Quantum Chemistry on Quantum Computer

Guoqing Zhou, Yuzi He

Quantum Computing

Qubit: superposition state

$$\alpha|0> + \beta|1>$$

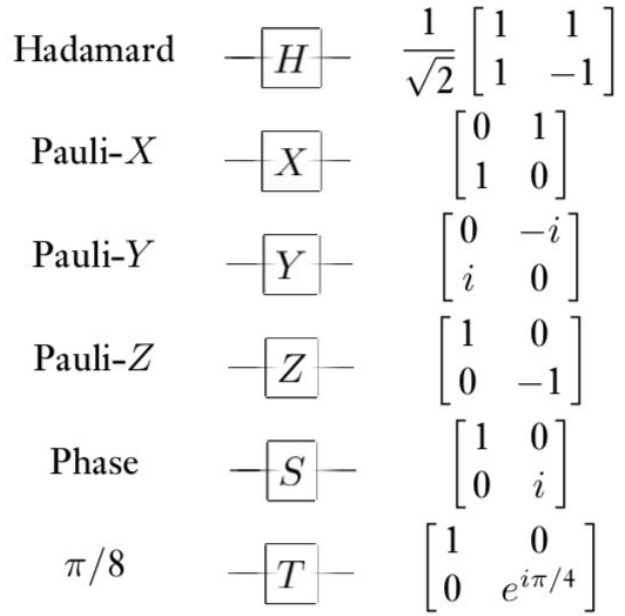
Quantum logical gate: Unitary Operator:

$$U^* U = 1$$

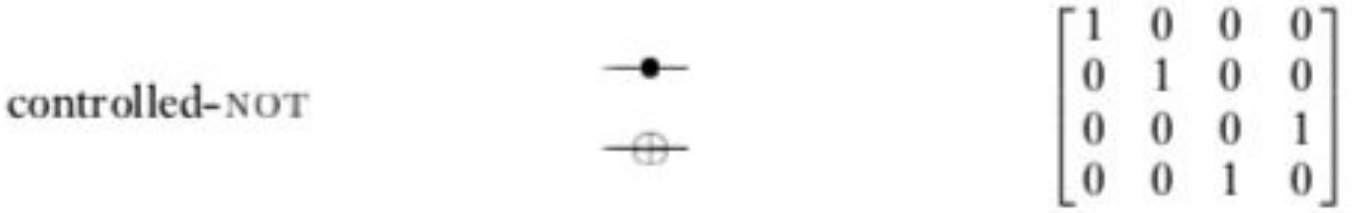
Physical Systems: ionic, photonic, superconducting and solid state systems.

Some Quantum Logical Gates

1 qubit:



2 qubits



Decompose the time evolution operator $\hat{U}$

Time evolution operator:

$$\hat{U}(t) = \exp(-i\hat{H}t)$$

1. Second-quantization
2. Transformation of the fermionic operators to spin variables
3. Exponentiation of the Hamiltonian
4. Circuit representations of the unitary propagator

1. Second quantization

Hartree-Fock Method

$$\hat{H} = \sum_{p,q} h_{pq} \hat{a}_p^+ \hat{a}_p + \frac{1}{2} \sum_{p,q,r,s} h_{pqrs} \hat{a}_p^+ \hat{a}_q^+ \hat{a}_r \hat{a}_s$$

$$h_{pq} = \int dx \chi_p^*(x) (-\frac{1}{2}\nabla^2 - \sum_\alpha \frac{Z_\alpha}{r_{\alpha x}}) \chi_q(x)$$

$$h_{pqrs} = \int dx_1 dx_2 \frac{\chi_p^*(x_1)\chi_q^*(x_2)\chi_r(x_2)\chi_s(x_1)}{r_{12}}$$

$\chi_q(x)$ **: single-particle basis**

Mapping from state space to qubits

|0> : occupied, |1> : unoccupied

Required N qubits for a system with N spin-orbitals

2. Transformation of the fermionic operators to spin variables: Third Quantization

Jordon-Wigner Method:

$$\hat{a}_j \rightarrow \mathbf{1}^{\otimes j-1} \otimes \hat{\sigma}^+ \otimes (\hat{\sigma}^z)^{\otimes N-j}$$

$$\hat{a}_j^+ \rightarrow \mathbf{1}^{\otimes j-1} \otimes \hat{\sigma}^- \otimes (\hat{\sigma}^z)^{\otimes N-j}$$

$$\hat{\sigma}^z = |0><0| + |1><1|$$

$$\hat{\sigma}^+ = |0><1|$$

$$\hat{\sigma}^- = |1><0|$$

Other Methods: Bravyi-Kitaev, Bravyi-Kitaev super fast

McClean, Jarrod R., et al. "OpenFermion: The Electronic Structure Package for Quantum Computers." *arXiv preprint arXiv:1710.07629* (2017).

