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Spin-gapped wave function as normal state in attractive Hubbard model

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Abstract

With the pseudogap in cuprate superconductors in mind, we study an attractive Hubbard model on the square lattice, in which the mechanism of superconductivity undergoes a crossover at $|U_c|/t$ from a BCS type to a Bose-Einstein condensation type, as the interaction strength $|U|/t$ increases. Correspondingly, for $|U|>U_c$, a normate, realized for $T>T_c$, is considered to exhibit gapped behavior. We try to construct such a state and study its properties using variational Monte Carlo method, which treats local correlation accurately and can connect the weak- and strong-correlation limits continuously. We introduce an intersite correlation factor between antiparallel spins in nearest-neighbor sites, in addition to the onsite (Gutzwiller) projection. This factor brings about a first-order transition from a metal to a spin-gapped phase at $|U|>U_c$ (bandwidth). For $|U|>U_c$, a gap opens in the spin degree of freedom, whereas the charge sector remains gapless. In this phase, conductivity is caused by a hopping of doublons.

Keywords: spin gap; pseudogap; normal state; attractive Hubbard model; variational Monte Carlo

1. Introduction

In connection with the evolution of superconducting (SC) properties and pseudogap as the doping rate decreases in the high-$T_c$ cuprates, we take notice of the attractive Hubbard model [1], in which a crossover of SC mechanism arises at $U=U_c$ from a BCS type to a Bose-Einstein-condensation (BEC) type as the interaction strength $|U|/t$ increases [2]. In the BEC regime ($|U|>U_c$), pseudogap behavior caused by preformed electron pairs, like that in the underdoped cuprates, is theoretically expected for $T>T_c$; actually such phenomena were recently observed in ultracold Fermi gases in continuum systems [3]. The attractive Hubbard model has been studied mainly in the context of superconductivity. In this work, we shed light on the properties of this anomalous normal state in two dimensions, using a variational Monte Carlo method. So far, $|U|/t$ dependence of normal-state properties was studied by quantum Monte Carlo (QMC) methods [4,5], dynamical mean field theories (DMFT) [6,7] and variation theories [8,9]. The QMC studies up to $|U|/t\sim 8$ showed that gap behavior in the density of state develops for $T>T_c$ as $|U|/t$ increases. The DMFT studies, by tracing the normal branch down to low temperatures, found that there exists a transition(s) at $|U|=|U_c|$ and $W$ (bandwidth), and a spin gap appears in the phase for $|U|>U_c$. However, the microscopic picture in the gapped phase is still unclear. In a variation theory using the Gutzwiller wave function $\Psi_g$ with the Gutzwiller approximation [8], the results parallel those for the repulsive Hubbard model. Namely, a Brinkman-Rice transition occurs and both kinetic and interaction energies vanish for $|U|>|U_c|$; thus, the transition is a metal-insulator type. In fact, it is known that a transition does not arise if $\Psi_g$ is exactly solved [10]. Later, a variational Monte Carlo study [9] showed that an intersite antiparallel-spin correlation is necessary to induce a transition from a metal to a gapped phase, but the

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properties in the strongly correlated phase were not fully revealed. In this work, we ascertain the significance of the antiparallel-spin binding factor, and clarify the character of the transition, as well as the properties for $|U| > |U_c|$. 

2. Method

We consider the single-band Hubbard model with an attractive interaction $(U \leq 0, t \geq 0)$ on the square lattice,

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^d c_{j\sigma} + c_{j\sigma}^d c_{i\sigma}) - |U| \sum_i n_{i\uparrow} n_{i\downarrow}. \tag{1}$$

Using a canonical transformation, it is shown that the ground state of Eq. (1) for $|U|/t > 0$ is always SC, and is degenerate with a CDW state at half filling ($n = N_e/N = 1$, $N_e$: electron number, $N$: site number) [11]. Here, we pursue a normal branch as a virtual state which may replace the SC state, using a VMC approach [10]. As a variational wave function, we adopt a simple two-body Jastrow form, $\Psi_Q = P \Phi_f$, where $\Phi_f$ is the Fermi sea. To construct the many-body part $P$, we refer to an effective Hamiltonian obtained by a strong-coupling expansion for $|U|/t \rightarrow \infty$ [12],

$$
\begin{align*}
H &\approx \sum_{\langle i,j \rangle} 2t \left[ \left( -b_j^\dagger b_j + n_j \right) + \sigma_j \right] + \frac{1}{2} \left( n_j \right), \tag{2}
\end{align*}
$$

