Ultra-Large Scale Simulations for Superfluid Irradiation Device toward Nuclear Application and Fundamental Issues in Nano-structured Superconductors

Project Representative

Masahiko Machida CCSE, Japan Atomic Energy Agency (JAEA) & CREST (JST)

Authors

Masahiko Machida [*1, 5], Atsushi Hiratsuka [*1, 5], Susumu Yamada [*1, 5], Narimasa Sasa [*1, 5], Masahiko Okumura [*1, 5], Toshiyuki Imamura [*2, 5], Tomio Koyama [*3, 5] and Masaru Kato [*4, 5]

＊1 CCSE, Japan Atomic Energy Agency (JAEA)

＊2 University of Electro-Communications

＊3 IMR, Tohoku University

＊4 Graduate school of Engineer, Osaka Prefecture University

＊5 CREST (JST)

This report describes simulation study results on the research for superconducting (superfluid) neutron detector device and related fundamental issues on nano-structured superconductors in the fiscal year 2008. At first, in order to examine a performance of a neutron detector using superfluid He^3, we make large-scale numerical simulations on non-equilibrium superfluid dynamics after a neutron capture below the superfluid transition temperature by solving the Gross-Pitaevskii equation. The simulations whose largest grid size is 2048^3 on the Earth Simulator successfully reproduce the vortex nucleation and reveal the non-equilibrium dynamics of decay superfluid turbulence. On the other hand, as a fundamental research issue of this project, we numerically investigate the ground state of a two-band Hubbard model by using the exact-diagonalization method developed with this project to examine a superconducting mechanism for iron-based high-Tc superconductors discovered by Hosono's group in February 2008. By employing the exact-diagonaliation as a large-scale numerical tool, we reveal that a robust and novel type of superconductivity widely emerges when the inter-band repulsion becomes stronger than the intra-band one. Although such a situation is un-usual in solid state matters, the atomic Fermi gases may easily create the situation.

Keywords: Gross-Pitaevskii Equation, Non-equilibrium Superfluidity, Neutron Detection, He^3, Two-band Hubbard Model, Atomic Fermi Gas, Exact Diagonalization

1. Introduction

After the discovery of an alloy superconductor MgB_2 [1], a large amount of experimental studies have been made in order to clarify fundamental aspects of MgB_2. As a result, several novel features including the highest transition temperature among metallic superconductors have been clarified, and many ideas toward applications using MgB_2 have been proposed. Among their ideas, an application suggested by Ishida et al. is 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 initially released as kinetic energy of the nuclear reaction products, and the energy is transformed into a heat, which leads to an instantaneous destruction of the superconducting state if the temperature is set to be lowered than the superconducting transition temperature. Thus, we expect that an event of the nuclear reaction is observable as an electrical signal in the superconducting current carrying state [2], since the destruction of superconductivity nucleates a normal hot spot along which an electrical resistance is generated. This idea is basically equivalent to the detection processes of superconducting Transition Edge Sensor (TES) for X-ray, Superconducting Single Photon Detector (SSPD) 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 and to provide helpful information for the experimental team making a neutron detecting device and examining its performance. We believe that the present simulation project enables to avoid

wasteful several trial experiments and to shorten the period of the development project [4].

In this fiscal year 2008, our simulation project team made a new simulation plan based on the successful results on the neutron detection in MgB_2. The plan is as follows. At first, we pay attention to a fact that He^3 atom taking a liquid form also reacts to a neutron like B^{10}. In a very low temperature, the liquid He^3 shows a phase transition into superfluid state, in which the nuclear reaction is expected to lead to an instantaneous destruction of the superfluidity like the superconductor detectors. In particular, since the superfluid He^3 has a very low heat capacity and a very high thermal conductivity, non-equilibrium processes after the destruction are regarded to be much more drastic than that of the superconductor. In fact, it is known that vortices emerge and their turbulent states appear after the reaction since the quenching speed is faster enough than the superfluid recovering speed [5]. In addition, the turbulent states decay and the vortices finally disappear after a sufficiently long time. The non-equilibrium process attracts two interests, i.e., an engineering interest related to a construction of its detection system, and a fundamental interest how the turbulent states decay. In this fiscal year, we then examine the dynamics of the decay turbulence.

