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Quantum computing for nuclear reactions

The 7th international workshop on Compound-Nuclear Reactions and Related Topics (CNR*24)
8-12 July 2024, IAEA Vienna

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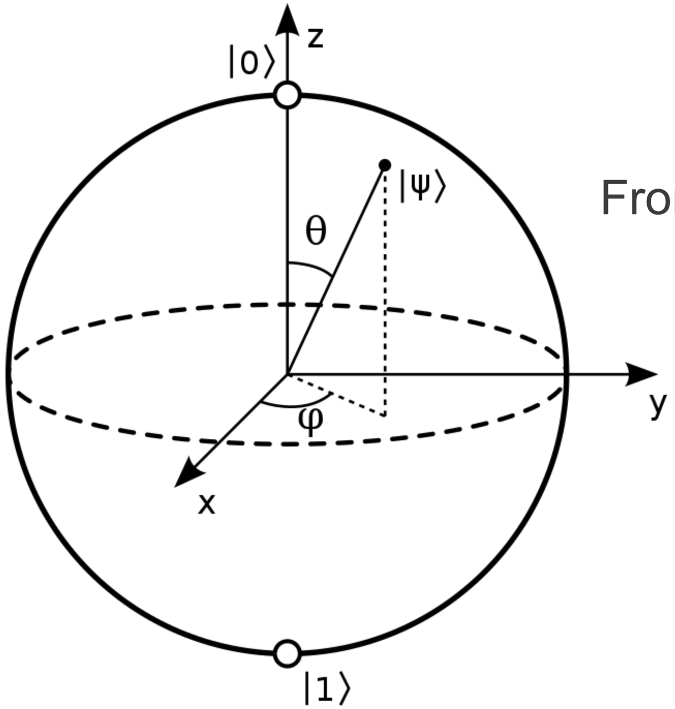
Outline
- Very brief introduction into quantum computing
- Quantum computing for nuclear physics
- Algorithms for state preparation, dynamics
- Summary and outlook

July 11, 2024

Quantum computing: qubit basics

Classical bit: 0 or 1



From Wikipedia

Quantum bit (qubit): cosθ|0>+sinθ|1>

Operations with single qubit gates:

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix};\ Y = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix};\ Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix};$$

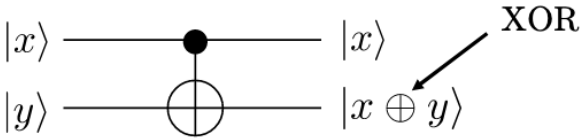
$$R_P(\theta) = \exp\left(-i\frac{\theta}{2}P\right);\ H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix};\ R_\phi = \begin{pmatrix} 1 & 0 \\ 0 & \exp(i\phi) \end{pmatrix}$$

swap gate

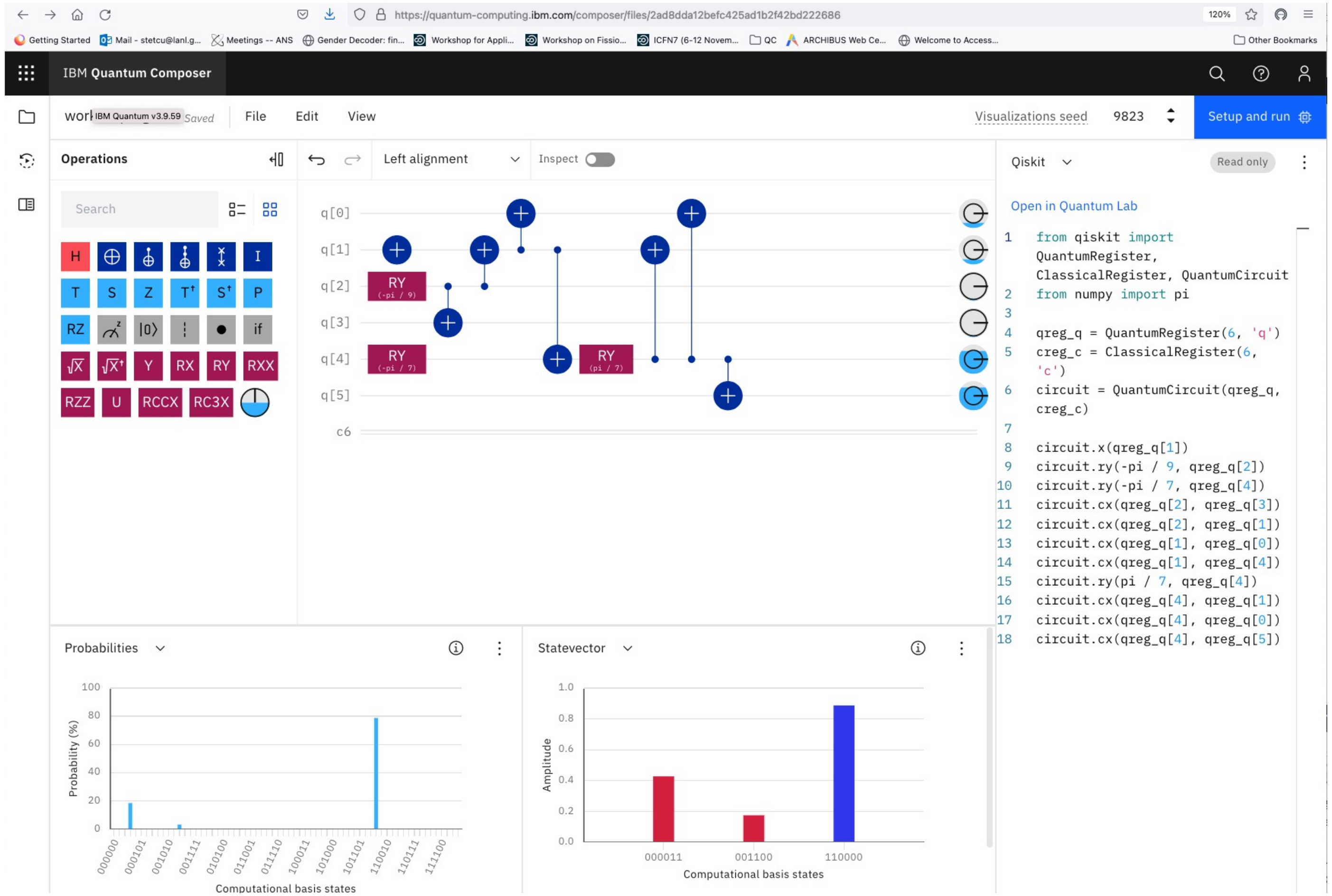
Qbit entanglement

(Others: Toffoli gates, C-Z, etc)