with $b_i = c_{i\sigma}^d c_{j\sigma} + n_i = (n_{i\uparrow} + n_{i\downarrow})/2$ and $\sigma_i = (n_{i\uparrow} - n_{i\downarrow})/2$. The first term in Eq. (2) represents a hopping of doublon, the second a nearest-neighbor (NN) density interaction, and the third a NN spin interaction. A binding factor between NN up- and down-spin sites $P_Q$ defined below must directly contribute to the spin term, and is probably effective also for the first and second terms indirectly through a NN doublon-holon pair, which is a configuration reached from a NN antiparallel spin pair by one hopping process. Thus, in addition to the onsite attractive (Gutzwiller) factor $P_g = \prod_j \left[ 1 - (1 - g) n_j n_{j\dagger} \right]$ of primary importance, we introduce $P_Q = \prod_j \left[ 1 - \mu Q_j \right]$ with,

$$
Q_j = s_j^\dagger \prod_r \left[ 1 - s_{j+r}^\dagger \right] + s_j^\dagger \prod_r \left[ 1 - s_{j+r}^\dagger \right], \tag{3}
$$

where $s_j^\dagger = n_{j\sigma} - (1 - n_{j\sigma})$, and $\sigma$ runs over the NN sites of the site $j$ [9]. This factor corresponds to the doublon-holon binding factor [13] used in the repulsive Hubbard model, and is crucial to induce a Mott transition [14]. Thus, the many-body part becomes $P = P_g P_Q$. In $\Psi_Q$, there are two variational parameters, $g (1 \leq g$ for the attractive case), which controls the number of doublons, and $\mu (0 \leq \mu \leq 1)$, which adjusts the strength of antiparallel spin binding. When $\mu = 0$ ($P_Q = 1$), the binding vanishes, and $\Psi_Q$ is reduced to the Gutzwiller wave function $\Psi_g = P_g \Phi_f$ [8], which is known not to exhibit Mott-type transitions [10]. On the other hand, for $\mu = 1$, an up-spin site is necessarily bound to a down-spin site(s). As mentioned, this projection, combined with $P_g$, encourages the hopping of doublons and doblon-holon attractive interaction.

We implement a series of VMC calculations, in which we use a simple linear optimization approach (substantially several million samples), with systems of up to $N = 32 \times 32$ and some electron densities, typically $n = 0.25, 0.5$ and $0.75$ with periodic-antiperiodic boundary conditions. In this article, we show the results only for $N = 20 \times 20$ and $n = 0.5$ (1/4 filling), because the dependence on $N$ and $n$ remains quantitative.

3. Results and discussions

![Fig. 1. (a) Momentum distribution function for various values of $|U|/t$; (b) Quasiparticle renormalization factor as function of $|U|/t$.](image-url)
As shown in a previous VMC study [9], by introducing $P_Q$, $\Psi_G$ greatly improves the variational energy on that of $\Psi_G$, and, in particular, induces a transition, which was regarded as a metal-insulator or Mott transition [9]. Let us start with a check of this transition. Figure 1(a) shows the momentum distribution function, $n(k) = \sum_{\omega} \langle c_{\omega k}^\dagger c_{\omega k} \rangle / 2$, along the path $\Gamma \rightarrow X \rightarrow M \rightarrow \Gamma$ for various values of $|U|/t$. As $|U|/t$ increases, the jump at the Fermi surface decreases, which corresponds to the quasiparticle renormalization factor $Z$ in the Fermi liquid theory. If $Z$ vanishes, we may consider some energy gap opens. As shown in Fig. 1(b), $Z$ vanishes at $|U| = |U_c| = 9.2t$ with a discontinuity, indicating that some first-order transition occurs and a gap opens. Next, we look at features of this transition. The solid circles in Fig. 2(a) show the $|U|/t$ dependence of doublon density $N_{j j}$, which is regarded as an order parameter of Mott transitions; $D$ exhibits a small jump at $U=U_c$, and tends to the fully onsite-paired value $D=0.25$ for $n=0.5$ as $|U|/t$ increases. The squares in Fig. 2(a) show the average distance from an up spin to its nearest down spin, and vice versa; for $|U|>|U_c|$, $r_{ud}$ is almost unity. Namely, even if an onsite singlet pair (doublon) is dissociated, its component spins cannot go away from each other beyond one lattice spacing. Thus, an independent-singlet-pair (or bosonic) picture is effective for a normal state in the strongly correlated phase ($|U|>U_c$). Now, we analyze the kinetic energy $E_{\text{kin}}$ into two parts, according as hopping processes vary the doublon number ($E_2$) or not ($E_1$) [15], as shown in Fig. 2(c). For

