Crossover of superconducting properties and kinetic-energy gain in two-dimensional Hubbard model

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Superconductivity in the Hubbard model on a square lattice near half filling is studied using an optimization (or correlated) variational Monte Carlo method. Second-order processes of the strong-coupling expansion are considered in the wave functions beyond the Gutzwiller factor. Superconductivity of $d_{x^2-y^2}$-wave is widely stable, and exhibits a crossover around $U = U_{co} \sim 12t$ from a BCS type to a new type. For $U > U_{co}$ ($U \ll U_{co}$), the energy gain in the superconducting state is derived from the kinetic (potential) energy. Condensation energy is large and $\propto \exp(-t/J)$ [tiny] on the strong [weak] coupling side of $U_{co}$. Cuprates belong to the strong-coupling regime.

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In a superconducting (SC) transition, conventional BCS superconductors follow a low-frequency sum rule of optical conductivity $\sigma_{1}(\omega)$ [1]. However, recent experiments have shown that cuprate superconductors violate this sum rule [2]. This violation implies a gain in kinetic energy ($K$) in the transition, because the sum of $\sigma_{1}(\omega)$ is proportional to $-K$ [2]. Such kinetic-energy-driven superconductivity [1] sharply contrasts with that of the conventional BCS superconductors, where the transition is induced by the lowering of potential energy [2].

The Hubbard model on a square lattice, $H = H_{t} + H_{U} = -t\sum_{\langle i,j \rangle,\sigma} (c_{i\sigma}^{\dagger}c_{j\sigma} + c_{j\sigma}^{\dagger}c_{i\sigma}) + U \sum_{j} n_{j\uparrow}n_{j\downarrow}$, is often used as a simple model which probablyseizes the essence of cuprates [1]. In spite of its importance, reliable knowledge is limited particularly in the intermediate and strong coupling regimes. It is still controversial whether superconductivity is realized in this model. In the strong coupling region, the Hubbard model is mapped to $t$-$J$-type models, where the $d_{x^2-y^2}$-wave superconductivity is concluded by exact diagonalization [7] and variational methods [8,9]. On the other hand, in the weak-coupling region, many quantum Monte Carlo (QMC) studies [10] came to negative conclusions for $U/t = 2$-4. Unfortunately, QMC is ineffective in larger-$U$ regimes due to the negative sign problem. In contrast, RPA calculations [11], fluctuation exchange approximations [12], renormalization-group [13,14] and perturbative [15,16] studies concluded $d_{x^2-y^2}$-wave superconductivity. Besides, variational Monte Carlo (VMC) studies using the Gutzwiller projection argued that an antiferromagnetic (AF) order prevails widely near half filling, and narrows the SC region [17,18].

The purpose of this letter is to resolve the above discrepancy, and to explore the possibility of the kinetic-energy-driven superconductivity in the two-dimensional Hubbard model. By carefully studying the wave functions with vital improvement on the Gutzwiller projection, it is found that the $d$-wave SC state is stabilized even in the weak coupling region, but its energy gain is too small to be observed in QMC. Furthermore, we find a crossover around $U_{co} \sim 12t$, over which the SC transition is induced by the lowering of kinetic energy. This indicates that the high-$T_{c}$ superconductivity should be understood in the context of strong correlation.

A VMC method [19] is useful to our purpose for its applicability to any $U/t$. Generally, a Jastrow-type function, $\Psi = P\Phi$, is used as a trial state, where $\Phi$ signifies a one-body (Hartree-Fock) state, and $P$ a correlation factor. For $P$, the Gutzwiller (onsite) factor [20], $P_{G} = \prod_{j} (1 - (1 - g) \delta_{n_{j\uparrow}n_{j\downarrow}})$, has been often chosen for its simplicity. Although $P_{G}$ is successful in $t$-$J$-type models [8,21], it brings about unfavorable results for the Hubbard model [10], which were expected to be remedied by improving $P_{G}$ [22,23]. Since the relationship between the Hubbard and $t$-$J$-type models is, $H_{t-J} = e^{iS}H_{Hub}e^{-iS}$ [24], which yields

$$\frac{\langle \Psi_{G}|H_{t-J}|\Psi_{G}\rangle}{\langle \Psi_{G}|\Psi_{G}\rangle} \sim \frac{\langle \Psi_{G}e^{iS}|H_{Hub}e^{-iS}\Psi_{G}\rangle}{\langle \Psi_{G}e^{iS}|e^{-iS}\Psi_{G}\rangle},$$

one can make improvements by applying the strong-coupling expansion, $e^{-iS}$, to $\Psi_{G} (= P_{G}\Phi)$.

