approx 0.4$

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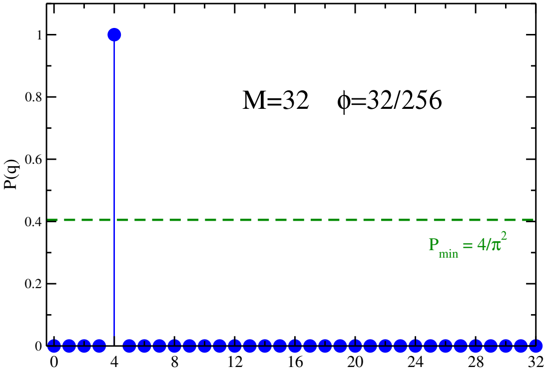

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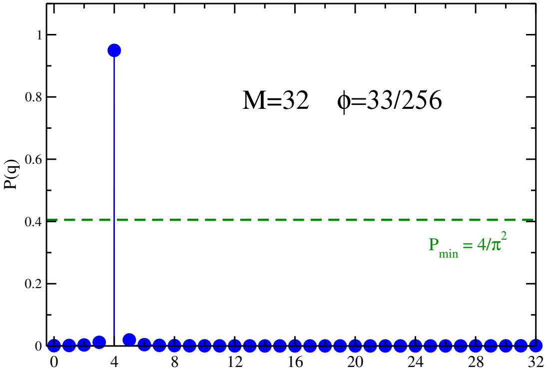

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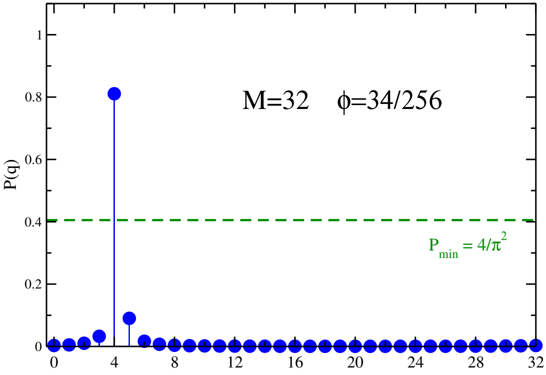

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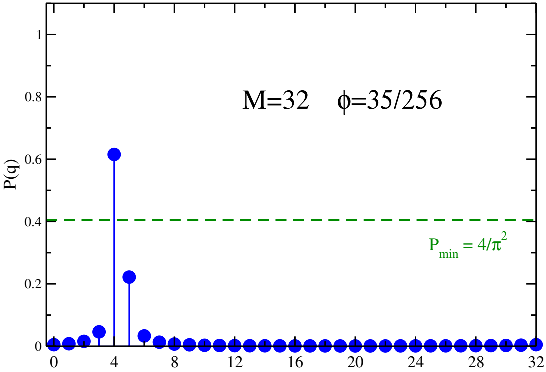

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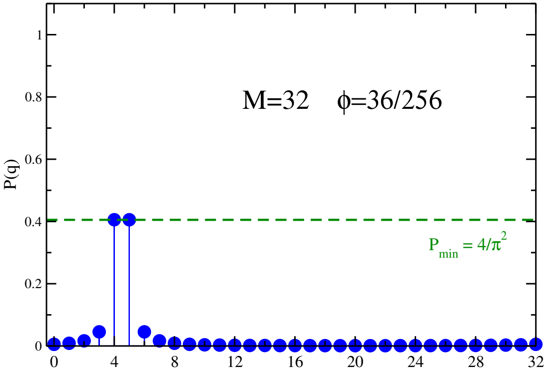

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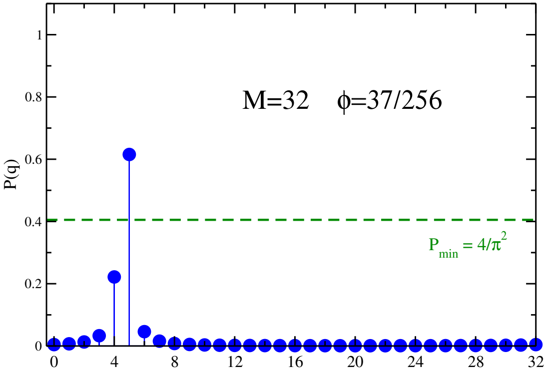

