CMPT 478/981 Spring 2025
Quantum Circuits & Compilation

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Today's agenda

- Paper discussion (Classical oracles)
- Time evolution ("Quantum" oracles)

Time evolution

Hamiltonian simulation

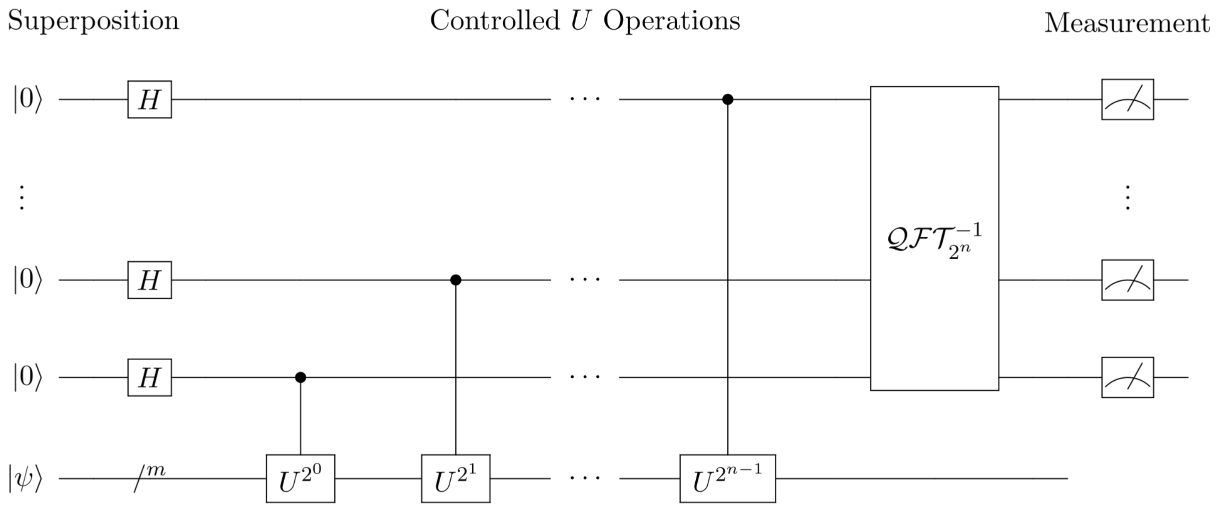
- Quantum computing's "killer app"
- Idea is to simulate a quantum mechanical system with a quantum computer
- Works by implementing the time evolution operator $U(t) = e^{-iHt}$ where H is a Hermitian matrix called the system's Hamiltonian
- Compilation of U(t) depends on the Hamiltonian but generic results exist

Theorem-ish (Lloyd, 1996)

A k-local Hamiltonian can be implemented in poly-time (ish)

Example: Ground state estimation

- Use phase estimation (i.e. Shor) to estimate an eigenvalue of Hamiltonian
- Replaces modular multiplication with time evolution operator U(t)



Implementing the time evolution operator

- In chemistry contexts, usually a fermionic Hamiltonian

$$H = \sum_{p,q} h_{pq} \hat{a}_p^\dagger \hat{a}_q + \sum_{p,q,r,s} g_{pqrs} \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s$$

- Apply a mapping to spin (Pauli) operators to get

$$H' = \sum_i s_i P_i + \sum_{i,j} d_{ij} P_i P_j + \ldots$$

- **Problem: Pauli terms don't commute, i.e. e^{A+B} =/= $e^A e^B$**

Classic solution: Product formulas

- Trotter formula gives limit of e^{A+B} as many alternations of fractions of $e^A e^B$

$$e^{i(A+B)t} = \lim_{n\to\infty} (e^{iA/n} e^{iB/n})^n$$

- Basic idea: select small enough n=epsilon to give good enough error bound
- Result is a **looooong,** repeating string of Pauli exponentials around small angles

Pauli exponentials

- Recall: Cliffords map Paulis to Paulis
- Given e^{-iPt} for Pauli P, diagonalize as $Ce^{-i(I \otimes I \otimes \ldots \otimes I \otimes Z)t}C^{\dagger}$
  - $\Rightarrow$ Implement as Clifford basis change + single-qubit Z rotation

