Quantum algorithms for strongly-correlated chemistry and physics problems

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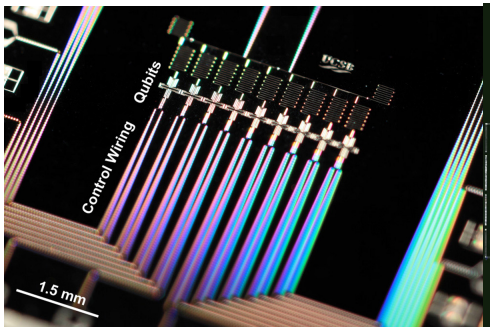
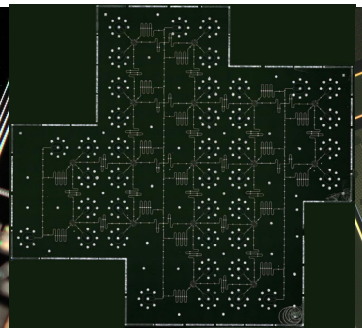
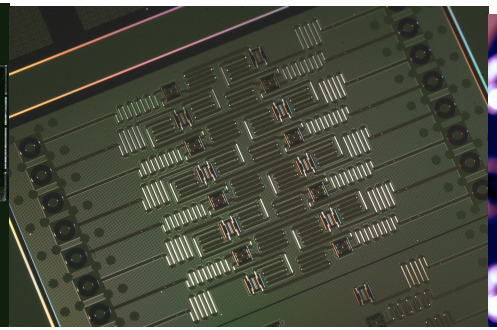
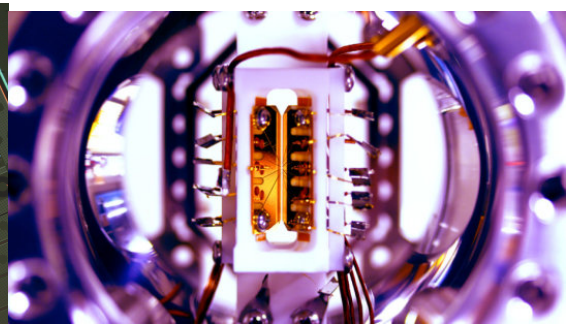
Outline

Quantum computing recap

- Replaces classical bit (either 0 or 1) with qubit (superposition of $|0\rangle$ and $|1\rangle$).
- N-qubit state requires $O(2^N)$ classical bits to describe.
- Will not *replace* traditional computers:
  - Cannot copy data (so no hard drives).
  - No advantage in performing basic mathematics.
  - More unstable / higher error rate.
- Instead, 'quantum speedup' for certain computational tasks.
- State of the art - 10-100 (physical) qubits, 100-1000 gates.

