Non-equilibrium Superconducting Dynamics after Neutron Capture in MgB_2 and Novel Superconductivity Confined inside Nano-scale Domains

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We perform large-scale numerical simulations on non-equilibrium superconducting dynamics after a neutron capture in MgB_2 by solving the time-dependent Ginzburg-Landau equation coupled with the Maxwell and the heat diffusion equations. The simulation results reveal that an electrical response accompanied by the non-equilibrium superconducting dynamics is sufficiently rapid to detect each neutron individually even in a large neutron flux yielding 10^5 counts per sec. On the other hand, we investigate a possibility of superconductivity confined in nano-scale domains by using exact diagonalization method. It is found that if the confined potential is strong enough to make an electron cluster inside a nano-scale region around a potential center and the Coulomb repulsion exceeds a critical value, then a Cooper pairing correlation develops around the electron cluster. This superfluidity can be easily confirmed in an atomic Fermi gas loaded on an optical lattice created by two laser beam interference.

Keywords: Nano-scale Superconductor, Non-equilibrium Superconductivity, Neutron Detection, Superconductivity Mechanism, MgB_2

1. Introduction

After the discovery of an alloy superconductor MgB_2 [1], a unique application using MgB_2 has been suggested by Ishida et al. [2]. The idea is as follows. A nuclear reaction between a neutron and ^{10}B releases a fixed energy. The energy transforms into a heat which leads to an instantaneous destruction of the superconducting state. Then, the moment is observable as the electrical signal [2] since the electrical resistance arises with the destruction of superconductivity. This is principally the same as the detection mechanism of the superconducting transition edge sensor (TES) for X-ray [3].

In this paper, we investigate how the superconductivity destructive region created by the nuclear reaction expands and shrinks inside the superconductor and estimate a time-resolution of MgB_2 strip geometry as a neutron detector by performing direct numerical simulations [4] of the time-dependent Ginzburg-Landau (TDGL) equation coupled with the Maxwell and the heat diffusion equations [5].

The nuclear reaction between the neutron and ^{10}B emits α particle with an energy of 1.47MeV. Then, the initial speed of the α particle is 2.7×10^6m/sec, and the speed is lost by the interaction with electrons and lattice ions inside MgB_2. In the atomic energy research, the traveling range of α particle inside solid state matters have been intensively investigated. According to their results [6, 7], we can assume it to be 3 μm and therefore, the time of flight to be 1.0×10^{-12} sec. Based on this assumption, we make a simple model in which the energy is lost with the same rate per second and calculate a time period from the initial nuclear-energy release to the recovery of superconductivity by installing the model onto the TDGL simulation code [5]. As a result, we find that the time period is short enough to individually detect each neutron even in 10^5 neutron flux per second which corresponds to the high-intensity neutron flux emitted from the pulse neutron source in J-PARC [8].

The superconductivity mechanism of High-T_c cuprate superconductors is now still elusive [9] although a tremendous of theoretical and experimental investigations have been made. This is because the superconductivity emerges on experimentally unexplored and theoretically difficult electronic-states, i.e., strongly-correlated electronic states.

The Hubbard model [10] has been regarded as a typical model showing strongly-correlated behaviors like the metal-insulator transition. Since the discovery of High-Tc superconductors, the model has been intensively investigated in order to clarify whether or not the model describes high temperature superconductivity exceeding 100K. However, the issue has been not resolved yet. This is because it is quite difficult to solve theoretically and numerically Hubbard model ($\geqq$2D) in thermo-dynamical limit.

On the other hand, we point out that the superconductivity still exists even if it is confined inside nano-scale domains. In fact, in atomic gas systems, the experimental success of Bose-Einstein condensation is performed on trapped finite systems. Recently, the experimental development in atomic physics is so rapid that superfluidity even in atomic Fermi gases has been confirmed [11]. Furthermore, we note that the interference of two lasers creates an optical lattice [12] which enables to experimentally study the Hubbard model. Although there has been still no experiment on the atomic Fermi gas loaded on an optical lattice, the theme is a quite big challenge inspiring all fundamental physicists. In this paper, in order to study superconductivity in confined systems, we numerically study the Hubbard model with a trap potential and explore a possibility of superfluidity [13].

