Enhancement of the $d_{x^2-y^2}$ pairing correlation in the two-dimensional Hubbard model: a quantum Monte Carlo study

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Quantum Monte Carlo is used to investigate the possibility of $d_{x^2-y^2}$ superconductivity in the two-dimensional repulsive Hubbard model. A small energy scale relevant to possible pairing requires a care (i.e., sufficiently small level separation between the $k$ points) to detect enhanced correlations in finite-size studies. The notion has also been success-
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If the one-band Hubbard model, a simplest of the repulsively correlated electron systems, superconducts in two dimensions (2D), the interest is not only conceptually generic but may be practical as well, which has in-deed been a challenge in the physics of high $T_c$ superconduc-
tivity. Some analytical calculations have suggested the occurrence of $d_{x^2-y^2}$-wave superconductivity in the 2D Hubbard model. Numerical calculations have also been performed extensively. Finite binding energy and pairing interaction vertex were found in those calculations. Variational Monte Carlo calculations show that the superconducting order lowers the variational energy. Quite recently, Hotta, Takada, and the present authors have shown that the pairing with excluded double occu-
pacities has an enhanced correlation. Nevertheless, there has been a reservation against the occurrence of superconductivity in the Hubbard model because the bare pairing correlation functions do not show any symptom of long-range behavior.

Now, quite a different avenue has emerged recently in the physics of ladders. While the weak-coupling theory for the two-leg Hubbard ladder predicts the dominant pairing correlation, the numerical calculations for small values of interaction gives enhancement of the pairing correlation only when the Fermi level for $U$(on-site repulsion)$= 0$ lies between a bonding and an antibonding band levels that are separated with a sufficiently small level offset. This is because the relevant energy scale (the spin gap in the case of ladders) is so small that one has to make the separation between the highest occupied level (HOL) and the lowest unoccupied one (LUL) smaller than that to detect the pairing correlation in finite-size studies. The notion has also been successfully applied to confirm the weak-coupling prediction that the three-leg Hubbard ladder can superconduct as well.

This view enables us to have a fresh look at the 2D Hubbard model. Interests here are two-fold: numerically, how will the QMC result behave when the care for a small LUL-HOL is taken. Physically, will the pair-tunneling mechanism remain relevant also in 2D. These are pre-
cisely the purpose of the present study. We have indeed found enhancements in the bare $d_{x^2-y^2}$ pairing correlation in cases where the Fermi level lies between slightly separated LUL ($\delta k, \pi - \delta k'$) and HOL ($\pi - \delta k'', \delta k$), between which the pair tunneling should occur.

It is instructive to start with the two-leg Hubbard ladder, given as,

$$
H = -t_x \sum_{x,y,\sigma} (c_{x,y,\sigma}^\dagger c_{x+1,y,\sigma} + \text{h.c.})
$$

$$
- t_y \sum_{x,\sigma} (c_{x,1,\sigma}^\dagger c_{x,2,\sigma} + \text{h.c.}) + U \sum_{x,y,n_x,y,n_{x,y,l},l} \delta_{n_x,y,l} \delta_{n_{x,y,l},l},
$$

where $x(= 1, \cdots, N)$, $y(= 1, 2)$, and $\sigma(= \uparrow, \downarrow)$ specifies the rungs, the chains, and the spins, respectively. According to the weak-coupling theory (perturbational renormalization + bosonization), a gap opens in the spin excitations due to the relevance of interband pair tunneling between the Fermi points $(k_x, k_y) = (\pm k_{FB}^0, 0), (\pm k_{FB}^0, \pi)$. This con-
comitantly makes the two-point correlation of the interchain singlet, $c_{i,1,\uparrow} c_{i,2,\downarrow} - c_{i,1,\downarrow} c_{i,2,\uparrow}$, decay slowly with distance. In k-space the dominant component of this pair reads

$$
\sum_{\sigma} \sigma (c_{k_{FB}^0,\sigma}^0 c_{-k_{FB}^0,\sigma}^0 - c_{k_{FB}^0,\sigma} c_{-k_{FB}^0,\sigma}^\dagger), (1)
$$

where $c_{k_{FB}^0,\sigma}^\dagger$ annihilates an electron with spin $\sigma$ at $k_x = k$ in band $\mu(= 0, \pi)$.

Now, when the band structure is such that $E_F$ intersects the bonding-band top and the antibonding-band bottom with $k_{FB}^0 \sim \pi, k_{FB}^0 \sim 0$, intrachain nearest-neighbor singlet pair also has a dominant Fourier-component equal to eqn.(1) with a phase shift $\pi$ relative to the interchain pairing. Thus, a linear combination, $\sum_{\sigma} \sigma (c_{i,1,\sigma} c_{i,2,\sigma} - c_{i,1,\sigma} c_{i,2,\sigma}^\dagger)$ which amounts to the $d_{x^2-y^2}$ pairing, should have a slow decay as well.