3: Exponentiation of hamiltonian

Trotter-Suzuki decomposition:

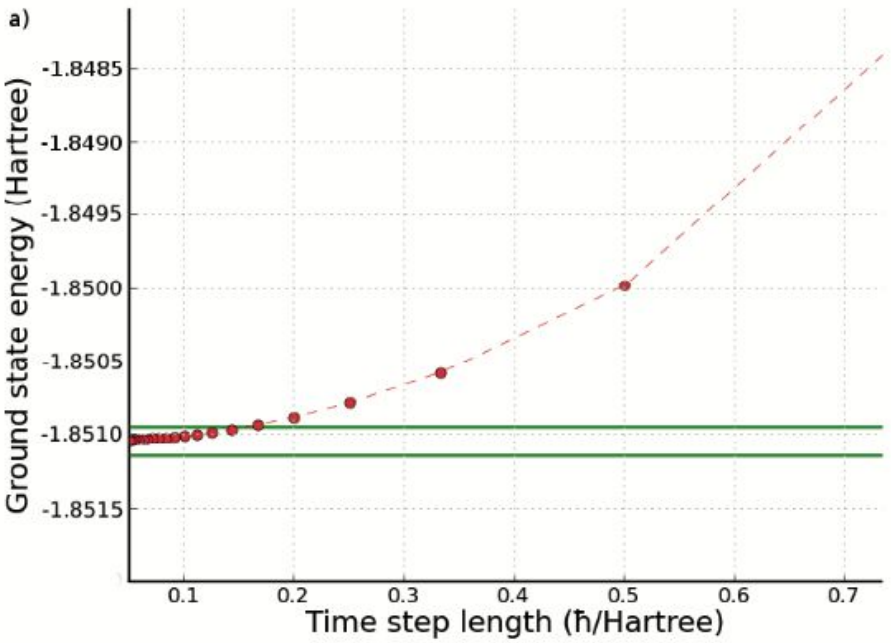
$$\hat{\mathbf{H}} = \sum_{i=1}^{N} \hat{h}_i$$

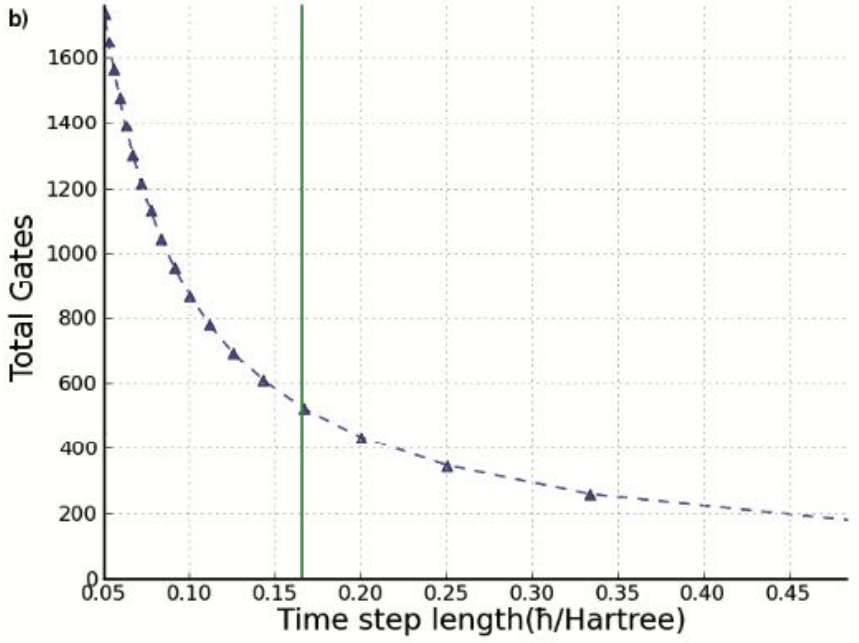
$$\hat{U}(t) = e^{-i\hat{H}t} = (e^{-i\hat{h}_1 dt} e^{-i\hat{h}_2 dt} \cdots e^{-i\hat{h}_N dt})^{\frac{t}{dt}} + O(dt^2)$$

