Variational Monte Carlo Study of Spin-Gapped Normal State and BCS-BEC Crossover in Two-Dimensional Attractive Hubbard Model

Shun TAMURA * and Hisatoshi YOKOYAMA

Department of Physics, Tohoku University, Sendai, 980-8578, Japan

We study the properties of normal, superconducting (SC), and CDW states for an attractive Hubbard model on the square lattice, using a variational Monte Carlo method. In trial wave functions, we introduce an interspinon binding factor, indispensable for inducing a spin-gap transition in the normal state, in addition to the onsite attractive and intersite repulsive factors. It is found that, in the normal state, as the interaction strength $|U|/t$ increases, a first-order spin-gap transition arises at $|U| \sim W$ (where $W$: bandwidth) from a Fermi liquid to a spin-gapped state, which is conductive as a result of the hopping of doublons. In the SC state, we confirm by the analysis of various quantities that the mechanism of superconductivity undergoes a smooth crossover at approximately $|U_\text{coh}| \sim |U_c|$ from a BCS type to a Bose-Einstein condensation (BEC) type, as $|U|/t$ increases. For $|U| < |U_\text{coh}|$, quantities such as the condensation energy, a SC correlation function and the condensate fraction of onsite pairs exhibit the behavior of $\sim \exp(-t/|U|)$, as expected from the BCS theory. For $|U| > |U_\text{coh}|$, quantities such as the energy gain in the SC transition and superfluid stiffness, which is related to the cost of phase coherence, behave as $\sim t^2/|U| \sim T_c$, as expected in a bosonic scheme. In this regime, SC transition is induced by a gain in kinetic energy, in contrast to the BCS theory. We refer to the relevance to the pseudogap in cuprate superconductors.

KEYWORDS: superconductivity, BCS-BEC crossover, pseudogap, superfluid stiffness, condensate fraction, CDW, attractive Hubbard model, square lattice, variational Monte Carlo method

1. Introduction

Since the pioneering effort by Eagles,1 many researchers have extensively and repeatedly addressed the transition of superconducting (SC) properties from a BCS type to a Bose-Einstein condensation (BEC) type as the strength of attractive potential between fermions is increased. Following early studies of the BCS-BEC crossover2,3 using continuum models with the superfluidity of 3He in mind, Nozières and Schmitt-Rink4 showed by approximation that the SC properties smoothly evolve with the correlation strength in an attractive Hubbard model (AHM). Later, stimulated by the discovery of high-$T_c$ cuprates with a small coherence length, numerous researchers have tackled AHM,5 especially in two dimensions (2D); now, in connection with the evolution of pseudogaps as the hopping rate $\delta$ decreases in the so-called underdoped regime,6 the problem of BCS-BEC crossover as a function of $\delta$ is a subject of urgency.7,8 Entering this century, we have become capable of directly observing phenomena of crossover9,10 and pseudogaps11,12 in traps of ultracold dilute alkali gases,13,14 for which physical parameters can be artificially tuned. Recent experimental advances have brought hope of obtaining similar observations on optical lattices.

In the above stream of research, AHM is one of the most important and basic lattice models for studying the evolution of SC properties according to the interaction strength $U/t$ ($U$: onsite interaction strength, $t$: hopping integral between nearest-neighbor sites). In early and later studies of AHM, mean-field-type5 and diagrammatic4,15-17 approaches were used; although they successfully treated the weakly correlated regime, where the original BCS theory is basically valid, and developed a conceptual framework of the BCS-BEC crossover, more reliable methods remain necessary to establish properties in the intermediately (unitary) and strongly correlated (BEC) regimes. First, as an unbiased way, quantum Monte Carlo (QMC) calculations were implemented in the weakly and intermediately correlated regimes ($|U| \lesssim W$, $W$: bandwidth), because QMC is free from the negative-sign problem for AHM, but statistical fluctuation increases with increasing $|U|/t$ and system size. In 2D, SC transition of the Berezinskii-Kosterlitz-Thouless type was confirmed and an $n$-dependent phase diagram was discussed ($n$: particle density).18 Then, it was shown in the normal state ($T > T_c$) for intermediate $|U|/t$’s that a thermal-activation-type behavior appears in magnetic susceptibility, but that the charge compressibility is almost $T$-independent.19 This spin-gap behavior was corroborated by a peak split in the density of state.20 The dynamical mean field theory (DMFT), which becomes exact in infinite dimensions and is applicable to an arbitrary interaction strength, is another important approach to AHM. Early DMFT studies addressed normal branches without introducing SC orders at low temperatures ($T < T_{c1}$21 and $T = 0^2$), and found that the normal state undergoes a first-order transition from a Fermi liquid to a gapped state at $|U|/W = 1-1.5$, as $|U|/t$ increases. Later, various properties of the SC phase were calculated,23-25 and the crossover was characterized by the SC gap and superfluid stiffness.26

Another effective approach to AHM is a many-body variation theory, which is applicable continuously in the entire range of correlation strengths and particle densities. In contrast to DMFT, the dimension and lattice form are realistically specified, and one can treat wave-number-dependent properties in low-lying states. Furthermore, since wave functions are explicitly given, this approach has advantages in forming a physical picture. Because an AHM of a bipartite lattice is mapped to a repulsive Hubbard model (RHM) by a canonical transformation,27-29 one can develop a theory relying on the knowledge of RHM. Thus, the well-known Gutzwiller wave function (GWF)30 became a primary trial function for the

*E-mail address: shun@cmpt-serv.phys.tohoku.ac.jp
normal state: first, its properties were studied\textsuperscript{31} using the so-called Gutzwiller approximation (GA).\textsuperscript{32} As known for RHM, although GWF itself is always metallic,\textsuperscript{33} additional GA induces a spurious metal-insulator (Brinkman-Rice) transition\textsuperscript{34} at finite $|U_{\text{IRL}}|/U$ in finite lattice dimensions. For $|U| > |U_{\text{IRL}}|$ in AHM, all the particles tightly form onsite singlet pairs, and hopping completely ceases, so that the Brinkman-Rice transition remains a metal-insulator (Mott) transition also in AHM. Later, approximations similar to GA, which may be correct in infinite dimensions, have also been applied to the SC state\textsuperscript{35–37} to discuss the BCS-BEC crossover. However, to avoid the ambiguity of GA in realistic dimensions and to make use of the merits of the variation method, we need to accurately estimate variational expectation values. This claim is satisfied by a variational Monte Carlo (VMC) method,\textsuperscript{33,38–40} which treats local correlation factors exactly without a minus sign problem. A decade ago, a VMC method was applied to a normal state in AHM to study a transition corresponding to the Mott transition in RHM by introducing a binding factor between adjacent antiparallel spinons.\textsuperscript{41} For simplicity, we call a singly occupied site a spinon. However, the interpretation of the transition was incorrect on account of the limitation of treated system sizes and an insufficient analysis. Recently, VMC has been applied to solving problems with optical lattices in a confinement potential.\textsuperscript{42}

In this study, on the basis of VMC calculations of high precision for normal, SC and CDW states, we modify the previous results\textsuperscript{41} and make features of the BCS-BEC crossover in AHM on the square lattice microscopically more clear. We mainly discuss the following points: (1) In both normal and SC states, a correlation between adjacent antiparallel spinons, in addition to the Gutzwiller correlation, is indispensable to qualitatively derive proper behavior. (2) In the normal state, which underlies the SC state, a first-order phase transition occurs at $|U_{\text{col}}| \sim W$ from a Fermi-liquid to a spin-gapped state. This transition is caused by the competition between the size of an antiparallel-spinon pair and the interpair distance, as in the case of Mott transitions in RHM.\textsuperscript{43,44} (3) The properties of SC noticeably change at approximately $|U_{\text{col}}| \sim |U_{\text{c}}|$, which are compared with those derived in a strongly correlated RHM with constant shifts:\textsuperscript{45} The rest of this paper is organized as follows: In §2, we explain the model and method used in this study. In §3, we provide a discussion of the spin-gap transition arising in the normal state, and of the features in the spin-gapped regime. In §4, we consider a BCS-BEC crossover from various points of view. In §5, we briefly summarize our main results.