Along this line, we employ $\Psi_{Q} = \prod_{j} [1 - \mu Q_{j}] \Psi_{G} = P_{Q}\Phi$ with $0 \leq \mu \leq 1$ in this work [25]. Here, $Q_{j}$ is an asymmetric projection $Q_{j}^{\tau} = d_{j} \prod_{\tau}(1 - e_{j+\tau})$ for less-than-half filling ($n < 1$, $n$: electron density), where $d_{j} = n_{j\uparrow}n_{j\downarrow}$, $e_{j} = (1 - n_{j\uparrow})(1 - n_{j\downarrow})$, and $\tau$ runs over all the nearest-neighbor sites. This factor takes account of virtual states in the second order of the strong-coupling expansion, as explained in Fig. 1. As a one-body function $\Phi$, we use the following: Fermi sea $\Phi_{F}$ for a normal state, a mean-field solution $\Phi_{AF}(\Delta)$ [26] for an AF state, and a fixed-$n$ BCS state with $d_{x^2-y^2}$-wave symmetry $\Phi_{SC}(\Delta, \zeta)$ for a SC state [27]. Here, $\Delta$ and $\zeta$ are variational parameters, although they denote gaps and chemical potential,
respectively, in the mean-field approximations.

Since our trial functions have up to four parameters to be optimized, the use of optimization VMC procedure is practically indispensable. Special treatment for the present calculations is that after the convergence of optimization, we continue iteration for a while, and average the data obtained during this excess process. Thereby, the accuracy in energy is markedly increased, sometimes to the order of $10^{-5}\cdot t$. We used lattices of $L \times L$ sites ($L = 6-16$) with closed shells and periodic-antiperiodic boundary conditions, and collected typically $2 \times 10^5-10^6$ samples, keeping the acceptance ratio 0.5.

![FIG. 1: Weight assignment of $P_Q$. A closed circle indicates a doubly-occupied (d-) site. (a) A configuration appearing for $U/t = \infty$. (b) A d-site arises by a single hopping process from (a) (a virtual state in the second order). (c) A d-site exists, and two hopping steps are needed to reach from (a) (a virtual state of the fourth order).](image)

First, we compare the total energy $E/t$ between $\Psi_Q$ and $\Psi_0$ [Fig 2(a)] for $n = 0.88$. In each state, $E/t$ is noticeably improved by the correlation factor $P_Q$, particularly in large-$U$ regimes. In Fig 2(b), the magnitude of the improvement is depicted for some values of $n$. The SC and normal states have large values which increase as $n$ approaches 1, whereas the value of the AF state is small and decreases as $n \to 1$. The improvements in the former states are caused by the lowering of kinetic energy $E_0 = \langle H_0 \rangle$ (not shown), because $P_Q$ promotes the hopping between neighboring sites by making the configurations like Fig 1(b) advantageous. In contrast, in the AF state, the binding effect between a d-site and an empty (e-) site is already included in $\Phi_{AF}$; the number of broken antiparallel-spin bonds increases in a Néel background when an e-site goes away from its partner d-site. Thus, the effect of $P_Q$ on $\Phi_{AF}$ is small and reduced as $n \to 1$. This result shows that the correlation factor $P_Q$ is essential for the normal and SC states. Henceforth, we focus on $\Psi_Q$.