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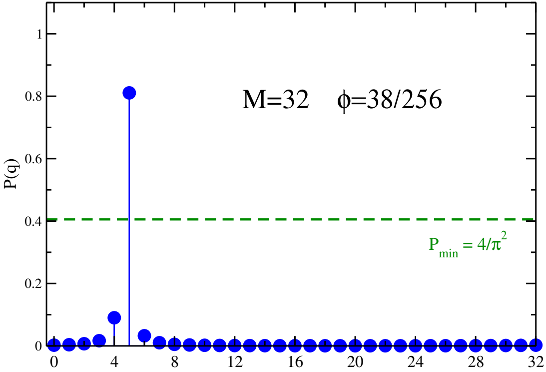

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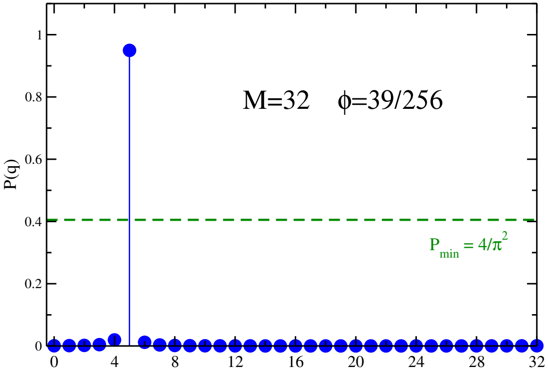

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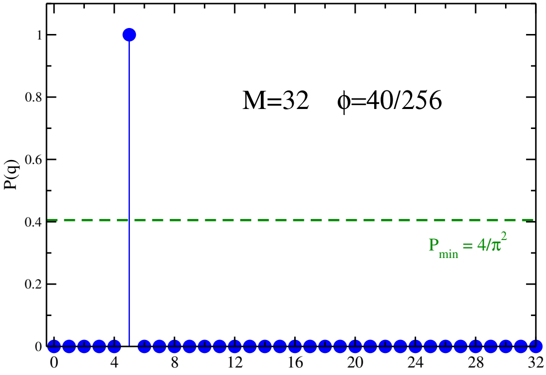
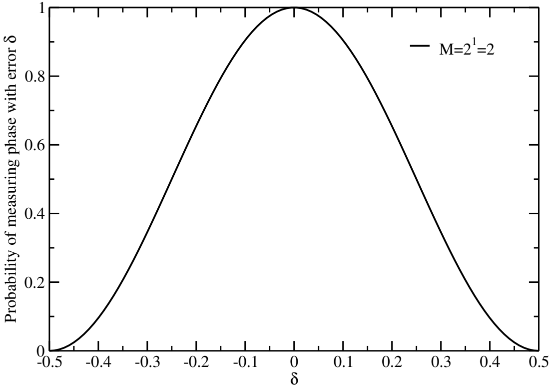


Final measurement: generic phase II

$$P(q) = \frac{1}{M^2}\frac{\sin^2\left(M\pi(\phi - q/M)\right)}{\sin^2\left(\pi(\phi - q/M)\right)}$$

- the best m-bit approximation to ϕ is p/M with $p = \lceil M\phi \rfloor$
- the probabilty of making an error $\delta = (q-p)/M$ is



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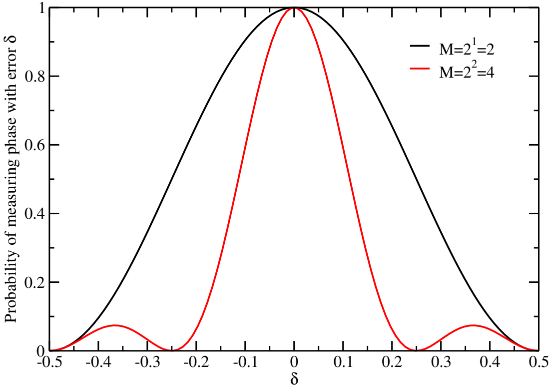