2. Formulation

In §2.1, we introduce AHM and briefly mention its relation to RHM. In §2.2, we discuss trial wave functions for normal, SC, and CDW phases. In §2.3, we briefly explain the setup of VMC calculations in this work.

2.1 Attractive Hubbard model

We consider a single-band attractive Hubbard model ($U \leq 0$) on a square lattice:

\begin{equation}
\mathcal{H} = \mathcal{H}_t + \mathcal{H}_U = \sum_{\text{ker}} \varepsilon_k c_{\text{ker}}^\dagger c_{\text{ker}} + U \sum_j n_{j\uparrow} n_{j\downarrow},
\end{equation}

where $n_{j\sigma} = c_{j\sigma}^\dagger c_{j\sigma}$, and $c_{\text{ker}}$ are fermion annihilation operators in the Wannier and Bloch representations, respectively, and

\begin{equation}
\varepsilon_k = -2t(\cos k_x + \cos k_y).
\end{equation}

We use the hopping integral $t$ and lattice constant as the units of energy and length, respectively. Because the lattice has a particle-hole symmetry at $n = N/N_z = 1$ ($N$: number of particles, $N_z$: number of lattice sites), and properties at half filling are deduced from the results of RHM using corresponding wave functions.\textsuperscript{46,47} As mentioned below, we mostly treat cases of $n < 1$. The chemical potential term $\zeta \sum_j n_{j\sigma}$ may be added to eq. (1) to adjust particle density, if necessary.

In the following, we summarize the relation of AHM to RHM. The attractive Hubbard Hamiltonian eq. (1) on a bipartite lattice satisfying the relation $\mathcal{H} = \mathcal{H}_t + \mathcal{H}_U$ is mapped to RHM with constant shifts:

\begin{equation}
\mathcal{H} = \sum_{\text{ker}} \varepsilon_k c_{\text{ker}}^\dagger c_{\text{ker}} + |U| \sum_j \tilde{n}_{j\uparrow} \tilde{n}_{j\downarrow} + U N \tilde{n}_{\uparrow} - h \sum_j \left( \tilde{S}_j^z + 1/2 \right),
\end{equation}

where $\tilde{n}_{j\sigma} = \tilde{c}_{j\sigma}^\dagger \tilde{c}_{j\sigma}$, $\tilde{S}_j^z = (\tilde{n}_{j\uparrow} - \tilde{n}_{j\downarrow})/2$ and $\tilde{n}_{\uparrow} = \tilde{N}_{\uparrow}/N$. A tilde denotes the representation transformed according to eq. (3). The chemical potential $\zeta$ and $n$ in AHM are related to the effective magnetic field as $h = 2\zeta$ and to the magnetization as $m = 1 - n$ in the $z$-direction in RHM, respectively. Therefore, unless the original AHM has a spin polarization ($m = 0$), the particle density in the transformed RHM is always at half filling ($\bar{n} = 1$). Also, the order parameters of CDW and onsite singlet pairing defined as

\begin{equation}
O_{\text{CDW}} = \frac{1}{N} \left| \sum_j e^{iQ_j r_j} (n_{j\uparrow} + n_{j\downarrow} - 1) \right|,
\end{equation}

\begin{equation}
O_{\text{SC}} = \frac{1}{N} \sum_j \langle c_{j\uparrow}^\dagger c_{j\downarrow} \rangle \quad \text{or} \quad \frac{1}{N} \sum_j \langle c_{j\uparrow} c_{j\downarrow} \rangle,
\end{equation}

in AHM are transformed into the forms of the $z$- and $xy$-components of the SDW order parameter:

\begin{equation}
\tilde{O}_{\text{SDW}} = \frac{1}{N} \left| \sum_j e^{iQ_j r_j} (\tilde{n}_{j\uparrow} - \tilde{n}_{j\downarrow}) \right|,
\end{equation}

\begin{equation}
\tilde{O}_{\text{SDW}} = \frac{1}{N} \sum_j \langle \tilde{c}_{j\uparrow}^\dagger \tilde{c}_{j\downarrow} \rangle \quad \text{or} \quad \frac{1}{N} \sum_j \langle \tilde{c}_{j\uparrow} \tilde{c}_{j\downarrow} \rangle,
\end{equation}

respectively, in RHM.\textsuperscript{29} It is widely accepted that, at $T = 0$, an antiferromagnetic (AFM) long-range order with equal magnitudes of $O_{\text{SDW}}$ for $x = x, y, z$ arises in the half-filled RHM on the square lattice for arbitrary $U (> 0)$, and that the AFM order in the $z$-direction is easily destroyed by a field applied in the $z$-direction $h$, whereas the AFM orders in the $xy$-plane survive. This implies that the ground state of AHM possesses a singlet pairing order for any $U$ and $n$ ($\zeta$), and simultaneously possesses a CDW order of the same magnitude at half filling $n = 1$ ($\zeta = 0$).\textsuperscript{29} This argument was confirmed by direct calculations for AHM.\textsuperscript{5} Although the above mapping holds unconditionally in exact treatments, when some approximation is applied, the validity of the mapping has to be verified.
individually for each specific treatment.

2.2 Trial wave functions

As a development of our previous study, we apply a many-body variation theory to the Hamiltonian eq. (1). As a trial wave function, a two-body Jastrow-type $\Psi = \mathcal{P}\Phi_\text{MF}$ was adopted, where $\Phi_\text{MF}$ is a one-body (mean-field) wave function and $\mathcal{P}$ is a many-body correlation (Jastrow) factor.

As the many-body part, we use the form $\mathcal{P} = \mathcal{P}_f\mathcal{P}_q\mathcal{P}_g$ in this work. The onsite (Gutzwiller) projector $\mathcal{P}_G = \prod_j \left[1 - (1 - g) d_j^\dagger d_j\right]$, (9)

with $d_j = n_{j\uparrow} n_{j\downarrow}$, is the most important. The variational parameter $g$ increases the number of doubly occupied sites (doublons), and ranges over $1 \geq g < \infty$ for $U \leq 0$; in the limit of $g \to \infty$, singly occupied sites (spinons) are not allowed in a nonmagnetic case. If we put $\bar{g} = 1/g$, the properties of $\mathcal{P}_G(\bar{g})$ for RHM are applicable to the present case $\mathcal{P}_G(g)$.41

To explain the importance of a binding factor between the up and down spinons $\mathcal{P}_Q$, it is convenient to refer to an effective Hamiltonian in the strong-correlation limit ($U/|J| \to 0$):49

$$\mathcal{H}_{\text{eff}} = \frac{2r^2}{|U|} \sum_{\sigma_1 \sigma_2} \left( -b^\dagger b_j + \rho_j \sigma_j + \sigma_i \sigma_j \right) + \text{H.c.} - \frac{1}{2},$$ (10)

with $b_j = c_\sigma_{j\uparrow} c_{\bar{\sigma}j\downarrow}$, $\rho_j = \frac{1}{2}(n_{j\uparrow} + n_{j\downarrow} - 1)$, $\sigma_i = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})$. (11)

The first term of eq. (10) indicates the hopping of doublons. The second is a repulsive interaction between doublons [or empty sites (holons)] and an attractive interaction between a doublon and a holon in nearest-neighbor (NN) sites. The third works as an AFM-Ising interaction. The expectation values of these terms can be reduced using antiparallel-spinon configurations in NN sites. To encourage such configurations, we introduce the attractive intersite correlation,41

$$\mathcal{P}_Q = \prod_j \left( 1 - \mu Q_j \right)$$ (12)

$$Q_j = s_j^\dagger \prod_{\tau} \left( 1 - s_{j+\tau}^\dagger \right) + s_j^\dagger \prod_{\tau} \left( 1 - s_{j+\tau}^\dagger \right)$$ (13)

where $s_j^{\uparrow} = n_{j\uparrow} (1 - n_{j\downarrow})$ (spinon projector), and $\tau$ runs over NN sites of the site $j$. In $\mathcal{P}_Q$, the parameter $\mu$ ($0 \leq \mu \leq 1$) controls the strength of binding between NN antiparallel spinons; for $\mu = 0$, spinons are free of binding, while in the limit $\mu \to 1$, antiparallel spinons are necessarily paired as nearest neighbors. As we will see later, $\mathcal{P}_Q$ is indispensable for a spin-gap transition41 and a proper description of the SC state. In fact, $\mathcal{P}_Q$ is the canonical transformation through eq. (3) of the doublon-holon binding factor often used to describe Mott transitions in RHM.50,51 A Mott transition in RHM corresponds to a spin-gap transition in AHM, as we will see in §3. Since $Q_j$ is a spin-dependent projector, the so-called spin contamination52 arises in the wave function, namely, $\Psi$ deviates from an eigenstate of $S^2 = \left( \sum_j S_j^2 \right)^2$. However, in this case, the expectation values of $S^2$ estimated using a VMC method are as small as 0.15 (2) in the SC (normal) state for $N = 200-300$ at its maximum at $U \sim W$. Because these values, particularly of the SC state, are much smaller than those of the AFM state, the spin contamination is considered to have little influence on the results.