The contents of this paper are as follows. In Section II, a model of the thermal-heat release with the motion of α particle after the neutron capture is given, and results of large-scale simulations incorporating the model are shown. In Section III, we examine a possibility of superconductivity in electron systems confined inside a nano-scale range and discuss physical significance of numerical results.

2. Non-equilibrium Superconducting Dynamics after the Neutron Capture in MgB$_2$

The boron B in MgB$_2$ has two isotopes, i.e., ^{10}B and ^{11}B, and ^{10}B has a quite large nuclear reaction cross- section for thermal neutrons. The nuclear reaction is described as follows,

$$^{10}\mathrm{B} + n + \longrightarrow {}^{7}Li + {}^{4}He\,(\alpha),$$

where, both ^{7}Li and ^{4}He are charged particles which strongly interact with the electron and lattice systems inside MgB$_2$ superconductor. In the nuclear reaction, ^{7}Li and α particles initially receive 0.84MeV and 1.47MeV, respectively. In this paper, we focus on the heat energy released by only the motion of α particle for simplicity. We note that the energy release process by ^{7}Li particle is principally equivalent with that of α particle and the inclusion of all the processes is easy.

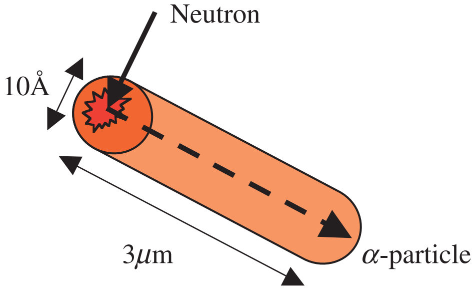

Fig. 1 A schematic figure for the motion of α particle after the neutron capture in MgB$_2$. The emission direction is randomly chosen . Li particle runs away in the opposite direction.

Figure 1 is a schematic figure for the flight of α particle inside MgB$_2$. The α particle takes 2.7×10^6m/sec as the initial speed, and pushes its way through the lattice and electronic barriers. Then, the running length until α particle being at rest is estimated to be about 3 μm inside MgB$_2$. This length scale is obtained by not only the empirical Bragg-Kleeman's law [6] but also a useful open code SRIM [7]. Thus, taking the length 3 μm and assuming the initial kinetic energy to be lost in a uniform rate per sec, we fix the time of flight of α particle to be 1.0×10^{-12}sec. This assumption further gives a simple model that the kinetic energy is also converted into thermal heat in the uniform rate during the time of flight. Although this modeling is not so sophisticated, it is valid enough to estimate the time resolution of electrical response after the neutron capture.

In order to simulate the dynamics of the superconducting state and the local temperature after the neutron capture together with the above model, we solve the TDGL equation coupled with the Maxwell [3] and the heat diffusion equations [4]. Figure 2(a) and (b) show snapshots of the superconducting order parameter at two moments in which α particle is just running inside and flying away to the outside, respectively.

From Fig. 2(a) and (b) it is found that since the heat propagation is much slower than the motion of α particle, the front line of the superconductivity destruction region expands like Cherenkov radiation. Fig. 2(c) is the voltage vs. the time (t) which shows the total electrical response after a neutron capture. In Fig. 2(c), it is found that after the nuclear reaction starts the negative dip of the voltage emerges. This is the electrical response to the heat energy release by the nuclear reaction. We find from Fig. 2(c) that the period from the initial response to the recovery of the superconductivity is about 10^{-7} sec. This result indicates that the system can principally detect 10^7 neutron individually per sec if the neutron flux is ideally narrow and uniform in its time domain. At the present, a resolution of more than 10^5 counts per sec is required in J-PARC [8]. The present simulation result guarantees that the detector using MgB$_2$ principally satisfies the condition.

