Quantum Chemistry on Quantum Computers

#4 Fermion–Qubit Transformation and Quantum Circuit Constructions

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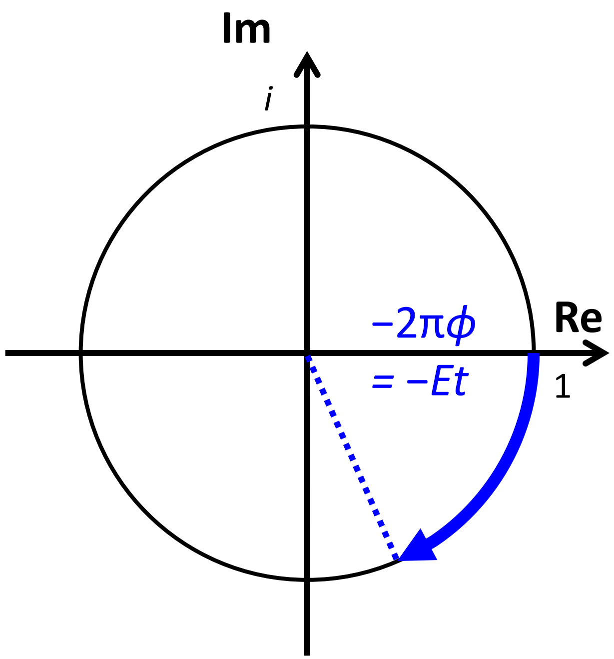
Basic idea of QPE for quantum chemistry

$$\exp(-iHt)|\Psi\rangle = \exp(-iEt)|\Psi\rangle = \exp(-i2\pi\phi)|\Psi\rangle$$

Time evolution of wave function → Phase shift depending on energy

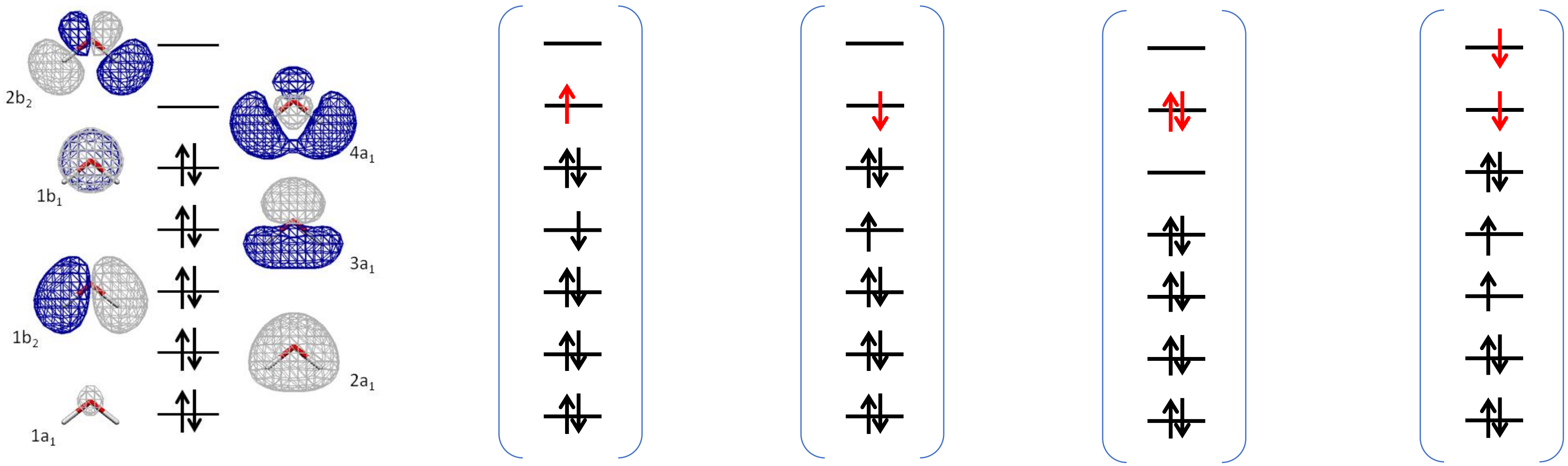


$$\boxed{Et = 2\pi\phi}$$

By determining the phase shift caused by the time evolution, we can extract the energy eigenvalue of the system!

CI expansion

Correlated wave function is expressed by the linear combination of Slater determinants



$$|\Psi_{\mathrm{HF}}\rangle = |2222200\rangle$$

$$|\Psi\rangle = c_0|2222200\rangle + c_1|222d2u0\rangle + c_2|222u2d0\rangle + c_3|2222020\rangle + c_4|22uu2dd\rangle + \cdots$$