Controlled-NOT (C-NOT) gate:



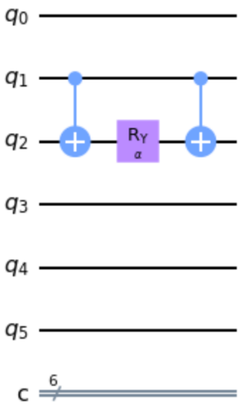
$$|0_0\rangle\langle 0_0|I_1 + |1_0\rangle\langle 1_0|X_1$$

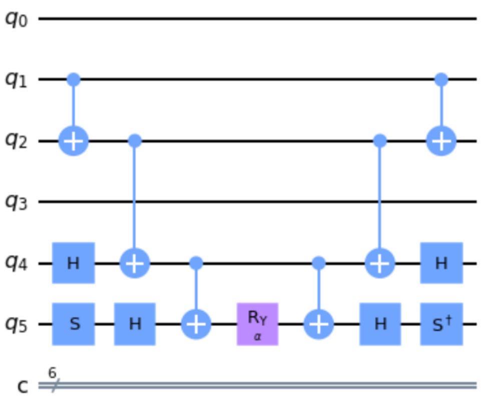


|HF> 2p-2h 2p-2h

$$A_0|000011\rangle + A_1|001100\rangle + A_2|110000\rangle$$

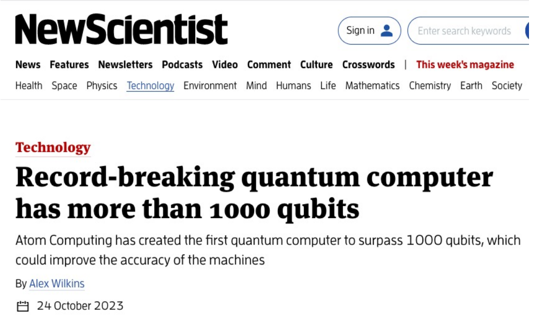
$$\exp(i\alpha Z_1 Z_2) \qquad \exp(i\alpha Z_1 Z_2 X_4 Y_5)$$





https://www.newscientist.com/article/2399246-record-breaking-quantum-computer-has-more-than-1000-qubits/

Status of quantum hardware



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Technology

Record-breaking quantum computer has more than 1000 qubits

Atom Computing has created the first quantum computer to surpass 1000 qubits, which could improve the accuracy of the machines

By Alex Wilkins

24 October 2023

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Technology

IBM's 'Condor' quantum computer has more than 1000 qubits

IBM has revealed two quantum computers. One is the second largest ever made and the other produces fewer errors than any quantum computer the company has built so far

By Karmela Padavic-Callaghan

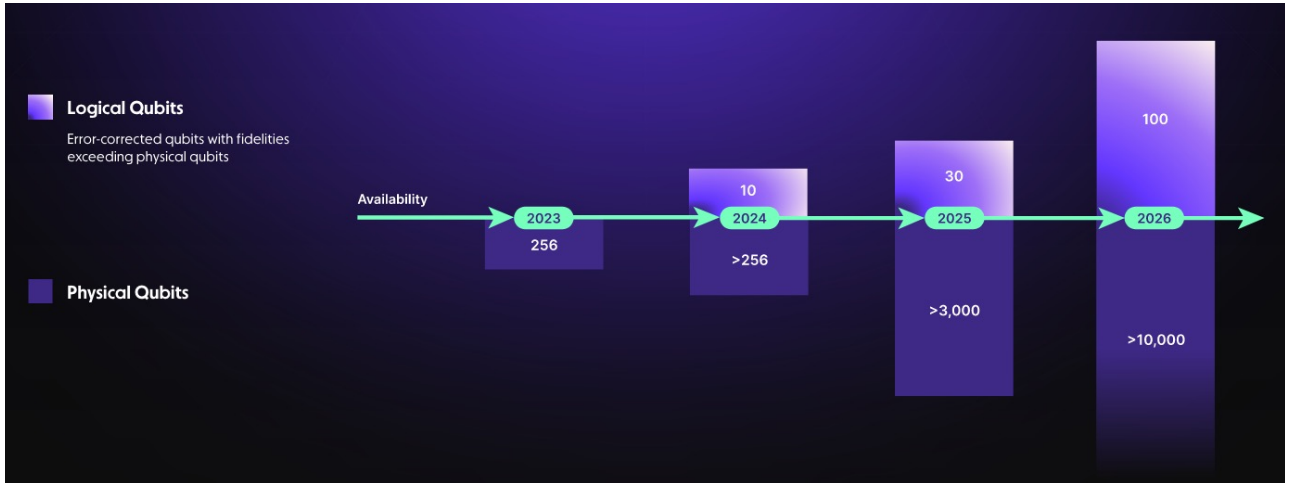
4 December 2023

Today: Noisy Intermediate-scale quantum (NISQ) devices

- Sensitive to environment, prone to decoherence
- Moderate gate fidelity
- Around 1,000 qubits
- Algorithms: quantum eigensolver (VQE) and quantum approximate optimization algorithm (QAOA), which offloads some of the work on classical processors; due to noise during circuit execution, they often require error mitigation techniques.

