Non-equilibrium Superconducting Dynamics after Neutron Capture Close to the Superconducting Transition Edge in MgB_2 and Novel Pairing in the Hubbard Model with Confinement Potential

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We perform large-scale numerical simulations on non-equilibrium superconducting dynamics after a neutron capture at the superconducting transition edge in MgB_2 by solving the time-dependent Ginzburg-Landau (TDGL) equation coupled with the Maxwell and the heat diffusion equations. The simulations are carried out under the voltage biased condition which is a typical operating situation for X-ray superconducting detectors, and a quick temporal response of the current associated with non-equilibrium dynamics after the release of the nuclear reaction energy is measured. On the other hand, we investigate a pairing mechanism in the Hubbard model with confinement potential, which is a model for strongly correlated electron systems confined inside a nano-domain and atomic Fermi gasses loaded on an optical lattice, by using exact diagonalization method. The calculation reveals that when the Coulomb repulsion exceeds a critical value and the confined potential is strong enough to make a Mott insulator region around the potential center, a Cooper pairing function develops between the both sides of the Mott region. This pairing is found to be strongly correlated to spin structure inside the Mott region, which shows a dimerized character of spin-singlet.

Keywords: Time-dependent Ginzburg-Landau Equation, Non-equilibrium Superconductivity, Neutron Detection, MgB_2, Hubbard Model, Optical Lattice, Cooper Pair, Spin-singlet

1. Introduction

After the discovery of an alloy superconductor MgB_2 [1], a tremendous number of experimental studies have been made in order to clarify basic aspects of MgB_2, and several intriguing features have been revealed. In addition, many applications using MgB_2 have been proposed due to its peculiarities. Among their several ideas, an application suggested by Ishida et al. is a quite attractive for the research field of the atomic energy science [2]. The idea is as follows. When a neutron hits on MgB_2 sample, a nuclear reaction occurs between a neutron and an isotope of B, i.e., ^{10}B with a high probability. Then, a fixed energy is released, and the energy transforms into a heat which leads to an instantaneous destruction of the superconducting state if MgB_2 is in the temperature below the transition temperature (39K). Thus, the moment of the nuclear reaction is easily found to be observable as the electrical signal [2], since the destruction of superconductivity nucleates a normal spot along which an electrical resistance is generated when the electrical current flows. This idea is principally equivalent to the detection mechanism of the famous superconducting transition edge sensor (TES) for X-ray and other ones [3].

In TES's, an essential operating condition is voltage-bias, in which the current responds to the thermal heat release and a dip structure emerges in the time sequence of the current due to the instantaneous superconductivity depression. In addition, the voltage bias makes it possible to automatically feedback to the initial state, which gives an excellent per-

formance as a detector. Thus, the condition employed in TES is found to be useful for the neutron detection in MgB_2, too. In this fiscal year, we have, therefore studied a theoretical framework [4] to trace the non-equilibrium state [5–8] under the voltage bias condition and developed a program to simulate the neutron detection under the case. Consequently, we have succeeded in performing preliminary simulations. The simulation results reveal that the response time is very short while the current response is correlated to the location in which the nuclear reaction occurs. This information is physically reasonable and important. We will perform more systematic studies in the next fiscal year project.

Various applications using the existing superconductors are known to be promising, while to raise the superconducting transition temperature (T_c) is a quite attractive issue for not only fundamental physics but also engineering scene, since all the superconductor applications now require a large energy cost to cool down the system. Thus, we have started to study the superconductivity mechanism to understand what a crucial factor is to lift up T_c since the last fiscal year [9]. As numerical methods to approach the issue in highly correlated electronic systems, three types of numerical methods have been so far suggested. These are called the exact diagonalization, the qunatum Monte calro, and the density matrix renormalization group methods, respectively. Among them, we paid an attention to a viewpoint of the exactness, and therefore, selected the exact diagonalization method as a main numerical approach in our project. Since the last fiscal year, we have faced the parallelization and the performance improvement for the exact diagonalization code, and developed an excellent high-performance one which shows ~16Tflops when using 512 nodes. Such a performance is much beyond our initial expectation since the diagonalization code frequently requires all-to-all communications which intrinsically drops the performance. In this report, we have to avoid describing the details of the code tuning due to lack of space, but we would like to remind that the tuning skills and techniques were selected as a finalist for the Gordon-Bell Prize in SC2005 [10].