As a factor supplementary to $\mathcal{P}_Q$, a repulsive correlation suited to eq. (10) should be considered. As a simple one, we check a repulsive factor between NN doublons:

$$\mathcal{P}_f = \prod_j \left[ 1 - f d_j (1 - \prod_{\tau} \tilde{d}_{j+\tau}^\dagger) \right],$$ (14)

where $f (0 \leq f \leq 1)$ is a parameter, $\tilde{d}_j = 1 - d_j$, and $\tau$ runs over NN sites of the site $j$. The projector $\mathcal{P}_f$ reduces the weight of configurations with adjacent doublons by $1 - f$; for $f \to 0$, the effect of $\mathcal{P}_f$ vanishes, and for $f \to 1$, a doublon cannot sit in a NN site of another doublon.

Now, we turn to the one-body part $\Phi$ of the wave function. For a normal state, we adopt the Fermi sea $\Phi_F$. Since general features of $\Psi_N = \mathcal{P}\Phi_F$ with $f = 0$ were studied in a previous paper,41 here we focus on the properties of the transition arising at $U \sim W$, which was regarded as a Mott transition.41

It is known that the BCS state $\Phi_{\text{BCS}}$ can be realized with the BCS-BEC crossover in some degree.2,4 it is natural to employ $\Phi_{\text{BCS}}$ for a SC state:

$$\Phi_{\text{BCS}} = \left( \sum_k a_k e_{k\uparrow}^\dagger e_{k\downarrow}^\dagger \right)^{N/2} |0\rangle,$$ (15)

where the particle number is fixed and

$$a_k = \frac{v_k}{\epsilon_k - \Delta_{p}} = \frac{\epsilon_k - \bar{\zeta} + \sqrt{(\epsilon_k - \bar{\zeta})^2 + \Delta_p^2}}{\Delta_p},$$ (16)

with $\Delta_p$ and $\bar{\zeta}$ being variational parameters corresponding to the SC gap $\Delta_{\text{SC}}$ and chemical potential $\zeta$, respectively, in the weakly correlated limit, and

$$\bar{\zeta}^2 (v_k^2) = \frac{1}{2} \left( 1 + \frac{\epsilon_k - \bar{\zeta}}{\sqrt{(\epsilon_k - \bar{\zeta})^2 + \Delta_p^2}} \right).$$

For $\Delta_p \to 0$, $\Phi_{\text{BCS}}$ is reduced to $\Phi_F$. Here, we assume $\Delta_p$ to be a homogeneous $s$ wave on account of the attractive contact potential. For RHM, a form similar to eq. (16) with a $d_{\bar{x},\bar{y}}$-wave pair potential was studied,46,53 where, as $\bar{x}$ decreases, what $\Delta_p$ means deviates from the SC gap, and represents a pseudogap.54,55 In contrast, in the present case, $\Delta_p$ seems to reflect the magnitude of $T_c$ for any $|U|/t$, except for $n \to 1$, for which $T_c$ is considered to vanish owing to the CDW order.

The correlated SC function $\Psi_{\text{SC}} = \mathcal{P}\Phi_{\text{BCS}}$ is mapped using eq. (3) to a projected AFM wave function ordered in the $x$-$y$ plane at $n = 1$.

In addition, we check a CDW wave function for $n \sim 1$:

$$\Phi_{\text{CDW}} = \prod_{k,\sigma} ( -a_k e_{k\sigma}^\dagger + \beta_k e_{k\sigma}^\dagger + \phi_k e_{k\sigma}^\dagger ) |0\rangle,$$ (17)

where the $k$ sum is taken in the Fermi sea, $Q = (\pi, \pi)$, and

$$\alpha_k (\beta_k) = \frac{1}{2} \left[ 1 - (-)^{\bar{\zeta}^2 k^2 + \Delta_p^2} \right],$$ (18)

with $\Delta_k$ being a parameter corresponding to the CDW gap. $\Psi_{\text{CDW}} = \mathcal{P}\Phi_{\text{CDW}}$ is mapped through eq. (3) to a projected AFM wave function ordered in the $z$-direction at $n = 1$. Because the AFM order is isotropic in RHM, $\Psi_{\text{SC}}$ and $\Psi_{\text{CDW}}$
should yield identical results at half filling.

2.3 Variational Monte Carlo method

In estimating variational expectation values with respect to \( \Psi \) discussed in §2.2, we use a VMC method,\textsuperscript{33,38-40} which gives virtually exact values for finite but relatively large systems. Since the number of variational parameters is not large, we execute rounds of linear optimization for each parameter with the other parameters fixed until the parameters as well as the energy converge (typically 3-5 rounds) with 2.5 \( \times \) 10\(^5\) particle configurations generated through a Metropolis algorithm. After the convergence, we continue to execute additional 20 to 30 rounds of iteration with successively renewed configuration sets. We determine the optimized values by averaging the data obtained in the additional rounds; in averaging, we exclude scattered data beyond the range of twice the standard deviation. Thus, the optimal value is an average of substantially more than several million samples. Physical quantities are computed with the optimized parameters thus obtained with 2.5 \( \times \) 10\(^5\) samples.

We use systems of \( L \times L \) sites of up to \( L = 32 \) for \( \Psi_N \) and \( L = 24 \) for \( \Psi_{SC} \) with the periodic-antiperiodic boundary conditions to reduce level degeneracy. We choose the particle densities to satisfy the closed-shell condition, and mainly study \( n = 0.25 \) (0.26), 0.5, and 0.75.

3. Spin-Gap Transition in Normal State

As mentioned in §2.1, the ground state of AHM is SC for any \( U/t \) and \( n \) (and CDW at \( n = 1 \)). Therefore, the normal state, we address in this section, is not the ground state of eq. (1). The significance to study \( \Psi_N \) is not only in a passive sense that a normal state appears when the SC state is destroyed by, e.g., magnetic field or impurities, but in that \( \Psi_N \) underlies \( \Psi_{SC} \), just as a SC transition is understood by the instability of the Fermi sphere against an infinitesimal attractive interaction in the BCS theory. Namely, normal states are deeply involved in the mechanism of SC transitions.

In §3.1, we show the improvement in energy by introducing \( \mathcal{P}_Q \) and \( \mathcal{P}_f \), and the energy gains using the SC and CDW states. In §3.2, we confirm the existence of a spin-gap transition in the normal state. In §3.3, we consider the mechanism of the spin-gap transition and other properties.