(Near) Future: Fault-tolerant hardware

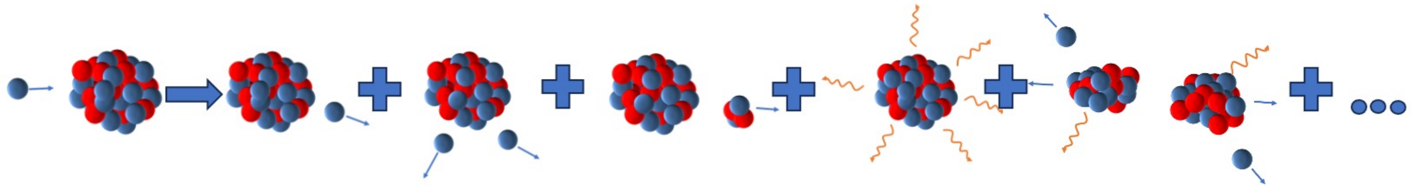
- Will perform calculations with arbitrarily low logical error rates
- Capable of handling (most of today's) algorithms that are impossible on NISQ devices
- **Logical qubit**: multiple physical qubits that are protecting themselves against errors) Unlike physical qubits, there are no hardware components of a quantum computer that specifically designate logical qubits.
- Logical qubits are intended to not fail.



https://www.quera.com/qec

Quantum Computing for Nuclear Physics at a Glance

- Quantum computing is designed to handle very well unitary transformations, hence reactions
- Limitation for classical computers: dynamics remains very difficult, as it involves a large number of degrees of freedom and many states
- Nuclear forces are short range, hence one possibly can reduce the mapping complexity
- Competing channels are ``easy”: on quantum hardware the states are superpositions of all energetically allowed channels.



- It is still an open question on whether the upcoming hardware would be able to extend enough the coherence time to execute the algorithms and extract the useful information (Forbes, December 2023: “All of the IBM roadmap developments and plans ultimately converge on 2033 in the form of 2,000 qubits and a billion quantum gates.”)
- Even if no full problem will be solved on quantum hardware, some of the hard calculations could be accelerated on quantum devices
- Algorithms could be developed to take advantage of executions that are easy on quantum hardware (e.g., restorations of broken symmetries)

Today’s reality

- Quantum computer simulators don’t usually claim to be able to simulate more than 40 qubits, and more than 40 qubits are needed.
- Computational advantages, by definition, are not going to be possible until quantum computers can at least outperform their simulators.
- Methods to improve NISQ results, like measurement error mitigation, require classical processing and, therefore, have scaling issues.
- Even if all else was absolutely perfect, NISQ qubits still don’t have the coherence to support algorithms that propose exponential computational advantages.
- Some modalities, such as neutral atoms, have the potential to scale up very quickly to thousands of qubits even before considering the use of interconnects.

Operator encoding

- We can only construct operators that involve elementary qubit + entanglement operators
- All operators will be written as sums of Pauli operators acting on individual qubits

$$\mathcal{O} = \sum_i c_i P_i \qquad P = ZXXIYXY$$

- Second quantization encoding: Jordan Wigner (occupation encoding):

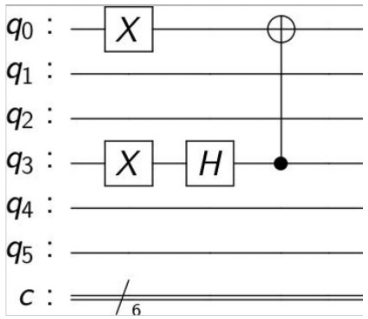
$$a_i = \frac{1}{2}\prod_{j=0}^{i-1}(-Z_j)(X_i + iY_i); \quad a_i^\dagger = \frac{1}{2}\prod_{j=0}^{i-1}(-Z_j)(X_i - iY_i)$$

$$H = \sum_{i,j} h_{i,j} a^\dagger a_j + \frac{1}{4}\sum_{ij;kl} V_{ij,kl} a_i^\dagger a_j^\dagger a_l a_k + \cdots = \sum_\alpha c_\alpha P_\alpha$$

- Number of qubits: the number of states
- Other types of second quantization encodings exist, some more efficient, but less transparent.

More efficient encoding

- **First-quantization mapping**
  - One single-particle state for each particle is mapped into a superposition of qubit states
  - Requires $\log_2(N_s)$ qubits, $N_p*\log_2(N_s)$ in total
  - Example: one particle in 8 states: |1> → |000>, |2>→|001>, |3>→|010>, |4>→|100>, |5>→|011>, |6>→|101>, |7>→|110>, |8>→|111>.
  - Initial state needs to be antisymmetrized (algorithms exist)



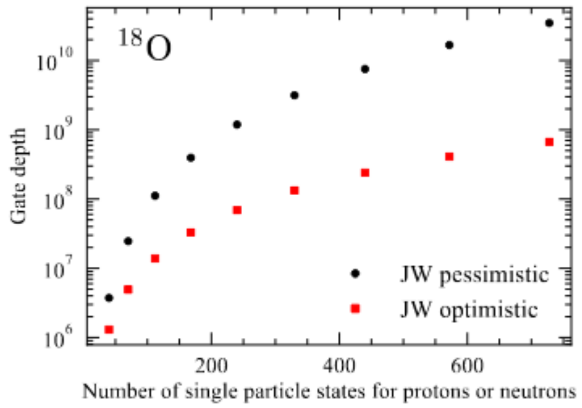
- **Hybrid efficient mapping: store already antisymetrized states as in first quantization**
  - Slater determinants are stored in combinations of one-qubit states
  - Requires $\log_2(N)$ qubits, where N is the number of antisymmetrized many-body states
  - Think about Shell Model: each state is stored in a superposition $|q_0 q_1 \ldots q_{Nq-1}>$, with q_k=0 or 1.
  - Operators are mapped from matrix elements

$$\mathcal{H} = \sum_{i,j} \langle v_j|\mathcal{H}|v_i\rangle |v_j\rangle\langle v_i| = \sum_{i,j} H_{ij} |q_0^i q_1^i \ldots q_{N_q-1}^i\rangle\langle q_0^j q_1^j \ldots q_{N_q-1}^j|$$