Our target model for the quest of superconductivity mechanisms [11] is the so-called Hubbard model [12]. The model has been regarded as a typical model capturing strongly-correlated behaviors like the metal-insulator transition. Since the discovery of High-T_c superconductors, the model has been intensively investigated in order to clarify whether or not the model describes high temperature superconductivity exceeding 100K [11]. However, the issue has been not resolved yet. This is because it is too quite difficult to numerically calculate the Hubbard model ($\geqq$ 2D) in large enough system sizes and to obtain a result which is conclusive in thermo-dynamical limit. Especially, the exact diagonalization method confronts a difficulty that the memory requirement exponentially increases with the number of fermions (electrons) [10]. However, it completely keeps the exactness in contrast to other two methods which require fundamental improvements to obtain reliable results. Namely, by using the exact diagonalization method, one can touch exact features of the model, although the model size is severely restricted [10]. Thus, we have studied the Hubbard model with confinement potential [9], which shows features intrinsic to finite systems. For example, it is known that the confinement potential nucleates the Mott insulator region at the center and the metallic one around the Mott region. Both of these are essential features of the Hubbard model [9], and the confinement potential makes it possible to study both of them in the spatially modulated co-existent systems [9]. On the other hand, we would like to point out that the system is realized in atomic Fermi gasses [13] by loading the gas on the optical lattice [14] created by the laser beam operation. This indicates that the obtained result can be experimentally confirmed in a direct way.

The contents of this report are as follows. In Section II, the numerical method to simulate the voltage bias condition is given, and preliminary results of large-scale simulations incorporating the nuclear reaction with the neutron in MgB_2 are demonstrated. In Section III, the spin structure accompanied by the development of the Cooper pair function are presented in the Hubbard model with confinement potential and the physical origin of the superconductivity in the confined system is discussed.

2. The Voltage-Bias Condition and the Non-equilibrium Dynamics in MgB_2

As a preparation to simulate the voltage bias condition used in TES's, we initially perform a simulation to obtain a profile of the temperature dependence of the resistance. We trace the dynamics of the superconducting state with increasing the heat bath temperature slowly and average the voltage for the time period which is 100 times longer than the relaxation time. The obtained profile is shown in Fig. 1(a). As seen in Fig. 1(a), the sharp transition from the superconducting state to normal one occurs at 38.7~37.8 which is below T_c (~40K), because the measured state is a current carrying one in which T_c is down depending on the magnitude of the flowing current. As a test, let us fix the voltage value to 100 (a.u.) as shown by the red line. The techniques for fixing the voltage are as follows. First, we note that the current is easily controllable by changing the boundary condition for the Maxwell equation [15], while the voltage is an observable quantity. Thus, the problem can be reduced to how one controls the current on the variation of the observable voltage value. As a current control method, we assume that the current feedback is written as $I_{feedback} \sim -A(V-V_{fix})$, where V_{fix} is the fixed target voltage and $I_{feedback}$ is added to the present current value to keep the voltage constant. Such a linear relation is valid

enough as long as sudden current variations are not supplied. The present case satisfies the condition. Figure 1(b) is a time evolution data of the current variation obtained by using the above relation. As seen in the figure, one finds that the voltage is fixed to be constant (V = 100 (a.u.)) after a time lug. This is the first success for realistic simulations as solving the TDGL equation, and indicates that a direct simulation for TES is possible. In the future, we will do a systematic study to raise the resolution in TES by applying this method.