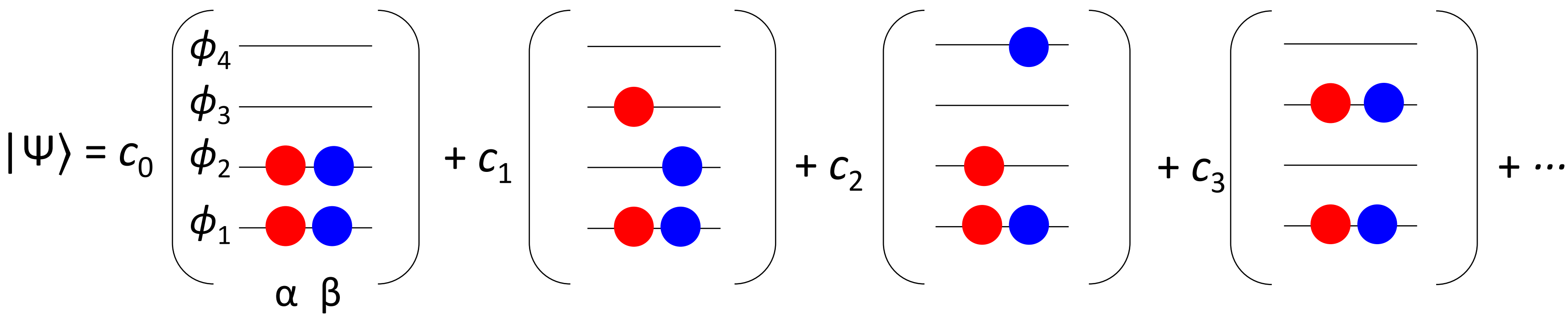
Quantum superposition states!

Mapping wave functions on qubits

<u>Direct mapping (DM)</u>:

Each qubit stores an occupation number of particular spin orbital.
($|1\rangle$ ... Occupied, $|0\rangle$ ... Unoccupied)

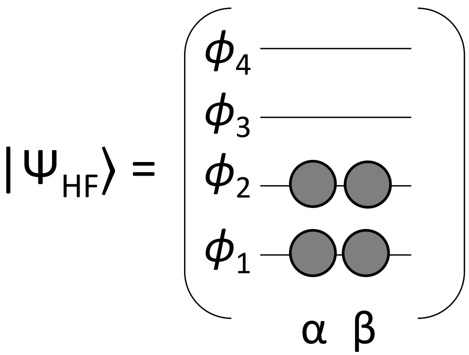
$$|\phi_{1\alpha}\phi_{1\beta}\phi_{2\alpha}\phi_{2\beta}\phi_{3\alpha}\phi_{3\beta}\phi_{4\alpha}\phi_{4\beta}\rangle$$

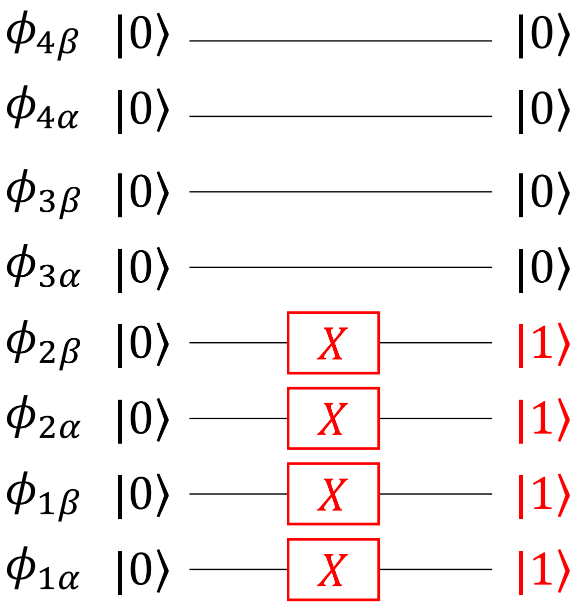


$$|\Psi_{\mathrm{JWT}}\rangle = c_0|11110000\rangle + c_1|11011000\rangle + c_2|11100001\rangle + c_3|11001100\rangle + \cdots$$

Mapping wave functions on qubits

By using direct mapping, the quantum state corresponding to HF state can be prepared by N_e of Pauli-X (NOT) gates, where N_e is the number of electrons in the active space.





Quantum Computations

Second quantized Hamiltonian → Qubit Hamiltonian

(Creation/annihilation operators → Strings of Pauli operators)

$$H = \sum_{p,q} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{p,q,r,s} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

$X_p = \sigma_p^x$, $Y_p = \sigma_p^y$, $Z_p = \sigma_p^z$

$$a_p^\dagger = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}_p = \frac{1}{2}(X_p - iY_p) = |1_p\rangle\langle 0_p|$$

$$a_q = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_p = \frac{1}{2}(X_q + iY_q) = |0_p\rangle\langle 1_p|$$

???

$$\{a_p^\dagger, a_q^\dagger\} = a_p^\dagger a_q^\dagger + a_q^\dagger a_p^\dagger = 0$$
$$\{a_p, a_q\} = a_p a_q + a_q a_p = 0$$
$$\{a_p^\dagger, a_q\} = a_p^\dagger a_q + a_q a_p^\dagger = \delta_{pq}$$

The creation and annihilation operators defined above do not satisfy the anticommutation relation!