  - Elementary qubit mapping table

$$|0\rangle\langle 0| = \frac{1}{2}(I+Z) \qquad |1\rangle\langle 1| = \frac{1}{2}(I-Z) \qquad |1\rangle\langle 0| = \frac{1}{2}(X-iY) \qquad |0\rangle\langle 1| = \frac{1}{2}(X+iY)$$

No free-lunch theorem



- **Second quantization mapping**
  - Requires a large number of qubits
  - Possibly large number of Pauli strings
- **First quantization mapping**
  - Anti-symmetrization adds to the overall depth of the circuit
  - The operators will have even a larger number of Pauli strings
- **Qubit-efficient mapping**
  - Large number of Pauli strings in the mapped operators
  - Pauli strings are very dense (many non-identity Pauli operators)

Shell	N_p	N_n	N_q^{JW}	N_{Pauli}^{JW}	N_q^{SM}	N_{Pauli}^{SM}
p	1	2	12	975	5	528
p	2	2	12	975	6	2,072
p	1	3	12	975	5	488
p	2	3	12	975	6	2,080
p	3	3	12	975	7	7,936
sd	1	2	24	12,869	7	8,252
sd	1	3	24	12,869	9	131,321
sd	2	2	24	12,869	10	523,720

- **(For time evolution one needs to also consider Trotter complications)**
- **Remain optimistic**
  - Largest shell model calculation ~10^9 states (could be mapped on ~30 qubits)
  - In the next couple of years 40-50 qubit (fault tolerant) machine will come online, so there is a good chance to go well over current computing capabilities

Measurements

- Quantum mechanics: measurement=projection on that state, there is no turning back!
- Need only to compute expectation values of general Pauli strings

$$\langle\Psi|P_\alpha|\Psi\rangle$$

- **Extra (ancilla) qubits can be used to prepare states and extract other quantities (e.g., overlaps); this is based on measurements with a desired outcome**

Initial state preparation

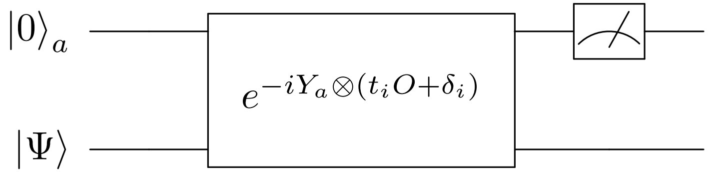
Classical algorithms:

- Direct diagonalization in a many body basis (Lanczos)
- Imaginary time evolution (MC techniques)
- Variational algorithms (UCC)

Quantum algorithms:

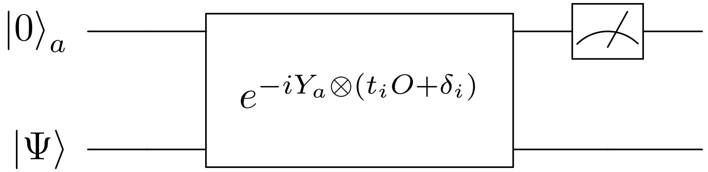
- Variational methods (UCC) – involve continuous interaction with a classical machine
- Filtering algorithms (e.g., Rodeo)
- Quantum Imaginary time evolution (QITE)
- Quantum Lanczos (QLANCZOS) – difficult to see how the state can be actually prepared

Toy example for preparing a state by projection



- **Main idea: couple with a ancilla qubit to manipulate the physical w.f. w/o touching it**
- **Assume only three states in a problem:**
  - *E_0=0, E_1, E_2=1.*
  - Chose $t_1 = \frac{\pi}{2E_1}$
  - Initial state: $\psi_0 = \sum_{i=0}^{2} C_i |E_i\rangle$
  - Perform time evolution $$\exp(-iHY_a t)\psi_0|0\rangle = (C_0|E_0\rangle + C_1\cos(\pi/2)|E_1\rangle + C_2\cos(\pi E_2/2E_1)|E_2\rangle)\,|0\rangle + (C_0\sin(0)|E_0\rangle + C_1\sin(\pi/2)|E_1\rangle + C_2\sin(\pi E_2/2E_1)|E_2\rangle)\,|1\rangle$$
  - Measure ancilla. If |0>, continue, if |1> start again
  - Continue with $t_2 = \frac{\pi}{2E_2} = \frac{\pi}{2}$
  - One can use approximate models for the spectrum (experiment, theory)
  - Success probability: $|C_0|^2$

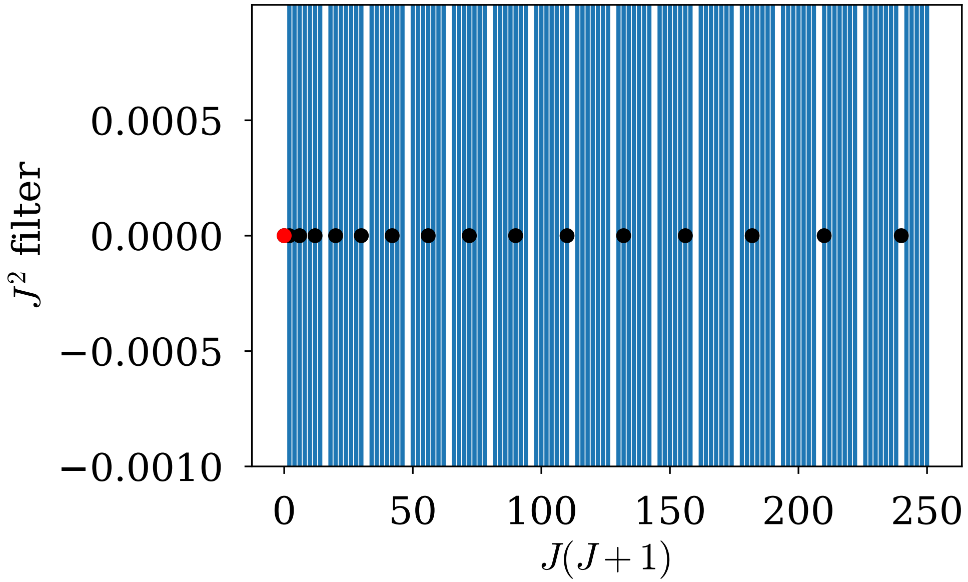
Symmetry projection



Arrange times and phases so that when one measures qubit *a* one produces the desired state