Next, let us show an actual time response of the current in the voltage biased condition after the nuclear reaction in MgB_2. Figure 2 is the time evolution of the measured current, in which the heat energy release due to the nuclear reaction starts at the vertical line. From the figure, it is found that the time evolution shows a dip structure after the heat energy release. The time period from the appearance of the dip to the recovery onto the steady current carrying state is found to be quite fast. This indicates that the condition employed in TES is also effective for the neutron detection in MgB_2.

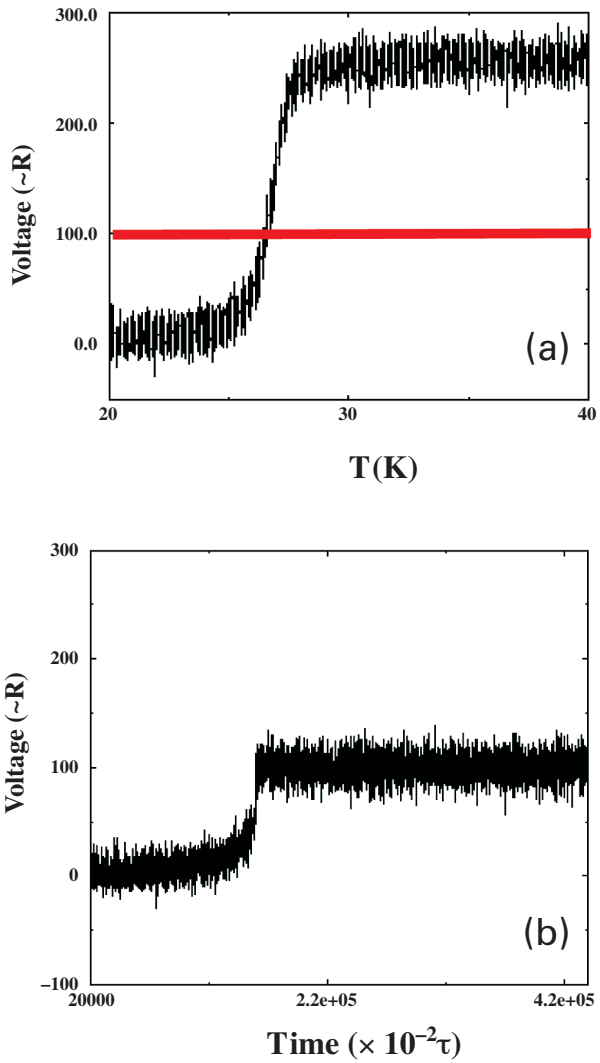

Fig. 1 (a) The voltage(arbitrary unit) vs. temperature. (b) The voltage (arbitrary unit) vs. time (τ; relatxation time ~10^{-12}sec).

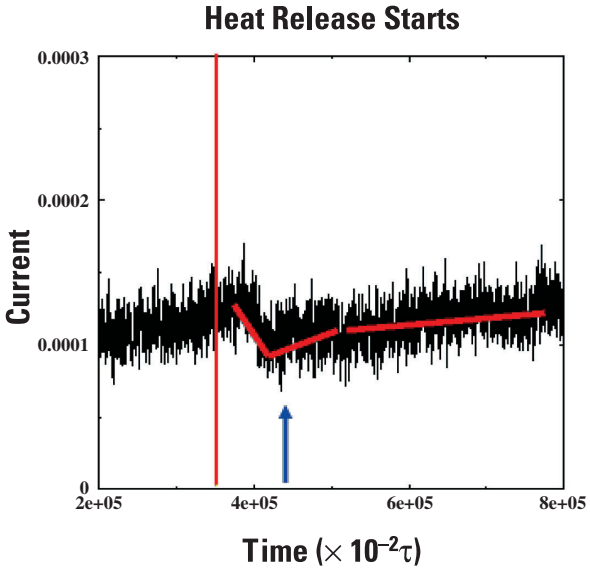

Fig. 2 The current vs. time. The time unit is $0.01\,\tau$ where $\tau \sim 1.0 \times 10^{-12}$ sec. The redline indicates when the heat release starts.