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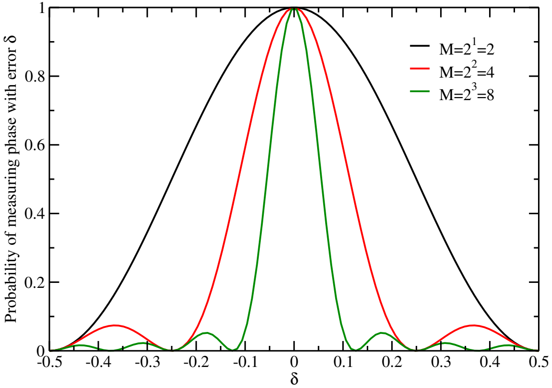

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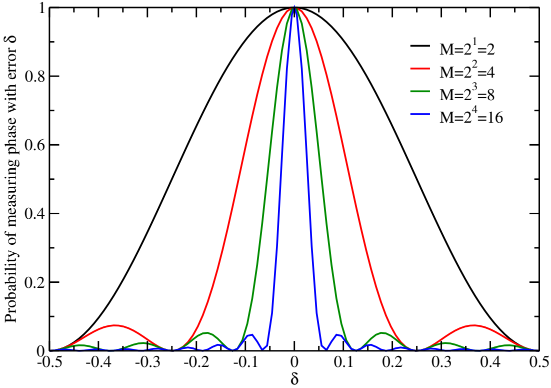

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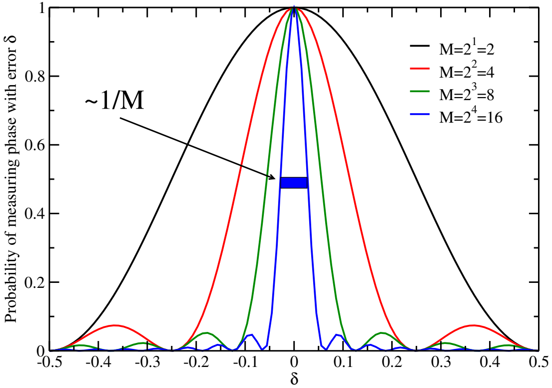
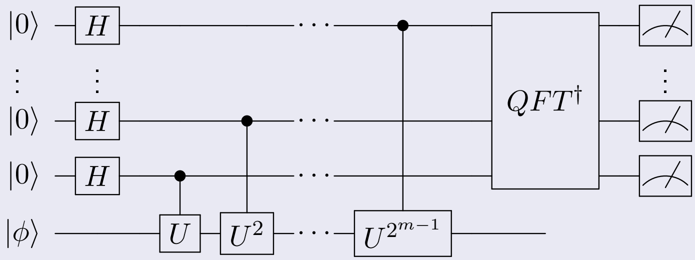


Quick recap of QPE for eigenstates



- given an eigenstate $|\phi\rangle$ QPE can provide an estimate for the phase ϕ with precision δ using $M \sim 1/\delta$ with probability $P > 4/\pi^2$

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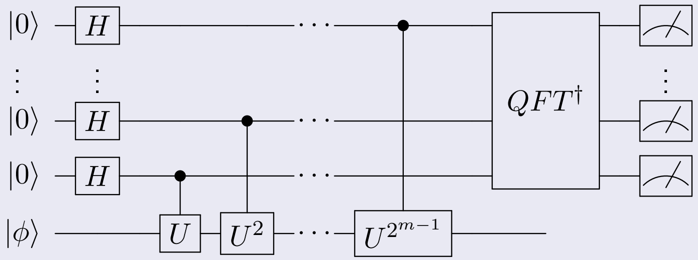

- given an eigenstate $|\phi\rangle$ QPE can provide an estimate for the phase ϕ with precision δ using $M \sim 1/\delta$ with probability $P > 4/\pi^2$
- this probability can be amplified to $1 - \epsilon$ using more ancilla qubits*

$$m' = m + \left\lceil \log\left(\frac{1}{2\epsilon} + 2\right) \right\rceil \quad \Rightarrow \quad M' \sim \frac{1}{\delta\epsilon}$$