Jordan–Wigner transformation

$$\{a_p^\dagger, a_q^\dagger\} = a_p^\dagger a_q^\dagger + a_q^\dagger a_p^\dagger = 0$$
$$\{a_p, a_q\} = a_p a_q + a_q a_p = 0$$
$$\{a_p^\dagger, a_q\} = a_p^\dagger a_q + a_q a_p^\dagger = \delta_{pq}$$

$$\Rightarrow$$

$$a_p^\dagger = \frac{1}{2}(X_p - iY_p) \otimes Z_{p-1} \otimes \cdots \otimes Z_0$$
$$a_q = \frac{1}{2}(X_q + iY_q) \otimes Z_{q-1} \otimes \cdots \otimes Z_0$$

Assume $p > q$

$$a_p^\dagger = \frac{1}{2}(X_p - iY_p) \otimes Z_{p-1} \otimes \cdots \otimes Z_q \otimes Z_{q-1} \otimes \cdots \otimes Z_0$$
$$a_q^\dagger = \frac{1}{2}(X_q - iY_q) \otimes Z_{q-1} \otimes \cdots \otimes Z_0$$

$$a_p^\dagger a_q^\dagger = \frac{1}{2}(X_p - iY_p) \otimes Z_{p-1} \otimes \cdots \otimes Z_{q+1} \otimes \left\{ Z_q \times \frac{1}{2}(X_q - iY_q) \right\}$$

Change $|0_q\rangle$ to $|1_q\rangle$ and then apply Z_q $\quad Z|1\rangle = -|1\rangle$

$$a_q^\dagger a_p^\dagger = \frac{1}{2}(X_p - iY_p) \otimes Z_{p-1} \otimes \cdots \otimes Z_{q+1} \otimes \left\{ \frac{1}{2}(X_q - iY_q) \times Z_q \right\}$$

Apply Z_q and then change $|0_q\rangle$ to $|1_q\rangle$ $\quad Z|0\rangle = |0\rangle$

Jordan–Wigner transformation

$$\boxed{\begin{aligned} a_p^\dagger &= \frac{1}{2}(X_p - iY_p)\otimes Z_{p-1}\otimes\cdots\otimes Z_0 \\ a_q &= \frac{1}{2}(X_q + iY_q)\otimes Z_{q-1}\otimes\cdots\otimes Z_0 \end{aligned}}$$

$$\begin{aligned} h_{pq}a_p^\dagger a_q &= \frac{h_{pq}}{4}(X_p - iY_p)\otimes Z_{p-1}\otimes\cdots\otimes Z_{q+1}\otimes(X_q + iY_q) \\ &= \frac{h_{pq}}{4}X_pZ_{p-1}Z_{p-2}\cdots Z_{q+1}X_q \\ &\quad +i\frac{h_{pq}}{4}X_pZ_{p-1}Z_{p-2}\cdots Z_{q+1}Y_q \\ &\quad -i\frac{h_{pq}}{4}Y_pZ_{p-1}Z_{p-2}\cdots Z_{q+1}X_q \\ &\quad +\frac{h_{pq}}{4}Y_pZ_{p-1}Z_{p-2}\cdots Z_{q+1}Y_q \end{aligned}$$

Real operators

Imaginary operators

$$h_{pq}(a_p^\dagger a_q + \underline{a_q^\dagger a_p}) = \frac{h_{pq}}{2}(X_pZ_{p-1}Z_{p-2}\cdots Z_{q+1}X_q + Y_pZ_{p-1}Z_{p-2}\cdots Z_{q+1}Y_q)$$

Complex conjugate of $a_p^\dagger a_q$

Jordan–Wigner transformation

$$
\boxed{
\begin{aligned}
a_p^\dagger &= \frac{1}{2}(X_p - iY_p)\otimes Z_{p-1}\otimes\cdots\otimes Z_0 \\
a_q &= \frac{1}{2}(X_q + iY_q)\otimes Z_{q-1}\otimes\cdots\otimes Z_0
\end{aligned}
}
$$

$$
h_{pq}\left(a_p^\dagger a_q + a_q^\dagger a_p\right) = \frac{h_{pq}}{2}\left(X_p Z_{p-1} Z_{p-2}\cdots Z_{q+1} X_q + Y_p Z_{p-1} Z_{p-2}\cdots Z_{q+1} Y_q\right)
$$

Electron occupancy is stored locally

Quantum state of particular qubit = Occupation number of particular spin orbital

Parity information is stored non-locally

We have to check quantum states of all the (p − 1)-th to (q + 1)-th qubits to know whether −1 should be applied or not, by the application of $h_{pq}\left(a_p^\dagger a_q + a_q^\dagger a_p\right)$

Number of Pauli operators in the Pauli strings: $O(N)$

Parity basis

Electron occupancy is stored non-locally, but Parity information is stored locally

Write f_i for occupation number of i-th spin orbital

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \end{pmatrix} = \begin{pmatrix} f_0 \\ f_0 + f_1 \\ f_0 + f_1 + f_2 \\ f_0 + f_1 + f_2 + f_3 \\ f_0 + f_1 + f_2 + f_3 + f_4 \\ f_0 + f_1 + f_2 + f_3 + f_4 + f_5 \\ f_0 + f_1 + f_2 + f_3 + f_4 + f_5 + f_6 \\ f_0 + f_1 + f_2 + f_3 + f_4 + f_5 + f_6 + f_7 \end{pmatrix}$$

Transformation matrix from occupation number basis to parity basis

Occupation number (Qubit rep. in JWT)