3. Pairing in Fermion-Hubbard Model with Confinement Potential

The Hubbard model [12] is one of the most intensively studied models by computers because it captures very rich varieties of strongly correlated many-body systems although the model expression is quite simple. Especially, since the discovery of High-T_c cuprate superconductors, an issue whether or not the Hubbard model with repulsive interaction can explain its high T_c has attracted many interests although the decisive conclusion has been not still attained [11]. In the last fiscal year, we studied the Hubbard model with confinement potential [9] motivated by the rapid advancement of atomic physics [13–14], and found that the model shows the Cooper pairing instability by confirming the negative binding energy and the development of the pairing function [9]. This result demonstrates a deep connection between the Hubbard model [12] and the pairing [9] although the system is a confined finite system. In this report, we show the mechanism of the Cooper pairing [16].

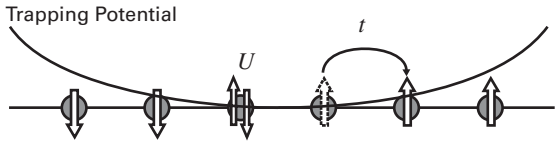

Fig. 3 A schematic figure for the fermion-Hubbard model with confinement potential.

Firstly, let us give the Hamiltonian of the Hubbard model with a confinement potential, [9]

$$H = -t \sum_{i,j,\sigma} \left(a^{\dagger}_{j\sigma} a_{j\sigma} + H.C. \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \left(\frac{2}{N} \right)^2 V \sum_{i,\sigma} n_{i\sigma} \left(i - \frac{N}{2} \right)^2 \quad (1)$$

where t, U, V, and N are the hopping parameter from i-th to j-th sites (normally j is the nearest neighbor site of i), the repulsive energy for the on-site double occupation of two fermions, the parameter characterizing the strength of the trapping potential, respectively, as schematically shown in Fig. 3, and the site number. We diagonalized the Hubbard Hamiltonian H (Eq.(1)) [10] and calculated the binding energy which is a probe for the Cooper pairing and the Cooper pair function by varying U(>0) and V [9] in the last fiscal-year project. Consequently, we found that U above a critical U_c changes the sign of the binding energy into the negative one and simultaneously develops the Cooper pair function under a confinement potential enough to gather all fermions into a central region [9]. Then, we also found that the particle distribution drastically varies at a boundary value U_c. Namely, as U exceeds over U_c, the distribution changes from the dome like shape around the trap center to the mesa one which is composed of the so-called Mott insulating core and metallic edges [9]. Above the critical value U_c, only the spin degree of freedom survives in the Mott core region [16], while the charge density can fluctuate only at the metallic edges [9, 16]. This situation is quite similar to underdoped case of High-T_c cuprate superconductors, in which nano-scale domain like structure of the Mott state is observable. In this fiscal year, motivated by these results and the similarity shown just above, we first study the spin structure of the Mott core region to approach the pairing mechanism [16]. One of our main interests is how the charge density fluctuation couples with the spin structure of the Mott core [16]. For the purpose, we calculate the spin correlation between neighboring sites $\langle S_i \cdot S_{i+1} \rangle$ and compare $\langle S_i \cdot S_{i+1} \rangle$ between N (n, n) and N+2 (n+1, n+1) [16].

Figure 4 shows i dependence of $\langle S_i \cdot S_{i+1} \rangle$ for N (n, n) and N+2 (n+1, n+1). Here, we note that these all results are obtained above the critical Uc, in which the central region is the Mott state and the signal of the pairing instability is observable. First, let us focus on the spin structure for N (n, n) (see the upper part of Fig. 4). We find that the neighboring spin correlation shows a zigzag structure [16]. By noticing that $\langle S_i \cdot S_{i+1} \rangle$ is –3/4 for the spin singlet, it is found that the spin singlet are spatially formed as the schematic figure. Next, let us compare the spin structure $\langle S_i \cdot S_{i+1} \rangle$ between N (n, n) and N+2 (n+1, n+1). From the schematic figures for N and N+2, it is found that the reformation of spin singlet pairs occurs by adding two fermions [16]. Through the reformation, the system obtains an energy gain because the formation of the spin singlet decreases the energy of the system [16]. Thus, the negative binding energy, i.e., the attractive interaction working between two fermions is found to be mainly originated from the reformation [16]. On the other hand, since the pairing function develops between both side edges in the same state [9], one finds that the ground state is approximately given by a linear combination as [16]