3.1 Energy improvement

First, we briefly look at the energy improvement by the projection factors \( \mathcal{P}_Q \) and \( \mathcal{P}_f \) in the normal, SC, and CDW states.

| \(|U|/t\) | 1 | 3 | 7 | 10 |
|---|---|---|---|---|
| \(\mathcal{P}_Q \Phi_N\) | -1.37536 | -1.55099 | -2.10435 | -2.7417 |
| \(\mathcal{P}_Q \Phi_{BCS}\) | -1.37536 | -1.55097 | -2.10440 | -2.7416 |
| \(\mathcal{P}_f \Phi_N\) | -1.37531 | -1.55686 | -2.17815 | -2.80500 |
| \(\mathcal{P}_f \Phi_{BCS}\) | -1.375355 | -1.55908 | -2.18444 | -2.81162 |

As studied in detail in ref. 41, the variational energy in the normal state is considerably improved by \( \mathcal{P}_Q \) on that of GWF, especially for large \(|U|/t\)'s (Table I). Moreover, it is known that the phase transition discussed in §3.2 does not arise without \( \mathcal{P}_Q \).\textsuperscript{33,41} Thus, the factor \( \mathcal{P}_Q \) is indispensable to appropriately describe the normal state. These aspects of \( \mathcal{P}_Q \) correspond to those of the doublon-holon (D-H) binding factor in RHM.\textsuperscript{47,51} On the other hand, the improvement by \( \mathcal{P}_f \) on \( \mathcal{P}_Q \Phi_Q \Phi \) is almost imperceptible for any \(|U|/t\) as shown in Table I. The optimized parameter \( f \) is nearly zero, namely, \( \mathcal{P}_f \) scarcely modifies the wave function.

In the SC state, the improvement in \( E/t \) by \( \mathcal{P}_Q \) on \( \mathcal{P}_Q \Phi_{BCS} \) is not as large as that for the normal state. This is because the effect of binding between up and down spinons, i.e., the effect of singlet pair creation, is already included in \( \Phi_{BCS} \) to some extent, as the one-body AFM state has some D-H binding effect for RHM.\textsuperscript{46} Further energy reduction by \( \mathcal{P}_f \) is again negligible for small \(|U|/t\)'s and remains relatively small in magnitude for larger \(|U|/t\)'s, as compared with the energy reduction by \( \mathcal{P}_Q \). The magnitude of energy reduction by \( \mathcal{P}_f \) is similarly small for \( n = 0.25 \) and 0.75.

Since we find that a short-range repulsive factor \( \mathcal{P}_f \) produces only negligible effects in all the cases we treat, we omit \( \mathcal{P}_f \) and use the form \( \mathcal{P} = \mathcal{P}_Q \equiv \mathcal{P}_Q \Phi_Q \) as the many-body factor in \( \Psi \) in the rest of this paper, unless otherwise specified.

Finally, we compare the energy gains using the SC and CDW states:

\[
\Delta E_{SC} (\Delta E_{CDW}) = E_N - E_{SC} (E_{CDW}),
\]

where \( E_N \), \( E_{SC} \), and \( E_{CDW} \) are the optimized energies per site for \( \Psi_N \), \( \Psi_{SC} \) and \( \Psi_{CDW} \), respectively. Figure 1 shows the \( n \) dependences of \( \Delta E_{SC} \) and \( \Delta E_{CDW} \) for large \( n \)'s. At half filling \((n = 1)\), the SC and CDW states are degenerate, but this degeneracy is immediately lifted for \( n < 1 \). \( \Delta E_{CDW} \) rapidly deteriorates and vanishes as \( n \) decreases, whereas \( \Delta E_{SC} \) preserves appreciable values for high densities and gradually decays until \( n = 0 \) (not shown). This feature of \( \Delta E \) coincides with what we discussed for the canonical transformation in §2.1.\textsuperscript{5}

In the remainder of this section, we will concentrate on \( \Psi_N \).
3.2 Spin-gap transition

In a previous VMC study using $\mathcal{P}_q \Phi_r$, a transition was detected with systems up to $L = 12$ at $U = U_c \sim 9t$. However, this transition was misinterpreted as a continuous metal-insulator transition. In this subsection and the next, we study the features of this transition more carefully.

First, we confirm the existence of a transition. In Fig. 2, we plot the momentum distribution function

$$n(k) = \frac{1}{2} \sum_{\sigma} \langle \epsilon^+_{k\sigma} \epsilon_{k\sigma} \rangle$$

for $|U|/t \sim 9$ and $n = 0.25$ ($L = 32$). For $|U|/t \leq 9.0$, $n(k)$ has discontinuities on the $\Gamma$-X and $\Gamma$-M segments, indicating that a Fermi surface exists and the state is a Fermi liquid. On the other hand, the discontinuity suddenly vanishes for $|U|/t \geq 9.05$, and $n(k)$ becomes a smooth function of $k$. It follows a certain gap opens and the state becomes a non-Fermi liquid for $|U| > |U_c|$, with $9.0 < |U_c|/t < 9.05$ in this case. Through similar analyses, we found $|U_c|/t \sim 0.875$ (0.83) for $n = 0.195$ (0.121) for $L = 32$; $|U_c|/t$ tends to gradually decrease with $n$. Thus, a transition from a Fermi liquid to a non-Fermi liquid certainly exists, as found in our previous study. According to similar analyses for $L = 24$ and 28 and $n \sim 0.25$, the system-size dependence of $|U_c|/t$ is very small at these values of $L$, but $|U_c|/t$ tends to increase slightly as $L$ increases. Such a feature is analogous to those of the Mott transitions in RHM induced by D-H binding factors.

Next, we check the order of this transition. In Fig. 3, the quasiparticle renormalization factor $Z$ is shown vs $U/t$; $Z$ is obtained using $Z = n(k_F - 0) - n(k_F + 0)$ on the $\Gamma$-X segment, where the values of $n(k)$ at $k_k \rightarrow k_F \pm 0$ are estimated using third-order least-squares fits of the data for $k < k_F$ and $k > k_F$, respectively. There exist clear discontinuities in $Z$ at $U = U_c$. The optimized spinon-binding parameter $\mu$ plotted in the inset of Fig. 3 also exhibits a large jump at $U = U_c$.

In fact, other physical quantities show a similar discontinuous behavior. Thus, we may safely conclude that this transition is not a continuous transition but a first-order phase transition. The reason why the previous study could not find the correct transition order is that the discontinuous behavior of $n(k)$ manifests itself only for $L \geq 18$. The critical value $|U_c|/t$ only slightly depends on $n$.

Now, we consider the features of $\Psi_q$ in the non-Fermi-liquid regime $|U| > |U_c|$. As shown in the inset of Fig. 3, the spinon-binding parameter $\mu$ approaches unity, suggesting that almost all up and down spinons are paired as singlets. In discussing gap formation, the small-$|q|$ behavior of the charge (density) and spin structure factors

$$N(q) = \frac{1}{N} \sum_{j,l} e^{-i q \tau_j} \langle n_j n_{j+l} \rangle - n^2$$

$$S(q) = \frac{1}{N} \sum_{j,l} e^{-i q \tau_j} \langle S^x_j S^y_{j+l} \rangle$$

provide us with useful information. Assuming that the lowest excitation occurs at $q = 0$, the energy gap in the spin sector between the ground state $\Psi_0$ and the first excited state $\Psi_q$ is given by the single-mode approximation (SMA) as

$$\Delta_S = \frac{\langle \Psi_q \mid (H - E_0) \mid \Psi_q \rangle}{\langle \Psi_q \mid \Psi_q \rangle} = \frac{\langle \Psi_q \mid S_{-q} \mid \Psi_q \rangle}{\langle \Psi_q \mid \Psi_q \rangle}$$

$$= -\frac{1}{8} \lim_{q \rightarrow 0} q^2 S^2$$

where $K$ denotes the kinetic energy, $|\Psi_q \rangle = S_q |\Psi_0 \rangle$, and

$$S_q = \frac{1}{\sqrt{N}} \sum_j e^{i q \tau_j} S^z_j$$

From eq. (23), we find that $\Delta_S$ vanishes if $S(\mathbf{q}) \propto q$ for $q \rightarrow 0$, whereas $\Delta_S$ becomes finite, if $S(\mathbf{q}) \propto q^2$ for $q \rightarrow 0$. The charge (density) gap $\Delta_N$ can be similarly treated.