Representation in parity basis

Number of Pauli operators in the Pauli strings: $O(N)$

Bravyi–Kitaev transformation

Both electron occupancy and parity are stored non-locally

Write f_i for occupation number of i-th spin orbital

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \end{pmatrix} = \begin{pmatrix} f_0 \\ f_0 + f_1 \\ f_2 \\ f_0 + f_1 + f_2 + f_3 \\ f_4 \\ f_4 + f_5 \\ f_6 \\ f_0 + f_1 + f_2 + f_3 + f_4 + f_5 + f_6 + f_7 \end{pmatrix}$$

Transformation matrix from occupation number basis to BKT

Occupation number (Qubit rep. in JWT)

Representation in BKT

Number of Pauli operators in the Pauli strings: $O(\log N)$

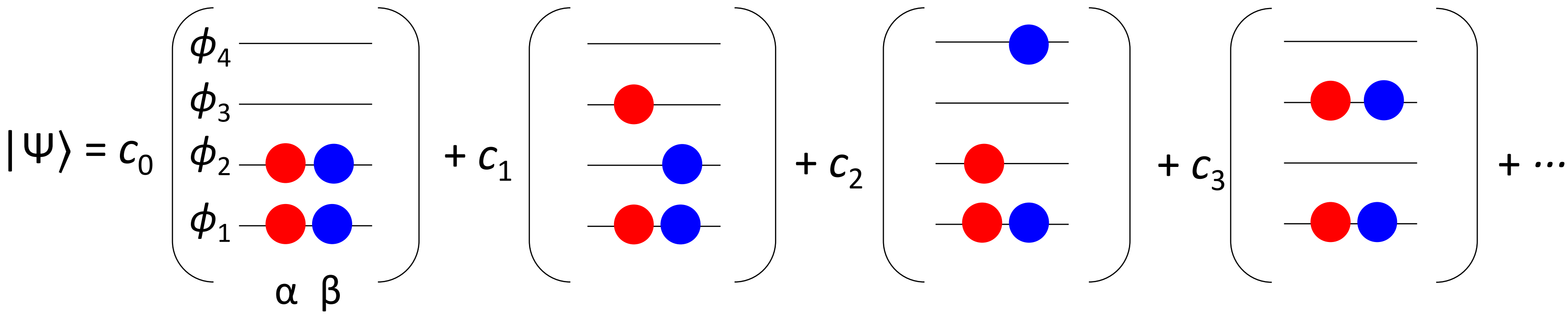
Bravyi–Kitaev transformation

Transformation matrix: $\beta_{2^0} = 1,\qquad \beta_{2^x} = \begin{pmatrix} \beta_{2^{x-1}} & \begin{matrix} 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{matrix} \\ \begin{matrix} 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \\ 1 & 1 & \cdots & 1 \end{matrix} & \beta_{2^{x-1}} \end{pmatrix}$

$$\beta_{2^3} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}$$

Compact mapping

The states of the simulated system and of the qubit system are simply enumerated and equated.



$$|\Psi\rangle = c_0|0000\rangle + c_1|0001\rangle + c_2|0010\rangle + c_3|0011\rangle + \cdots$$

- Requires less qubits than JWT, parity basis, and BKT. ${}_{N}\mathbf{C}_{Norb} \ll 2^N$.
- Only symmetry-adapted subspace can be explored.
- Transformation from fermionic to qubit Hamiltonians is not straightforward.

Fermion–Qubit transformation using OpenFermion

Using OpenFermion (python library for simulating fermionic systems), we can easily generate qubit Hamiltonians from fermionic Hamiltonian.

https://github.com/quantumlib/OpenFermion

$$H = v + h_0 a_0^\dagger a_0 + h_1 a_1^\dagger a_1 + h_{01}\left(a_1^\dagger a_0 + a_0^\dagger a_1\right)$$

```
import openfermion
from openfermion.ops import *
from openfermion.transfoms import *

hamiltonian = (FermionOperator((), v) +
               FermionOperator(((0, 1), (0, 0)), h0) +
               FermionOperator(((1, 1), (1, 0)), h1) +
               FermionOperator(((1, 1), (0, 0)), h01) +
               FermionOperator(((0, 1), (1, 0)), h01))
```

1 means creation

0 means annihilation

Indices of qubits

MO integrals

```
h_jwt = jordan_wigner(hamiltonian)  # Apply Jordan-Wigner transformation
h_jwt.compress()                    # Hamiltonian is real. Remove zero imaginary
```

Quantum circuits for time evolution operator

H_2, STO-3G basis set (4 spin orbitals), BKT

$$H = f_0\mathbf{1} + f_1 Z_0 + f_2 Z_1 + f_3 Z_2 + f_1 Z_0 Z_1 + f_4 Z_0 Z_2 + f_5 Z_1 Z_3 + f_6 X_0 Z_1 X_2 + f_6 Y_0 Z_1 Y_2$$
$$+ f_7 Z_0 Z_1 Z_2 + f_4 Z_0 Z_2 Z_3 + f_3 Z_1 Z_2 Z_3 + f_6 X_0 Z_1 X_2 Z_3 + f_6 Y_0 Z_1 Y_2 Z_3 + f_7 Z_0 Z_1 Z_2 Z_3$$