$$|\Psi\rangle = a\,|(\uparrow\downarrow)(\uparrow\downarrow)\ldots(\uparrow\downarrow)\rangle + b\,|s(\uparrow\downarrow)\ldots(\uparrow\downarrow)s'\rangle$$

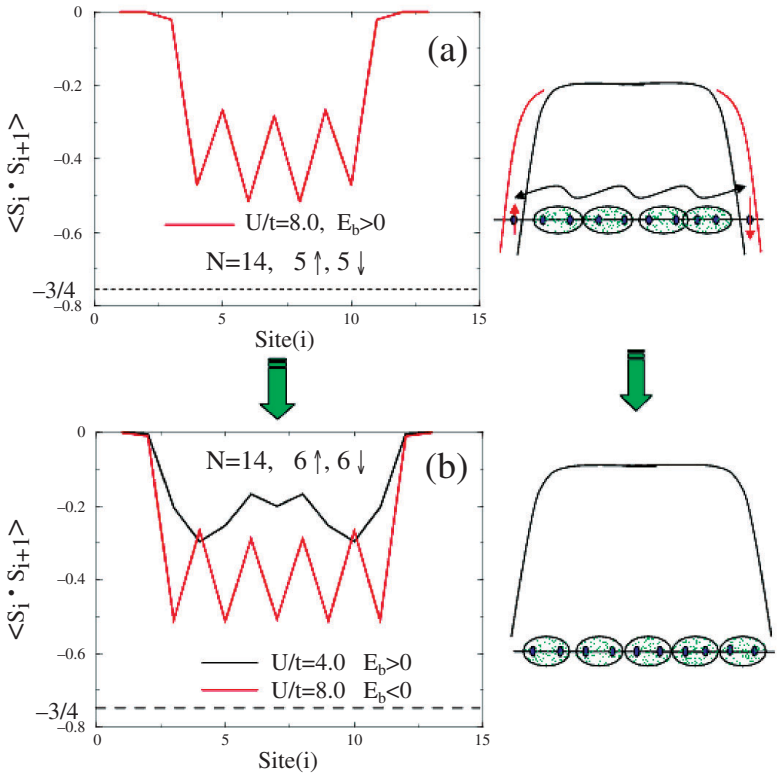

Fig. 4 The site depdendences of $\langle S_i \cdot S_{i+1} \rangle$ for (a) 14 (5↑, 5↓). and (b) for 14 (6↑, 6↓). The right figures are schematic figures for the spin structures obtained from (a) and (b), respectively.

In Eq. (2), the first part brings out the zigzag spin structure [16] and the second part gives the development of the Cooper pair function [9]. In fact, we numerically check the dominance of the two terms from the ground state wave function, and moreover confirm that the dominance of the second term in the trapped system becomes more significant than that of uniform or open system [16]. This is because the non-uniformity of the trap enhances the weight of the second term.

We point out that the present mechanism of the pairing is unique in the sense that the pair remotely develops and the Mott core mediates the pairing, i.e., the same kind of fermions play different roles through the spatial difference of hole concentration. This becomes possible only in the strongly correlated fermion system trapped inside the confinement potential. This situation partly has a close similarity to the spatially modulated phases or the stripe phases of high T_c superconductivity [11]. For example, the Mott domains in the stripe phases periodically emerge in atomic scales. Then, the system is strongly affected by the periodical potential which is self-organized over the extent of the emerging Mott domain. A part of such a situation is quite analogous to the present case [9, 16].

