Experimental Simulation of a Pairing Hamiltonian on an NMR Quantum Computer

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Abstract

We have developed a concrete quantum simulation scheme and experimentally simulated a pairing model on an NMR quantum computer. The design of our experiment includes choosing an appropriate initial state in order to make our scheme scalable in near future, and the accomplishment of our experiment makes use of twice Fourier transforms so that our method is applicable to other physical models. Our results show that the experimental simulation can give the spectrum of the simulated Hamiltonian. Consequently, the potential power of a quantum computer on the simulation of complex physical systems is verified.

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I. INTRODUCTION

Quantum computer (QC) can offer attractive ability in accelerating the computation. The most appealing feature from the classical computer, as Feynman[1] noted, is that QC can be used to simulate the physical behavior of a real system. Lloyd[2] later confirmed this idea in a two-state array. Recently, Somaroo et al.[3] presented a general scheme for the quantum simulation with a physical system to simulate another. At present, among the physical realizations of QC, nuclear magnetic resonance (NMR) has shown the greatest achievements (for a review see e.g.,[4, 5]) though it uses the nuclear spin ensemble[6, 7]. With NMR technique, some interesting physical issues have been simulated successfully, including a four-level truncated quantum harmonic oscillator[3], a natural decoherence of a two-spin system[8], a two-qubit correlation function of the Fano-Anderson model[9], a three-spin effective Hamiltonian[10], and the migration of excitation in an eight-state quantum system[11].

Quantum simulation utilizes a physical system, commonly referred to as a QC, which is easier to control and measure, to simulate the dynamics of another one, which is rather a complex system, also called the simulated system. Quantum simulation is expected to solve the problems in quantum many-body theory which is dealt with more difficult by the classical methods. The simulated system we will discuss is the BCS model[12, 13] which is of wide interest in condensed matter and gives a phenomenal explanation to superconductivity. In BCS model, one of the key problem is to find the energy gap, i.e., the energy required at least to excite a quasiparticle from the Fermi surface[14]. In fact, some approximate methods[15, 16] have been proposed to calculate the energy gap for a given BCS Hamiltonian. However, if we realize the quantum simulation, one can get the accurate result within a polynomial time and resources[17].

In this paper, we show that QC can be used to simulate the property of a superconductor, such as the BCS model. Based on a concrete scheme of quantum simulation on NMR QC which includes a method for choosing an appropriate working initial state and the usage of twice Fourier transforms[18], we experimentally obtained the spectrum of the BCS Hamiltonian, which coincided with the theoretic expectations. In Ref. [19], authors had mentioned that the energy spectrum can be obtained by a fast Fourier transform after the measurement. In this paper, we deepen this point and show how to implement the
II. SCHEME OF QUANTUM SIMULATION ON AN NMR QC

For a complete quantum simulation procedure, there are three mainly qualitative steps – Hamiltonian mapping, the experimental simulation, and again mapping back to the simulated system. We will obey these three steps to describe our quantum simulation scheme of the BCS model in the following.

Firstly, the mapping from the BCS Hamiltonian to the Pauli operators.

The reduced Hamiltonian of the BCS model is a pairing Hamiltonian \[ H_{\text{BCS}} = \hbar \sum_{m=1}^{N} \frac{\varepsilon_m}{2} (n_m + n_{-m}) + V \sum_{m,l=1}^{N} c_{m}^{\dagger} c_{-l} c_{l}^{\dagger} c_{-m}, \] where \( \varepsilon_m \) denotes the free electron energy from the Fermi surface; \( V \) the coupling coefficient where it is simplified as a constant \[21]; \( n_{\pm m} \equiv c_{\pm m}^{\dagger} c_{\pm m} \) the electron number operators; \( c_{m}^{\dagger} \) (\( c_{m}^{\dagger} \)) the fermionic creation (annihilation) operator; \( m = 1, 2, \cdots, N \) represent all of relevant quantum numbers, and the electron pairs are labelled by the the quantum number \( m \) and \(-m\), according to the Cooper pair situation where the paired electrons have equal energies but opposite momenta and spins: \( m = (\vec{k}, \uparrow) \) and \(-m = (\vec{k}, \downarrow)\). For a typical metal superconductor, \( \hbar \varepsilon_m \sim 10^{-2} \text{ eV} \), \( \hbar V \sim 10^{-6} \text{ eV} \).\[20]\]

Our interested physical property of the BCS superconductor is the spectrum of the Hamiltonian \[11\], because an important parameter in superconductor — energy gap can be followed from it \[22\]. The energy gap in superconductor is the energy difference between the ground state of the element excitation to its first excited state. A lot of analytical and numerical methods (see \[23\] for a review) have been developed to obtain the energy gap through the diagonalization of the BCS Hamiltonian. However, these methods are complicated and use some unproved approximations. In this paper, we show that the quantum simulation on a QC can solve it in a practical and direct way with reduced resources.