In Fig. 4, we show $S(q)$ and $N(q)$ for some values of $|U|/t$ near $U = U_c$. In the vicinity of $\mathbf{q} = 0$, as $|U|/t$ increases, $S(\mathbf{q})$ abruptly changes its behavior from linear to quadratic at $U = U_c$, as shown in the inset of Fig. 4(b). Thus, it is very likely that the spin gap is generated in the non-Fermi-liquid regime. In Fig. 5, we plot the spin gap estimated using eq. (23) for the segment of $0, 0 \rightarrow (\pi, 0)$ of $S(\mathbf{q})$; the magni-
3. Picture of transition and spin-gapped state

To deepen our understanding of the above spin-gap transition, let us look at some other quantities. Figure 6(a) shows the doublon density

\[ D = \frac{1}{N_s} \sum_j (b_j^\dagger b_j). \quad (25) \]

As \(|U|/t\) increases, \(D\) increases in the Fermi-liquid state owing to the attractive correlation of \(P_G\), but it reaches almost its full value \((n/2)\) at \(U = U_c\). The main panel of Fig. 6(b) shows the average distance from an up (down) spinon to its nearest down (up) spinon \(r_{ud}\). Here, we measure distance \(r\) by the stepwise (so-called Manhattan) metric. As \(|U|/t\) increases in a small-\(|U|/t\) regime, \(r_{ud}\) increases because the densities of up and down spinons decrease owing to doublon formation, and the binding correlation of \(P_G\) is still weak, as in the inset of Fig. 3. However, \(r_{ud}\) abruptly drops when \(U\) approaches \(U_c\), and converges to unity for \(|U| > |U_c|\), because an up spinon and a down spinon are tightly bound within NN sites \((\mu \rightarrow 1)\). Consequently, for \(|U| > |U_c|\), almost all particles form onsite pairs, and even if a doublon resolves into spinons, they remain an adjacent pair and do not itinerate as isolated spinons.

Thus, we notice that this spin-gap transition can be understood in parallel with a recently proposed picture of Mott transitions owing to the D-H binding.\(^{43,44}\) Here, we postulate that antiparallel spinon pairs with a pair domain of size \(\xi_{cd}\) are created by the attractive correlation of \(P_G\). We can appropriately define this binding length \(\xi_{cd}\) and also the minimum distance...
from a spinon to its nearest parallel spinon $\xi_{uu}$ as

$$\xi_{ud} = r_{ud} + \sigma_{ud}, \quad (26)$$

$$\xi_{uu} = r_{uu} - \sigma_{uu}, \quad (27)$$

where $r_{ud}$ is the average distance from an up (down) spinon to its nearest up (down) spinon, and $\sigma_{ud}$ and $\sigma_{uu}$ are the standard deviations of $r_{ud}$ and $r_{uu}$, respectively. In the spin-gapped phase, the relation $\xi_{ud} < \xi_{uu}$ holds, indicating that the domains of pairs do not usually overlap, at least, not in sequence. Consequently, almost all pairs are isolated and an up spinon and a down spinon are confined within $\xi_{ad}$, resulting in singlet pairs of small lengths with finite excitation gaps. In contrast, in the Fermi-liquid phase, $\xi_{ud}$ becomes longer than $\xi_{uu}$, indicating that the domains of spinon pairs overlap with one another. Then, an up spinon in a pair can exchange a partner down spinon with a down spinon in an adjacent pair. As a result, an up spinon and a down spinon can move independently by exchanging their partner, as shown in long arrows in Fig. 7, and definite singlet pairs cannot be specified. Thus, as $|U|/t$ is varied, a spin-gap transition takes place when $\xi_{ud}$ becomes equivalent to $\xi_{uu}$, which is expected to be a monotonically increasing function of $|U|/t$.

Figure 8 shows $\xi_{ud}$ and $\xi_{uu}$ estimated from the VMC results as functions of $|U|/t$ for three particle densities. As expected from Fig. 6(b), $\xi_{ud}$ abruptly drops at $U = U_c$, whereas $\xi_{ud}$ monotonically increases as $|U|/t$ increases with a small jump at the transition point. As a result, $\xi_{ud}$ and $\xi_{uu}$ intersect each other at $U = U_c$ for any $n$. Thus, the scheme illustrated in Fig. 7 is justified to some extent.

Finally, we discuss the itinerancy of particles. To this end, it is convenient to decompose the kinetic energy $E_{\text{kin}}$ into two parts ($E_{\text{kin}} = E_1 + E_2$), namely, the contribution of the hopping processes that do (do not) change the number of doublons $E_1$ ($E_2$),\textsuperscript{58} as shown in the lower part of Fig. 9. In the main panel of Fig. 9, $E_1$, $E_2$, and $E_{\text{kin}}$ are depicted as functions of $|U|/t$. For $|U| < |U_c|$, both $E_1$ and $E_2$ contribute to $E_{\text{kin}}$ because isolated spinons are independently mobile, whereas in the spin-gapped phase, $E_1$ almost vanishes ($E_{\text{kin}} \sim E_2$) for any particle density. In this case, the independent motion of a spinon not accompanied by an antiparallel spinon is strongly suppressed.

On the other hand, the contribution of the dissociation of a doublon into a spinon pair and their reunion, $E_2$, remains appreciable and is proportional to $-t^2/|U|$ for large $|U|/t$'s. This point is in sharp contrast to a feature of the Brinkman-Rice transition\textsuperscript{34} derived using the Gutzwiller approximation;\textsuperscript{52} in this case, the motion of particles is completely prohibited for $|U| > |U_{BR}| = 8(E(U = 0)),\textsuperscript{31}$ so that the state becomes insulating, and a charge (Mott) gap opens.

The above feature of $E_1 = 0$ ($|U| > |U_c|$) for any $n$ is distinct from that of the D-H binding state for strongly correlated RHM, where $E_1$ is $n$-dependent ($\sim 1 - n$) near half filling.\textsuperscript{53} Thus, in doped Mott insulators in RHM, doped holes or particles play a role of carriers, and bound D-H pairs are localized and not involved in conduction. On the other hand, in AHM, the motion of a doublon, which is composed of two single
4.1 Energy gain and kinetic-energy-driven transition

First, we discuss the BCS-BEC crossover from the point of view of the energy difference per site between the normal ($\Psi_N$) and SC ($\Psi_{SC}$) states $\Delta E (\geq 0)$ defined in eq. (19). In Fig. 11(a), the $|U|/t$ dependence of $\Delta E/t$ is shown; $\Delta E/t$ increases as $\exp(-t/|U|)$ corresponding to the BCS theory for small $|U|/t$'s, reaches a maximum at $|U| = |U_{col}| \sim 8.7t$, and then decreases for $|U| > |U_{col}|$ as $\sim t/|U|$. As we will see later, various properties of SC actually exhibit qualitative changes at approximately this $|U_{col}|/t$ from a BCS type to a BEC type. Note that normal-state properties are deeply involved in the crossover; $|U_{col}|/t$ is affected by the spin-gap transition point $|U_c|/t$ in $\Psi_N$, where $E_N$ exhibits a cusp, resulting in $U_{col} \sim U_c$. Recall that the normal state $\Psi_N$, underlying $\Psi_{SC}$, is a Fermi liquid for $|U| < |U_c|$, but $\Psi_N$ becomes a spin-gapped state in the absence of a Fermi surface, as shown in Fig. 2 for $|U|/t \geq 9.05$. Namely, for $|U| > |U_{col}|$, a SC transition cannot be interpreted by the instability of the Fermi surface against an attractive interaction. In this relation, $\Delta E$ means the condensation energy for $|U|/t \sim 0$ according to the BCS theory, but $\Delta E$ probably deviates from the condensation energy observed experimentally for $|U| \geq |U_{col}|$, as in the case of high-$T_c$ cuprates.\textsuperscript{53}