At first, the simulation team prepares a seed of the vortices, in which superfluid order is mostly destroyed and the phase of the depressed order is randomly distributed [6]. This assumption is reasonable since the starting situation corresponds to a normal region created by the heat energy release after the nuclear reaction. Starting with the initial condition, we numerically solve the Gross-Pitaevskii equation and examine the dynamics of the macroscopic superfluid wave function [7]. For this purpose, we employ the spectral method, which is frequently used in the numerical studies for normal isotropic and homogeneous turbulence [8]. The largest mesh size that we perform in this project is 2048^3, which is the world-record in the simulation field of the superfluid turbulence.

Another topic of our simulation project is a microscopic calculation on superconducting mechanism. Just before this fiscal year, since a new type of high-Tc superconductor, i.e., iron-based superconductor was discovered by Prof. Hosono's group [9], a main target has been a numerical study for the superconducting mechanism of the iron-based superconductors. We modify the exact diagonalization code to study the mechanism and perform large-scale calculations by mainly using 256 nodes. In iron-based superconductors, it is well-known that multi-orbitals of Fe atom have essential roles on electronic structures around the Fermi surface. Thus, it is crucial to theoretically treat a multi-band Hubbard model in order to examine the electronic origin as the pairing mechanism. In this present project, we use a two-band Hubbard model to do exact diagonalization and examine the binding energy, the spin gap energy, and the electron density profiles in various parameter ranges. Consequently, we find that a robust pairing occurs when the inter-band repulsive interaction U' becomes larger than the intra-band one U[10]. Then, the binding energy shows a very large negative value, and the spin gap energy is largely positive. Moreover, it is found that the pairing emerges in a very wide parameter range as long as U' is larger than U. We believe that the result is attractive for not only superconductivity but also atomic gas research field. This is because the atomic gas field also explores a more high-Tc superfluid mechanism.

The employed exact diagonalization code has been updated by our project team since the fiscal year 2004 [11]. The initial step of this project was to select the best effective numerical scheme and to parallelize the calculation code. Consequently, we successfully found an effective algorithm and implemented its parallel program on the Earth Simulator. So far, since we have improved the code step by step, we now have a sufficiently highly-parallelized code. In the latest code, an alternative numerical scheme called "preconditioned conjugate gradient method (PCG)" is employed instead of the traditional Lanczos one, since the PCG scheme runs about 5 ~ 12 times faster than Lanczos one on the Earth Simulator [12]. This result indicates that PCG method is much more effective in large-scale parallel calculations than the traditional and widely used Lanczos scheme. In addition, our parallel diagonalization code usually shows the performance exceeding above 50% of the peak on the Earth Simulator. These results are applicable to other wide fields, which require a fast parallelized matrix-diagonalization code. These works were nominated as finalists of Gordon Bell Prize in both 2005 [11] and 2006 [12] years. Generally, since the matrix diagonalization code repeats all-to-all communications, the performance basically drops down due to the heavy communication. However, we have successfully improved the code by effectively overlapping communication steps with floating operations. Since there is no room to describe the details of such tuning techniques in this annual report, we would like to also point out another point that a combination of three-level tuning, i.e., the inter-node and the intra-node parallelization and the vector parallelization is crucial in improving the performance on the Earth Simulator [12].

The contents of this report are as follows. In Section II, the numerical method to simulate Gross-Pitavskii is briefly described and the numerical results are given. In Section III, the two-band Hubbard model is derived for iron-based superconductors, and the numerical results are shown. See Ref [13] and [10] for more details of results in Section II and III, respectively.

2. Simulations for the Gross-Pitaevskii equation

In this section, we briefly introduce the quantum turbulence and explain the numerical method to perform numerical simulations for Gross-Pitaevskii equation. Subsequently, we give typical simulation results in the decay turbulence condition.

Now, let us first concentrate on vortex dynamics in superfluid. Vortex dynamics and turbulence due to their complex motions are quite important issues for not only fundamental physicists but also engineers. Especially, understanding and predicting the turbulence are crucial for various engineering fields, e.g., construction of power plants from nuclear to wind energy. The classical turbulent flow of normal fluids has still remained unsolved, while quantum fluids have offered another challenging target, "Quantum Turbulence", which may be more fundamental but significant in a sense [6].