Large enhancement of the inter-chain pairing correla-
tion has in fact been found by exact diagonalizations and by density matrix renormalization group when $E_F$ lies close to the $k$-points $(0, \pi)$ and $(\pi, 0)$. Although the $d_{x^2-y^2}$-like nature of the pairing was suggested, the $d_{x^2-y^2}$
pairing correlation itself has not been calculated. So, in our quest for 2D, we first calculate the correlation function with QMC.

Here we employ the ground-state, canonical-ensemble QMC where we take the free Fermi sea as the trial state. In most cases, we have taken the projection imaginary time $\tau$ to be $50/t_F$ or larger to ensure the convergence. We assume periodic boundary condition $c_{N+1} = c_1$. We set $t_F = 1$ hereafter.

We consider the case of 56 electrons in a $30 \times 2$ lattice $(n = 0.93)$ with $t_y = 1.975$, where HOL is $(0, \pi)$ and LUL’s are $(\pm14\pi/15, 0)$ for $U = 0$. We have deliberately made the LUL deviate from exactly $(0, \pi)$ because, although we have stressed that the interactions around $(0, \pi)$ and $(0, \pi)$ favors a $d_{x^2-y^2}$ pairing, the system becomes insulating if $E_F$ at $U = 0$ (denoted by $E_F^0$ hereafter) lies exactly between $(0, \pi)$ and $(0, \pi)$, for which the equality $\delta k = \pi$ brings about the interband umklapp processes.

In Fig. 1 we show the $d_{x^2-y^2}$ pairing correlation $P(r)$ defined by $P(r) = \sum_{x | y = 0} (O^\dagger(x + \delta x, y + \delta y)O(x, y))$, where $O(x, y) = \sum_{\delta x, \delta y} \sigma(c_{x,y,\sigma}c_{x+y,\sigma-\sigma-\sigma-\sigma-\sigma-\sigma-\sigma-\sigma-\sigma-\sigma})$, with $c_{x,y} \equiv c_{x,1}, c_{x,0} \equiv c_{x,2}$. $P(r)$ for $U = 1$ has an overall enhancement over the noninteracting result, and decays slowly.

Here we have tuned $t_y$ to make the LUL-HOL gap (denoted by $\Delta \varepsilon^0$ hereafter) as small as 0.006. This procedure is important, at least for small $U$, in detecting an enhanced pairing correlation in finite systems, as stressed in ref. 14 and in our previous publications. We can in fact see this in Fig. 1 where a 2 % change into $t_y = 1.93$ washes out the enhancement. This may seem surprisingly sensitive, but the change in $t_y$ is accompanied by a more than one order of magnitude increase in $\Delta \varepsilon^0 \to 0.1$ (without changing the $U = 0$ ground state).

Now we are in position to move on to the 2D Hubbard model. Here we consider the isotropic case of $t_y \approx t_x$ and $x, y = 1, \cdots, N$ with periodic boundary condition in both directions, where the $k$-points around $(0, \pi)$ and $(\pi, 0)$ are close in energy. Our expectation from the study on ladders is that the pair tunneling processes between $(\delta k, \pi - \delta k')$ and $(\pi - \delta k, \delta k')$ may result in $d_{x^2-y^2}$ pairing, $\sum_{k} \left[ \cos(k_x) - \cos(k_y) \right] c_{k}c_{k}$ in 2D, but an enhanced pairing correlation may be detected only when $\Delta \varepsilon^0$ between those levels is small. Apart from such an argument, the importance of the interactions around $(0, \pi)$ and $(\pi, 0)$ in the 2D Hubbard model has been suggested by various authors.

In the present approach, one should be able to detect the effect of a spin (or superconducting) gap due to the tunneling processes in the situation where $E_F^0$ situates between closely lying levels of $(\delta k, \pi - \delta k')$ and $(\pi - \delta k, \delta k')$, where $\delta k$’s are small.

We first take 46 electrons in $8 \times 8$ sites ($n = 0.72$) with $t_y = 0.999$. For this band filling, $E_F^0$ lies between the levels of $(0, \pm3\pi/4)$ and $(\pm3\pi/4, 0)$. We have taken $t_y = 0.999$, because the number of electrons considered here would have an open shell (with a degeneracy in the free-electron Fermi sea) for $t_y = 1$, which will destabilize QMC convergence. Taking $t_y = 0.999$ lifts the degeneracy between $(k_1, k_2)$ and $(k_2, k_1)$ to give a tiny $(< 0.01)$ but finite $\Delta \varepsilon^0$.

In Fig. 2 we plot the $d_{x^2-y^2}$ pairing correlation, where the correlation for $U = 1$ is clearly seen to be enhanced over that for $U = 0$ especially at large distances, resulting in a slower decay. A similar result is shown in the inset for a larger system ($10 \times 10$ with 78 electrons), where $E_F^0$ lies between $(0, \pm4\pi/5)$ and $(\pm4\pi/5, 0)$. Also shown in Fig. 2(a) is a result for $t_y = 0.95$, where $\Delta \varepsilon^0$ blows up to $\sim 0.17$, and the enhancement vanishes in accordance with the expectations from the ladders.