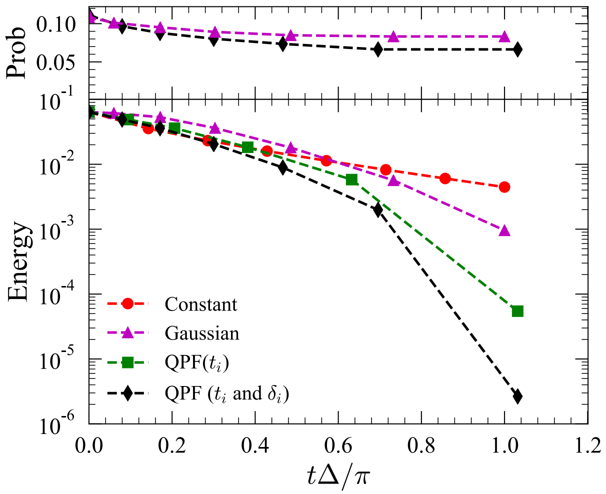
$$|\psi\rangle \otimes |0\rangle_a \to |\psi(t_i)\rangle = \cos(t_i O + \delta_i)|\psi\rangle \otimes |0\rangle_a + \sin(t_i O + \delta_i)|\psi\rangle \otimes |1\rangle_a.$$

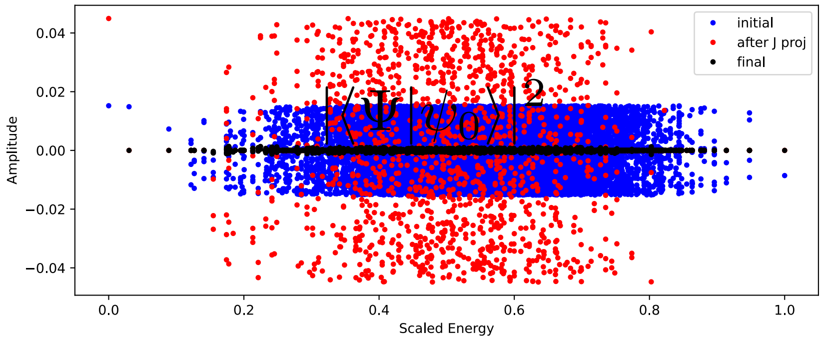
- **Replace O with a symmetry operator (e.g., J^2):**
  - Time series $\pi/4$ (eliminates: J=1,2,5,6,9,10,13,14,…), $\pi/8$ (J=3,4,11,12,…), $\pi/16$ (J=7,8,24,25,…)
  - Same types of series can be used to project on other symmetries (total momentum, J_z, particle number, etc)
  - This is an essential step: it increases the effective gap, thus reducing the time necessary to filter out the energy

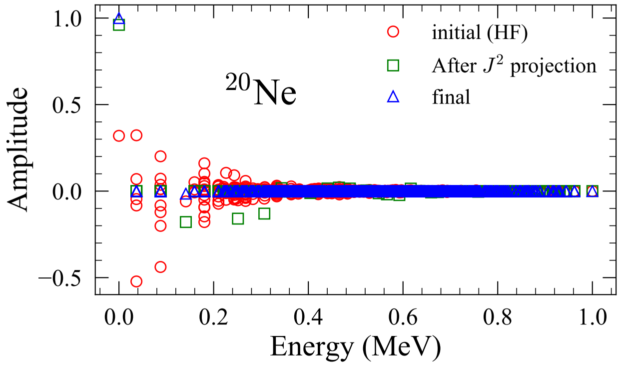


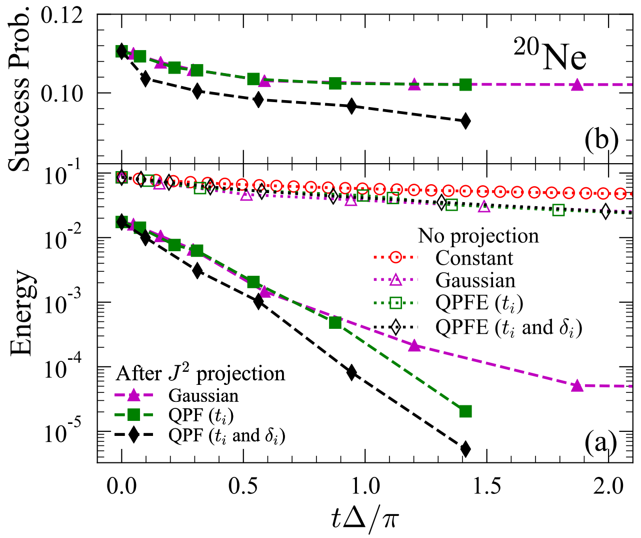
Quantum Filtering Projection (QFP)

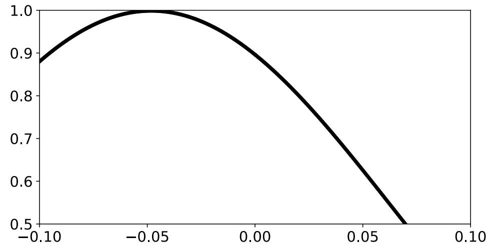
- **After projection apply the same circuit and series of measurements with the Hamiltonian**
  - Apply the same type of filtering for the Hamiltonian, but now one can optimize in advance the times and phases
  - The optimization algorithm does not require full knowledge of the spectrum, but general features (gap, average level spacing); when using phases, measurements of qubit *a* in |1> state can provide information to further optimize the times and phases
  - Success probability converges to $|\langle\Psi|\psi_0\rangle|^2$
  - Optimization can include noise model to produce a better series of times and phases