Recall that the normal state $\Psi_N$ exhibits a cusp, resulting in $U_{col} \sim U_c$. In the latter case, the low-energy excitations in $\Psi_N$ are drawn in (b) and (c), respectively. In the BCS theory, a SC transition is induced by lowering $E_{int}$ at the cost of smaller loss in $E_{kin}$. On the other hand, it is known in a large-$U/t$ regime of RHM that a SC transition occurs by reducing $E_{kin}$ with a loss in $E_{int}\textsuperscript{46,53}$. In the latter case, the low-frequency sum rule of optical conductivity $\sigma_1(\omega)$\textsuperscript{63} should be broken, namely, high-frequency excitations in $\sigma_1(\omega)$ arise, because the sum of $\sigma_1(\omega)$ is proportional to $-E_{kin}\textsuperscript{62}$ on a...
square lattice. In Figs. 11(b) and 11(c), we show $\Delta E_{\text{kin}}$ and $\Delta E_{\text{int}}$, respectively, for AHM. For $|U| \leq |U_{\text{col}}|$, $E_{\text{int}}$ ($E_{\text{kin}}$) has a gain (loss) by the SC transition in accordance with the BCS theory. Meanwhile, for $|U| \geq |U_{\text{col}}|$, the situation is reverse; the SC transition is driven by a gain in kinetic energy. Correspondingly, the hopping of doublons (carriers) $|E_D|$ becomes more enhanced in $\Psi_{\text{SC}}$ than in $\Psi_N$ in the BEC regime, as shown in the inset of Fig. 10. Kinetic-energy-driven (SC or magnetic) transitions may be rather general in strongly correlated systems.46,53,63 As mentioned previously, this reversal of driven force will be experimentally found if $\sigma_1(\omega)$ is accurately measured in cold-atom systems. In fact, similar results were reached for AHM in infinite dimensions by DMFT.26,64

Let us consider this SC transition in the light of the variational parameters. At the level of one-body wave function, $\Phi_{\text{BCS}}$ improves the energy over $\Phi_N$ by creating onsite Cooper pairs through the pair potential $\Delta_P$ (Fig. 21), in accordance with the BCS theory. Therefore, in the BCS regime, the number of doublons is expected to be more in the SC state than in the normal state. This is actually shown in Fig. 6(a). Since the increase in $D$ hinders the motion of particles, the kinetic energy is suppressed in the SC state, as in Fig. 11(b). As $|U|$ increases, however, $D$ of $\Psi_N$ increases more rapidly and surpasses that of $\Psi_{\text{SC}}$ at $|U_{\text{col}}|$. This reversal is brought about mainly by the correlation factor $\mathcal{P}$. In Fig. 12, we compare the optimized parameters in $\mathcal{P}$ between the normal and SC states. The onsite attractive factor $g$ is certainly larger in $\Psi_N$, especially near $U = U_{\text{col}}$. The antiparallel-spinon binding factor $\mu$ mainly works for the suppression of overgrown $D$ by $g$ in the BEC regime in order to gain $E_{\text{kin}}$.

In a one-body framework, when the chemical potential ($\zeta$) is situated in an energy band, low-energy excitation in the SC phase is described by Bogoliubov’s quasiparticles, whereas when $\zeta$ becomes lower than the band bottom $\varepsilon_1$, the statistics of the system becomes bosonic. Thus, the BCS-BEC crossover point is roughly estimated using $\zeta = \varepsilon_1$. We estimate $\zeta$ for $\Psi_{\text{SC}}$ from $\zeta = \partial E_{\text{SC}}/\partial n$ (strictly finite differences). Within statistical error, $E_{\text{SC}}$ is almost a linear function of $n$ for $0.5 < n < 1.0$, so that the $\zeta$ obtained in this range becomes independent of $n$. In Fig. 13, we plot the thus-estimated $\zeta$ as a function of $|U|/t$ with the value at half filling i.e., $\zeta = U/2t$. $\zeta$ reaches the band bottom $\varepsilon_1 = -4t$ at $|U|/t \sim 7.9$. The behavior of $\zeta$ here is consistent with those obtained by DMFT.23,24

![Fig. 12](image1.png)

**Fig. 12.** (Color online) Optimized variational parameters, (a) Gutzwiller (onsite) factor $g$ and (b) NN antiparallel-spinon factor $\mu$ for $\Psi_n$ and $\Psi_{\text{SC}}$ are shown as functions of $|U|/t$. The symbols are common in (a) and (b). The arrows indicate the spin-gap transition points in $\Psi_N$.

Finally, let us look at the momentum distribution function for $\Psi_{\text{SC}}$ as $|U|/t$ varies. The dashed line indicates $|U|/t = \infty$.

![Fig. 13](image2.png)

**Fig. 13.** (Color online) The chemical potential estimated from $E_{\text{SC}}/t$ at higher particle densities ($0.5 \leq n \leq 1.0$) is shown by dots as a function of $|U|/t$. The dash-dotted line denotes the value at half filling: $\zeta = U/2$. The dashed line indicates the band bottom $\varepsilon_L = -4t$.

4.2 Pair correlation function and helicity modulus

As mentioned in §1, a previous study of Toschi et al.26 using DMFT argued that appropriate quantities that trace the strength of SC ($T_c$) in the BCS and BEC regimes are the gap $\Delta_{\text{SC}} = \langle c^*_1 c_1 \rangle$ and the superfluid stiffness $D_s$, respectively. $\Delta_{\text{SC}}$ indicates the cost of creating a Cooper pair, while $D_s$ characterizes the cost of realizing phase coherence. In this subsection, we start with the quantities corresponding to $\Delta_{\text{SC}}$ and $D_s$.

As an appropriate index of off-diagonal-long-range order (ODLRO) in the present scheme, we consider a SC correlation.

![Fig. 14](image3.png)

**Fig. 14.** (Color online) Evolution of momentum distribution function for $\Psi_{\text{SC}}$ as $|U|/t$ varies. The dashed line indicates $|U|/t = \infty$. 
by the BCS theory. In this regime, the optimized
tered to approximate the gap, as will be argued; we confirmed
QMC study, of
The magnitude of ODLRO is given by the long-distance value
calculations with finite systems, we must check the
along a typical path on the lattice. Since
3\frac{1}{2}\text{--wave pairing}, \Psi_N's \text{ are bound to vanish for } L \to \infty.
function of onsite pairing,\textsuperscript{66} defined as
\[ P(\mathbf{r}_t) = \frac{1}{N_c} \sum_j \langle b_j^\dagger b_{j+t} \rangle. \] (30)
The magnitude of ODLRO is given by the long-distance value
of \( P(\mathbf{r}_t) \), i.e., \( P_\infty = \lim_{|\mathbf{r}| \to \infty} P(\mathbf{r}_t) \sim \Delta_{SC}^2 \). In the present VMC
calculations with finite systems, we must check the \( r_t \) dependence
of \( P(\mathbf{r}_t) \). In Fig. 15, we plot \( P(\mathbf{r}_t) \) for various \( |U|/t \)'s along a typical path on the lattice. Since \( P(\mathbf{r}) \) is substantially
constant for \( |r| \geq 2 \) for any value of \( |U|/t \), consistently with a
QMC study,\textsuperscript{57} it is appropriate to put \( P(\mathbf{r}) \) with the most
distant \( \mathbf{r} = (L/2, L/2) \) at \( P_\infty \), and check its system-size de-
pendence. In Fig. 16, we plot the thus-estimated \( P_\infty \) as a function
of \( 1/L \) for three values of \( |U|/t \). In the SC state, the system-
size dependence of \( P_\infty \) is very weak for any \( |U|/t \), and fitted
well by a first-order least-squares method. Thus, we may dis-
cuss \( P_\infty \) with a finite but large \( L \). Figure 17 shows the \( |U|/t \) dependence of \( P_\infty \) for \( L = 20 \). In the BCS regime \((|U| \lesssim |U_{\text{co}}|)\),
\( P_\infty \) increases as \( \sim \exp(-t/|U|) \) as \( |U|/t \) increases, as predicted
by the BCS theory. In this regime, the optimized \( \Delta_\text{P} \) is consid-
ered to approximate the gap, as will be argued; we confirmed
using the data shown in Fig. 21 that the relation \( P_\infty \sim \Delta_\text{P}^2 \)
holds. On the other hand, in the BEC regime, \( P_\infty \) tends to con-
verge at a finite value as \( |U|/t \) increases, in accordance with the
result of \( \Delta_{SC} \) obtained using DMFT.\textsuperscript{23,24} Thus, the behav-
ior of \( P_\infty \) or \( \Delta_{SC} \) in this regime does not coincide with the
behavior of \( T_c \sim \ell^2/|U| \), which was naturally expected\textsuperscript{4} and
actually obtained by DMFT.\textsuperscript{7,25,26}
Incidentally, a similar SC correlation function with the NN
d_{\text{\text{3--wave pairing}} \Psi_N} \text{ has been calculated for RHM in 2D by}
VMC with the same class of trial functions.\textsuperscript{53} In the strongly
correlated regime (typically \( U/t = 12 \)), where the cuprates
are considered to be properly described, \( P_\infty \) behaves as the
so-called dome shape as a function of doping rate \( \delta = (1 - n) \).
This dome shape closely agrees with the \( \delta \) dependence of \( T_c \)
experimentally observed for the cuprates. If the framework
of \( \text{BSC-BEC crossover} \) as a function of \( \delta \) is applicable to this
case, \( P_\infty \) decreases and scales with \( T_c \) as the parameter
approaches the BEC limit \( (\delta \to 0) \). Consequently, the behavior
of \( P_\infty \) in RHM does not fully correspond to that of \( P_\infty \) in this study.