In the quantum turbulence, there remain various interesting questions. The typical one is how quantum effects simplify the turbulent flows. In order to challenge the problem, Kobayashi and Tsubota performed direct numerical simulations for a modified version of the Gross-Pitaevskii equation by using the spectral method and found the Kolmogorov spectrum as a statistical feature of the turbulent state similar to the classical turbulent flow [14]. The spectral method is widely used for simulation studies on normal fluid dynamics. Especially, it has been well-known that the method is frequently employed in fundamental numerical studies on the turbulence under isotropic and homogeneous conditions, which are realized by imposing a periodic boundary condition [8]. We note that Yokokawa et al., reported their development and interesting results on the Earth Simulator [8].

In this fiscal year, our project team challenges to a mission in terms of decay quantum turbulence. The mission is divided into two steps, one of which is to construct a parallel code to analyze the dynamics in decay turbulent states in larger scale, and another of which is to confirm the scale invariant property of the characteristic spectrum as seen in the classical turbulence and to find particular features intrinsic to superfluid if it is present. We think that the second step is quite important for further understanding of quantum turbulence and non-equilibrium dynamics after the nuclear reaction. In order to carry out the purpose, we constructed a code simulating the modified Gross-Pitaevskii equation [5, 14] and parallelized the code on the Earth Simulator. By using the code, we have already succeeded in reproducing the results of Kobayashi and Tsubota on 256^3 and 512^3 grids [5, 14] and also performed huge scale simulations on larger grid sizes, e.g., 1024^3 and 2048^3[13].

Let us show typical simulation results. Figure 1 is an energy spectrum, i.e., a snapshot of the relation k vs. E(k) obtained through a decay simulation with 512^3 grids. The result clearly indicates that a part of energy spectrum obeys the Kolmogorov law, which is $E(k) \propto k^{-3/5}$. Although this is a reconfirmation of results of Kobayashi and Tsubota, we successfully found that the relation continues up to 2048^3 grid sizes. This clearly indicates that the Kolmogorov law is universal for quantum turbulence. Thus, it is found that quantization effect, i.e., vortex quantization intrinsic to quantum turbulence is directly irrelevant to its universal features.

On the other hand, we find that there is a peculiarity in the spectrum. The feature is a hump structure observed in a high-k range. Now, we search the reason why the structure emerges. One of possibility is ascribed to a bottleneck effect due to Kelvin wave cascade on the conserved quantized vortex. In addition, we note that such a clear structure has been not observed in normal fluid turbulence.

Figure 2 shows a typical snapshot picture of a vortex profile when the Kolmogorov spectrum like Fig.1 is observed.
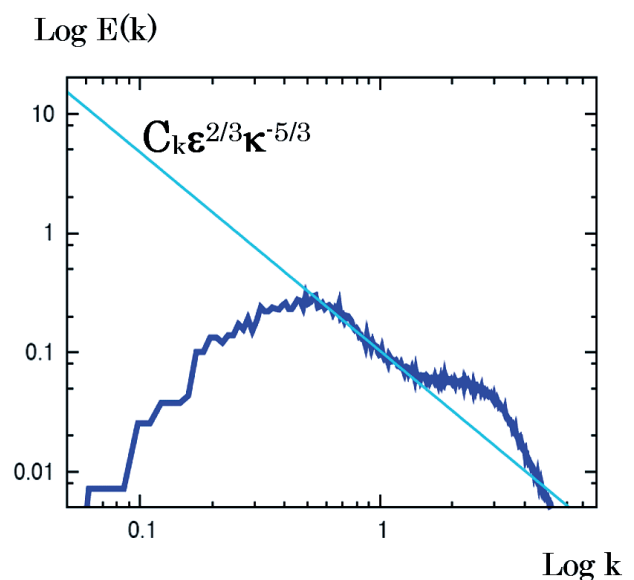

Fig. 1 A energy spectrum (k vs. E(k)) when vortices nucleated at the initial stage develop sufficiently. The used grid size is 512^3. The guiding line corresponds to the Kolmogorov scaling.
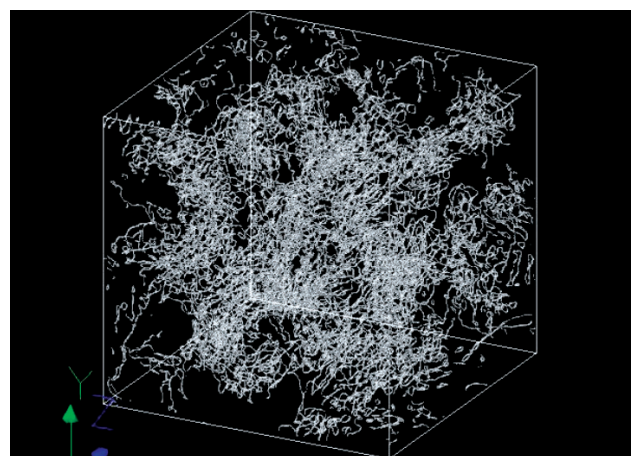

Fig. 2 A snapshot of vortex profiles in the simulation region (512^3) when the energy spectrum is like Fig. 1.