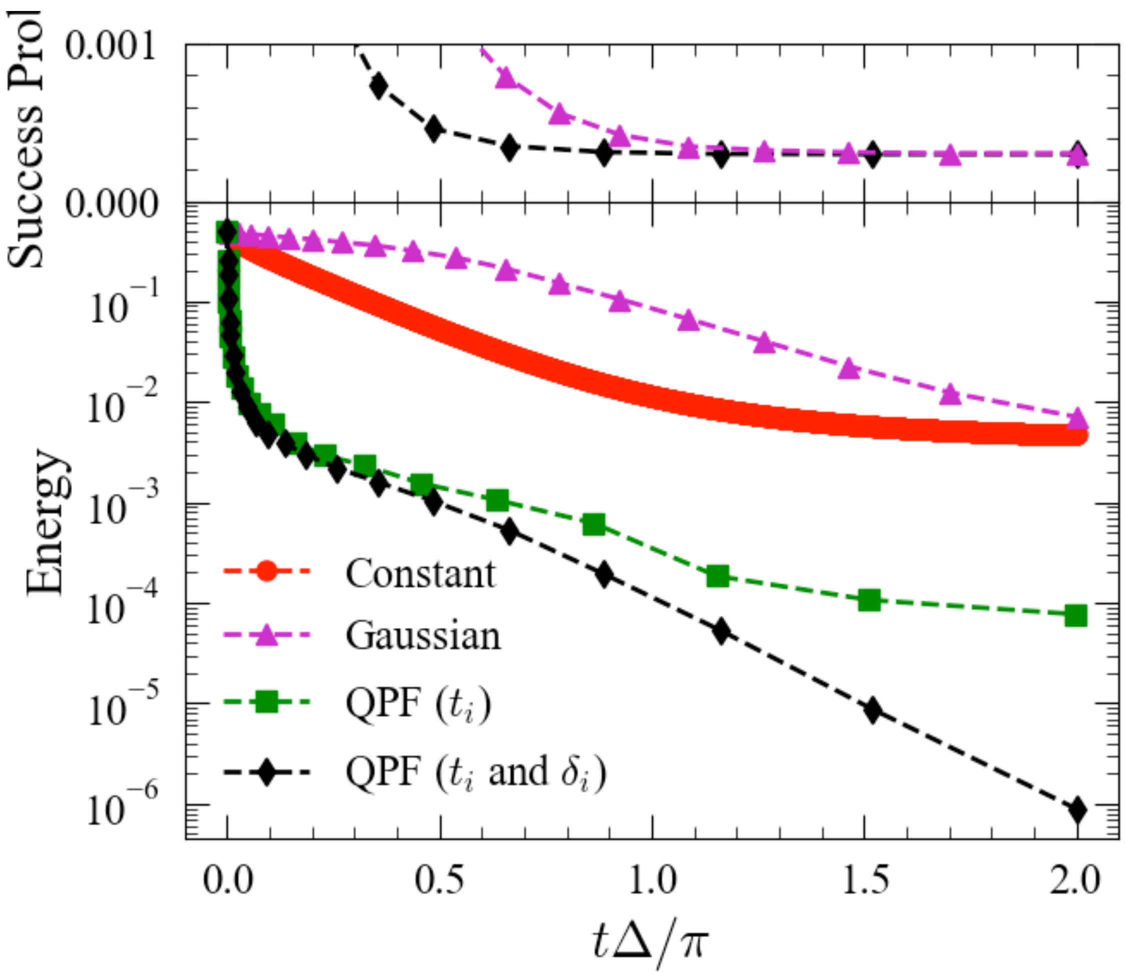






Small gap

- Random Hamiltonian
- Delta=0.001



Nucleons on a lattice

- **Implementation on a (cubic) lattice**
  - Lattice is the best suited to treat both bound and continuum states
  - Lattice dimensions: $L_x=N_x a$, $L_y=N_y a$, $L_z=N_z a$ (a=lattice constant), $N_{xyz}=N_x N_y N_z$
  - Momentum basis states: $|\vec{p}_1\vec{p}_2\ldots\vec{p}_A\rangle$ with $\vec{p}_1+\vec{p}_2+\ldots+\vec{p}_A=\vec{0}$
  - Each basis state will be mapped into qubit states $|\vec{p}_1\vec{p}_2\ldots\vec{p}_A\rangle \rightarrow |\{0,1\}_q^N\rangle$
  - Number of qubits $N_q=\log_2(N_s)$, where N_s=number of antisymmetric states with zero CM momentum
    - 1D example with Nx=4, s.p. states $\{0, \pi/2a, -\pi/a, -\pi/2a\}$

$$|\pi/2a,-\pi/2a\rangle \otimes |\pi/2a,-\pi/2a\rangle \rightarrow |000\rangle, |0,\pi/2a\rangle \otimes |0,-\pi/2a\rangle \rightarrow |001\rangle,$$
$$|\pi/a,-\pi/2a\rangle \otimes |0,-\pi/2a\rangle \rightarrow |010\rangle, |0,-\pi/2a\rangle \otimes |0,\pi/2a\rangle \rightarrow |011\rangle,$$
$$|0,-\pi/2a\rangle \otimes |\pi/a,-\pi/2a\rangle \rightarrow |100\rangle$$

- **Deuteron:**
  - N_{xyz} states (no antisymmetrization): $|\vec{k},-\vec{k}\rangle$
  - Same contact interaction in both L=0 channels
  - $N_q=\log_2(N_{xyz})$
  - State preparation and simple reaction (electron scattering) on N_x=8, N_y=8, N_z=8 lattice, N_q=9 qubits