Now, we turn to the helicity modulus \( \rho_\text{h} \), which is related to
superfluid stiffness $D_s$ with $\rho_s = D_s / 4 \pi c^2$. In the SC state, $D_s$ is equivalent to the strength of the delta-function component at $\omega = 0$ in the optical conductivity $\sigma_1(\omega)$ and represents the superfluid weight. We calculate $\rho_s$ as the coefficient of the quadratic term in the increment in energy when the phase of order parameter $\Delta_j$ is twisted by $\mathbf{q}$ as $\Delta_j = |\Delta| e^{i \mathbf{q} \cdot \mathbf{r}_j}$; 

$$E(\mathbf{q}) - E(0) = 2 \rho_s |\mathbf{q}|^2 + O(|\mathbf{q}|^4), \quad (31)$$

following the prescription of Denteneer et al.\textsuperscript{70} In Fig. 18, the $|U|/t$ dependence of the $\rho_s$ thus obtained is plotted for three particle densities. The resultant $\rho_s$ here is almost independent of the $\mathbf{q}$ used ($|\mathbf{q}| \sim 0.1$), and the system size dependence is negligible within the symbols between $L = 12$ and 20. Regardless of $n$, $\rho_s$ is a monotonically decreasing function of $|U|/t$. The behavior in the BCS regime is distinct from that of $T_c \sim \text{exp}(-t/|U|)$, but $\rho_s$ scales with $T_c \sim t^2/|U|$ in the BEC regime, indicating the strength of SC in the BEC regime is determined not by the cost of creating a pair but by the cost of realizing phase coherence. The present result of $\rho_s$ is consistent with the previous results obtained by a VMC method with $\mathcal{P}_G \Phi_{BCS}$,\textsuperscript{70} QMC,\textsuperscript{20} and DMFT.\textsuperscript{23,24,26}

\[ \rho_0 = \frac{1}{D} n_D(0) = \frac{1}{DN_s} \sum_{j,\ell} \langle b^\dagger_{j\ell} b_{j\ell+1} \rangle. \quad (32) \]

In Fig. 20, the $|U|/t$ dependence of $\rho_0$ is depicted for three particle densities. The behavior of $\rho_0$ for small $|U|/t$’s is $\rho_0 \sim \text{exp}(-t/|U|)$ and has a meaning similar to $P_\infty$. In the BEC regime ($|U| > |U_\infty|$), $\rho_0$ is almost constant, indicating that a picture of hard-core bosons is justified in the entire regime of BEC. The suppression of $\rho_0$ with increasing $n$ is primarily because a high density enhances the effect of onsite interaction.

Finally, we consider the pairing gap parameter $\Delta_p$ given in eq. (16). In Fig. 21, we show the $|U|/t$ dependence of the optimized $\Delta_p$. For $|U| < |U_\infty|$, it is natural that $\Delta_p$ represents the SC gap of $\propto \text{exp}(-t/|U|)$, as expected from the BCS theory. In the BCS theory, $\Delta_{SC}$ should continue to linearly increase like $\Delta_s$ in Fig. 19. However, the $\Delta_p$ of $\Psi_{SC}$ exhibits a peak

![Fig. 19](image)

Fig. 19. (Color online) Spin gap of SC state estimated similarly to that in Fig. 5 by single-mode approximation. The dash-dotted straight line indicates an extrapolation from large-$|U|/t$ values for $n = 0.5$. In the remainder of this subsection, we discuss some quantities related to $P(\mathbf{r})$ and $\rho_s$. First, we take up the small-$|\mathbf{q}|$ behavior of spin and charge structure factors, eqs. (21) and (22). Like for the normal state, $N(\mathbf{q}) \sim |\mathbf{q}|$ for $|\mathbf{q}| \to 0$ for any $|U|/t$, showing that $\Psi_{SC}$ is conductive in particle density. On the other hand, $S(\mathbf{q}) \sim |\mathbf{q}|^2$ for any $|U|/t$ ($> 0$) in contrast to the case of $\Psi_N$, indicating that a spin gap opens owing to pair formation. We estimate the spin gap $\Delta_s$ for $\Psi_{SC}$ using SMA [eq. (23)], and show the $|U|/t$ dependence in Fig. 19. Although we do not display the data for small $|U|/t$’s owing to the relatively large errors due to the use of a finite system ($L = 20$), $\Delta_s$ seems to be proportional to $\text{exp}(-t/|U|)$ for small $|U|/t$’s. On the other hand, $\Delta_s$ is proportional to $|U|/t$, and has a magnitude similar to that of $\Psi_N$. $\Delta_s$ is almost independent of $n$. Thus, $\Delta_s$ is a quantity that scales with $T_c$ in the BCS regime.

Next, let us consider the condensate fraction $\rho_0$. We may regard $b^\dagger_j$ as a creation operator of a hard-core spinless boson at the site $j$; $b^\dagger_j$ satisfies the Bose commutation relation except for the same site. Following Bose systems,\textsuperscript{44} we define a quantity corresponding to the condensate fraction or the $k = 0$ element of momentum distribution function $n_D(k)$ for $b^\dagger_j$:

![Fig. 20](image)

Fig. 20. (Color online) Condensate fractions of hard core bosons (or doublons) for three particle densities as functions of $|U|/t$. The dash-dotted line is a visual guide of $\propto \text{exp}(-t/|U|)$ for $n = 0.26$.\n
$\rho_0 = \frac{1}{D} n_D(0) = \frac{1}{DN_s} \sum_{j,\ell} \langle b^\dagger_{j\ell} b_{j\ell+1} \rangle. \quad (32) \]

In Fig. 20, the $|U|/t$ dependence of $\rho_0$ is depicted for three particle densities. The behavior of $\rho_0$ for small $|U|/t$’s is $\rho_0 \sim \text{exp}(-t/|U|)$ and has a meaning similar to $P_\infty$. In the BEC regime ($|U| > |U_\infty|$), $\rho_0$ is almost constant, indicating that a picture of hard-core bosons is justified in the entire regime of BEC. The suppression of $\rho_0$ with increasing $n$ is primarily because a high density enhances the effect of onsite interaction.

![Fig. 21](image)

Fig. 21. (Color online) Optimized gap parameter $\Delta_p$ for several $n$’s as function of $|U|/t$. The dash-dotted line is a visual guide of $\propto \text{exp}(-t/|U|)$. The inset shows a comparison of the optimized values of $\Delta_p$ between $\mathcal{P}_G \Phi_{BCS}$ and $\mathcal{P}_G \Phi_{BCS}$ for $n = 0.5$.
at $U \sim U_{co}$, and then decreases as $|U|/t$ increases, similarly to $\Delta E$ [Fig. 11(a)]. In the BEC regime, it is probable that $\Delta \rho$ obeys $2r^2/|U| = J$, because $J$ is the sole energy scale for $|U|/t \to \infty$, according to eq. (10). It seems that $\Delta E$ and $\Delta \rho$ scale $T_c$ in AHM.

In the inset of Fig. 21, we compare the optimized $\Delta \rho$'s between $\Psi_{SC}$ and $\mathcal{P}_G \Phi_{BCS}$. Although the two $\Delta \rho$'s behave similarly in the BCS regime, the $\Delta \rho$ of $\mathcal{P}_G \Phi_{BCS}$ monotonically increases unlike the $\Delta \rho$ of $\Psi_{SC}$ in the BEC regime. It follows that the binding correlation between antiparallel spins is also significant for $\Psi_{SC}$, especially in the BEC regime.

