November 9

Intro to Trotterization

- **Fermionic simulations can be mapped to unitaries**
  Recall that $u, u^\dagger$ are not unitaries

  Observe however H is hermitian ($H = H^\dagger$, follows from p, q, r, s being symmetric). Now from this we know that for H (hermitian), e^{-iH} is unitary.

  In order to get e^{-iH} to a gate form, Jordan-Wigner came up with definitions for $a, a^\dagger$. Consider our X, Y (Pauli) gates.
  $X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, $Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$. And now define,
  $a^\dagger = \frac{X-iY}{2} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$ and by definition $a = \frac{X+iY}{2} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$

  Now substitute the $a, a^\dagger$ and you'll see that H simplifies to,

  $H = \Sigma_{pq} h_{pq} \Sigma_{(\sigma_p, \sigma_q \in X, +/-iY)} \sigma_p \sigma_q + \Sigma_{pqrs} h_{pqrs} \Sigma_{(\sigma_p, \sigma_q, \sigma_r, \sigma_s \in X, +/-iY)} \sigma_p \sigma_q \sigma_r \sigma_s,$

  and h_{pq}, h_{pqrs} are the coefficients (probability?) that the Pauli strings are chosen.

  Now from the (lie-trotter-suzuki) product formulas we get,

  $e^{-i\sum_j^m H_j t} = \Pi_j^m e^{iH_j t} + O(m^2 t^2)$.
  O(m^2t^2) is the error term and observe how if m is big, the error scales in a bad way so instead trotter said we will break it into small (r) chunks and apply it r times (or "trotterize" it) - this helps it scale in a better way.
  $e^{-i\sum_j^m H_j t} = (\Pi_j^m e^{iH_j \frac{t}{r}})^r + O(\frac{m^2 t^2}{r})$.

- **Energy Level Derivation**
  We know that $H|\Psi_g >= E_0|\Psi_g >$, and now I'm claiming that $e^{-iHt}|\Psi_g >= e^{-iE_0 t}|\Psi_g >$.

  Proof: $e^{-iHt}|\Psi_g >= \Sigma_{k=0}\infty \frac{(-iHt)^k}{k!} e^{-iHt}|\Psi_g >= \Sigma_{k=0}\infty \frac{(-iE_0 t)^k}{k!} e^{-iHt}|\Psi_g >= e^{-iE_0 t}\Psi_g >$

  Now, just use QPE to extract this E_0 we embedded into the phase.

- **Review**
  You're given hamiltonian H and initial state $|\Psi_g >$. In order to simulate it, you will:

- convert hamiltonian into a sum of paul strings (X, Y, Z)
- separate the strings. implement their exponential forms
- use QPE to extract energy

The simulation problem (calm down, you don't need to fully understand this)

- Problem is that if t, m are large, the error $O(\frac{m^2t^2}{r})$ scales in a bad manner. Therefore, we can:
  - trotterize with large r's
  - employ higher-order trotter-suzuki formulas
  - reduce hamiltonian complexity
- how to prepare the initial state $|\Psi(x)>$?
  - hardware-informed techniques: what's easy to implement?
  - inspired from what truly is. It's called Unitary coupled cluster (UCC).

    $$T = \sum_{i=1}^{k} T_i, T_1 = \sum_{pq} h_{pq} a_p^\dagger a_q, T_2 = \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s \Rightarrow |\psi(\vec{h})\rangle = e^T|0\rangle$$

    Other methods include UCCS, UCCSD, UCCSDT.
- simulation in practice (caveats)
  - born-oppenheimer approximation - assumption: electrons are independent of the motion of nucleus
  - space complexity and connectivity - assume full connectivity if qubits
- alternatives
  - variational quantum eigensolvers
  - adiabatic simulation - set a physical hamiltonian within the qubits and observe the final state