Hamiltonian Simulation Part 2: Fermionic Simulation and Trotterization

Christopher Kang for CSE 490Q Au20

November 3rd

Learning Goals

1. **Understanding the premise of fermionic Hamiltonian simulation**
   a) Problem mapping
   b) Fermionic operators
2. **Understanding Trotterization**
   a) Jordan-Wigner transform and relevant circuits
   b) Error scaling and asymptotic bounds with the Lie-Trotter-Suzuki Formula
3. **Understanding the simulation pipeline**
   a) Full problem I/O
   b) State preparation

I: Problem & Relevance

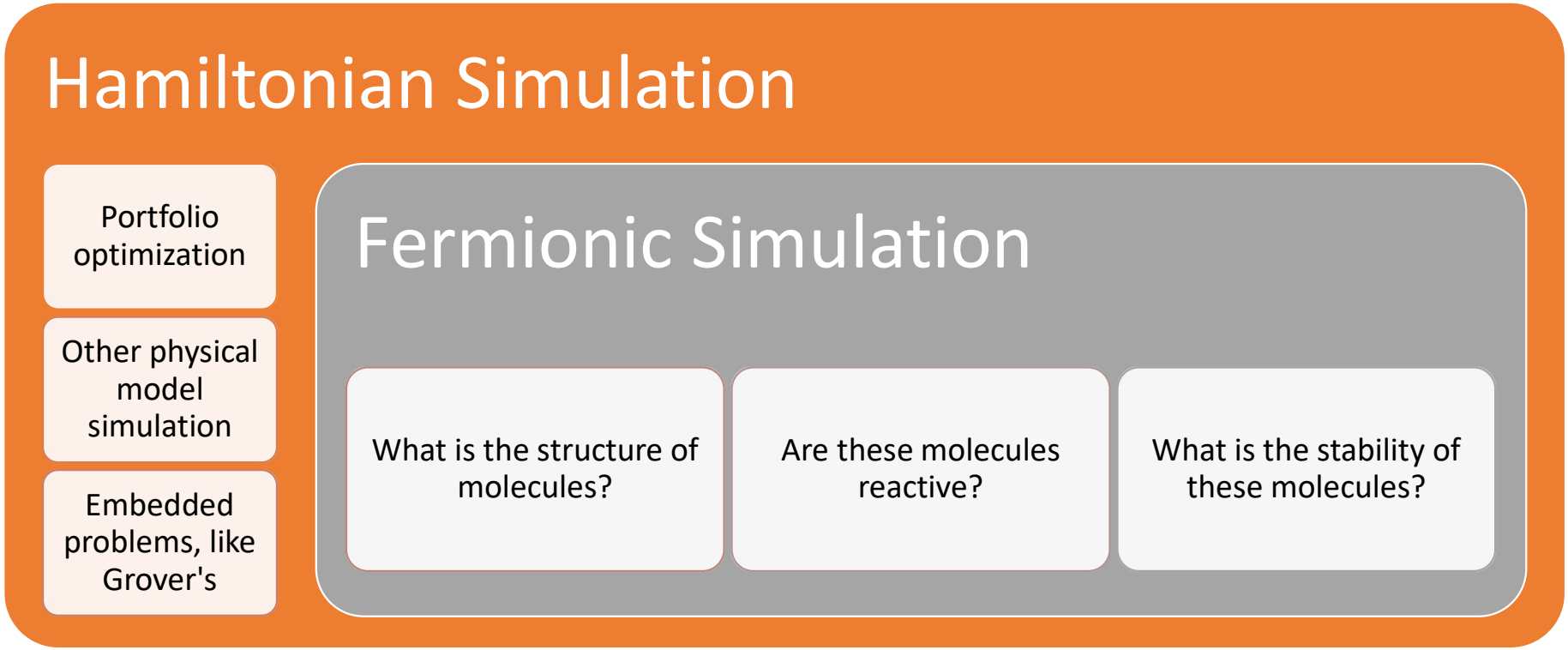
Introducing the context of Hamiltonian simulation, it's modern-relevance, and why quantum computers are necessary

Problem setup / relevance / classical algs

Questions

1. What is the problem of fermionic Hamiltonian simulation / its relevance?
2. What is the structure of a fermionic Hamiltonian?
3. Why do traditional algorithms fail?

