SPECTRUM SEARCH ALGORITHM ON QUANTUM COMPUTATION

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ABSTRACT

Spectrum search algorithm was designed by combining imaginary time evolution and Grover search algorithm. The Grover algorithm was used to eliminate the known states from the fully-mixed state. By iteratively applying the eilination algorithm and imaginary evolution, we can obtain full spectrum of the general Hamiltonian including degeneracy states.

Keywords Spectrum search · Imaginary time evloution · Grover algorithm · Quantum simulation

1 Introduction

Spectrum search is a fundamental routine in physics to analysis the given quantum system. In the research, two algorithms were combined to construct the spectrum search algorithm of the given quantum system; imaginary time evolution, and Grover search algorithm. Theoretically, the composed algorithm aims the time-independent Hamiltonian system, and could measure the full spectrum of the system by iteratively applying the algorithm from the ground to the higher energy state , without affected by degeneracy of the system.

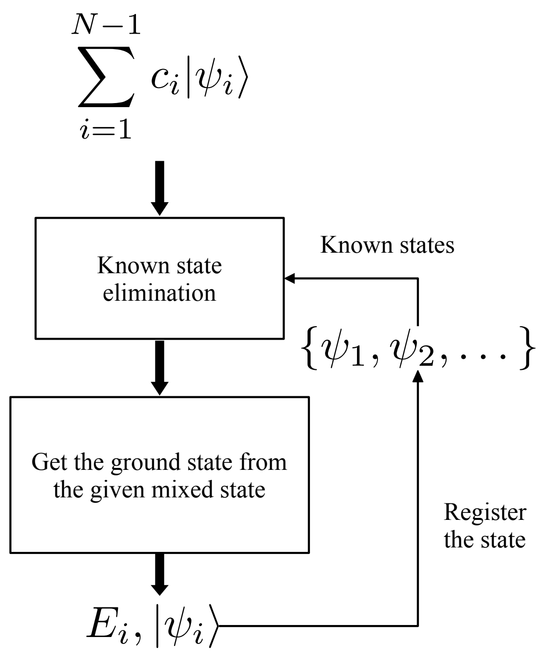

Figure 1: Schematics of the algorithm flow.

2 Background knowledges

2.1 Spectrum theory

In the finite dimension, any given system Hamiltonians has a finite Hermit matrix form, and their time evolution operator is unitary, U, with

$$U = e^{-iHt} \tag{1}$$

form.

Theorem 1. *For a given Hermit matrix H and eigen vector, $\mathbf{v}$ with*

$$H\mathbf{v} = \lambda\mathbf{v} \tag{2}$$

then, $\mathbf{v}$ is an eigenvector of the unitary matrix, $U = \exp(-iH)$ and its eigen values is $\exp(-i\lambda)$.

$$\exp(-iH)\mathbf{v} = \exp(-i\lambda)\mathbf{v} \tag{3}$$

Theorem 2. *Spectrum theorem*

- *For a given Hermit matrix H, it has an orthonormal eigen-basis.*
- *For a given Unitary matrix U, it has an orthonormal eigen-basis.*

The orthogonality plays significant role in the below section. All state we want to find is mutually orthogonal to each other.

2.2 Imaginary quantum evolution

Imaginary time evolution is frequently used in quantum system simulation in statistical physics. The reason is that from the given governing equation; Schrödinger equation, we can directly obtain a progress to reach the ground state of the system. From the time-independent Schrödinger equation,

$$i\hbar\frac{\partial}{\partial}|\psi\rangle = H|\psi\rangle \tag{4}$$

takes $\tau = it$ then, $df/d\tau = (dt/d\tau)df/dt = idf/dt$, thus,

$$\frac{\partial}{\partial\tau}|\psi\rangle = H|\psi\rangle \tag{5}$$
$$|\psi(\tau)\rangle = e^{-\tau H}|\psi(0)\rangle \tag{6}$$

From the Eq (5), we get a general solution,

$$|\Psi\rangle = \sum_i c_i(0)e^{-E_i\tau}|\psi_i\rangle \tag{7}$$

The terms are decaying and does not oscillate. Therefore, with sufficient long time, τ, we get

$$|\Psi(\tau) \approx_{\tau\to\infty} c_g(0)e^{-E_g\tau}|\psi_g\rangle \tag{8}$$

However, the imaginary time evolution cannot be directly implemented in common gate model computer. Since, it is a non-unitary transformation, $\exp(-H\tau)^\dagger = \exp(-H\tau)$, Hermit. Therefore, the implementation of ITE is also a challenge in the quantum computation. There are several ways, one is approximate the non-unitary gate with unitary gate. It is a common method by VQE, we can approximate unitary process to reach the same result of the imaginary time steps. The other methods are a block-encoding, embeding the non-unitary gate into unitary gate, or using a measurement based approach. The method we used in the implementation was non-unitary Trotter circuit suggested by Leadbeater et al**?**. Once we get a proper ITE routine, then the quantum computer could find a ground state from the *given* states.