Hamiltonian mapping

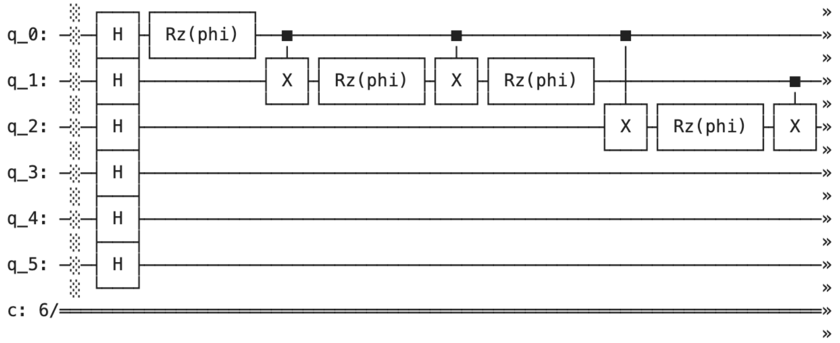
- **Kinetic energy:**
  - Diagonal in momentum space, will reduce to mapping |0><0| and |1><1| only, hence I and Z Paulis
  - Due to the values of the momentum on the lattice, even though all possible combinations of I and Z are possible (N_{xyz}=512), only a small number survives (19 for N_{xyz}=512)
  - All commuting (no Trotter errors)

- **Interaction:**
  - In momentum space, the contact interaction is a constant all states to all states

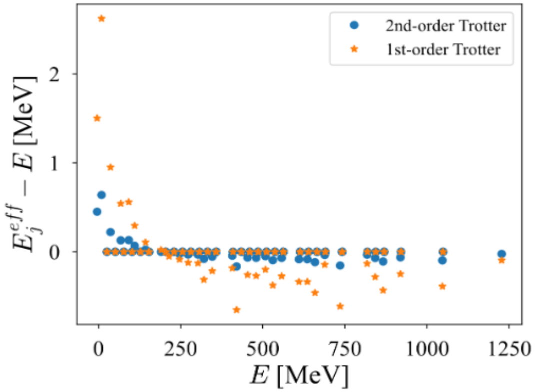
$$V = C_0(I+X)^{\otimes N_q} = C_0 H(I+Z)^{\otimes N_q} H$$

  - All strings commute, but now all possible combinations of I and X are possible, which complicates an evolution circuit

Time evolution



- **Trotter approximation (T and V do not commute)**
  - First order $\exp\left(-i(T+V)t\right) \approx \exp(-iTt)\exp(-iVt)$
  - Second order $\exp\left(-i(T+V)t\right) \approx \exp(-iTt/2)\exp(-iVt)\exp(-iTt/2)$



$$\exp\left(i\theta ZZZ\right) =$$

- **Circuit implementation**
  - Exp(-iVt) can be implemented with 18 CNOTs and 18 Rotations
  - exp(-iVt) naively requires $2 - 2^{N_q+1} + N_q 2^{N_q}$ CNOTs and $2^{N_q} - 1$ Z rotations

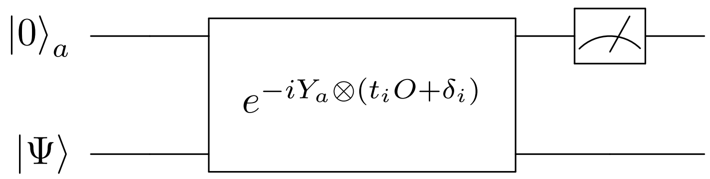
    Efficient implementation $2^{N_q} - 2$ CNOTs and $2^{N_q} - 1$ Z rotations

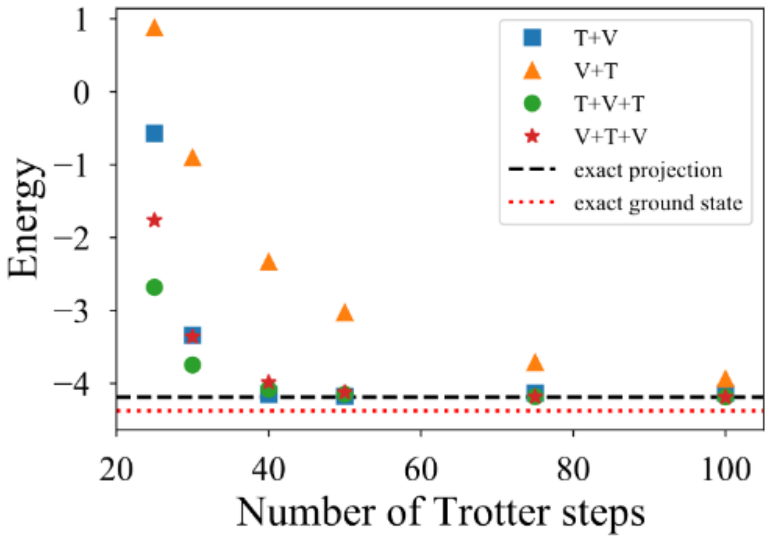
    (order of the terms in V given by the Gray code)

J. Welch et al., New J. Phys. **16**, 033040 (2014)

State preparation

- Initial state: |0,0> (0.87 amplitude in the exact ground state)
- Remove only one excited state using the projection algorithm
- Time to evolve $t = \dfrac{\pi}{2(E_1 - E0)}, \delta = 0$





- Circuit for removing one excited state would require 21,440 CNOTs and 21240 Z rotations
- Use Qiskit implementation (not scalable): 510 CNOTs and 2,035 Z rotations

Inclusive response calculation (dynamics/simple reaction)

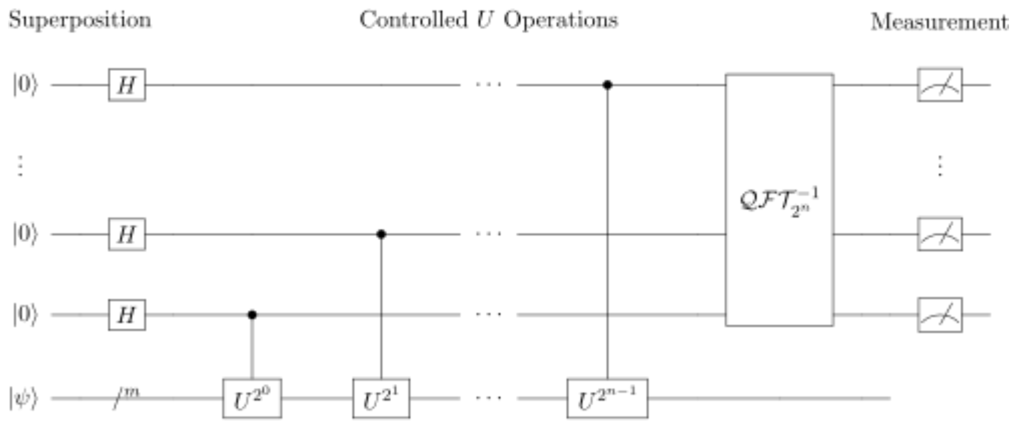
R. Weiss, A. Baroni, J. Carlson, and I. Stetcu, arXiv:2404.00202 (2024)