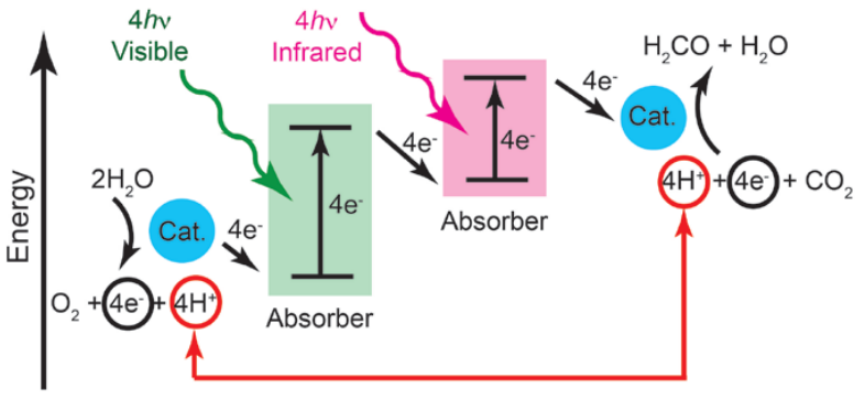


Google | Intel/QuTech | IBM | JQI Maryland

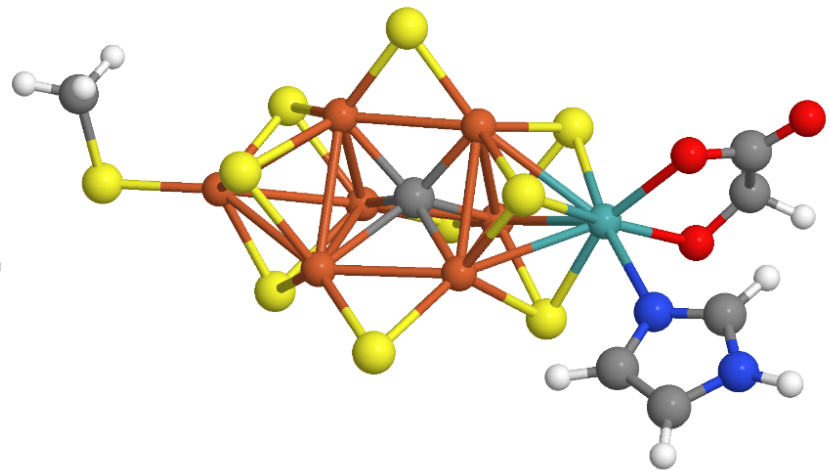
Representing quantum systems on a quantum computer

- Hamiltonian of a quantum system naturally maps to quantum computer.
- N spin orbitals/N spins $\rightarrow$ N qubits ($= 2^N$-dimensional Hilbert space).
- Need orthonormal wavefunctions.
- Need to rewrite Hamiltonian in qubit basis (e.g. via Jordan-Wigner).
- Largest cost - number of terms in Hamiltonian.



Purchase *et al*, 2014,

FeMoco

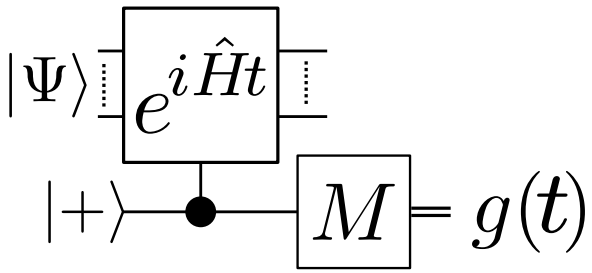


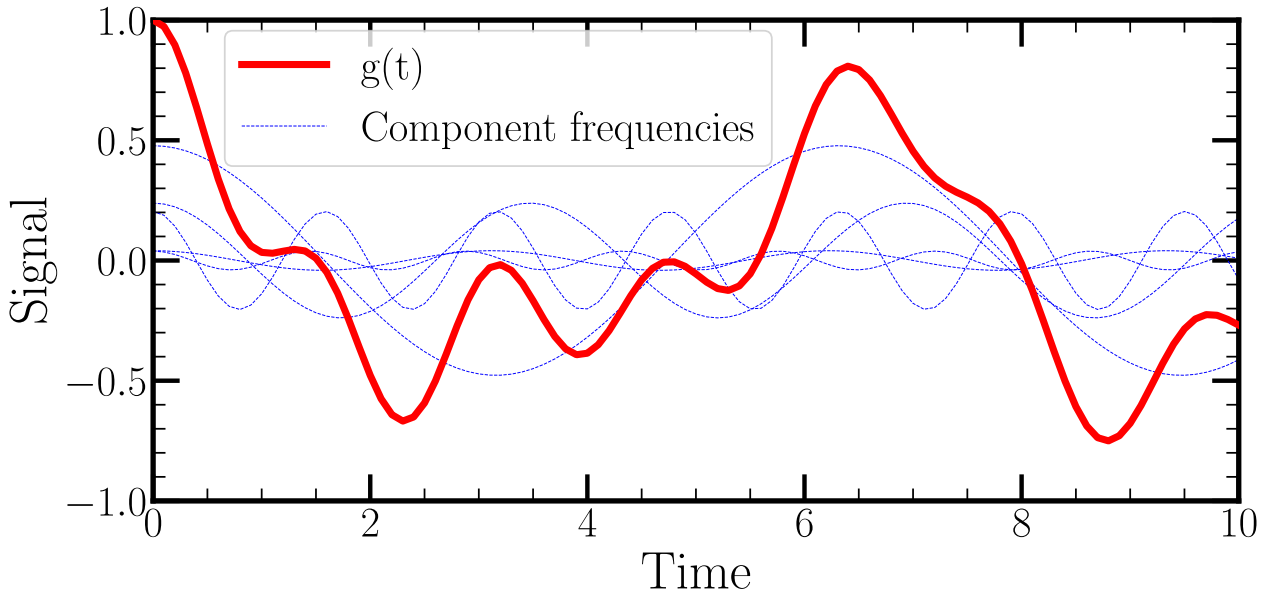
Reiher *et al*, 2017.