In BKT, allowed configurations are
$|1000\rangle$ and $|0010\rangle$
The 2nd and 4th qubits are always $|0\rangle$

$$H = g_1\mathbf{1} + g_2 Z_0 + g_3 Z_1 + g_4 Z_0 Z_1 + g_5 X_0 X_1 + g_6 Y_0 Y_1$$

Time evolution operator

$$U = \exp(-iHt) = \exp\{-i(g_1\mathbf{1} + g_2 Z_0 + g_3 Z_1 + g_4 Z_0 Z_1 + g_5 X_0 X_1 + g_6 Y_0 Y_1)t\}$$

Trotter decomposition

$$\xrightarrow{} \big[\exp(-ig_1\mathbf{1}t/N)\exp(-ig_2 Z_0 t/N)\exp(-ig_3 Z_1 t/N)$$
$$\times \exp(-ig_4 Z_0 Z_1 t/N)\exp(-ig_5 X_0 X_1 t/N)\exp(-ig_6 Y_0 Y_1 t/N)\big]^N$$

Quantum circuits for time evolution operator

$$U = \exp(-iHt) \approx \left[\exp(-ig_1 \mathbf{1} t/N) \exp(-ig_2 Z_0 t/N) \exp(-ig_3 Z_1 t/N) \times \exp(-ig_4 Z_0 Z_1 t/N) \exp(-ig_5 X_0 X_1 t/N) \exp(-ig_6 Y_0 Y_1 t/N)\right]^N$$

Construct quantum circuit corresponding to each exponential term and then combine them

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RESEARCH ARTICLE

Simulation of electronic structure Hamiltonians using quantum computers

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Quantum circuits for time evolution operator

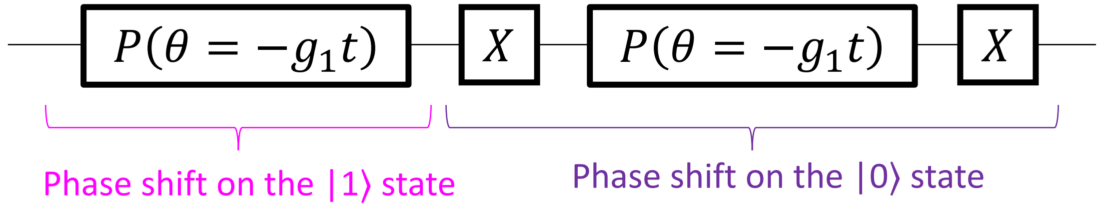
$$U = \exp(-iHt) \approx \left[\exp(-ig_1\mathbf{1}t/N)\exp(-ig_2Z_0t/N)\exp(-ig_3Z_1t/N)\right.$$
$$\left.\times \exp(-ig_4Z_0Z_1t/N)\exp(-ig_5X_0X_1t/N)\exp(-ig_6Y_0Y_1t/N)\right]^N$$

$\exp(-ig_1\mathbf{1}t)$ term

- Global phase shift independent on the quantum state.
- Constant contribution to the phase shift.

If you have to simulate this term, you can use the following circuit.

Any one of the qubit used for wave function storage



$$P(\theta) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{pmatrix}$$

Quantum circuits for time evolution operator

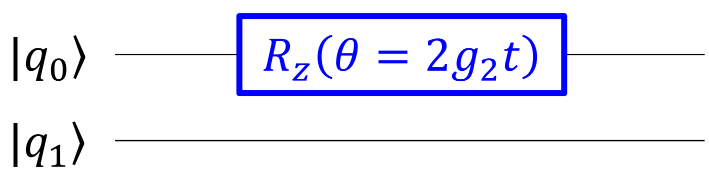
$$U = \exp(-iHt) \approx \left[\exp(-ig_1 \mathbf{1} t/N) \exp(-ig_2 Z_0 t/N) \exp(-ig_3 Z_1 t/N) \right.$$
$$\left. \times \exp(-ig_4 Z_0 Z_1 t/N) \exp(-ig_5 X_0 X_1 t/N) \exp(-ig_6 Y_0 Y_1 t/N)\right]^N$$

$\exp(-ig_2 Z_0 t)$ term

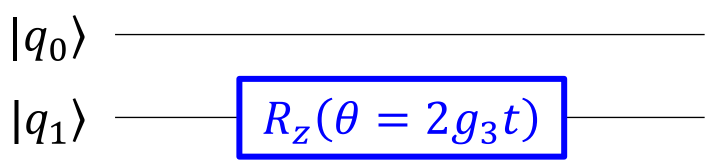
$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\exp(-ig_2 Z_0 t)|0\rangle = \exp(-ig_2 t)\,|0\rangle$$
$$\exp(-ig_2 Z_0 t)|1\rangle = \exp(+ig_2 t)\,|1\rangle$$

$$R_z(\theta) = \begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix}$$



$\exp(-ig_3 Z_1 t)$ term



Quantum circuits for time evolution operator

$\exp(-ig_4 Z_0 Z_1 t)$ term

$$Z_0 \otimes Z_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\exp(-ig_4 Z_0 Z_1 t)|00\rangle = \exp(-ig_4 t)\,|00\rangle$$
$$\exp(-ig_4 Z_0 Z_1 t)|01\rangle = \exp(+ig_4 t)\,|01\rangle$$
$$\exp(-ig_4 Z_0 Z_1 t)|10\rangle = \exp(+ig_4 t)\,|10\rangle$$
$$\exp(-ig_4 Z_0 Z_1 t)|11\rangle = \exp(-ig_4 t)\,|11\rangle$$