2.3 Mixed state

There weakness also arise from that if the ground state was not in the given mixed state, one cannot find the proper ground state. Even the state is mixed completely in computational basis, in the eigen basis of the Hamiltonian, it could be just a few combination or a basis itself. For example, $\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)^{\otimes n}$ has full eigen states of the n-qubit system in computational basis, however, for $H = \sum_i X^i$. It is just an eigen-basis with ground energy.

The fully mixed state representation in computational basis is not hard to obtain, just add all column of the given matrix, we get a fully mixed state in the eigen basis of the matrix. Unfortunately, the preparation of the such state on QC is an another challenge, and this topic would not be analyzed in this research.

Even though the mixed state preparation problem, the property of the ITE is very powerful. Without changing the Hamiltonian, if the given state only consists of excited states of the system, we get a lowest energy state and it would be a specific excited state of the original Hamiltonian. For example, If we want to get a 2nd excited state from the system, only thing we have to do is preparing the mixed state in which the ground and 1st excited states are not combined and just apply the ITE routine. Thus, if we can efficiently eliminate the known ground states from the mixed state, we have a spectrum search algorithm with imaginary time evolution. We already know the algorithm modifying amplitude of state to the desired state, *Grover algorithm*.

3 Spectrum Search algorithm

In the original Grover algorithm, the object was search the proper state, however, in here our object is *eliminating the known state* from the given mixed state. More specificially, if the eigen-states of the given Hamiltonain, H, was $\{|\psi_i\rangle\}_{i=1}^n$, and we know $|\psi_1\rangle$, we want to get the next state

$$|\Psi\rangle = \sum_{i\neq 1} c_i|\psi_i\rangle\,, c_i \neq \forall i \tag{9}$$

$|\Psi\rangle$ and $|\psi_1\rangle$ are orthonormal by the spectrum theorem of Hermit matrix. If we have a proper oracle gate, we can obtain the $|\Psi\rangle$ state by using Grover iteration. In fact, the oracle gate in the situation is defined with $e(iH')$ form, naturally.

3.1 Qauntnum oracle

With the given ground state, $|\psi_g\rangle$, and the combination of all the other specturm, $|\Psi\rangle$, define a H' as

$$H' = I - |\psi_g\rangle\langle\psi_g| \tag{10}$$

then,

$$H'|\psi\rangle = \begin{cases} 0|\psi\rangle & \text{if } |\psi\rangle = |\psi_g\rangle \\ 1|\psi\rangle & \text{if } |\psi\rangle = |\Psi\rangle \end{cases} \tag{11}$$

and by the Theorem 1,

$$\exp(i\pi H')|\psi\rangle = \begin{cases} 1|\psi\rangle & \text{if } |\psi\rangle = |\psi_g\rangle \\ -1|\psi\rangle & \text{if } |\psi\rangle = |\Psi\rangle \end{cases} \tag{12}$$

The state $|\Psi\rangle$ is a state we want to get after the Grover iteration. Therefore, Eq (12) satisfies the oracle gate required in the iteration. In addition, the implementation of the oracle is well-analyed already; Trotterization.

$$U_\omega = \exp(-i\pi(I - |\psi_g\rangle\langle\psi_g|)) \tag{13}$$

However, the Grover algorithm only increases the probability to be orthogonal to the given state. For the precise spectrum search, we have to ensure the perfectly orthogonal to the known state, unless we still get a same ground state by ITE.

3.2 Measurement

Consider the POM, $M_0 = |\psi_0\rangle\langle\psi_0|$, after the measurement, the remained state would be

$$\frac{M_0|\psi\rangle}{\sqrt{\langle\psi|M_0^\dagger M_0|\psi\rangle}} = \begin{cases} |\psi_g\rangle & \text{if } \langle M_0\rangle \neq 0 \\ |\Psi\rangle & \text{if } \langle M_0\rangle = 0 \end{cases} \tag{14}$$

thus, applying the M_0 to get a 0 value, we can ensure the $|\psi_0\rangle$ is totally eliminated from the state. The remaning thing is applying the imaginary evolution, we will get a 1st exicted state or, if the system has a degeneracy in the ground state, we get an another ground state.

3.3 i-th state

By iteratively applying the result, we want the algorithm to eliminate the state from the mixed state and get full-eigen state.

$$\begin{aligned} &[\{\psi_1, \psi_2, \psi_3, \psi_4\}_{unknown}, \{\}_{known}] \\ &\rightarrow [\{\psi_3, \psi_4\}_{unknown}, \{\psi_1, \psi_2\}_{known}] \end{aligned} \tag{15}$$

The oracle must be chose differently in each intermediate steps. Since the spectrum states are all orthogonal, we can assure a linear combination of the known states still orthogonal to all the other states, thus we can generalize the Eq (10) as

$$H' = I - \sum_{i\in J} |\psi_i\rangle\langle\psi_i| \tag{16}$$

where, $|\psi_i\rangle$ are knwon state $\forall i\ inJ$. There eigen states are same with the original H and the eigen values are only $0, 1$. If $i \in J$, the eigen value is 0 and otherwise the value is 1. Consequently, the oracle and measurement are also

$$U_\omega = \exp(-\pi i H') \tag{17}$$

$$M_0 = \sum_{i\in J} |\psi_i\rangle\langle\psi_i| \tag{18}$$

By iteratively applying the algorithm, we can extract the spectrum and the their energy from bottom to the top in the finite Hilbert space. At the last step, we don't have to apply the ITE after we eliminate all the other state. The remained state would be a last eigen-state.