Approximation becomes exact as:

$$T_n = t/dt \to \infty$$

3: Exponentiation of hamiltonian





Error with respect to the time step, and number of quantum logical gates required with given time step for the calculation of Hydrogen molecules

4: Circuit representation of the unitary propagator

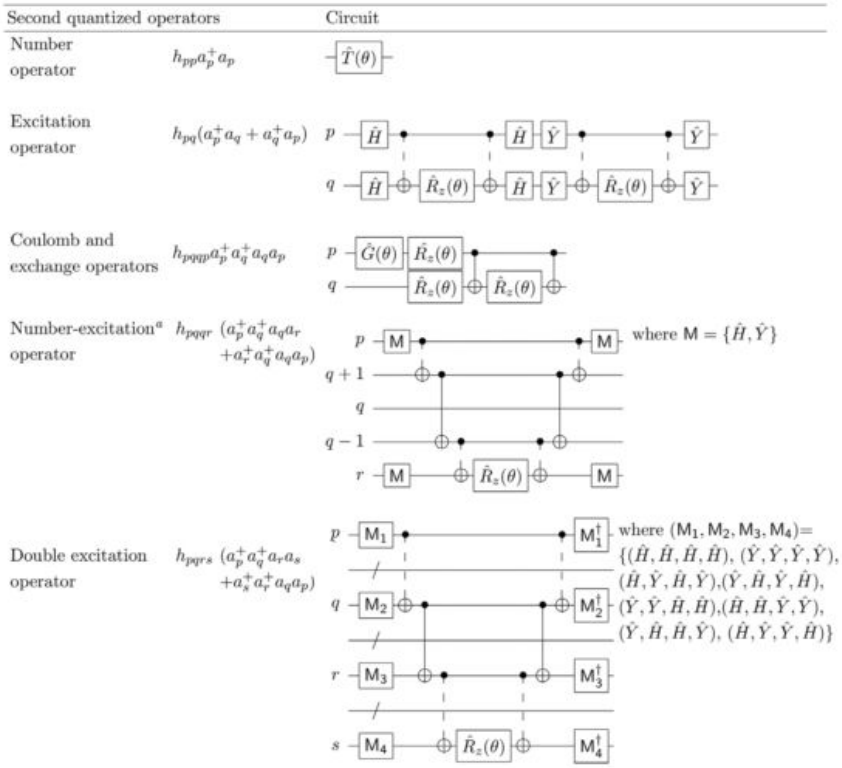
Unitary operator: $\hat{U}(dt)$

Controlled Unitary: $c - \hat{U}(dt)$

Control qubit is 1, then propagate

$$|1, \psi > \rightarrow \hat{U}|1, \psi >$$

If it is 0, don't propagate



Require $O(N^5)$ quantum logical gates without considering error correction.

Calculation of Hydrogen molecule

Bisis: STO-3G, |1s>, with spin, there are 6 spin-orbitals

Due to the symmetries, Hamiltonian is block-diagonal, with dimensions 1, 1, 2, 2

The problem is reduced to estimate the eigenvalues of 2 by 2 matrices.

The iterative phase estimation algorithm (IPEA) is used to evaluate the energy.

Eigenstates preparation:

for hydrogen molecules, known from symmetry requirement.

Generally, one can use adiabatic state preparation technique

Quantum Phase Estimation

In this section, I will explain the the method used to estimate quantum phase in detail.

