Ultra-Large Scale Simulations for Superconductor MgB_2 Device toward Nuclear Application and Fundamental Issues in Nano-superconductivity and Atomic Fermi Gas Loaded on Optical Lattice

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We performed 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 equation coupled with the Maxwell and the heat diffusion equations. The simulations were executed under the current-biased condition in order to explain experimental results carried out in JRR-3, JAEA and the temperature and the current dependences of the experimentally observed signals were successfully reproduced. On the other hand, we investigated issues about microscopic matter-density inhomogeneities through the attractive Hubbard model with confinement potential, which is a model for nano-size domain of strongly-coupled superconductors and atomic Fermi gas loaded on an optical lattice. The calculations revealed that microscopic density inhomogeneities, whose characteristic variation length is the lattice constant, universally appear in the presence of strong attractive interaction and confinement potential breaking the translational symmetry. This type of inhomogeneity is easily observable for the optical lattice systems in atomic Fermi gases.

Keywords: Time-dependent Ginzburg-Landau Equation, Non-equilibrium Superconductivity, Neutron Detector, MgB_2, Hubbard Model, Optical Lattice, Inhomogeneity

1. Introduction

After the discovery of an alloy superconductor MgB_2 [1], a large amount of experimental studies have been made in order to explore fundamental aspects of MgB_2. As a result, several novel features have been clarified. In addition, many applications using MgB_2 have been proposed. Among their ideas, an application suggested by Ishida et al. is a quite attractive for 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 nuclear energy is released, and the energy transforms into a heat which leads to an instantaneous destruction of the superconducting state if MgB_2 is set to be in the superconducting state. Thus, an event of the nuclear reaction is easily found to be observable as an 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]. Thus, a main aim of our project using the Earth Simulator is to simulate the process from the nuclear reaction to the electrical signal generation [4–6] and to provide helpful information on making a real neutron detecting device. We believe that our simulation enables to avoid wasteful trial experiments.

In this fiscal year 2006, our project team performed simulations, in order to explain experimental results jointly carried out by Osaka Pref. Univ. and Quantum Beam Science Directorate, JAEA. The experiments, which were made on

JRR-3, JAEA in 2006, succeeded in observing the electrical signal for the first time by exposing MgB_2 sample to the neutron irradiation. The characteristic response time for the single detecting event is an order of 10 ns, which is almost consistent with our predicted data obtained through our 2004 and 2005 year's project. In addition to the fundamental signal data, experimentalists measured the temperature and the applied current dependences of the signal appearance. Thus, we also numerically tried to examine the temperature and the applied current dependence in this fiscal year 2006. These all simulations were performed under the current-biased condition, and the obtained results show a good agreement with the experimental results. We will perform more systematic studies in the next fiscal year 2007.

Various applications using the conventional and high-Tc cuprate superconductors are known to be promising. On the other hand, an attempt to raise the superconducting transition temperature (T_c) [7] is a quite attractive issue for not only fundamental physicists but also engineers, 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 fiscal year 2004 [8, 9]. An initial step for us is to develop numerical schemes [10, 11] to approach the issue. This is to make parallel programs executable on large-scale parallel supercomputers like the Earth Simulator. At first, we have focused on the exact diagonalization, and we found an alternative numerical scheme called "preconditioned conjugate gradient method (PCG)" instead of the traditional Lanczos one. The PCG scheme runs about 5~12 times faster than Lanczos [10, 11]. Moreover, our parallel diagonalization code usually shows the performance exceeding above 50% of the peak [10, 11]. This result is also applicable to other wide fields, which need a fast parallelized diagonalization code. Thus, our team was selected as one of finalists of Gordon Bell Prize for both 2005 [10] and 2006 [11] years.

Our target model for the quest of superconductivity microscopic mechanism and related topics is the so-called Hubbard model [12]. The model has been regarded as a typical one capturing strongly-correlated behaviors like the metal-insulator transition. In addition, since the discovery of High-Tc superconductors, whether it can describe d-wave high temperature superconductivity exceeding 100K [7] or not, has been intensively studied. However, the issue has been not resolved enough yet. This is because it is too quite difficult to numerically calculate the Hubbard model (≧2D) in large system sizes enough to obtain a conclusive result in the thermo-dynamical limit. Especially, the exact diagonalization scheme confronts a crucial difficulty that the necessary memory space exponentially increases with the number of fermions (electrons) and sites, although it completely keeps exactness in contrast to other methods, which require more fundamental improvements to obtain reliable results. Thus, we studied the Hubbard model with confinement potential [8, 9] by using the parallelized exact-diagonalization code. The model is for atomic gas systems and partly nano domains of supercondutors, in which finiteness is an intrinsic feature.

The contents of this report are as follows. In Section II, the numerical results under the current-biased condition are presented and compared with experimental results. In Section III, the exact diagonalization results for the attractive Hubbard model with the confinement potential are given and the origin of the observed matter-density oscillation is briefly discussed.