In variational theories with $d_{x^2-y^2}$-wave SC states for cuprates, the $d_{x^2-y^2}$-wave gap parameter $\Delta_d$, corresponding to $\Delta_p$ here, is considered to represent a singlet-pairing gap (not necessarily SC gap). The optimized $\Delta_d$ monotonically increases as the doping rate, the relevant parameter of the crossover, approaches the BEC limit ($\delta \to 0$), in contrast to $T_c$. The behavior of $\Delta_d$ here is distinct from that of $\Delta_d$ again, we should be careful to consider the cuprate in the point of view of the BCS-BEC crossover.

4.3 Coherence length and intuitive picture

The BCS-BEC crossover has been typically explained by whether or not a domain of a Cooper pair overlaps with a domain of another pair, as in Fig. 7. To discuss this more quantitatively, we need to estimate a pair size $\xi_{pair}$ corresponding to the coherence length and a distance between Cooper pairs $\tilde{\xi}_{uu}$. As for $\xi_{pair}$, it is reasonable to refer to the BCS expression of Pippard’s coherence length,

$$\xi_0 = \frac{\hbar \nu_F}{\pi |\Delta_{BCS}|},$$

(33)

in the BCS regime. In the present study, $\nu_F$ is a constant for any $|U|/t$, because the renormalization of $k_F$ by $|U|/t$ is not introduced. Thus, we assume $\xi_{pair} = \alpha/\Delta_p$, where $\alpha$ is a constant determined so that $\xi_{pair}$ can be smoothly connected to the form on the BEC side. In the BEC regime, eq. (33) does not work, because $\nu_F$ cannot be defined. Thus, following eq. (26), we naively assume $\xi_{pair} = \tilde{\xi}_{ud} = \tilde{r}_{ud} + \tilde{\sigma}_{ud}$, where $\tilde{r}_{ud}$ and $\tilde{\sigma}_{ud}$ denote the average distance between a spin (not necessarily of a spinon) and its nearest antiparallel spin and the standard deviation of $\tilde{r}_{ud}$, respectively. Note that $\tilde{r}_{ud}$ ($\tilde{\sigma}_{ud}$) is different from $r_{ud}$ ($\sigma_{ud}$) in eq. (26) in that spins that constitute doublons are taken into account. Similarly, following eq. (27), we estimate an interpair distance as the average minimum distance between a spin and its nearest parallel spin, $\tilde{\xi}_{uu} = \tilde{r}_{uu} - \tilde{\sigma}_{uu}$.

In Fig. 22, the $|U|/t$ dependences of $\xi_{pair}$ and $\tilde{\xi}_{uu}$ thus estimated are compared for $n = 0.5$. The pair size $\xi_{pair}$ is a monotonically decreasing function of $|U|/t$, whereas the interpair distance $\tilde{\xi}_{uu}$ is almost independent of $|U|/t$. Consequently, $\xi_{pair}$ crosses $\tilde{\xi}_{uu}$ at $|U| = |U|_c \sim 6.2$ at this particle concentration. Thus, for $|U| < |U|_c$, Cooper pairs penetrate each other ($\xi_{pair} > \tilde{\xi}_{uu}$) as in the Fermi liquid phase in Fig. 7. On the other hand, for $|U| > |U|_c$, a pair becomes almost a point hard-core boson ($\xi_{pair} \sim 0$), and is isolated from other pairs ($\xi_{pair} < \tilde{\xi}_{uu}$). Similarly, we estimated $|U|/t$ for other values of $n$, and found $|U|/t \sim 6t$ irrespective of particle densities. Since the above estimation of $U_k$ is rather broad, we consider that $U_k$ should be identical to $U_{co}$

Finally, we point out the difference in pairing manner between the spin-gap transition at $U_c$ in the normal state (§3.3) and the crossover at $\sim U_{co}$ in the SC state. Bound spinon pairs in the normal state ($|U| > |U|_c$) dissociate into independent spinons immediately when the pair domains overlap with each other at $U = U_c$. On the other hand, Cooper pairs in the SC state remain paired, even if pair domains come to considerably overlap for $|U| \ll |U|_{co}$ in the BCS regime; there is no critical change at $U = U_{co}$. Consequently, a phase transition (crossover) arises and a spin gap closes (survives) on the weakly correlated side in the normal (SC) state. The stability of Cooper pairs against mutual overlap is a current topic.

5. Conclusions

Using a variational Monte Carlo (VMC) method, we studied the features of a spin-gap transition in a normal state and of the BCS-BEC crossover in a superconducting (SC) state in the attractive Hubbard model (AHM) on the square lattice. We summarize the main results below.

(1) In the normal state, we revealed that, unlike the simple Gutzwiller wave function (GWF), a wave function with an antiparallel-spinon binding correlation $P_Q$ [eqs. (12) and (13)] undergoes a first-order transition from a Fermi liquid to a spin-gapped phase at $|U|_c/|U| \sim 9$. In the spin-gapped phase, particle density current can flow through the hopping of doublons. The pseudogap phase above $T_c$ for $|U| \gtrsim |U|_c$ may be deduced from the properties of this wave function. The mechanism of this spin-gap transition is understood to be similar to that of a Mott transition in a repulsive Hubbard model (RHM) induced by a doublon-holon binding correlation. We would also like to realize a variational normal state that is spin-gapped and conductive in RHM.

(2) We first applied VMC to the SC state of AHM, and confirmed that, as $|U|/t$ increases, the mechanism of superconductivity undergoes a crossover at approximately $|U|_{co} \sim |U|_c$ from an BCS type to a Bose-Einstein condensation (BEC) type. $P_Q$ is again needed to suppress the gap, which is greatly overestimated in GWF for $|U| \gtrsim |U|_{co}$. In the weak-correlation regime ($|U| < |U|_{co}$), the strength of SC ($T_c$) is scaled with quantities related to the SC gap as $\sim \exp(-t/|U|)$, as expected from the BCS theory. For $|U| > |U|_{co}$, the superfluid stiff-
ness, which is related to the cost of phase coherence, scales with $T_c$, as $r^2/|U|$. Such typical features of this crossover are captured by the energy gain in the SC transition $\Delta E$ in the whole range of $|U|/t$. In the BEC regime, the SC transition is induced by a gain in kinetic energy; this aspect is in contrast to the BCS theory, but is in accord with the magnetic and SC transitions in strongly correlated RHM.\(^{46,53}\) Most features are consistent with the framework of BCS-BEC crossover that previous studies provided.

(3) The physics of a spin–gap transition in the normal state and the BCS-BEC crossover in the SC state are explained in a semiquantitative manner by a simple idea of the competition between the pair size $\xi_{ad}$ and the interpair distance $\xi_{un}$, as shown in Fig. 7. This idea is equivalent to that of Mott transitions in RHM.\(^{45,44}\) In which a doublon-holon pair corresponds to the singlet pair here.

(4) In connection with that observed high-$T_c$ cuprates, the $|U|/t$ dependence of the pair correlation function $P_{\infty}$ and the gap parameter $\Delta_\rho$ studied here qualitatively differ from the doping rate ($\delta$) dependence of the corresponding quantities ($P_{\infty}$ and $\Delta_\rho$) in the strongly correlated RHMs, when the relevant parameters ($|U|/t$ and $\delta$) are in the respective BCS regimes. Furthermore, in a strongly correlated RHMs, the $d_{x^2−y^2}$-wave SC transition is always kinetic-energy-driven, regardless of $n$.\(^{53}\) We will address this subject more carefully in upcoming publications.

Acknowledgments

The authors thank Tomoaki Miyagawa for helpful discussions. This work is partially supported by Grant-in-Aids from the Ministry of Education, Culture, Sports, Science, and Technology, Japan.

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The principal feature of the BCS-BEC crossover is a change in the mechanism of SC transition, which arises owing to the competition between the SC and normal states. Therefore, the BCS-BEC crossover is not necessarily a problem of the SC state alone; some quantities such as $\Delta E$ may reflect the properties of the normal state.

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