In Ref. \[14, 17\], authors had mapped the Hamiltonian \[11\] into the qubit space based on the isomorphic algebras of spin-fermion connection. The mapped Hamiltonian is also known measurement of the spectrum on an NMR QC.
as the spin-analogy,

$$H_p = \hbar \sum_{m=1}^{N} \frac{\varepsilon_m}{2} \sigma_z^m + \frac{V}{2} \sum_{l>m=1}^{N} (\sigma_x^m \sigma_x^l + \sigma_y^m \sigma_y^l),$$

where $\sigma_x, \sigma_y, \sigma_z$ denote the Pauli operators.

Secondly, experimental simulation.

The details of the experimental simulation will be presented in the next section. Here we emphasize two problems.

One is how to choose a working initial state for the quantum simulation. In order to get the spectrum of $H_p$, one should select an appropriate initial state which can lead to a nonzero absorptive spectrum after the whole procedure of quantum simulation. Note that it is nontrivial to find such a state. In a recent work [18], we proposed a general method of the selection of an initial state for $N$-qubit quantum simulation of BCS model. This method guarantees the existence of the absorptive peaks in the $H_p$ spectrum and the correspondence between the peaks and the $H_p$ energy levels is clearly known.

The other problem is how to obtain the spectrum of a Hamiltonian by quantum simulation on an NMR QC. We propose that the simulation scheme has to include twice Fourier transforms ($ft$s) — the first $ft$ is from temporal-domain to frequency-domain of the NMR free induction decay (FID), and the second $ft$ is of the NMR amplitudes of a peak.

To validate this point, let us briefly review the procedure of the NMR measure (the first $ft$). NMR internal Hamiltonian in a lab frame is

$$H_{int}^{lab} = \frac{1}{2} \left( \sum_{i=1}^{N} \omega_0^i \sigma_z^i + \sum_{j>i=1}^{N} \pi J \sigma_z^i \sigma_z^j \right).$$

NMR measure process under such an internal Hamiltonian is

$$S_{NMR}(\omega) \propto ft[Tr(e^{-iH_{int}^{lab}t} \rho_{fin} e^{iH_{int}^{lab}t} \sum_{i=1}^{N} \sigma^+_i)],$$

where we label the evolution time during the NMR measure as $t$; $S_{NMR}(\omega)$ the NMR frequency-domain spectrum; $\rho_{fin}$ the state before the measurement, i.e., the state after a unitary evolution, which is, in our case, the evolution with $H_p$; $\sigma^+_i$ the project operator, $\sigma^+_i = \sigma_x^i + i \sigma_y^i$; $Tr$ the trace operation; $ft$ the Fourier transform applied for the NMR measured signal which is the function of NMR measure time $t$. 

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Eq. (4) implies that after the NMR measure, the spectrum is just that of NMR Hamiltonian self, but not the spectrum of the simulated Hamiltonian. Thus whatever the initial state or the evolution is, the spectrum is unchanged after the NMR measurement. From only NMR measure, we can not get the knowledge of the simulated Hamiltonian. However, the amplitude in NMR spectrum includes the information of the $H_p$ evolution time. If we select a series of discrete $H_p$ evolution time, and measure the corresponding amplitudes of the each spectrum, then apply another $ft$ on these amplitudes, the result will be the spectrum of the Hamiltonian simulated. A more formal mathematic derivation for this procedure refers to [18].

From the above discussion, due to the characteristic of NMR measurement, twice Fourier transforms are required to get the spectrum of the simulated Hamiltonian when performing the quantum simulation. The first $ft$ is the NMR measure applied for the NMR measure time, which obtains the NMR energy spectrum, and the second $ft$ is applied for the simulated Hamiltonian evolution time, which obtains the spectrum of $H_p$.

Thirdly, mapping back to the simulated system.