*see eg. Nielsen & Chuang

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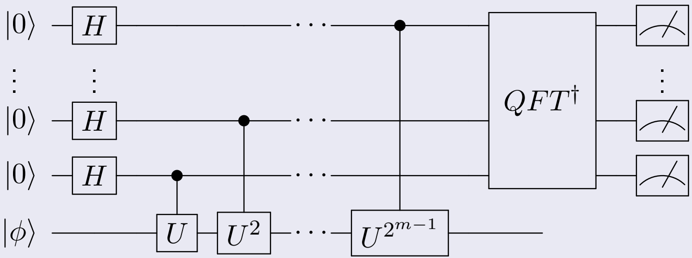

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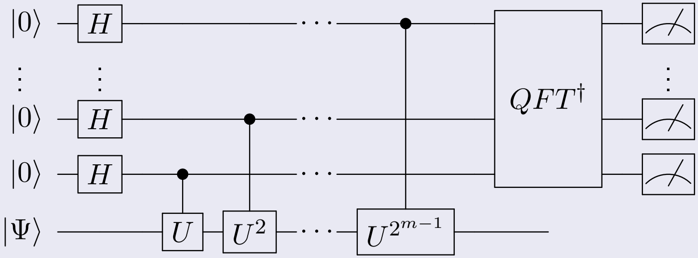
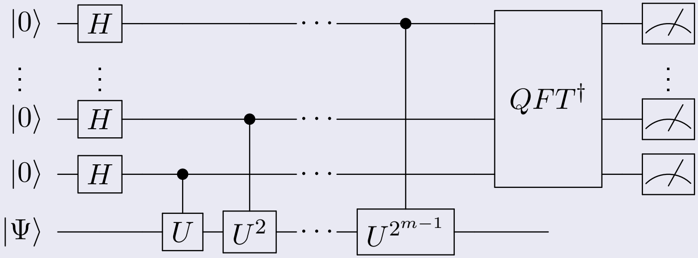
*see eg. Nielsen & Chuang

- we can also repeat this $O(\log(1/\eta))$ times and take a majority vote to increase the probability to $1 - \eta$ (see Chernoff bound)

QPE on general states



QPE on general states



If we start with a generic state $|\Psi\rangle = \sum_j c_j |\phi_j\rangle$ we find

$$|\Phi_3\rangle = \sum_j c_j \sum_{q=0}^{2^m-1} \left(\frac{1}{2^m} \sum_{k=0}^{2^m-1} \exp\left(i \frac{2\pi k}{2^m} \left(2^m \phi_j - q\right)\right)\right) |q\rangle \otimes |\phi_j\rangle$$

The new probability becomes

$$P(q) = \frac{1}{M^2} \sum_j |c_j|^2 \frac{\sin^2\left(M\pi(\phi_j - q/M)\right)}{\sin^2\left(\pi(\phi_j - q/M)\right)}$$

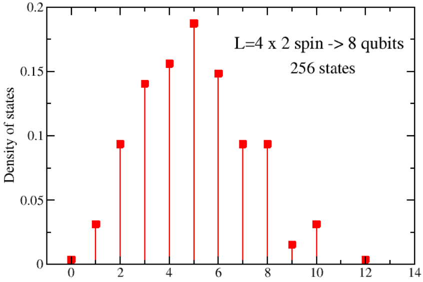
EXAMPLE: Spectrum of 1D Hubbard model

example taken from Ovrum & Horth-Jensen (2007)

$$H_H = \sum_i^L \sum_{\sigma=\uparrow,\downarrow} \left[\epsilon a^\dagger_{i,\sigma} a_{i,\sigma} - t \left(a^\dagger_{i+1,\sigma} a_{i,\sigma} + a^\dagger_{i,\sigma} a_{i+1,\sigma} \right) \right] + U \sum_i^L n_{i,\uparrow} n_{i,\downarrow}$$

- we can estimate the spectrum using QPE with random initial states
- consider simple case with $t = 0$, $\epsilon = U = 1$

Ovrum&Horth-Jensen (2007)