Our focus: Fermionic Simulation



What is the problem?

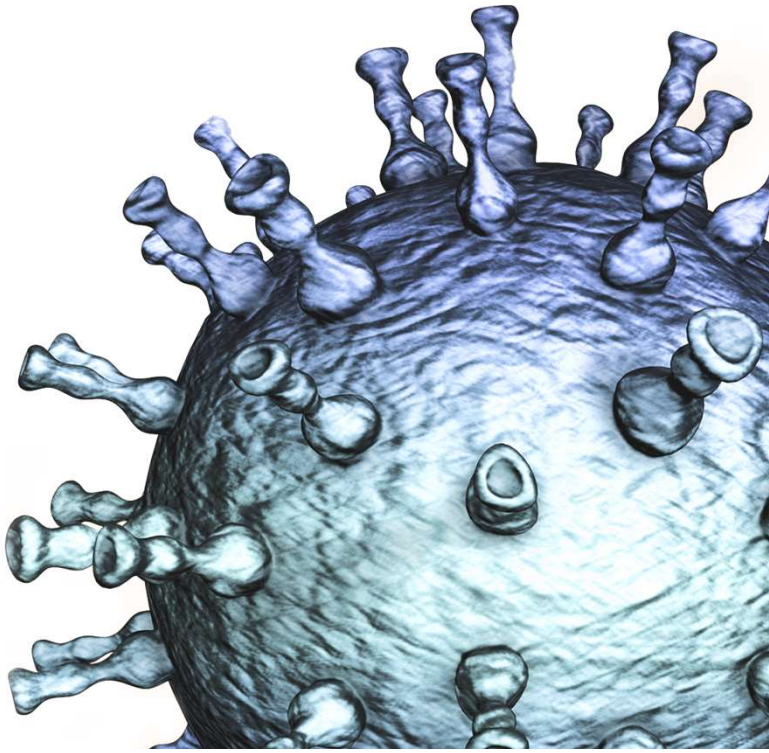
Key Chemistry Problem

- **Inputs**
  - *Fermionic Hamiltonian* (composition of annihilation/creation operators)
  - *Initial state constraints*, can parametrize this state as $|\psi(\vec{x})\rangle$
- **Output**
  - *Energy level of the state*, which we can use to identify…
  - *Eigenvectors* which represent ground electron configurations
- **Simplified**: Where did the electrons come from, where did they go? (Where did they come from configuration-eyed Joe)?

Case study: Vaccine Development

- **Context**
  - We are interested in **rapid vaccine development**
  - We have a few candidate molecules, but are unsure of which would be the best
  - We need to narrow down the candidates for clinical testing
- **Potential solution**
  - Simulating sample drugs would be cheaper, but would it be faster?

(Bottom right: rendering of the influenza virus)



Math of problem

- Given fermionic Hamiltonian H and parametrized state $|\psi(\vec{x})\rangle$, what $\vec{x}$ minimizes λ in:

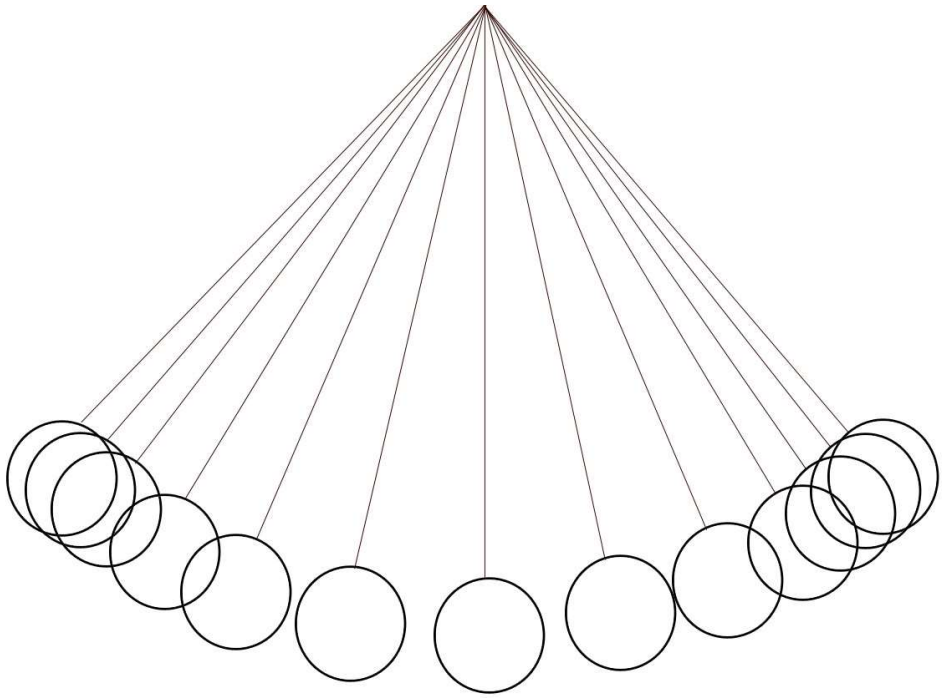
$$H|\psi(\vec{x})\rangle = \lambda|\psi(\vec{x})\rangle$$