2. The Non-equilibrium Dynamics under the Current-biased Condition in MgB_2

Recently, the experiments to test the neutron detection were made at JRR-3, JAEA. The employed condition was the so-called current bias, in which the fixed transport current is applied and the voltage is measured as the event counter for the nuclear reaction. The signal was actually measured in voltage vs. time, and the signal shape was principally pulse like one. The pulse width, i.e., the time-scale characterizing the event, is an order of 10 nsec, which coincides with our prediction. However, since we expected the detection in the voltage-biased condition, we had not data enough to compare with the experimental results. Thus, we performed numerical simulations under the current-biased condition, again. Our typical signal data (voltage vs. time) is shown in Fig. 1, where the temperature is 38K (Tc = 39K) and the bias current is 0.001, which is normalized by the critical current density at T = 0. It is found from Fig. 1 that the signal is divided into a rapid rising and a relatively slow decay, which well looks like the experimental data.

Figure 2 presents a temperature dependence of the signal. Since we use the same initial seed for random number to create noises for both the superconducting order parameter and the electric field, the time fluctuating component are quite similar. The signal height decreases with decreasing the temperature, and becomes comparable to the noise level at T = 35K. Figure 2 just demonstrates such a case. The experimental results also show the same behavior. From these results, we conclude that the developed simulation code[4–6] well reproduces the experimental results. In the next fiscal year, we will perform more systematic simulations in order to understand the relationship between the non-equilibrium dynamics and the signal shape and to optimize the detecting conditions. The simulation will have a key role on optimizing the detector.

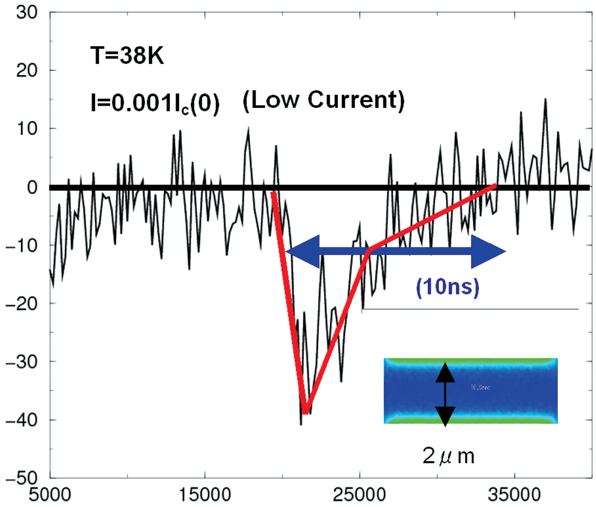

Fig. 1 (a) The voltage (a.u.) vs. time (a.u.). The inset is the simulated geometry.

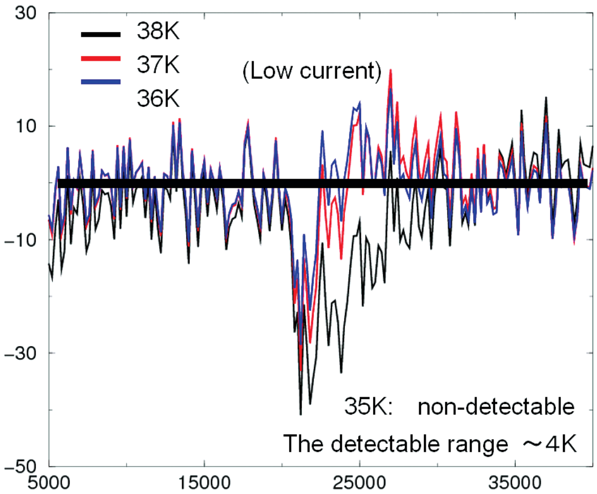

Fig. 2 The voltage (a.u.) vs. time (a.u.) for three temperature.

3. Attractive 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 simple. From the fiscal year 2004 to 2005, we studied the repulsive fermion-Hubbard model with confinement potential (see Fig. 3)[8, 9] motivated by the rapid advancement of atomic gas physics [13–14], and found that the model shows the Cooper pairing instability by confirming the negative binding energy and the development of the pair function [8, 9]. This result demonstrates a deep connection between the Hubbard model [12] and the superfluidity [8, 9] although the system is a confined finite system. In this fiscal year 2006, we turn to the attractive fermion-Hubbard model with confinement potential [15]. This is because the superfluidity of the atomic gas loaded on an optical lattice was experimentally observed [16], and its experimental situation can be modeled by the attractive Hubbard model rather than the repulsive one.

Firstly, let us describe the Hamiltonian of the Hubbard model with a harmonic-well potential, [8]

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

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 on-site attractive interaction energy, the parameter characterizing the strength of the trapping potential as schematically shown in Fig. 3, and the site number, respectively. We diagonalize the Hubbard Hamiltonian H (Eq.(1)) [8, 9] and calculate the site dependence of the fermion density <n(i)>.