![Figure 2](image)

**Fig. 2.** (a) The doublon density (left axis) and average distance between up spin and its nearest down spin (right axis) are shown as functions of $|U|/t$; (b) kinetic energy $E_{\text{kin}}$ and its components $E_1$ and $E_2$ as functions of $|U|/t$. $E_1$ indicates the contribution from the hopping which do not change the number of doublons, and $E_2$ that of otherwise; (c) Schematic pictures of hopping processes in $E_1$ and $E_2$ discussed in (b).
[U]>|U|c, E1 almost vanishes, indicating that electrons cannot move unless a doublon is created or dissociated. This behavior is reflected in the effective model Eq. (2), in which electrons can move only through the doublon hopping. From these results, we suspect that the present transition is not a metal-insulator transition. Then, let us consider this transition in the light of correlation functions. In Figs. 3(a) and 3(b), we plot the charge \[N(q)\] and spin \[S(q)\] correlation functions, respectively, defined as

\[
N(q) = \frac{1}{N} \sum_{j \neq j'} \exp(-i \mathbf{q} \cdot \mathbf{r}_j) \langle n_{j \uparrow} n_{j' \downarrow} \rangle - n^2,
\]

\[
S(q) = \frac{1}{N} \sum_{j \neq j'} \exp(-i \mathbf{q} \cdot \mathbf{r}_j) \langle \hat{S}^\dagger_{j \uparrow} \hat{S}_{j' \downarrow} \rangle.
\]

Here we are interested in the small-\(|q|\) behavior of \[N(q)\] and \[S(q)\], because it is known within the single mode approximation (SMA) [16] that \[N(q)\] is linear in \(|q|\) for \(|q|\to 0\) if the charge excitation is gapless, whereas the small-\(|q|\) behavior becomes quadratic in \(|q|\) in a gapped case. As in Fig. 3(a), \[N(q)\] is linear for small \(|q|\) regardless of the value of \(|U|/t\), meaning that the charge excitation is gapless and can be conductive. On the other hand, the small-\(|q|\) behavior of \[S(q)\] abruptly changes at \(|U|=|U|c\) from linear to seemingly quadratic as \(|U|/t\) increases, as in Figs. 3(b) and its magnification 3(c). Thus, a gap opens in the spin sector in the strongly correlated phase, and is estimated with a SMA formula \[\Delta = -\lim_{q \to 0} q^2 E_{\text{kin}} / [8S(q)]\], as shown in Fig. 3(d). We find that the spin gap for \(|U|=|U|c\) is proportional to \(|U|/t\).

Finally, we consider the conductivity in the present wave function. In Fig. 4, we show expectation values of the single electron hopping \[|E_{\text{kin}}|/t\] and doublon hopping \[|E_D|/J = \sum_{j \neq j'} \langle b_j^\dagger b_{j'} \rangle\] with \(J=2t^2/U\). In the spin-gap phase, while \[|E_{\text{kin}}|/t\] decreases as \(|U|/t\) increases, \[|E_D|/J\] tends to a constant value. Since, once doublons are generated, there is no factor which prevents them from moving around independently, it is natural to think that the conductivity due to doublon hopping remains finite, although it may decay proportionally to \(J\), as \(|U|/t\) increases.

![Fig. 4. Expectation values of single electron hopping (dot) and of doublon hopping (square) as a function of \(|U|/t\).](image)

4.Summary

We revealed that a wave function with an antiparallel-spin binding correlation \(P_D\) with Eq. (3) undergoes a transition from a metal to a spin-gapped phase, in which charge current can flow. The conductivity in the spin-gapped phase is caused by the doublon hopping. Through a canonical transformation [11], the physics corresponds to that of the Mott transition in the repulsive Hubbard model [14]. The present result suggests that features in the pseudogap phase appearing above SC \(T_c\) for \(|U|>U_c\) can be deduced from the properties of this wave function. As a future problem, it is intriguing to extend this approach to the repulsive Hubbard, with the pseudogap in cuprates in mind.

References