In such a moment, we can find that vortices are strongly entangled. More details of the simulation results will be published as a journal paper[13].

3. Exact Diagonalization Studies for Iron-based Superconductors: Two-band Hubbard Model

The Hubbard model [15] 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. In the fiscal year 2008, we studied the pairing mechanism on the two-band repulsive Hubbard model by using the exact diagonalization technique [11–12, 16] motivated by the rapid advancement of research for iron-based high-Tc superconductors [9].

There have been now debates how many bands are essential to study the superconductivity mechanism in iron-based superconductors. However, it is widely accepted that the most effective bands around Fermi surface are mainly two degenerate bands, i.e., d_{xz} and d_{yz} orbitals on Fe atoms. Thus, we believe that an exact analysis in the effective two-band model is significant enough to give important information on the pairing mechanism. Figure 3 is a schematic picture of sites and bands of the two-band Hubbard models. Due to the numerical resource limitation, the system is a ladder with 2 × 5 sites, and the number of the total sites is 20 due to two-bands. In the case, the half-filling condition mostly requires memory resource. We use 256 nodes to execute the code at the half-filling. The present two-band Hubbard model is composed of the kinetic energy term and the interaction one. The former is characterized by four hopping matrix elements whose values are given by a comparison with Fermi surface derived from the first-principle electronic structure calculation [17]. In this report, we do not describe details of the parameters. See Ref. for more details of them [10]. As for the interaction energy term, we consider three parameters, the intra-band Coulomb repulsion U, the inter-band one U', and the exchange correlation J. In this study, we note that we drop off the pair inter-band hopping. In iron-based superconductors, these interaction parameters can be also derived from the first-principle cal-
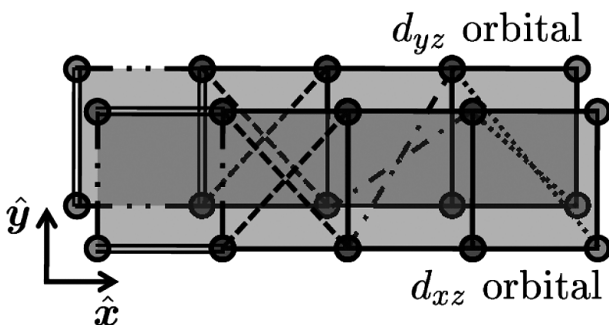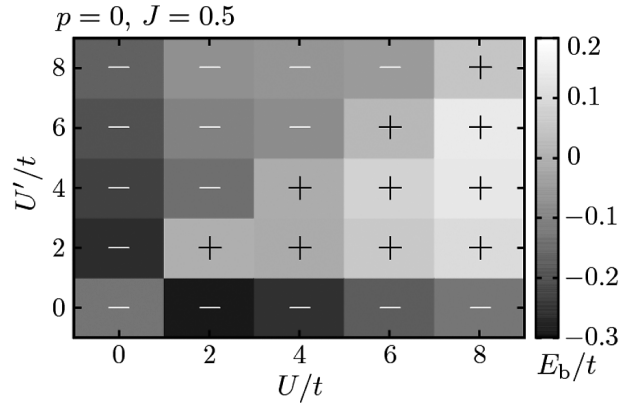

Fig. 4 A calculation result of the binding energy in U–U' range at J = 0.5. The doping rate p = 0.1.

culation, while the parameters still remain unsettled because the first principle calculation can not partly reproduce the experimental results [18]. Thus, we vary the three parameters in their possible wide ranges and explore the parameter region, in which the pairing can occur.