Figure 4 presents a typical result of U/t dependence of <n(i)>, in which V/t = 1, and N = 16 . As seen in the figure, it is found that <n(i)> shows zigzag structures in a wide range of |U/t| [15]. Also, one finds that the periodicity of such a zigzag oscillation is almost the lattice constant. We confirm that this kind of microscopic inhomogeneous character universally appears in a wide range of parameters if the translational symmetry is broken [15]. We would like to point out that these inhomogeneous microscopic inhomogeneities are very similar to the observation results in the surface of High-Tc superconductors. We predict that these features can be easily confirmed by atomic gases loaded in optical lattices, while similar patterns are also observable in condensed matter systems due to its universality. See Ref.

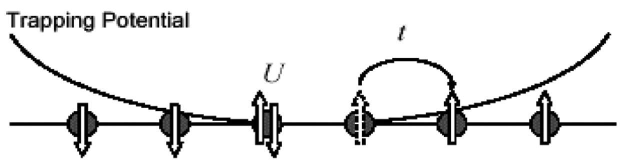

Fig. 3 A schematic figure for the fermion-Hubbard model with confinement potential.

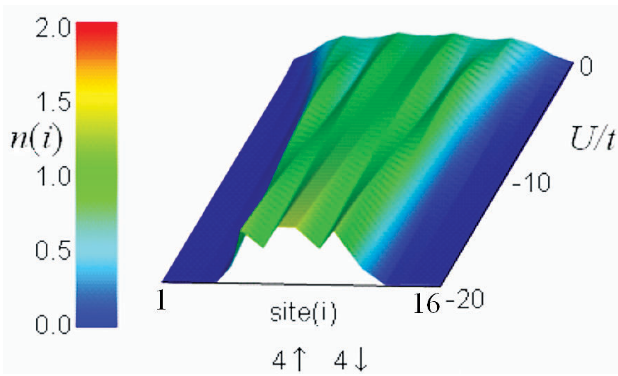

Fig. 4 The U/t dependence of the matter density profile n(i) for the fermion-Hubbard model with a harmonic potential (V./t=1).

[15] for more details of numerical simulations and theoretical analysis on why such a structural pattern appears.

4. Summary and Conclusion

We numerically studied two topics related to superconductivity. The main result in the first topic was a comparison between numerical simulations and experimental results. Consequently, we successfully reproduced experimental results. This implies that our numerical framework is valid and useful. In the next fiscal year, we will perform more systematic simulations to clarify non-equilibrium dynamics and to optimize detector performance. On the second topic, we further developed the highly-parallelized code for the exact diagonalization. The paper about its technical points was selected as a 2006 year's finalist of Gordon Bell Prize. In this year, we concentrated on the attractive Hubbard model with confinement potential and found that microscopic density oscillation universally appears in a wide variety of the model parameters. We predict that the observed oscillating patterns can be easily confirmed in atomic Fermi gas loaded on optical lattices. Moreover, we believe that the result has a relationship with the observation of inhomogeneities seen in High-Tc cuprate superconductors. In the next fiscal year, we will develop a new code using the dense matrix diagonalization and challenge new fundamental and fruitful issues.

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MgB_2超伝導体デバイスの中性子捕獲後の非平衡ダイナミクスと引力ハバードモデルでの非一様状態の形成

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1. プロジェクトの概要（計画）

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計画した。

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) 異種超伝導体をモザイク状に配置するなどにより得られるナノ量子デバイスのシミュレーション研究。

テーマ1)では、コンソーシアム内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やそれの中性原子版である原子ガスの研究を行う。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やジョセフソン接合等の大規模シミュレーションを行う。

2. 得られた成果（2006年度）の概要

今年度得られた成果の一つは、①テーマ1)に関し、実験グループがJRR-3（原子力機構）にて初期的実験に成功し、中性子検出と見られるシグナルを得たことと、その応答時間は10nsecのオーダーであり、昨年度までのシミュレーション結果と一致したことである。また、実験で得られたシグナルの温度依存性や電流依存性を再現するため初期的シミュレーションを実施したが、その結果もほぼ実験と一致した。これらの成果は、当プロジェクトで開発してきたシミュレーションコードが正しく動作していることの証拠であり、今後の研究進展が大いに期待できる。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、強い引力を及ぼしあう系の非一様基底状態の発見であり、光学格子上の原子ガスで容易に検証可能である他、広いパラメータ領域で実現することから、超伝導体のナノスケール・ドメイン内においても観察できる可能性が高い。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、この熱変換の様子について、電流バイアス条件下で観測に成功した実験結果を再現すべく、シミュレーションを行った。シミュレーションで得られたシグナル（電圧）の形状は、実験と良く一致した他、温度依存性、電流値依存性についてもほぼ一致する結果を得ることができた。

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）の対角化を行った。本年度は、強い引力が働く引力ハバードモデルの大規模計算を行い、広いパラメータ範囲で非一様な状態（粒子密度分布が非一様）が現れることを見出した。[1]。

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