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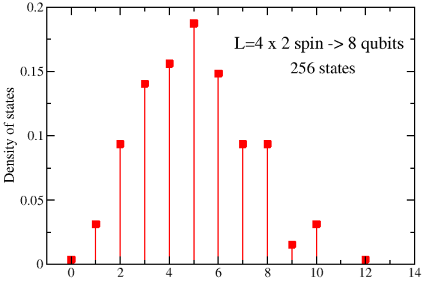
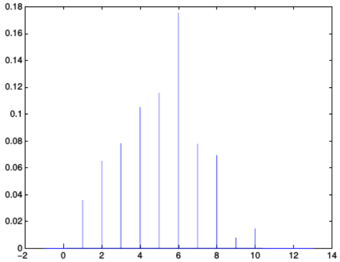


$m = 16$ ancilla qubits



Time evolution for Hubbard model

$$H'_H = \sum_i^L \sum_{\sigma=\uparrow,\downarrow} n_{i,\sigma} + \sum_i^L n_{i,\uparrow} n_{i,\downarrow} \qquad n_{i,\sigma} = a^\dagger_{i,\sigma} a_{i,\sigma}$$

- using Jordan-Wigner transformation we can map this into $2L$ qubits

$1\uparrow$ $1\downarrow$ $2\uparrow$ $2\downarrow$ $3\uparrow$ $3\downarrow$ $4\uparrow$ $4\downarrow$

$$n_{i,\uparrow} = \frac{\mathbb{1} + Z_{2i-1}}{2} \quad n_{i,\downarrow} = \frac{\mathbb{1} + Z_{2i}}{2}$$

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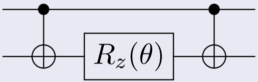
$$n_{i,\uparrow} = \frac{\mathbb{1} + Z_{2i-1}}{2} \qquad n_{i,\downarrow} = \frac{\mathbb{1} + Z_{2i}}{2}$$

$$H_{JW} = h_0 + h_1 \sum_{j=1}^{2L} Z_j + h_2 \sum_{j<k=1}^{2L} Z_j Z_k$$

- propagator $U(\tau)$ can be obtained using one and two-qubit Z rotatations

EXERCISE

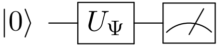
Show that $U_2 = e^{-i\frac{\theta}{2} Z_1 Z_2}$ is



Measuring an observable: single qubit case

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

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

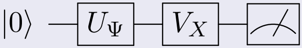


We now need to repeat calculation M times to estimate the probabilities

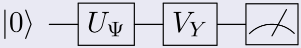
$$P(0) = |\langle 0|\Psi\rangle|^2 \sim \frac{\sum_k \delta_{s_k,0}}{M} \qquad Var\left[P(0)\right] \sim \frac{v_0}{M} \longrightarrow 0\ .$$

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 $V_Y = SV_X = SH$

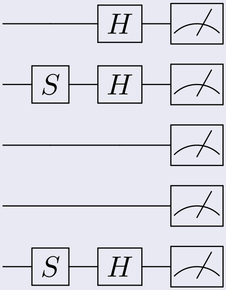
Measuring an observable: the Pauli group

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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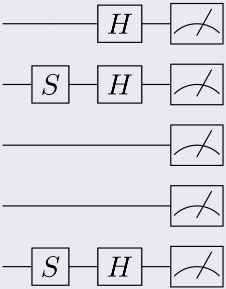
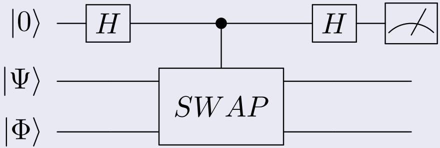


- naive estimator has total error $\propto \sqrt{N_K/M}$
- we can measure multiple terms together!

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

EXAMPLE 2: 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

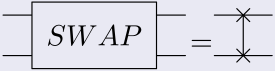


Buhrman, Cleve, Watrous & de Wolf (2001)

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

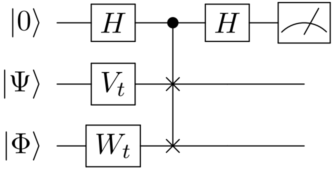
The SWAP gate

$$\text{SWAP}\,|\Psi\rangle\otimes|\Phi\rangle = |\Phi\rangle\otimes|\Psi\rangle$$



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

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!