3.4 Summary of the algorithm

1. Preparte the mixed state of the given H, by as summation of the all columns.
2. Applying $H^{\otimes n}$ to $|0\rangle^{\otimes n}$ get a full mixed state.
3. Using imaginary time evolution, obtain a ground state energy, E_g.
4. Measure the ground state, $|\psi_g\rangle$. The state preparation is conducted by imaginary time evolution.
5. Define a oracle gate as $U_w = \exp(-\pi i|\psi_g\rangle\langle\psi_g|)$, the circuit implementation archieved by Trotterization.
6. Applying n-time Grover iteration.
7. Measure the state, $M_0 = |\psi_g\rangle\langle\psi_g|$.
8. If the result was 0, apply the imaginary time evolution with H, we will get a 1st excited state of the system.
9. Go back to 3 and repeat until the all specturm are measured, replacing $|\psi_g\rangle \rightarrow \sum |\psi_i\rangle$.

3.5 About the degeneracy

During the state preparation step, the Grover iteration only consider the orthogonoality of the given states and does not consider the what energy states they have. Therefore, even the system has some degeneracy, the state prepation is not affected, and we can get full state without considering the degeneracy.

4 Conlcusion

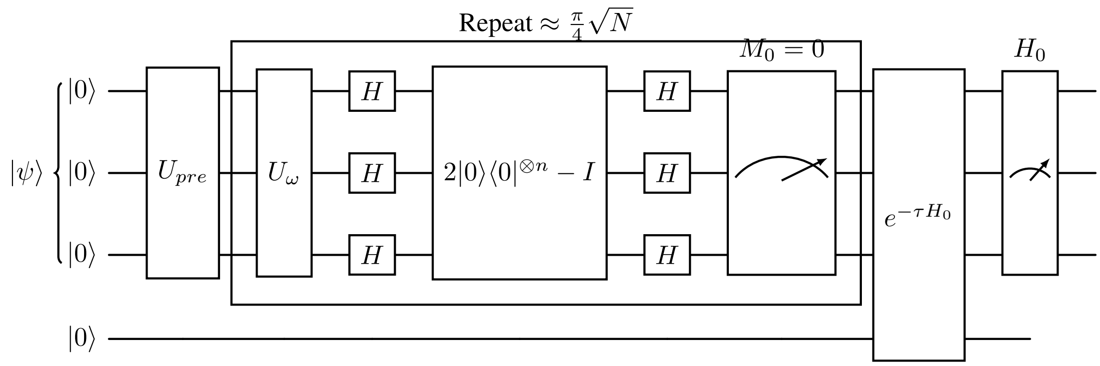

Figure 2: Schema of the algorithm on circuit. U_{pre} is a mixed state preparation algorithm. U_ω is a quantum oracle defined in Eq (12, 17). M_0 is defined in Eq (18.) For $i = 0$ step, the Grover, repeated circuit, becomes identity gate, and the last step, the ITE routine becomes identity.

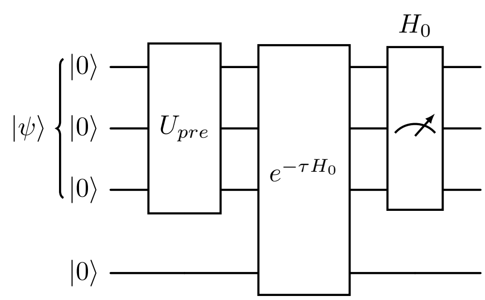

Figure 3: $i = 0$ step.

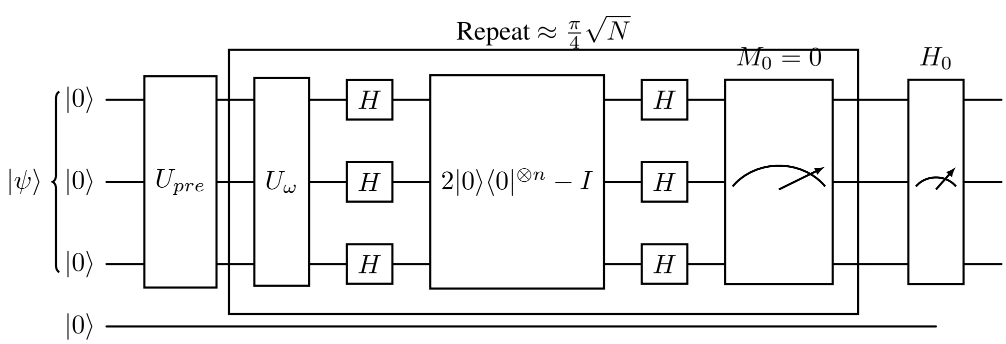

Figure 4: $i = N - 1$ step.