• **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,

  $a^\dagger = \frac{X - iY}{2}$ 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,

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

  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,

  $e^{-i \sum_j H_j t} = \prod_j e^{i H_j t} + O(m^2 t^2)$.

  $O(m^2 t^2)$ 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.

  $e^{-i \sum_j H_j t} = (\prod_j e^{i H_j \frac{t}{r}})^r + O(\frac{m^2 t^2}{r})$.

• **Energy Level Derivation**

  We know that $H|\Psi_g> = E_0|\Psi_g>$, and now I’m claiming that $e^{-i H t} |\Psi_g> = e^{-i E_0 t} |\Psi_g>.$

  Proof: $e^{-i H t} |\Psi_g> = \sum_{k=0}^\infty \frac{(-i H t)^k}{k!} e^{-i H t} |\Psi_g> = \sum_{k=0}^\infty \frac{(-i E_0 t)^k}{k!} e^{-i H t} |\Psi_g> = e^{-i E_0 t} |\Psi_g>.$

  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 $O(m^2t^2)$ 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 $|\Psi(x)\rangle$?
  – hardware-informed techniques: what’s easy to implement?
  – inspired from what truly is. It’s called Unitary coupled cluster (UCC).

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

  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