- Note that energy from a quantum-mechanical perspective is a bit weird; **we set energy as the eigenvalue of a specific eigenstate** (λ).

Energy

- In a perfect pendulum, the system should have the same energy no matter where it's at
- Two quantities affect energy: **position** ($\vec{x}$) and **momentum** (p)
- Our Hamiltonian expresses dynamics – so, the eigenvalue accounts both

Energy operator, more info



What is the structure of the Hamiltonian?

Fermionic Operators + Mapping

- Two goals: create an electron or destroy an electron
  - "Creation" vs "Annihilation" operators
- Create: $a^\dagger$, destroy: a

$$a^\dagger = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, a = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

- Consider $|0\rangle$ as an unoccupied orbital and $|1\rangle$ occupied. Then,

$$a^\dagger|0\rangle = |1\rangle, a|1\rangle = |0\rangle$$

- (Confirm this for yourself)

Fermionic Hamiltonian

- Hamiltonian takes the following form:

$$H = \sum_{pq} h_{pq} a_p^\dagger a_q + \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

- "One-body terms", "Two-body terms"
  - One-body terms are just one electron making a jump; two-body terms are two electrons switching, jumping, etc.
- h_{pq}, h_{pqrs} are real-valued coefficients that assign likelihoods of specific jumps (for our purposes)

Test Your Knowledge

- Given:

$$H = a_0^\dagger a_1 + a_1^\dagger a_0, |\psi_0\rangle = |01\rangle, |\psi_1\rangle = \frac{1}{\sqrt{2}}[|01\rangle + |10\rangle]$$

- **Question**: What is $H|\psi_0\rangle$? $H|\psi_1\rangle$? Which is the stable state?
- **Answer**:
  - $H|\psi_0\rangle = |10\rangle$, unstable
  - $H|\psi_1\rangle = |\psi_1\rangle$, the stable state, energy of 1

Why do traditional algorithms fail?

Why do classical algorithms fail?

- H grows quickly
  - Increases the complexity of the Hamiltonian, as there are now more both one-body, two-body terms
- $|\psi(x)\rangle$ grows quickly
  - Each additional orbital doubles the number of potential configurations

- **Fun fact:** One *ab initio* ("from the beginning") simulation is Full Configuration Interaction (FCI), which scales **exponentially!**

Review:

Check your knowledge

1. What is the problem of fermionic Hamiltonian simulation / its relevance?
2. What is the structure of a fermionic Hamiltonian?
3. Why do traditional algorithms fail?

Going further

- What is $a^\dagger|1\rangle$? $a|0\rangle$? Does this answer make sense?
- Suppose that we know there are n orbitals and e electrons. How many potential electron configurations are there?