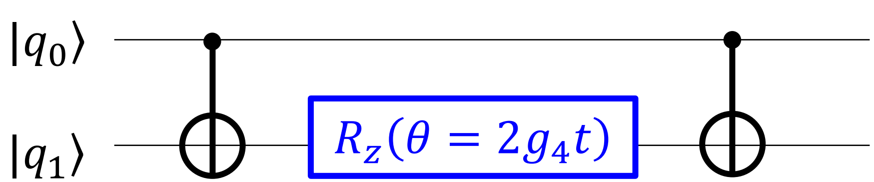
Apply phase shift $\exp(-ig_4 t)$ if the number of qubits in the $|1\rangle$ state is even.

Apply phase shift $\exp(+ig_4 t)$ if the number of qubits in the $|1\rangle$ state is odd.

Use a CNOT gate to collect the number of qubits in the $|1\rangle$ state!

CNOT[0,1] $|00\rangle$ = $|00\rangle$
CNOT[0,1] $|01\rangle$ = $|01\rangle$
CNOT[0,1] $|10\rangle$ = $|11\rangle$
CNOT[0,1] $|11\rangle$ = $|10\rangle$

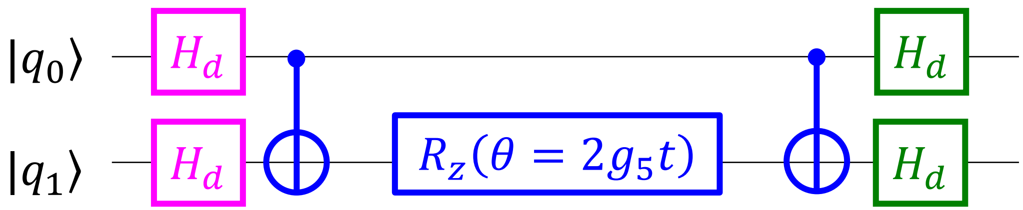
Second qubit is $|0\rangle$ … Apply $\exp(-ig_4 t)$ Second qubit is $|1\rangle$ … Apply $\exp(+ig_4 t)$



Quantum circuits for time evolution operator

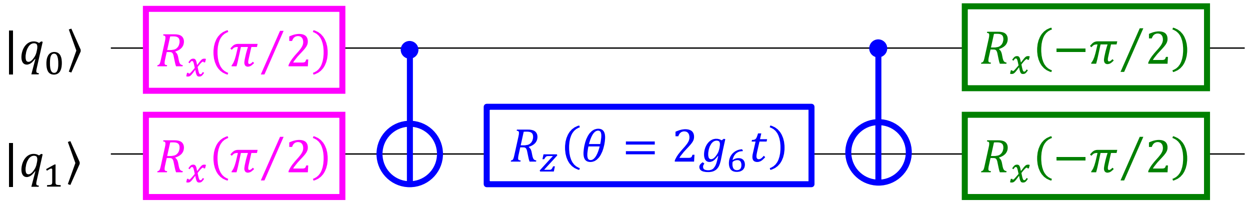
$\exp(-ig_5 X_0 X_1 t)$ term

1) Transform from X basis to Z basis
2) Apply $\exp(-ig_5 Z_0 Z_1 t)$ term
3) Reverse transform from Z basis to X basis