Quantum phase estimation

- Want system eigenenergies - solutions to $H|\Psi\rangle = E|\Psi\rangle$.
- Can imprint multiple E as frequencies of an ancilla qubit ('phase kickback').
- Extract in postprocessing like identifying notes in a chord.

$$|\Psi\rangle = \sum_j a_j |E_j\rangle \quad \rightarrow \quad g(t) = \sum_j |a_j|^2 e^{iE_j t}$$



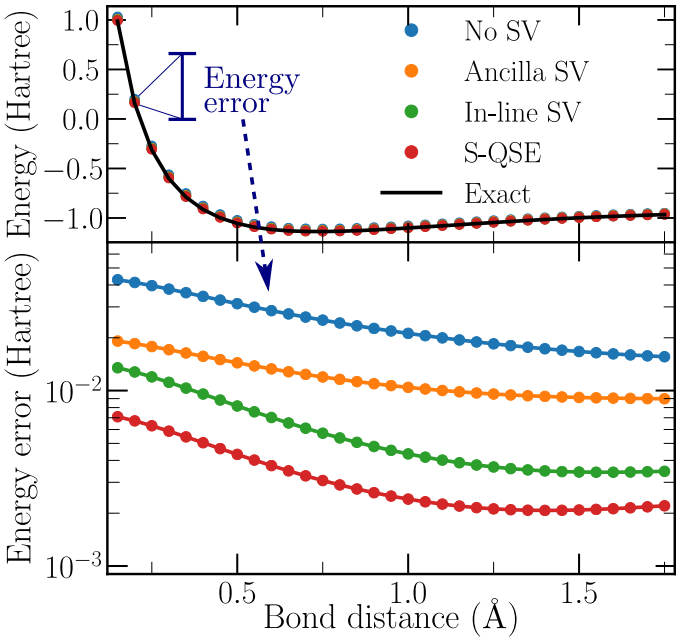


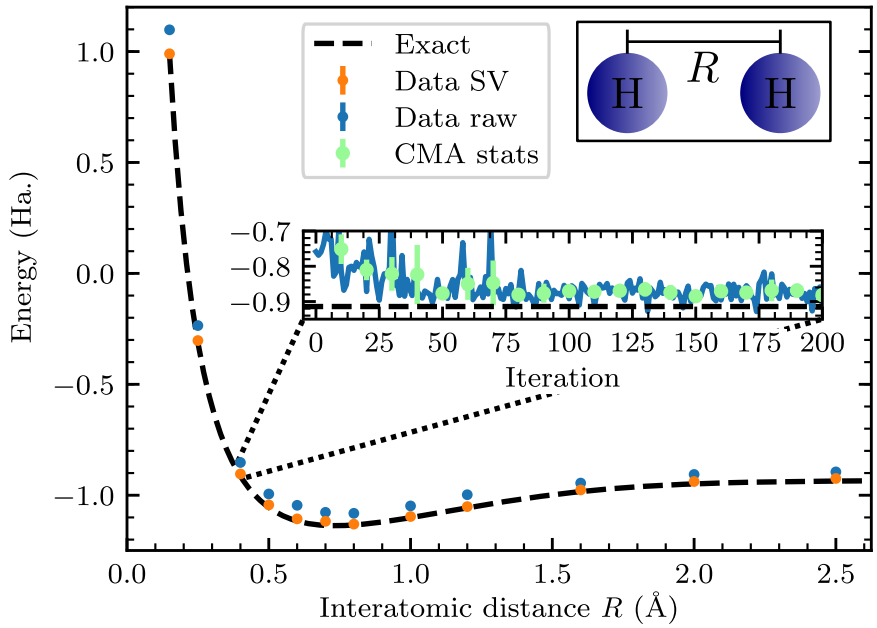
Variational quantum eigensolvers

- Approximate (ground state) ansatz $|\Psi(\vec{\theta})\rangle$ generated on a quantum register

$$|\Psi(\vec{\theta})\rangle = U(\vec{\theta})|\Psi_0\rangle.$$