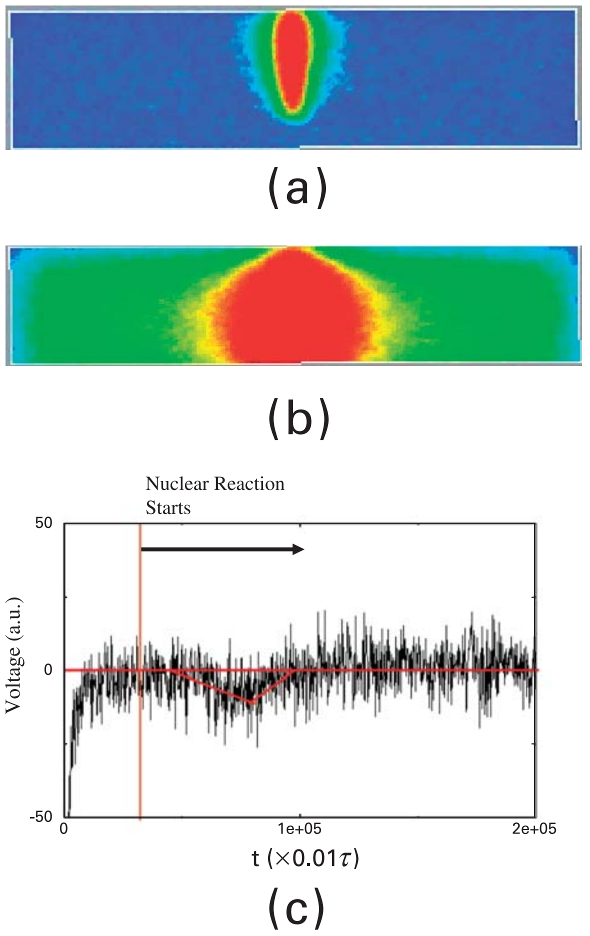

Fig. 2 (a) The snapshot of the order parameter distribution. The red color indicates the complete depression of the amplitude of the superconducting order-parameter. In this case, the nuclear reaction occurs at the top center surface. The moving α particle is located at the front of the depressed region. (b) The snapshot after α particle ran away into the outside. (c) The voltage vs. time (t). The time unit is 0.01 τ where $\tau \sim 1.0 \times 10^{-12}$ sec.

3. Exact Diagonalization for Fermion-Hubbard Model with Confined Potential

The Hubbard model [10] is one of the most intensively studied models by computers because it owns very rich physics although the model expression is quite simple. The Hamiltonian of the Hubbard model with a trap potential is given as [13]

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

where t, U, and V 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, and the parameter characterizing the strength of the trapping potential, respectively, as schematically shown in Fig. 1.

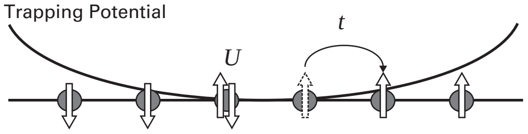

Fig.3 A schematic figure for the confined fermion-Hubbard model.

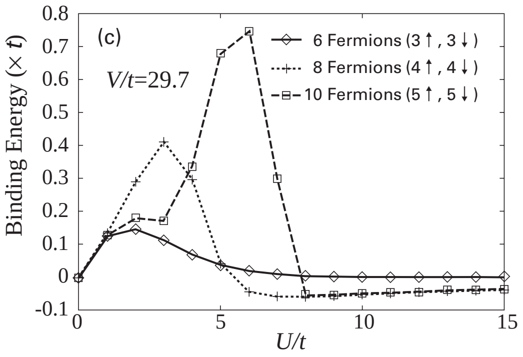

Fig. 4 E_b vs. U/t for three cases. V/t is fixed to 29.7.