$\exp(-ig_6 Y_0 Y_1 t)$ term

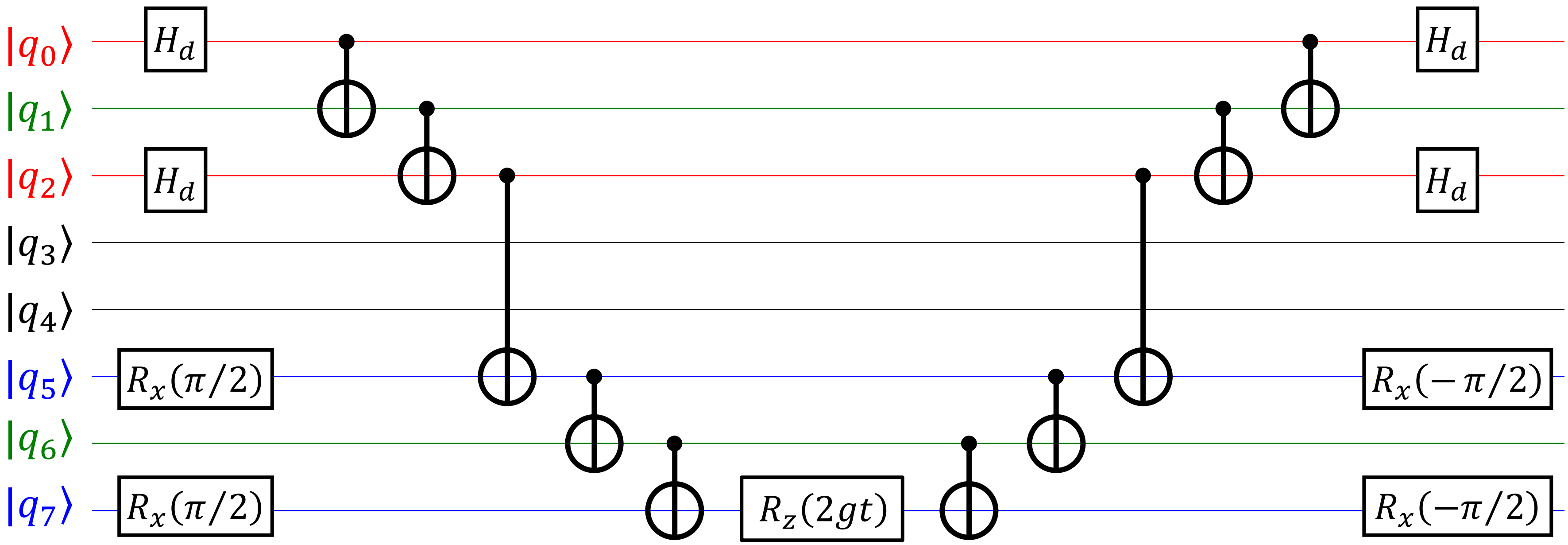
1) Transform from Y basis to Z basis
2) Apply $\exp(-ig_6 Z_0 Z_1 t)$ term
3) Reverse transform from Z basis to Y basis



Quantum circuits for time evolution operator

General procedure

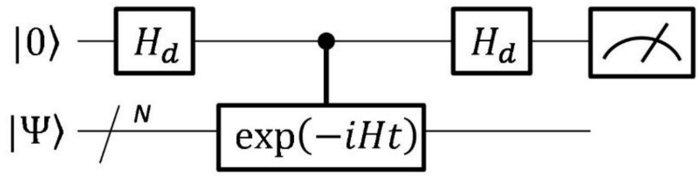
$\exp(-igX_0Z_1X_2Y_5Z_6Y_7t)$ as an example



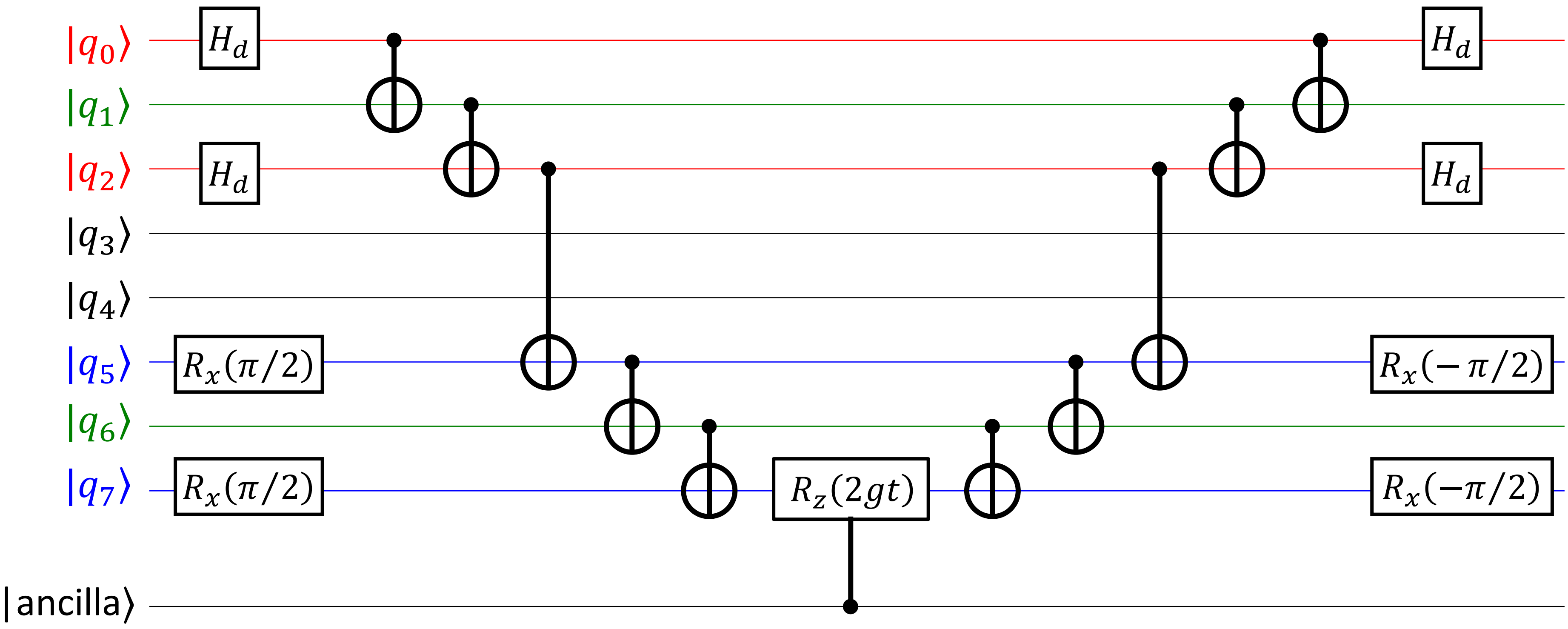
1) Apply Hadamard gate to the qubits those Pauli-X will act
2) Apply $R_x(\pi/2)$ gate to the qubits those Pauli-Y will act
3) Connect all qubits those Pauli operator will act by CNOT ladder
4) Apply $R_z(2gt)$ gate to the qubit in the bottom of CNOT ladder
5) Apply CNOT ladder in the reversed order to all qubits those Pauli operator will act
6) Apply $R_x(-\pi/2)$ gate to the qubits those Pauli-Y will act
7) Apply Hadamard gate to the qubits those Pauli-X will act