- Low depth circuits, error mitigation possible - more feasible for near-term.

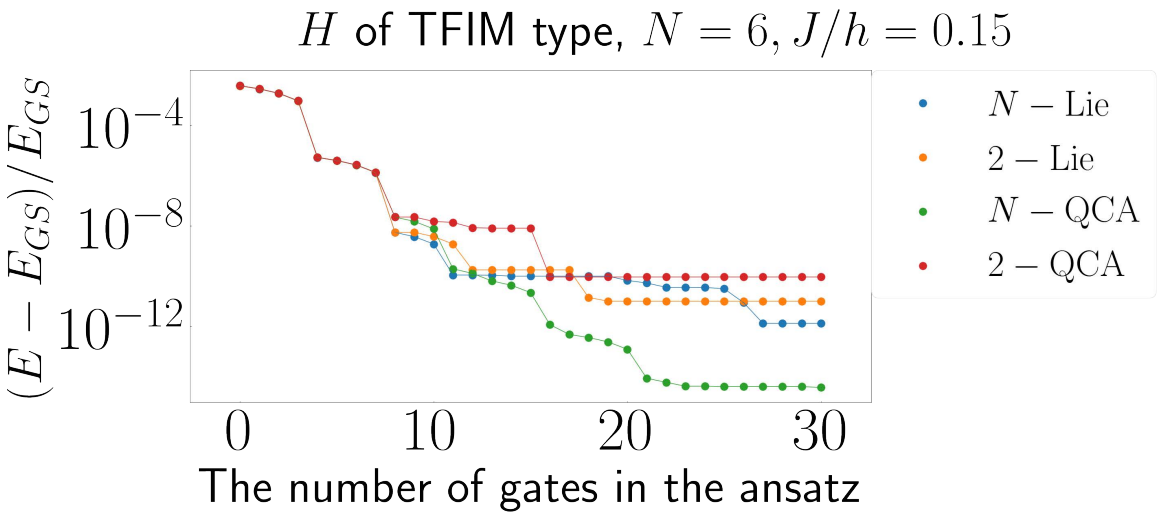




VQE design

- Typically write $U(\vec{\theta}) = \prod_i e^{iT_i\theta_i}$.
- Most popular choice - unitary coupled cluster - $T_i = \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_k \hat{c}_l + \text{h.c.}$.
- Can estimate relevance of T_i terms via perturbation theory on interaction JV

$$|\Psi(\vec{\theta})\rangle = |\Psi_0\rangle + O(\theta) + O(\theta^2) + \dots$$
$$\sim |GS(J)\rangle = |\Psi_0\rangle + O(J) + O(J^2) + \dots$$