Suppose we have obtained a eigenstate of a given hamiltonian *H*

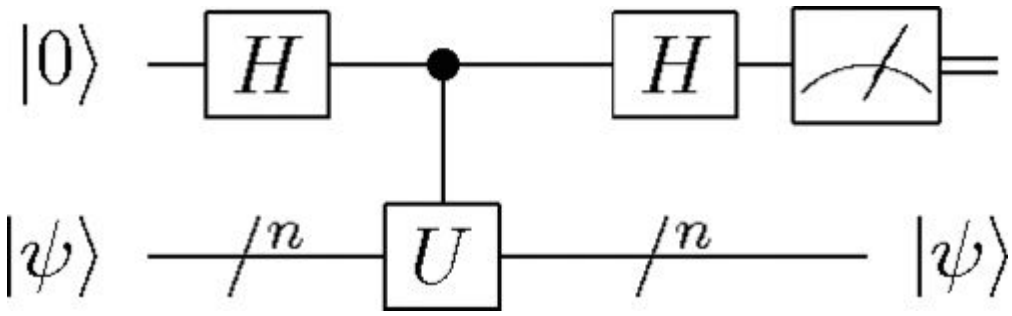
Under the time translation operator, the eigenstate will behave as *U = exp(-* i*Ht/ħ)*,

$$U\left|\psi\right\rangle = e^{-iEt/\hbar}\left|\psi\right\rangle = e^{i2\pi\phi}\left|\psi\right\rangle$$

This indicates that by measuring phase angle and the time interval which the operator *U* is applied, we are able get the eigen energy *E.*

Naive Version of Iterative Phase Estimation Algorithm (IPEA)

Consider the following quantum circuit:



Right before measuring, the state is $\frac{1}{2}[(1+e^{i2\pi\phi})|0\rangle+(1-e^{i2\pi\phi})|1\rangle]|\Psi\rangle$

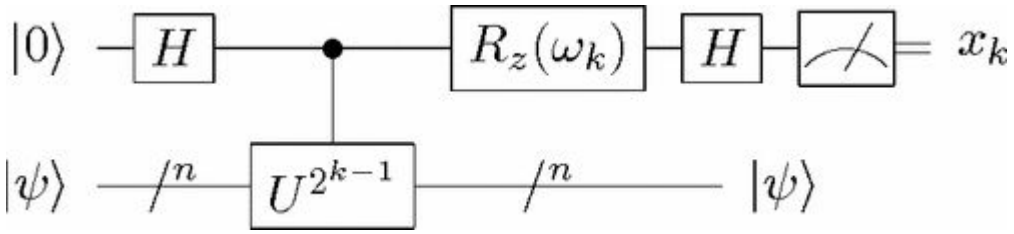
Which implies the probability of getting state 0 is $P_0=\cos^2(\pi\phi)$

Assume *N* experiment, the accuracy of P0 is 1/sqrt(N). For m digits of phase angle,

We need 2^(2m) measurements.

Kitaev's Imporved IPEA

Assume we can apply U multiple times. Rz is can adjust the phase between 0, 1.



By definition phase angle satisfis $0 \leq \phi < 2\pi$

We expand it into binary digits, ex. 0.f1f2f3f3f5…, fi = 0, 1

If we do the measurement now, the probability of getting 0 is given by

$$P_0 = \cos^2(\pi(2^{k-1} - \omega_k))$$

Kitaev's Imporved IPEA (Cont.)

We plug in the binary form of the phase angle,

$$2^{k-1}\phi - \omega_k = (f_1 f_2 \dots f_{k-1} . f_k f_{k+1} \dots) - \omega_k$$

Let $\omega_k = (0.0 f_{k+1} f_{k+1})$

$$P_0 = \cos^2(\pi(2^{k-1}\phi - \omega_k)) = \cos^2(\pi(0.f_k))$$

This probability is dermistic.

Method: Start from the last digit of the phase, repeat measurements.

Put the previous results into phase adjuster Rz. Repeat till the first digits is recovered.

Kitaev's Imporved IPEA Accuracy

In real life, the binary expansion of phase angle is not exact.

The reminder is $\delta 2^{-m}, 0 \leq \delta < 1$

Assuming all previous measurements are correct, the probability of current measurement to be correct is

$$P_k = \cos^2(\pi 2^{k-m-1}\delta)$$

The probability of correctly measuring all m digits are given by

$$P(\delta) = \prod_{k=1}^{m} P_k = \frac{\sin^2(\pi\delta)}{2^{2m}\sin^2(\pi 2^{-m}\delta)},$$

This probability is lower bounded by $P(1/2) = 4/\pi^2$