Quantum circuits for *controlled*-time evolution operator

In QPE, we have to simulate time evolution **conditional on the ancillary qubit**.

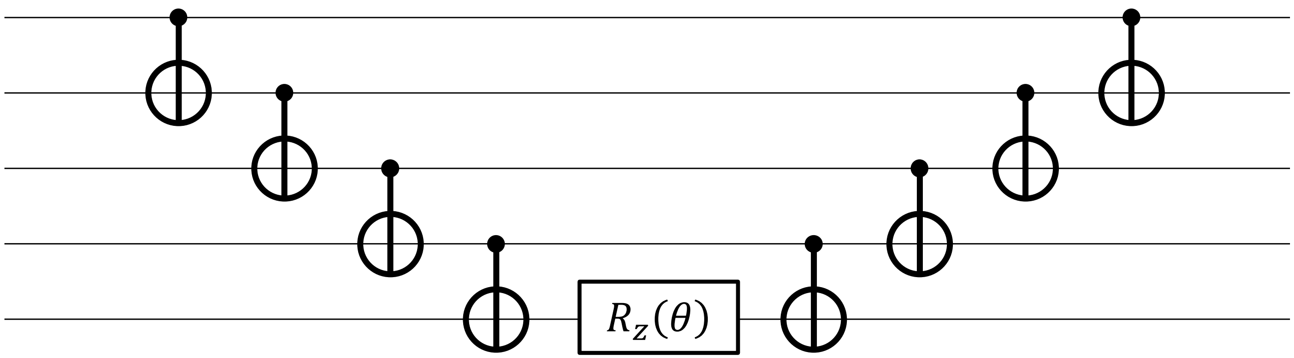


controlled- $\exp(-igX_0Z_1X_2Y_5Z_6Y_7t)$

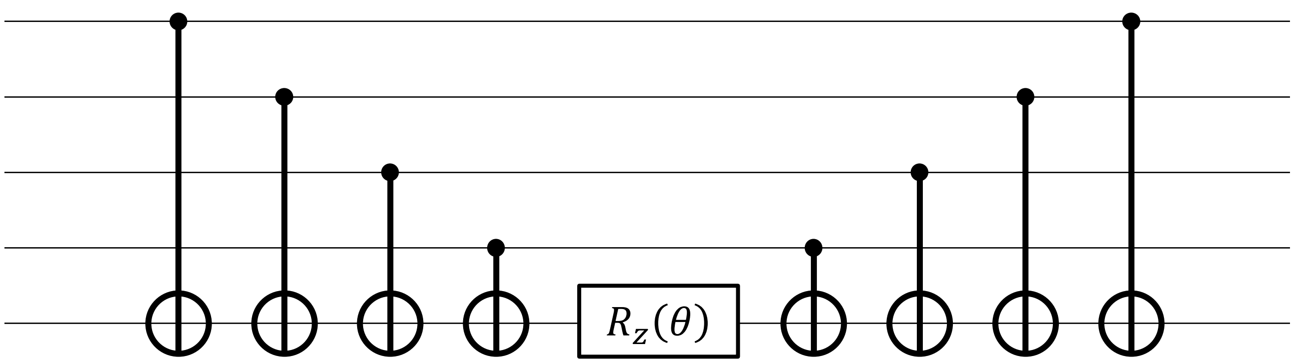


Quantum circuits for time evolution operator

(a)



(b)



- Quantum circuits (a) and (b) depicted above are equivalent
- The quantum circuits in (a) is often used, because it contains no CNOT gates acting on the non-nearest neighbor qubits.

An exercise

We have a qubit Hamiltonian of the form

$$H = 0.5X_0X_1 + 0.5Y_0Y_1$$

1) Construct a quantum circuit on IBM-Q for the time evolution operator with $t = \pi$

$$U = \exp(-iHt) \approx \exp(-0.5iX_0X_1t) \times \exp(-0.5iY_0Y_1t)$$

2) Simulate the time evolution circuit with following conditions.

- Start from the $|10\rangle$ state by adding an X gate before the time evolution circuit
- Measure two qubits after time evolution
- Set evolution time $t = \pi/4$, $\pi/2$, $3\pi/4$, and π
- Run the circuit on IBM-Q simulator_statevector and check the measurement outcome.
- Run the circuit on any IBM-Q machine (not simulators) and check the measurement outcome.