Next, we consider the energy difference between the normal and the ordered states (condensation energy), $\Delta E = E^{\text{norm}} - E^{\text{order}}$, which is plotted in Fig 3. At half filling, the AF state is dominant for any value of $U$ as anticipated, and has a peak at $U = U^\text{AF} \sim 8t$, which originates in a metal-insulator (Mott) transition of the normal state [20]. Phase-transition behavior was found in $\Psi_Q^{SC}$, although $\Psi_Q^{SC}$ does not give the lowest variational energy for $n = 1$. As shown in Fig 3, $\Delta E$ for the SC state abruptly increases at $U = U_{SI} \sim 6.5t$, and the increase there becomes sharper as $L$ increases (not shown). Note that this behavior is inherent in the SC state, and $E^{\text{norm}}$ is smooth near $U_{SI}$. Around $U_{SI}$, the quasiparticle renormalization factor $Z$ for $\Psi_Q^{SC}$ vanishes (Fig 3), and the small-$q$ behavior of the charge structure factor $N(q)$ changes from linear to $q^2$-like (not shown). Therefore, we consider that a superconductor-insulator transition takes place, and $\Psi_Q^{SC}$ becomes insulating for $U > U_{SI}$. Actually, the parameter $g$ exhibits a cusp, and $\Delta$ and $\mu$ drastically change at $U = U_{SI}$. The insulating behavior with $\Delta E \propto t^2/U$ is consistent with the aspect of $t$-$J$-type models [24, 31].

When $n$ deviates from half filling, the behavior of $\Delta E$ is no longer a transition, but becomes a crossover. The inset of Fig 3 shows a close-up of $\Delta E$ of the small-$U$ region for $n = 0.88$. It is found that $\Delta E$ is very small for $U \lesssim 6.5t$ ($\sim 10^{-4}t$ at $U = 4t$), and behaves mildly.

FIG. 2: (a) Comparison of total energy among various functions. For instance, ‘Q/norm’ indicates $\Psi = \Psi_Q\Psi_e$. (b) Energy improvement by $\Psi_Q$ on $\Psi_Q$ in each state for several values of $n$. Solid (open, half-solid) symbols indicate the d-wave (AF, normal) state. For $n \lesssim 0.85$, the AF phase is not stabilized for any $U/t$.

FIG. 3: Energy difference (condensation energy) between the d-wave (AF) and the normal states, estimated by $\Psi_Q$.

Solid (open) symbols denote the SC (AF) state. Additional lines for $n = 1$ and $n = 0.88$ are $\propto t/U$ (dashed), and exp($-t/U$) (dash-dotted), respectively. Shown in inset is magnification of the small-$U$ region for $n = 0.88$. Additional lines are $\propto (U/t)^2$ (dashed) and exp($-t/U$) (dash-dotted). An arrow for $n = 1$ indicates $U_{SI}/t$, and those for $n < 1 U_{CO}$ at which $\Delta E$ has a maximum.
like a power-law function. It is probable that due to this imperceptibly weak superconductivity, many QMC studies for \( U/t = 2-4 \) overlooked signs of SC order. At \( U \sim 6.5t \), an exponential-like rapid increase occurs which again originates in \( \Psi_Q^{\text{SC}} \), and then \( \Delta E \) reaches a maximum at \( U = U_{\text{co}} \) as indicated by arrows in Fig. 3. As we will explain shortly, the SC properties for \( U > U_{\text{co}} \) qualitatively differ from those for \( U < U_{\text{co}} \). For \( U > U_{\text{co}} \), \( \Delta E \) is nicely fitted by the form \( \exp(-U/t) \) [or \( \exp(-t/J) \)], which means that the effective attractive interaction is \( J = 4t^2/U \); a viewpoint from \( t-J \)-type models is justified. In this region, the SC state is fairly stable relative on the SC state than on the AF state. We expect this behavior to considerably large \( U/t \). As \( n \) decreases, the difference between the two regimes tends to be vague.