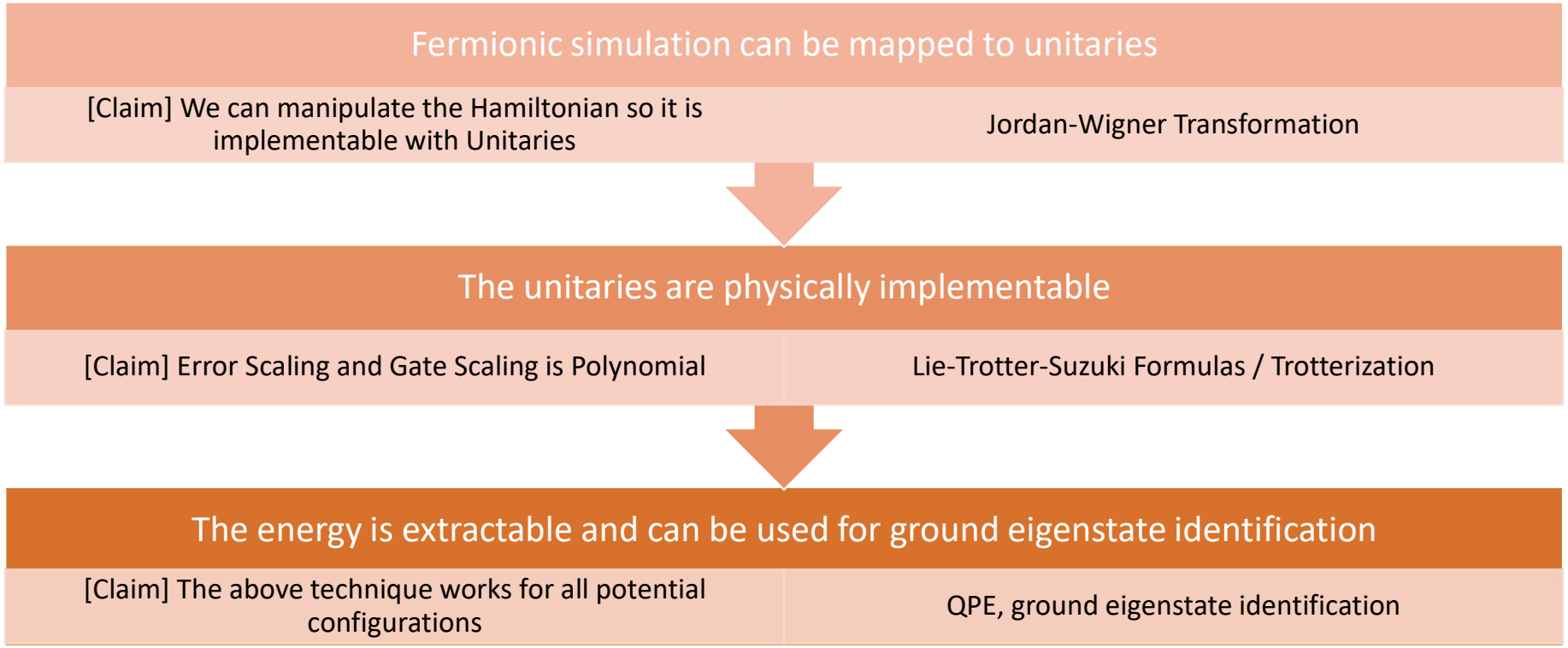
II: Introduction to Trotterization

Leveraging the Jordan-Wigner transformation, discussing the role of QPE in energy estimation, deriving some elementary bounds

Overview

- Physicists want to know the minimal energy λ associated with a Hamiltonian H
- They ask CS majors to simulate the associated energy of a given $|\psi\rangle$ via Trotterized QPE
- We can then generalize the technique to search for the best $|\psi\rangle$

Overview


Fermionic simulation can be mapped to unitaries
[Claim] We can manipulate the Hamiltonian so it is implementable with Unitaries
Jordan-Wigner Transformation
The unitaries are physically implementable
[Claim] Error Scaling and Gate Scaling is Polynomial
Lie-Trotter-Suzuki Formulas / Trotterization
The energy is extractable and can be used for ground eigenstate identification
[Claim] The above technique works for all potential configurations
QPE, ground eigenstate identification

Fermionic simulation can be mapped to unitaries

Mapping

- Recall $a^\dagger, a$ – they were not unitary!
- How do we implement these nonunitaries? Hamiltonian may not be:

$$H = \sum_{pq} h_{pq} a_p^\dagger a_q + \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

- **Observation**: H Hermitian ($H = H^\dagger$ by premise that $pq, pqrs$ symmetric)

Mapping pt2

- $a^{\dagger}, a$ not unitary, but we constrain H Hermitian by symmetry of $pq, pqrs$. Note-
- **Fact**: For some Hermitian matrix A, e^{-i} unitary.
- Thus,

$$e^{-\mathrm{iAt}}$$

- Unitary, *plus* it implements the time evolution of the state!