After the simulation, we are able to get the spectrum of $H_p$. However, we have to remap it back into the BCS physical system and formulate the energy gap, which is the final aim of quantum simulation. In other words, we would like to know how the $H_p$ spectrum corresponds to the energy gap in BCS model. The derivation of the relationship between the eigenvalues of $H_p$ and the energy gap can be found in Ref. [18] by the diagonalization of the spin-analogy Hamiltonian submatrices [24] and numerical calculations [20]. The energy gap is a function of eigenvalues corresponding to states $|01\rangle$ and $|10\rangle$ which span a subspace with one spin-up states, i.e., one Cooper pair [17]. Thus, if we obtain the eigenvalues of the $H_p$ through the quantum simulation, the energy gap in BCS superconductor can be deduced.

III. EXPERIMENTAL IMPLEMENTATION

We performed the experiment on a Bruker AVANCE 400 MHz spectrometer, keeping the temperature at 300K. The spin system is $^{13}$C-labeled Chloroform (Cambridge Isotopes) dissolved in $6d$ acetone. Spins $^{13}C$ and $^1H$ are the two qubits and labeled as qubits 1 and 2. The coupling constant is $J = 214.9$Hz.

Our simulation can be described with 4 stages.
1) Prepare for the working initial state.

The simplest initial state for a two-qubit system is $|\psi\rangle_{ini} = |00\rangle + |01\rangle$. We began with a pseudopure state based on spatial averaging \cite{27, 28}, and then apply a Hadamard gate on the second qubit, say $H_2$, to obtain the working initial state,

$$|00\rangle \xrightarrow{H_2} |00\rangle + |01\rangle.$$ \hfill (5)

2) Realize the unitary transformation.

In this paper, we consider a 2-qubit system and its evolution with $H_p$. The Hamiltonian is

$$H_p = \frac{\hbar}{2}[\varepsilon_1 \sigma_1^z + \varepsilon_2 \sigma_2^z + V(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y)],$$ \hfill (6)

and the corresponding propagator is

$$U_p(\tau) = e^{-iH_p\tau/\hbar} = e^{-i\frac{\hbar}{2}[\varepsilon_1 \sigma_1^z + \varepsilon_2 \sigma_2^z + V(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y)]\tau},$$ \hfill (7)

where we label the evolution time with $H_p$ as $\tau$. Note that we want to investigate whether the NMR control technique is adapted to be a testbed for the quantum simulation. In order to check the level of experimental accuracy to perform this simulation without any error in the unitary decomposition, we choose a special case of the Hamiltonian \hfill (7) – set the parameters $\varepsilon_1 = \varepsilon_2 = \varepsilon$, so as to the four terms in Eq. \hfill (7) are commuted with each other. Then Eq. \hfill (7) can be decomposed exactly into

$$U(\tau) = e^{-i\frac{\hbar}{2}\varepsilon \sigma_1^z \tau} \cdot e^{-i\frac{\hbar}{2}\varepsilon \sigma_2^z \tau} \cdot e^{-i\frac{\hbar}{2}V \sigma_1^x \sigma_2^x \tau} \cdot e^{-i\frac{\hbar}{2}V \sigma_1^y \sigma_2^y \tau}.$$ \hfill (8)

Actually, even if $\varepsilon_1 \neq \varepsilon_2$, there is no any important difference for our simulation procedure.

Experimentally we set both of the spins at their resonance frequency respectively and use $z$-rotations to realize the first two terms in Eq. \hfill (5), and then, use J-coupling evolutions to realize the last two terms. With the experimental one-qubit and two-qubit gates, Eq. \hfill (8) can be expressed into
FIG. 1: Quantum network to realize the evolution of 2-qubit BCS Hamiltonian. Horizontal lines represent qubits 1 and 2. Time goes from left to right. The boxes marked by X, -X, Y, -Y denote the π/2 rotations along the respective directions, and \((\theta_i)_z\) \((i = 1, 2)\) the rotation along z direction with the angle \(\theta_i\). The combination of two dots and a vertical line denotes the J-coupling evolution, i.e., the Ising gate, namely \(e^{-i\frac{\pi}{4}\sigma_1^x}\sigma_2^x\tau_3\).