Figure 4 is a result of variation of the binding energy on U − U' space at a fixed J = 0.5. Here, we note that the attractive interaction works between two electrons when the binding energy is negative due to its definition [16]. However, it is noted that the negative binding energy does not necessarily guarantee superconductivity but the condition is just a requirement for superconductivity. From Fig. 4, it is found that the negative binding condition is widely satisfied when U' becomes larger than U. Although such a situation may be unusual, it is peculiar to multi-band systems. In addition, the robustness and the strong binding are quite attractive for the future exploration of high-Tc superconductors. We suggest that the novel mechanism may be directly confirmed in atomic Fermi gases, in which various parameters are more controllable.

4. Summary and Conclusion

We numerically studied two kinds of topics related to radiation detector and superconductivity mechanism. The main result in terms of the first topic was the success of parallel large-scale simulations for vortex nucleation and its decay quantum turbulence in superfluid He[3]. We confirmed that the superfluid turbulence satisfies the Kolmogorov scaling of the energy spectrum in a wide range of the wave vector like normal fluid turbulence. Furthermore, we found a unique feature peculiar to quantum turbulence. The result in terms of the second topic is that a robust and strong electron binding emerges when the inter-band Coulomb repulsion becomes larger than the intra-band one. The possibility is quite attractive for not only superconductivity research but also other fields like atomic gas research.

Fig. 3 A schematic figure for the present two-band Hubbard model as the computational region (2-legs × 5 sites).

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He³超流動中性子捕獲後の渦糸ダイナミクスと
2-バンドハバードモデルでの鉄系化合物超伝導の解析

プロジェクト責任者

町田　昌彦　　日本原子力研究開発機構　システム計算科学センター

著者

町田　昌彦*1, 5，平塚　　篤*1, 5，山田　　進*1, 5，佐々　成正*1, 5，奥村　雅彦*1, 5，
今村　俊幸*2, 5，小山　富男*3, 5，加藤　　勝*4, 5

＊1　日本原子力研究開発機構　システム計算科学センター

＊2　電気通信大学

＊3　東北大学　金属材料研究所

＊4　大阪府立大学　工学研究科

＊5　CREST（科学技術振興機構）

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2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（新たな放射線デバイス開発のための研究も含む）。

2) 1) のテーマを基礎からサポートし、かつ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。

　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他、新たなデバイス開発のためのシミュレーションを行う。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等を行う。

2. 得られた成果（2008年度）の概要

　1) に関しては、2007年度に原子炉JRR-3（原子力機構）にて超伝導体MgB_2に対する初期的検出実験が成功し、中性子検出と見られるシグナルが得られ、その応答時間（10nsecのオーダー）は、シミュレーション結果と一致した他、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ことにも成功した。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、超伝導放射線検出シミュレーションの枠組みがほぼ完成の域に到達したことを意味している。そこで、2008年度は、もう一つの超高精度検出器として期待されている超流動He³の中性子衝突による核反応後のダイナミクスのシミュレーションに挑戦した。2) に関しては、2007年度までにナノスケールに閉じ込められた多電子の基底状態を厳密に探索できる超並列行列対角化手法を開発してきたが、今年度はこの手法を2008年2月に発見された鉄系化合物超伝導体の超伝導機構探索に利用し、広いパラメータ領域で実現可能な新奇な超伝導状態が存在することを見出すことに成功した。こうした超伝導状態については、原子ガスでも対応物を構成することが可能であり、直接の検証が可能である。以下に両テーマの具体的な成果の概要を記す。

① 超流動体He³に中性子が照射されると、He³は核反応を起こし、一定の運動エネルギーを持った³Hとプロトン粒子が射出される。この際、射出粒子は物質内の原子と衝突を繰り返し、そのエネルギーは、一定の飛程距離内で熱へと変換される。本年度は、この熱変換後の様子をモデル化し、超流動がランダムに破壊されたとして、その後の超流動回復過程をシミュレーションした。その結果、実験で確かめられている渦糸生成とその渦糸の減衰乱流過程をシミュレーションすることに成功し、超流動乱流状態特有の現象を見出すことに成功している。

② 2008年2月に東工大・細野教授らのグループが鉄化合物高温超伝導体を発見したことに動機づけられ、これまでに開発してきた超並列厳密対角化法[1]を用いて、其の有力な単純化モデルである2-バンド・ハバードモデルの解析を行った。その結果、軌道間の斥力相互作用が軌道内のそれより一般に大きいとき、強力な超伝導が実現可能であることが分かった。こうした条件を満たす例は未だ幾つかの研究を除いて例がないが、極めて強力な状態を構成できるため、原子ガス等での直接観察[1]も可能であると考えられる。

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