The unitaries are physically implementable

Jordan-Wigner Transformation

- **Question**: How do we get from e^{-iHt} to a gate form?
- **Answer**: Jordan + Wigner use a clever physics transformation:

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

- X, Y are our fundamental gates!! (Termed “Pauli” gates)

JW-Part 2

- What is the Hamiltonian after JW?

$$H = \sum_{pq} h_{pq} a_p^\dagger a_q + \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s \Rightarrow$$

$$\sum_{pq} h_{pq} a_p^\dagger a_q = \sum_{pq} h_{pq} (X_p X_q \pm i X_p Y_q \pm i Y_p X_q \mp Y_p Y_q)$$

- Try it yourself: can you identify the two-body term?

$$\sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s = ?$$

JW Part 3

- So, we can roughly do this:

$$H = \sum_{pq} h_{pq} \sum_{\sigma_p, \sigma_q \in \{X, \pm iY\}} \sigma_p \sigma_q + \sum_{pqrs} h_{pqrs} \sum_{\sigma_p, \sigma_q, \sigma_r, \sigma_s \in \{X, \pm iY\}} \sigma_p \sigma_q \sigma_r \sigma_z$$

- Where $h_{pq}, h_{pqrs} \in \mathbb{R}$, coefficients of the Pauli/σ strings chosen appropriately

- **Key question**: Uh, now where do we go? e^{-iHt} still not directly implementable on quantum chips!

Implementation?

- We don't have a $e^{-iH_0 t}$ gate!
- **Fact**: We have gates that can implement $e^{-iXt}, e^{-iY}, e^{-iZt}$
- **First idea**: Can we split the Hamiltonian? So,

$$e^{-it(a_1^\dagger a_2 + a_2^\dagger a_1)} = e^{-i\,(a_1^\dagger a_2)} e^{-it(a_2^\dagger a_1)}$$

And then implement a series of $e^{-iX}, e^{-iYt}, e^{-iZt}$?

- **Smart** 😳: "These are matrices! We are not guaranteed:"

$$e^{X+Y} = e^X e^Y$$

- What are we going to do?

Trotterization

- **Fact**: Lie-Trotter-Suzuki Product formulas

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

- If $t \ll 1$, error is minimal. Otherwise, we need to "Trotterize"

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

- Select $r \in \mathcal{O}(m^2 t^2)$ so that error is minimal (r is Trotter step size).

"Simulating Hamiltonian Dynamics," Microsoft Q# documentation

Implementation!

- So, if we can implement $e^{-i\sigma_p\sigma_q t}$ and $e^{-i\sigma_p\sigma_q\sigma_r\sigma_z t}$ for $\sigma \in \{X, Y, Z, I\}$, we can implement the Hamiltonian
- These may not seem implementable, **but they actually are!**
  - And you will implement them in a future homework assignment, with help from a paper by Whitfield, et al. 😁
- Each of these gates is implementable in linear gate complexity, so our time complexity scales with respect to m the size of H

The energy is extractable and can be used for ground eigenstate identification

Energy Level Derivations

- **Claim**: Given a fermionic Hamiltonian H and ground eigenstate $|\psi_g\rangle$ with $H|\psi_g\rangle = E_0|\psi_g\rangle$:

$$e^{-iHt}|\psi_g\rangle = e^{-iE_0 t}|\psi_g\rangle$$

- **Proof**: Recall the definition of a matrix exponential:

$$e^{-iHt}|\psi_g\rangle = \sum_{k=0}^{\infty} \frac{(-iHt)^k}{k!}|\psi_g\rangle = \sum_{k=0}^{\infty} \frac{(-iE_0 t)^k}{k!}|\psi_g\rangle = e^{-iE_0 t}|\psi_g\rangle$$

- **Implication**: QPE can be used to extract the energy level!