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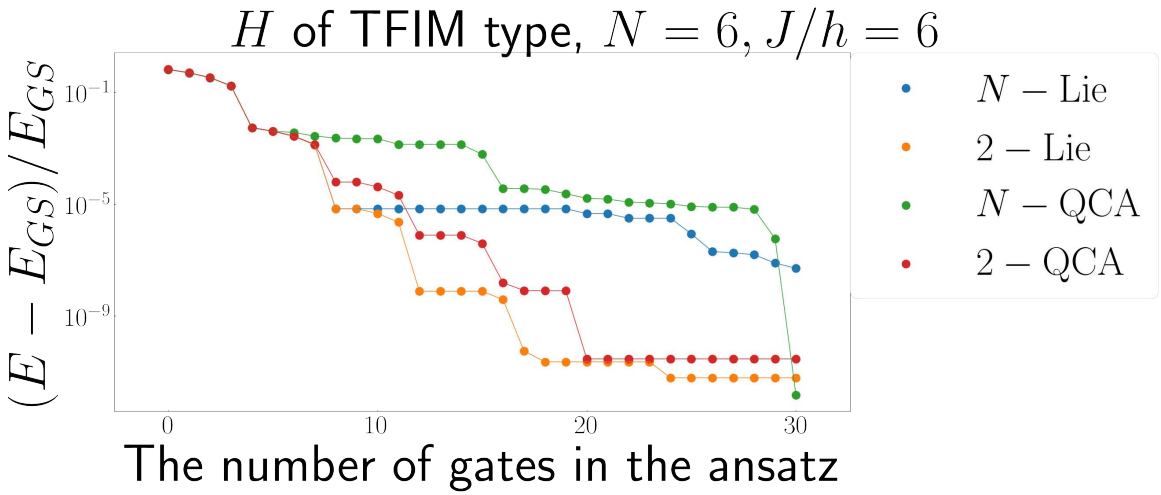

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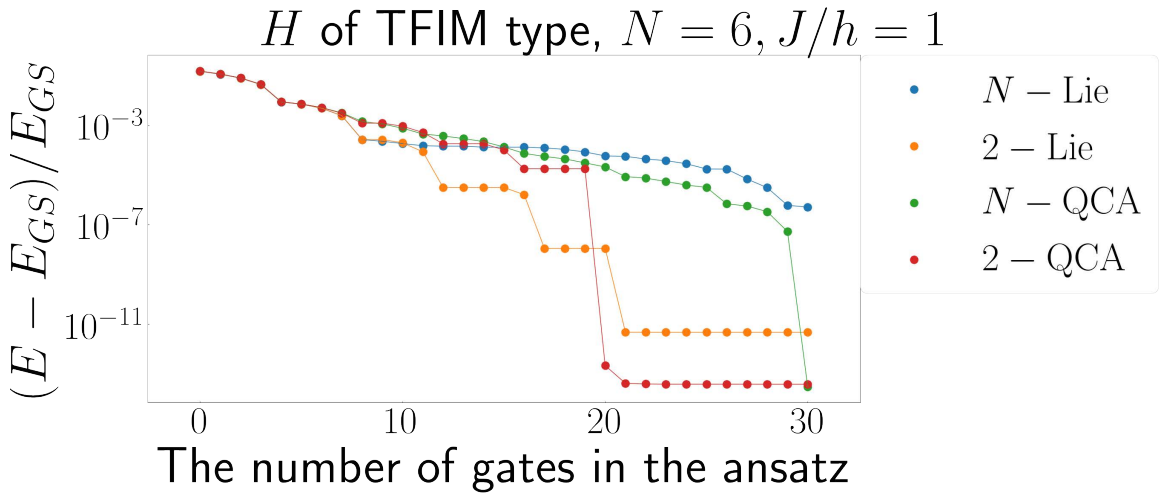


Hamiltonian simulation

- Want to evolve register by e^{iHt} for complex Hamiltonians H.
- Essential part of various other quantum algorithms (in particular QPE).
- Various methods exist
  - Trotterization - $e^{j\sum_i h_j t} \approx \prod_j e^{ih_j t}$.
  - Random quantum walks
  - Qubitization (reaches provable lower bounds in scaling)
- All methods suffer from rather large scaling and constant factors (error correction expected to be needed).