Pauli partitioning

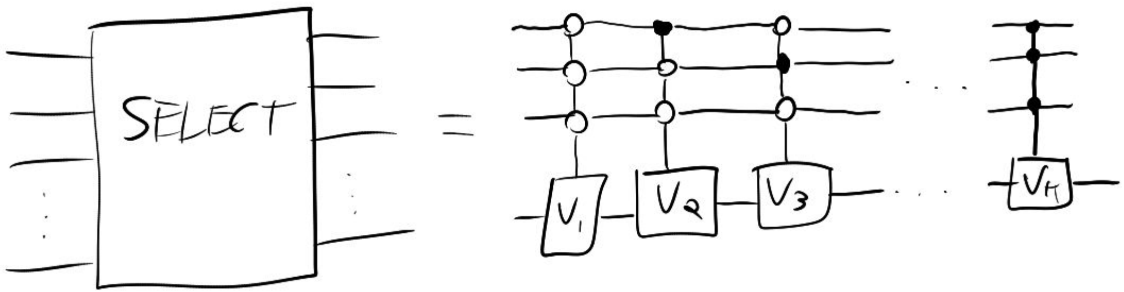
- Important optimization in both NISQ & FTQEC regimes
- Problem: Given a spin Hamiltonian H, break up into minimal number of commuting subsets of Paulis
  - E.g. H = ZXZ + IZI + IIX + XZX → {ZXZ}, {IZI, IIX, XZX}
- Commuting subset can be simultaneously diagonalized!
  - Map first Pauli to ZI…I
  - Remaining Paulis only have Z in first qubit, so iterate on next n-1 qubits
  - Result is a set of tensor products of Z
    - → Exponential is a phase polynomial! More on optimizing those later…

Implementing commuting Paulis

- Result is some set {P} of Z-type Paulis
  - $e^{-iaZiZjZk}|x\rangle = e^{-ia(xi \oplus xj \oplus xk)}|x\rangle$, i.e. Phase polynomial!
- How to iterate through linear functions of n bits?
  - Gray code!
- In general don't need all linear functions, so can we do better?
  - Heuristically, yes (Gray-synth, Amy Azimzadeh & Mosca "On the CNOT-complexity of CNOT-phase circuits)
  - NP-hard in special cases
  - Complexity of general case still unknown

Modern solutions: linear combinations of unitaries

- Modern alternative to product formulas is to use Linear Combination of Unitaries (LCU) in various ways
- Basic idea: to implement the sum aU + bV of unitaries
  - (PREPARE) Prepare a register in the state a|0> + b|1>
  - (SELECT) Apply a quantum multiplexor which sends |0>|ψ> → |0>U|ψ> and |1>|ψ> → |1>V|ψ>



Hamiltonian simulation “algorithms”

- = methods of compiling a unitary circuit approximating time evolution
- Product-formula based
  - Product formulas
  - Multi-product formulas
  - Higher-order product formulas
  - QDrift
- LCU-based
  - Taylor series approximation
  - Quantum Signal Processing
  - Qubitization

Compiling time evolution operators

- Non-trivial task to automate due to
  - calculation of error bounds
  - calculation of e.g. roots of high degree polynomials (QSP)
  - combinatorial explosion of parameters & combinations of techniques
    - Jordan-Wigner vs Bravyi-Kitaev vs direct Fermionic Hamiltonian
    - ~6-7 algorithmic frameworks each with choices within
    - Possibility to combine techniques for separate parts of the Hamiltonian
    - Different models of Hamiltonians & qubit reduction techniques

- Goal for compilers is to automate at least some of the frequent tasks
  - LCU/block encodings
  - Grouping & compiling sequences of Pauli exponentials

Readings for next week

- Posted to the website
  - Childs et al., *Toward the first quantum simulation with quantum speedup*. arxiv.org:1711.10980
    - Focus on the main paper & understand the high-level structure of the various algorithms
    - You may skip over the derivation and analysis of error bounds
  - Nam, Su, Maslov, *Approximate Quantum Fourier Transform with O(nlog(n)) T gates*. arXiv:1803.04933
    - Pay attention here to the **use of an adder to implement the phase gates**
  - Campbell, *A random compiler for fast Hamiltonian simulation*. arXiv:1811.08017
- As before send me a short (paragraph or two) summary of **ONE (1)** paper of your choice before next class and be prepared to give a short summary of any of the papers in class