- **Algorithm based on Quantum Phase Estimate algorithm**
  - Rogero and Carlson, Phys. Rev. C **100**, 034610 (2019)

- **Compute** $S(\omega) = \sum_{\nu} |\langle \Psi_\nu | O | \Psi_0 \rangle|^2 \delta(E_\nu - E_0 - \omega)$

- **Transition Operator:** $O = \exp(i\vec{q}\cdot\vec{r}_p) = \exp(i\vec{q}\cdot\vec{r}/2)\exp(i\vec{q}\cdot\vec{R}_{CM})$
- $\frac{1}{2}\vec{q}\cdot\vec{r}$ **Hermitian operator, mapped into 16 Pauli strings, so** $O|\Psi_0\rangle$ **can be created**

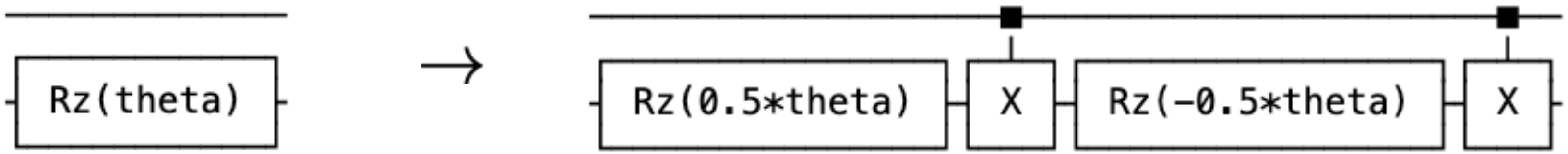
https://en.wikipedia.org/wiki/Quantum_phase_estimation_algorithm

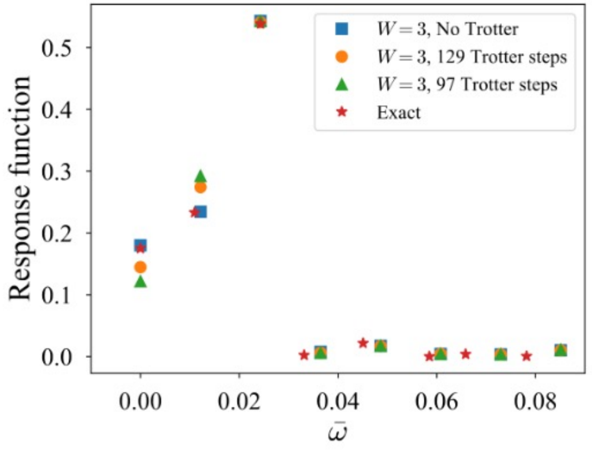


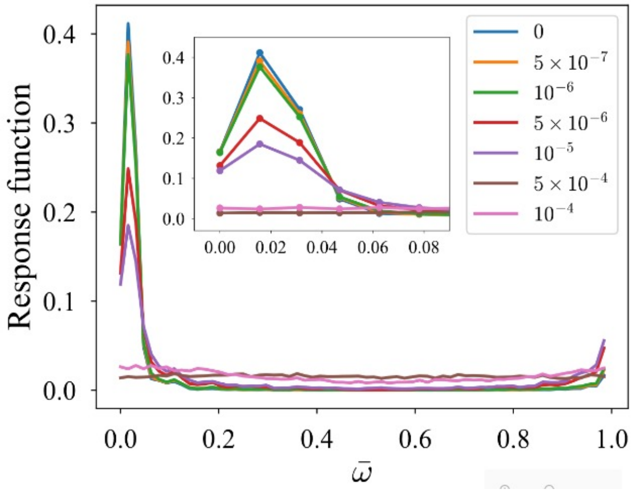
- **Phase estimate algorithm**
  - Identifies eigenvalues from the measurement of ancilla qubits
  - The probability of each state is given by the measurement probability of each string of ancillas
  - Energy resolution given by the number of ancilla qubits
- **Somewhat similar to the classical Lanczos algorithm for transitions**

Circuit simulation

- **Use 3-6 ancilla qubits**
- **Any Z rotation transforms into a Controlled rotation, introducing 1 extra rotation and 2 CNOTs**







Noise model with 6 ancilla

- 15 qubits (9+6)
- 126 Trotter steps (2nd order)
- Depolarizing errors for CNOTs
- 2E5 CNOTs
- 1.37E5 Z rotations
- Averaging 1,000 simulations per value of depolarizing error

R. Weiss, A. Baroni, J. Carlson, and I. Stetcu, arXiv:2404.00202 (2024)

Currently working with QuEra for implementing it on their hardware

Summary and outlook

- **Quantum computing can become a powerful method to describe the dynamics (reactions) of strongly interacting quantum many-body systems**
- **The hardware is continuously improving, with systems capable of surpassing classical capabilities in the next few years**
- **Description of dynamics has three steps that need to be performed with sufficient accuracy:**
  - State preparation
  - Time evolution
  - Computation of physical observables (measurements)
- **Nuclear physics is well suited to this approach (short-range interactions, many states need to be included, many competing channels)**
- **Our investigation using realistic gives a feeling of the computational burden that quantum hardware needs to be able to handle to solve nuclear reactions**
- **Still a long road ahead (hardware, algorithms)**

Collaborators: J. Carlson (LANL), A. Baroni (ORNL), R. Weiss (LANL)
Funding: Work made possible with support by Advanced Simulations and Computing Program (ASC-PEM).