Whitfield *et al* 2009, Berry *et al* 2014, Low and Chuang 2017

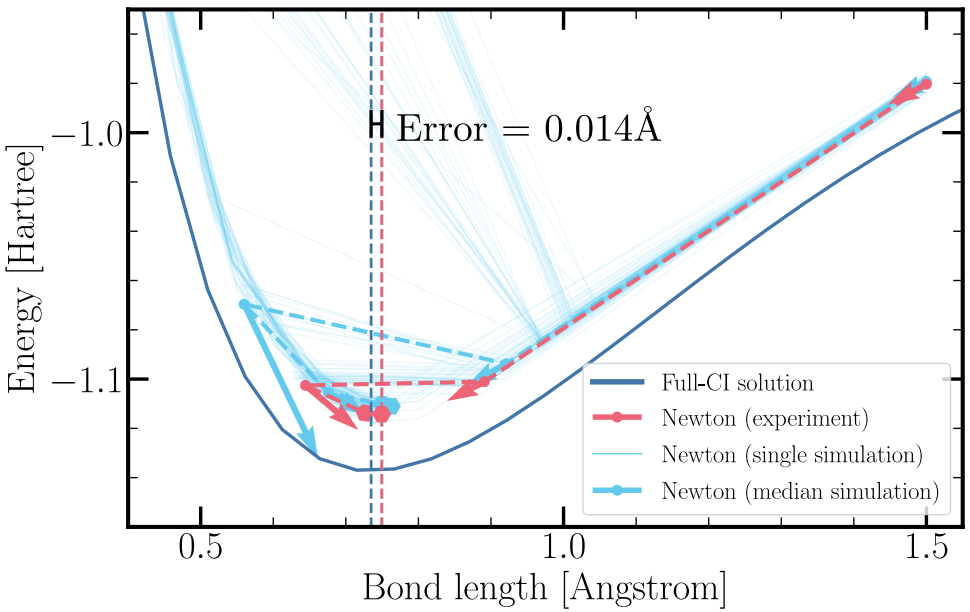
Excited state estimation

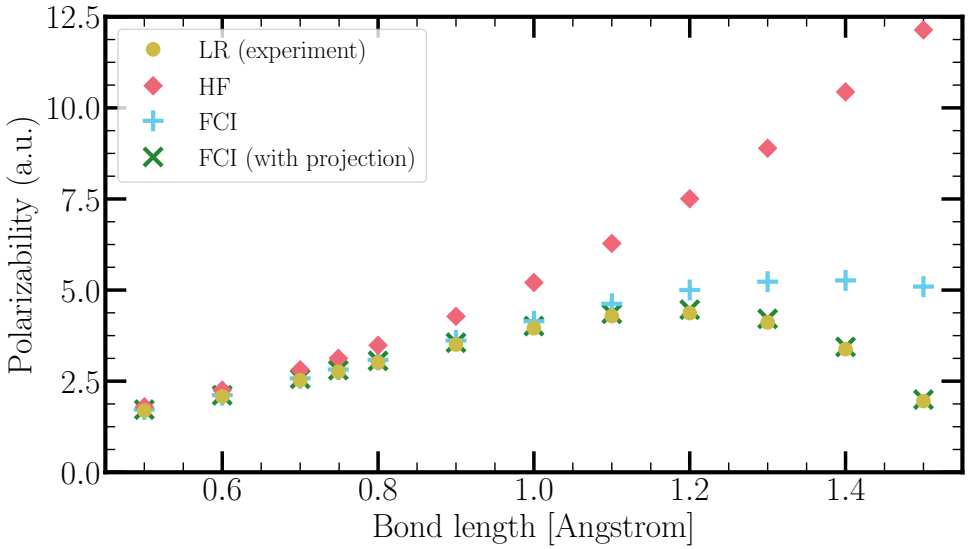
- Various methods to approximate $|\Psi_j\rangle$ above the ground state.
- *Quantum subspace expansion (QSE)* - $|\Psi_j\rangle \sim \hat{E}_j|\Psi_0\rangle$.
- *Witness-assisted variational eigenspectra solver (WAVES)* - measure phase accumulation with single-ancilla to optimize $\hat{E}_j|\Psi(\vec{\theta})\rangle$ as an eigenstate.
- *Overlap-based methods*: add penalty terms to VQE to minimize overlap with ground state.
- *Folded-spectrum methods*: calculate $(H - \alpha I)^2$ as function of α.