4. Summary and Conclusion

We numerically studied two kinds of topics related to superconductivity. The main result in terms of the first topic was the construction of the simulation framework and its large-scale simulation program in order to simulate the voltage-biased condition employed in TES. We successfully finished test simulations and actually confirmed the automatic rapid response of the current at the transition edge. For the second topic, we calculated the spin structure in order to clarify the mechanism of the Cooper pairing which was observed in the Hubbard model with the confinement potential.

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MgB_2超伝導体の転移点近傍での中性子捕獲後の非平衡ダイナミクスと閉じ込めハバードモデルでの超伝導ペア形成

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1. プロジェクトの概要

最近発達してきた超伝導ナノファブリケーションのテクニックにより全く新しいタイプの超伝導デバイス開発の可能性が開けてきた。これを受けて本プロジェクトでは、以下の3つの新しい超伝導デバイス開発に関連したシミュレーション研究を行った。

1）中性子飛来の時系列を検出する超伝導デバイス開発のための研究。
2）1）のテーマを基礎からサポートし、かつ新しいナノスケールでの新奇超伝導物理現象を探索するための研究。
3）高温超伝導体と金属超伝導体とをモザイク状に配置するなど、ナノ量子ドットデバイスのシミュレーション研究。

テーマ1）では、コンソーシアムの複数の実験グループと協力し、高精度中性子検出デバイスを提案するための試行シミュレーションを実施する。テーマ2）では、ナノスケールでの超伝導発現機構やその微視的状態を明らかにするため、ナノ超伝導体の基底状態の探索を行う。テーマ3）では、量子コンピュータ・キュビットモデルとして有力視されている異なる超伝導体界面に現れる縮退半磁束のダイナミクスを大規模シミュレーションする。

2. 得られた成果（2005年度）の概要

今年度得られた成果の一つは、①テーマ1）の超伝導体MgB_2の中性子捕獲後の超伝導非平衡ダイナミクスのシミュレーションを超伝導転移点近傍かつ電圧バイアス条件下で実施することに成功し、超伝導放射線検出器一般のシミュレーションを原理的に可能とした点である。もう一つの成果は②テーマ2）に関連してナノスケールに閉じ込められた強相関電子系が示す新しいタイプの超伝導ペア形成のメカニズムを同定したことである。以下に具体的な成果の概要を記す。

① 超伝導体MgB_2に中性子が照射されるとB（ボロン）の同位体^{10}Bは核反応を起こし、一定の運動エネルギーを持ったα粒子が射出される。この際、荷電粒子であるα粒子は物質内で原子と衝突を繰り返し、そのエネルギーは熱へと変換される。本年度は、この熱変換を最も効率良く電気信号に変えることができる超伝導転移点近傍でのシミュレーションに挑戦した他、その際、初期状態への自動フィードバックを可能にする電圧一定のバイアス条件をシミュレーションできるようにプログラムを改良した。実際、テスト計算により、電圧バイアスでの自動フィードバックを再現することに成功し、検出過程は極めて高速であることを見出した [1]。

② 一般に酸化物高温超伝導体に代表されるような電子相関の極めて強い系の代表的理論的モデルとしてハバードモデルがあるが、当プロジェクトではこのハバードモデルに対し、調和振動子型のポテンシャルを付加し、フェルミオン粒子（電子）を中心部に閉じ込める派生モデルに着目し、その超大規模ハミルトニアン行列（最大で千数百億次元に達する）の対角化を行うことで超伝導に必須のペア形成が起こることを見出している。本年度は、この超伝導ペア形成の機構を解明するため、スピン構造を計算した。その結果、ポテンシャル中心部ではスピン・シングレットの交替形成が見出され、粒子の付加と共にそのシングレット・ボンドが組み替わることでエネルギー利得を得ているという事実を見出し、それが粒子間引力の源であることを突き止めた [2]。

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