We diagonalize the Hubbard Hamiltonian H and calculate an binding energy which is a probe for superfluidity by varying U (> 0) and V[13]. We discuss a condition in which Cooper pair develops based on the binding energy given by $E_b = E_g\,(n+1\uparrow, n+1\downarrow) + E_g\,(n\uparrow, n\downarrow) - 2E_g\,(n\uparrow, n+1\downarrow)$ where $E_g\,(n\uparrow, n\downarrow)$ is the ground state energy for n up-spin and n down-spin fermions. If E_b is negative, then an attractive interaction works between two fermions, which leads to an instability of cooper pair formation. Figure 4 shows E_b vs U/t for three cases in which the total number of fermions varies from $N_F = 6$ (3↑, 3↓) to 10 (5↑, 5↓) and V/t is fixed to be 29.7 in all cases. From Fig. 4 it is found that E_b goes to negative above a critical U_c (~8) and the negative amplitude increases with increasing N_F. We confirm that U/t dependence of E_b almost converges at $N_F = 10$ although results of $N_F > 10$ are not shown here. These results mean that a large U/t (>U_c) leads to a superfluidity associated with attractive interaction between two particles under sufficient particles

Next, let us focus on a change of the particle distributions around U_c. Figure 5(a) and (b) show those as $U<U_c$ and $U>U_c$, respectively. When $U<U_c$, the distribution is like a dome-shape. This means that particles concentrate in the central area since V is dominant over U. When $U>U_c$ the shape changes into a flat mountain like mesa[13]. This means that the Mott state (1 fermion per site) emerges reflecting a strong correlation effect due to large U. In addition, we find that particle fluctuations occur only around the Mott cluster, i.e., particles clings to the wing of the Mott cluster and the attractive interaction works between their particles. This remote pairing via the Mott cluster is intrinsic to confined systems which is the first observation in a history of superfluid and superconductivity [13].

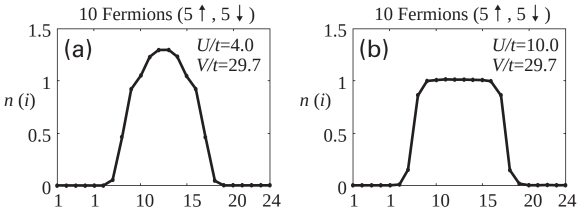

Fig. 5 Particle distributions for U/t =4.0 (U<Uc) and U/t=10.0 (U>Uc).

4. Summary and Conclusion

We performed two kinds of large scale simulations related to superconductivity. The first one is to examine the non-equilibrium superconducting dynamics after the neutron capture in MgB_2, and the second one is the exploration of superconductivity confined inside the nano-domains. As a result of the use of the Earth Simulator, we succeeded in roughly estimating a time resolution of the MgB_2 neutron detector and finding a new type of superconductivity peculiar to the confined systems.

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MgB_2超伝導体の中性子捕獲後の非平衡ダイナミクスとナノスケールに閉じ込められた系での新しい超伝導

プロジェクト責任者

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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した。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った。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した。

2. 得られた成果（2004年度）の概要

今年度得られた最も大きな成果はテーマ1）に関連して行った超伝導体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による中性子検出の時間分解能の見積もりとテーマ2）に関連する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状態の発見である。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、α粒子の物質内の飛距離は3μm程度と見積もられることから、飛行時間と運動エネルギーから熱エネルギーへの変換過程のモデル化が可能となる[1]。本年度はこのモデルを、超伝導の非平衡ダイナミクスを記述する時間依存のギンツブルク・ランダウ方程式のシミュレーションに組み込むことで、捕獲後の時間変化を詳細にシミュレーションし、その結果、中性子検出の時間分解能が極めて高いことを見出した。

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モデルを有限に閉じ込めるために調和振動子型のポテンシャルを付加し、ポテンシャルが超伝導にどのような寄与を及ぼすかを超大規模行列（最大で千数百億次元に達する）の対角化を行うことで調べることとした。その結果、閉じ込めポテンシャルが有効に働き、ポテンシャル中心にモットコアと呼ぶ、1格子当たり1フェルミ粒子の状態を介して互いに隔たった周辺部で遠隔のペアリング相関が発達するという全く新しいタイプの超伝導状態を発見することに成功した。この超伝導は、固体で実現することは現状では難しいが、トラップされたフェルミ原子ガスにおいては近い将来実現可能である[2]。

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