Before the SC properties, let us discuss the phase diagram. As shown in the inset of Fig. 3, due to the sudden increase of \( \Delta E_{\text{AF}} \) for \( n < 1 \), the stable phase switches from SC to AF, but the SC phase is retrieved at a larger \( U/t \) (Fig. 3). The obtained phase diagram in the \( U/t-n \) plane is shown in Fig. 4(a). The AF state is stabilized near half filling where the nesting condition is satisfied, and occupies the maximum range of \( n \) at \( U \sim 6t \). If we use \( \Psi_Q \) instead of \( \Psi_Q \), the AF region becomes larger. This implies that the improvement by \( e^{-iS} \) is more effective on the SC state than on the AF state. We expect that the higher-order improvements enlarge the SC region.

We turn to the SC properties in \( \Psi_Q^{\text{SC}} \). Figure 5 shows the difference of kinetic energy \( \Delta E_k = E_k^{\text{norm}} - E_k^{\text{SC}} \) and potential energy \( \Delta E_U \). Apparently, the mechanism of energy gain changes at \( U \sim U_{\text{co}} \). For \( U < U_{\text{co}} \), the energy gain is due to the lowering of \( E_U (\Delta E_U > 0) \), as in the BCS superconductors. Inversely, for \( U > U_{\text{co}} \), kinetic-energy gain occurs (\( E_k \) is lower in the SC state), agreeing with cuprates. This qualitative change is a crossover and not a phase transition. These aspects do not depend on \( n \) qualitatively, although the magnitude of both \( \Delta E_k \) and \( \Delta E_U \) decreases, as \( n \) decreases. The lowering of \( E_k \) has been found also by a dynamical cluster approximation.

The momentum distribution function \( n(k) \) gives another evidence for the crossover. Since there are nodes in the \( d_{x^2-y^2} \)-wave state, \( n(k) \) has a discontinuity at \( k = k_F \) in the \( y = \pm x (\Gamma-M) \)-direction [Fig. 4(b)]. The magnitude of this jump represents the renormalization factor \( Z \), which is related to the inverse of the electron effective mass. The estimated \( Z \) for \( \Psi_{\text{norm}} \) and \( \Psi_{\text{SC}} \) are plotted in Fig. 6. For \( U < U_{\text{co}} \), the normal state has a larger value than the SC state, whereas this relation is reversed for \( U > U_{\text{co}} \) (see also inset). For \( U > U_{\text{co}} \), electrons are hard to move (or heavy) in the normal state, hampered by the strong correlation. On the other hand, in the SC state,
the coherence somewhat relieves the suppressed mobility, and thus the energy gain occurs in $E_0$.

This kind of crossover from weak- to strong-coupling regimes is not restricted to the present case. The attractive Hubbard model exhibits similar behavior in the s-wave SC transition for any electron density [24]. Hence, the kinetic-energy-driven superconductivity arises, not because the model has repulsive interaction, but the interaction is strong enough. The VMC calculations for the $t$-$J$ model showed that the exchange (hopping) energy is lowered (raised) in the $d_{x^2-y^2}$-wave SC state (see Table I in ref. [3], and also [24]). Since the kinetic part of the Hubbard model induces the exchange term ($J = 4t^2/U$), the results of $t$-$J$-type models are compatible with the present results in the Hubbard model for $U \gtrsim U_{co}$.

The magnitude of condensation energy in our calculation is larger than that obtained experimentally [35]. We anticipate that further refinement on the wave functions, especially on $\Psi_{\text{norm}}$, leads to a better outcome.

In summary, we have studied the two-dimensional Hubbard model near half filling, based on evolved VMC calculations. It is shown that the $d_{x^2-y^2}$-wave SC state is stabilized in the Hubbard model if the variational states are improved. Furthermore, we find a crossover at around $U_{co}/t = 11$-$13$. For $U \gtrsim U_{co}$, the SC state is similar to the conventional BCS state, but for $U \gtrsim U_{co}$, the SC transition is caused by lowering the kinetic energy. Recent experiments of $\tau_1(\omega)$ for cuprates [2] accord with the characteristics of this strong-coupling region. Extended description will be given elsewhere [18]. The authors thank D.S. Hirashima for helpful comment. This work is partly supported by Grant-in-Aids from the Ministry of Education etc. of Japan, and by the Supercomputer Center, ISSP, University of Tokyo.

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