Full Pathway

I. Identify the Hamiltonian

II. Prepare a parametrized state $|\psi(\vec{x})\rangle$ with randomly chosen $\vec{x}$ and appropriate ψ

III. Use Trotterized Quantum Phase Estimation to estimate the associated energy.

IV. Leverage classical optimization schemes to tune $\vec{x}$ to minimize the energy from QPE (and repeat from II)

Ground eigenstate identification

- **Claim**: QPE can be used for ground eigenvectors and will have noticeable effects when non-ground eigenvectors are used.
- **Proof**: Suppose we are given a non-ground eigenvector $|\psi_0\rangle = c_g|\psi_g\rangle + \sum_i c_i|\psi_i\rangle$ where $|\psi_g\rangle$ is the ground eigenvector, $|\psi_i\rangle$ are eigenvectors, and $c_g, c_i \in \mathbb{C}$.
- Then, by Trotterization, we will yield

$$e^{-iHt}|\psi_0\rangle = c_g e^{-iE_g t}|\psi_g\rangle + \sum_i c_i e^{-iE_i t}|\psi_i\rangle$$

- QPE will thus extract E_g, E_i with some probability. By minimality, $\forall i, E_g < E_i$. Thus, check that we don't have high E_i.

Review

- **Question**: You are given a Hamiltonian H and initial state $|\psi\rangle$. Describe, high level and step by step, the process of simulation

- **Answer**:
  1. Convert the Hamiltonian to a sum of Pauli-strings (X, Y, Z)
  2. Separate the strings and implement their exponentiated form
  3. Apply QPE to estimate the energy

III. The Simulation Pipeline

Summarizing our work, selecting hyperparameters, state preparation, implementing

Disclaimer

- This section is more for curiosity, you don’t need to fully understand concepts discussed

Overview

Algorithm Optimization	• What do we do when t large? • What do we do as H grows?
State Preparation Techniques	• What strategies exist for state preparation? • What is the asymptotic cost?
Simulation in Practice	• What is the pipeline / alternatives? • What are the caveats of this approach?

Algorithm Optimization

Overcoming challenges

- **Challenge**: If t large, $\mathcal{O}\left(\frac{m^2t^2}{r}\right)$ grows quickly
- **Challenge**: If m large, $\mathcal{O}\left(\frac{m^2t^2}{r}\right)$ grows quickly
- **Solutions**:
  - Select sufficiently large r (with $r \in \mathcal{O}(m^2t^2)$ at cost of gates)
  - Employ higher-order Trotter Suzuki Formulas (at cost of gates)
  - Reduce Hamiltonian complexity (reduces m at cost of accuracy)

State Preparation Techniques

Ansatz Preparation

- Our $|\psi(\vec{x})\rangle$ is called the "Ansatz" (German for ~initial guess)
- **Challenge**: How do we select ψ so that $|\psi(\vec{x})\rangle$ physically relevant?
- **Solution**: Employ theoretical chemists!
  - **Hardware-Informed Techniques**: Essentially, what's easy for my quantum computer to implement?
  - **Unitary Coupled Cluster (UCC)**: Physically-Inspired; what is realistic for an electron configuration? Takes the following forms:

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

  - T_k generalize to higher orders
  - Fun names like UCCS (singles), UCCSD (doubles), UCCSDT (triples) ….

Simulation in Practice

Caveats / Alternatives

- **Fundamental Caveats to Simulation**
  - **Born-Oppenheimer Approximation** – we assume electronic configuration can emerge independent of motion in the nucleus. This may affect structure/reactivity estimates
  - **Space complexity and connectivity** – we assume full connectivity of qubits in implementation and the number of qubits required, while linear with respect to number of orbitals, still is large
- **Alternatives**
  - **Variational Quantum Eigensolvers** (VQEs) – happy to talk 1:1 about these, outside the scope of our lecture
  - **Adiabatic Simulation** – set a physical Hamiltonian within the qubits and observe the final state they evolve into

Vocabulary

- **Annihilation operator**: operator deleting an electron from an orbital
- **Creation operator**: operator creating an electron in an orbital
- **Fermion**: general class of subatomic particle that includes electrons
- **Fermionic Hamiltonian**: matrix describing the dynamics of the electronic configuration
- **Trotterization**: An approach which segments an exponentiated matrix into a series of smaller exponentiated matrices with minimal error

The Hamiltonian is a ~Derivative for a DifEq

- Aside: True simulation problem says:

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

- We are saying that H is a discretization and

Review Questions

Explicit knowledge

- What are the two basic fermionic operators and their matrices?
-

Deeper knowledge

- Why do the fermionic operator matrices make sense?
- What is $a^\dagger|1\rangle$ or $a|0\rangle$? Why does the answer make sense?