McClean *et al* 2017, Santagati *et al* 2018, Endo *et al* 2018, Higgott *et al* 2018, McClean *et al* 2016

Gradient estimation

- Want to estimate $\frac{\partial^n E_0}{\partial\lambda_1\partial\lambda_2\ldots}$ for some system parameters λ_i.
- λ_i might be
  - the position of an atom in a molecule
  - a coupling strength
  - an external perturbation (e.g. electric field)



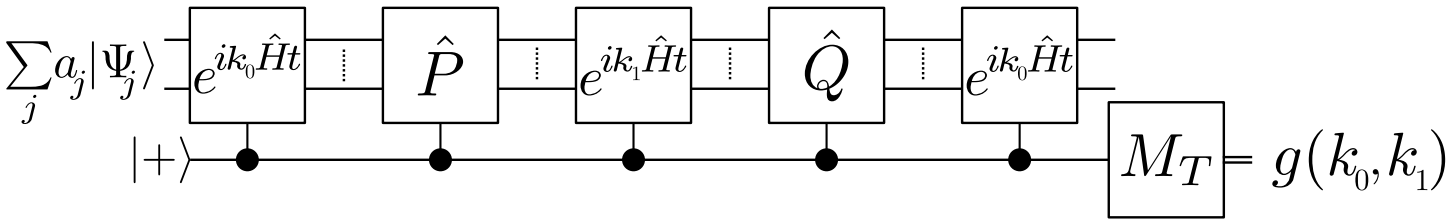


Gradient estimation - how?

- Perturbation theory - e.g. for second order

$$\frac{\partial^2 E_0}{\partial\lambda_1\partial\lambda_2} = \langle\Psi_0|\frac{\partial^2\hat{H}}{\partial\lambda_1\partial\lambda_2}|\Psi_0\rangle + \sum_{j\neq 0} 2\,\mathrm{Re}\left[\langle\Psi_0|\frac{\partial\hat{H}}{\partial\lambda_1}|\Psi_j\rangle\langle\Psi_j|\frac{\partial\hat{H}}{\partial\lambda_2}|\Psi_0\rangle\right]\frac{1}{E_0 - E_j}$$

- Phase and Propagator Estimation (PPE) - simultaneously measure $\langle\Psi_0|\frac{\partial\hat{H}}{\partial\lambda_1}|\Psi_j\rangle\langle\Psi_j|\frac{\partial\hat{H}}{\partial\lambda_2}|\Psi_0\rangle$ and energies E_j of the corresponding eigenstates $|\Psi_j\rangle$.



$$g(k_0, k_1) = \sum_{j,m,n} a_m^* a_n \langle\Psi_m|\hat{P}|\Psi_j\rangle\langle\Psi_j|\hat{Q}|\Psi_n\rangle e^{ik_0 t(E_m+E_n)} e^{ik_1 tE_j}$$

- Eigenstate Truncation Approximation (ETA) - take a set $|\tilde{\Psi}_j\rangle$ of approximate excited states and measure expectation values directly.

So when do we get all of this?

- $\sim 50 - 100$ qubits required before impossible to simulate classically.
- Simplest algorithms $\sim N - N^2$ depth - ~ 2500 gates required.
- Current state of the art: $\sim 20 - 50$ qubits, ~ 100 gates before decoherence.
- No known optimized circuits for near-term quantum computers yet. (?)
- With error correction, number of qubits increases to $\sim 10^5 - 10^6$.
- Error correction clock cycle also incredibly slow ($\sim 10 - 100$ μs for superconducting qubits, $\sim 10 - 100$ ms for ion traps).

The take-home

- Quantum computers should have an exponential advantage in simulating strongly correlated quantum systems.
- Algorithms are known for (incomplete list!):
  - Ground and excited state preparation
  - Time evolution
  - Gradient estimation
- Still some time before implementation.
- Algorithm optimization and near-term target identification highly desired!

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