\[
U(\tau) = e^{-i\frac{\omega_1}{2}\sigma_1^z\tau_1} \cdot e^{-i\frac{\omega_2}{2}\sigma_2^z\tau_2} \\
e^{-i\frac{\pi}{4}\sigma_1^x} e^{-i\frac{\pi}{4}\sigma_2^x} e^{-i\frac{\pi}{4}\sigma_1^y \sigma_2^y} e^{-i\frac{\pi}{4}\sigma_1^x} e^{-i\frac{\pi}{4}\sigma_2^x} \\
e^{i\frac{\pi}{4}\sigma_1^x} e^{i\frac{\pi}{4}\sigma_2^x} e^{i\frac{\pi}{4}\sigma_1^y \sigma_2^y} e^{i\frac{\pi}{4}\sigma_1^x} e^{i\frac{\pi}{4}\sigma_2^x}, \tag{9}
\]

where \(\tau_3\) is the J-coupling evolution time; \(\tau_1, \tau_2\) are the z-pulse widths; the r.f. powers \(\omega_1\) and \(\omega_2\) can be specified by the 90 degree pulse widths of two spins respectively [20]. The z pulse \(e^{-i\frac{\pi}{4}\sigma_1^y}\) on spin \(i\) \((i = 1, 2)\) with the rotation angle \(\theta_i\) is implemented using the combination of \(x\) and \(y\) pulses \(\left(\frac{\pi}{2}\right)_x - (\theta)_y - \left(\frac{\pi}{2}\right)_x\) and the rotation angle is \(\theta_i = \omega_i\tau_i\). The corresponding network to realize \(U(\tau)\) is shown in Fig. 1.

The parameters in Eq. (9) and Eq. (8) satisfy

\[
\omega_1\tau_1 = \omega_2\tau_2 = \varepsilon\tau, \quad \pi J\tau_3 = V\tau. \tag{10}
\]

According to the values of the parameters in BCS Hamiltonian (2), we set \(\varepsilon_m/2\pi \sim 10^4\) Hz, \(V/2\pi \sim 1\) Hz in the experimental simulation. For the \(H_p\) evolution time \(\tau\) in Eq. (8), we select 64 different values — the initial value is 0, the maximal value is \(\frac{63}{2\pi}\) s, and the increment is \(\frac{1}{2\pi}\) s. The NMR experimental evolution time \(\{\tau_1, \tau_2, \tau_3\}\) can be calculated from the evolution time \(\tau\) using the Eq. (10). That means we repeat the experiments for 64 times
TABLE I: Discrete sets of values of the evolution time used in experiment. $\tau_1$ is the $z$-pulse width of qubit 1 ($^{13}C$), $\tau_2$ is the $z$-pulse width of qubit 2 ($^1H$), and $\tau_3$ is the J-coupling evolution time. Note the periods of $\tau_1$, $\tau_2$, $\tau_3$ are $\sim 40 \mu s$, $\sim 40 \mu s$, $\sim 10$ ms, respectively. When the values exceed their respective periods, their values can be shortened. See text for details.

|       | $\tau_1$ | $\tau_2$ | $\tau_3$ |
|-------|----------|----------|----------|
| initial values | 0        | 0        | 0        |
| increment | 17.6 $\mu s$ | 18.0 $\mu s$ | 1.4805 ms |
| final values | 19.7 $\mu s$ | 20.1 $\mu s$ | 0.2489 ms |

with the 64 sets of evolution time $\{\tau_1, \tau_2, \tau_3\}$. In experiment, the receiver phases are set with the same phase as that of the measurement of the first set $\{\tau_1, \tau_2, \tau_3\}$. We obtain the relative amplitudes of the final states by integrating the peaks.

Since the decoherence time $[28]$ ($T_2$ relaxation time) of the two qubits $^1H$ and $^{13}C$ is no more than 3.3 s and 0.4 s, respectively, the whole evolution time should be controlled within the decoherence time. However, the values of evolution time in the latter sets $\{\tau_1, \tau_2, \tau_3\}$ are so long to exceed the decoherence time. To solve this problem, we experimentally use a technique to shorten the evolution time based on the fact that both the $z$-rotation and the J-coupling evolution are the periodic rotations with the period $2\pi$. Therefore, the $z$-pulse width and the J-coupling evolution time longer than one period can be shortened less than one period.

More specifically, the period of $z$-pulse is $2\pi$ radian, and since we use the hard pulses in heteronuclear system, the value of one period is $\sim 40 \mu s$. The period of J-coupling evolution is $2/J$. In our system, this value is $\sim 10$ ms. Note that compared with the J-coupling evolution time, the $z$-pulse width is so small and can be ignored. So the experiment time mainly depends on the J-coupling evolution time. Further note that there are two segments of the J-coupling evolution in our network (Fig. 11), the whole time of our experiment is about 20 ms, which is well within the decoherence time. In our experiment, the $z$-pulse width and the J-coupling evolution time are listed in table 11.

After the evolution, the final state is

$$\langle \psi \rangle_{fin} = e^{-iH_p\tau} \langle \psi \rangle_{ini} = e^{-i\varepsilon \tau} |00\rangle + \cos(V\tau) |01\rangle - i \sin(V\tau) |10\rangle.$$  \hspace{1cm} (11)
This state implies that there are two peaks appeared in NMR spectrum – one corresponds to the transition $|00\rangle \leftrightarrow |10\rangle$, and the other corresponds to $|00\rangle \leftrightarrow |01\rangle$ depended on the nonvanishing coefficients.

3) The 1st ft. Since NMR spectrum of the eigenvalues is unchanged, the positions of the peaks include no useful information. What we need is to record the amplitudes of the peaks. For the initial state we select, there are two peaks in the final spectrum, as shown in Eq. (11) — one is the peak of $^{13}C$, another is the peak of $^1H$. We measure the peaks of $^1H$, and record the real and imagery parts of the amplitudes corresponding to the different evolution time through the integration of the peaks. By substituting Eq. (11) into Eq. (4), the amplitudes of the peak of $^{13}C$ and $^1H$ theoretically satisfied the equations

\begin{align}
Amp_1 &= i \sin(V\tau)[\cos(\varepsilon\tau) + i \sin(\varepsilon\tau)], \\
Amp_2 &= \cos(V\tau)[\cos(\varepsilon\tau) + i \sin(\varepsilon\tau)],
\end{align}

respectively. The measured amplitudes fit the Eq. (13). The real and imaginary parts of the experimentally measured amplitudes are shown in Fig. 2.

4) The 2nd ft. Apply a discrete $ft$ on the amplitudes, and obtain the spectrum of $H_p$, shown in Fig. 3. The distance of the two peaks is 2 Hz from the figure. The value is same as the theoretical result which can trivially diagonalize the Hamiltonian (2) and calculate the energy difference corresponding to the eigenstate $\{|01\rangle, |10\rangle\}$. The difference of the eigenvalues is just the information we want to know from the Hamiltonian $H_p$. Since $H_p$ is the mapped one from the BCS Hamiltonian, we can remap the eigenvalues of $H_p$ to get the energy gap in BCS Hamiltonian [18]. The errors mainly arise as a result of the imperfect pulses and delays as well as the variability of the measurement.

IV. CONCLUSION

In this paper, a concrete experimental scheme of quantum simulation on NMR QC is presented. Two important components in our scheme are the selection of an appropriate working initial state and the usage of twice Fourier transforms. Based on this scheme, we simulate the evolution of the BCS Hamiltonian with an experimental technique to reduce the system evolution within the decoherence time. The simulation results show the BCS energy
FIG. 2: The real (a) and the imaginary parts (b) of the NMR measured amplitudes. The solid lines are fitted to the theoretical expectation. The stars are the experimental data. Note the horizontal axes is the evolution time $\tau$, from 0 to $63/2\pi$ s.

spectrum agrees with the theoretical value. This provides a practical method to obtain the characteristic of the complex physical system, and shows the potential power of the QC in quantum simulation.

It is believed that quantum simulation is possible to solve the quantum dynamics. The ability to perform an efficient quantum simulation requires many degrees of freedom (perhaps $10^{\sim}100$ qubits in the next generation QC [17]). In this paper, we are putting our research on those issues associated with problems that are difficult for quantum many-body theory to solve on classical computer. Although a 2-qubit quantum simulation of BCS model is shown in experiment, the fact that even small numbers of qubits leads to new insight into the mechanism of QC how to perform quantum simulation, and permit accurate prediction of the dynamics of complex quantum system if the technique developed future.

Clearly, a number of challenges for the efficient simulation of physical system still remain at present [9]. Can we find the physical results in the simulated system after the algebras remapping? How can we realize a complex network of multi-qubit system with the enough accuracy? Can we find the a physical simulation problem that a QC can solve but not
FIG. 3: The spectrum of the Hamiltonian $H_p$ obtained by the second Fourier transform. The solid line is fitted to the theoretical expectation. The distance between two peaks shows the difference of the eigenvalues of $H_p$ is 2 Hz, which is same as the theoretical calculation.

the classical computer today? Nevertheless, we are sure that the concept presented here establishes a very first step to simulate a real physical system on QC.

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Note added. – After this work was completed, we became aware of a similar work appeared in quant-ph/0410106 by C. Negrevergne, R. Somma, G. Ortiz, E. Knill, and R. Laflamme,
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