In the above situation, LUL and HOL are taken to be $(0, \pi - \delta k)$ and $(\pi - \delta k, 0)$ with $\Delta \varepsilon^0 < 0.01$, while the other levels lie more than $\sim 0.1$ away from $E_F^0$. One might thus raise a criticism that the scattering processes involving the states away from $E_F^0$ are unduly neglected. Some of these processes may favor the pairing, while others may not. We can in fact focus on the scattering processes that do not favor $d_{x^2-y^2}$ pairing by taking a LUL state on the $\Gamma$-M ($|k_x| = |k_y|$) line, and situate all the others except a certain HOL away from $E_F^0$. There, $d_{x^2-y^2}$ pairing should not to be favored since the $d_{x^2-y^2}$ gap function has nodal lines along $\Gamma$-M. To realize such a situation, we introduce the next nearest-neighbor hopping $t' = -0.24$ in a $10 \times 10$ lattice with 74 electrons where we take $t_y = 1$ this time. $E_F^0$ now lies between LUL $(\pm2\pi/5, \pm2\pi/5)$ along $\Gamma$-M line and HOL $(\pm4\pi/5, 0)$, with $\Delta \varepsilon^0 \sim 0.01$. 

FIG. 1. QMC result for the $d_{x^2-y^2}$ pairing correlation, $P(r)$, in a $30 \times 2$ Hubbard ladder with 56 electrons with $U = 1$ and $t_y = 1.975$ ($\square$) or $t_y = 1.93$ ($\bigcirc$). The error bars are smaller than the symbols. The dashed line represents the noninteracting case.
We can see from the inset of Fig. 3 that the $d_{x^2-y^2}$ correlation is indeed no longer enhanced for $U = 1$.

We have then to investigate the case where both the scatterings which do and do not favor $d_{x^2-y^2}$ pairing are taken into account on an equal footing. To realize such a situation, we can in fact take an $8 \times 8$ lattice with 60 electrons with $t_y = 0.999$ and $t' = 0$. In this case, the energies of the occupied levels $(0, \pi)$ and $(\pm \pi/4, \pm 3\pi/4)$ are within 0.01 to those of the unoccupied levels $(0, 0)$, $(\pm 3\pi/4, \pm \pi/4)$, and $(\pm \pi/2, \pm \pi/2)$, so that the scatterings between, e.g., $(0, \pi)$ and $(3\pi/4, \pi/4)$, which favors $d_{x^2-y^2}$ pairing, and those between, e.g., $(0, \pi)$ and $(\pi/2, \pi/2)$, which do not, coexist. In Fig. 3(b) we can see that the $d_{x^2-y^2}$ correlation for $U = 1$ is enhanced over the non-interacting result, so that the coexistence is not detrimental. A similar $k$-space configuration may be realized by taking 92 electrons in a $10 \times 10$ system ($n = 0.92$), for which an enhanced $d_{x^2-y^2}$ correlation is obtained as well (Fig. 4).

Our final important finding is the band-filling dependence. We have calculated $S \equiv \sum_{r \geq 3} P(r)$, which is a measure of the long-range part of the correlation, for the $10 \times 10$ lattice with $t_y = 0.999$ and $t' = 0$ for various $n = 1, 0.92, 0.78$, and 0.46. $\Delta S^0$ is kept to be $< 0.01$ throughout. The summation is restricted to $r \geq 3$ in order to eliminate short-range contributions. For $n = 0.46$ (46 electrons) LUL/HOL is $(0, \pm 3\pi/5)$ and $(\pm 3\pi/5, 0)$, which significantly deviate from $(0, \pi)$ and $(\pi, 0)$. The result, displayed in Fig. 5, shows that the enhancement in $S$ for $U = 1$ has a maximum around a finite doping. Although some enhancement over the $U = 0$ result remains at $n = 0.46$, the absolute value of $S$ becomes small reflecting the rounded-off Fermi surface for small $n$. Thus the message here is that the $d_{x^2-y^2}$ pairing is favored near, but not exactly at, half-filling.

To conclude, we have obtained an enhancement of $d_{x^2-y^2}$-wave pairing correlation in the 2D Hubbard model. Special care has been taken on $\Delta S^0$ between the HOL $(\delta k, \pi - \delta k')$ and LUL $(\pi - \delta k'', \delta k''')$, as motivated from the studies on ladders. Analytical approaches for the 2D Hubbard model show that the relevant energy scale for superconductivity, $\Delta_S$, is $O(0.01t)$ in this light it is natural that $\Delta S^0$ has to be smaller than $\sim O(0.01t)$ if one wishes to detect enhanced pairing correlations in finite systems.

Although the $d_{x^2-y^2}$ correlation is shown to be enhanced only when $\Delta S^0$ is small, this result does not necessarily imply that a high density of states around the Fermi level is a prerequisite to superconductivity in the thermodynamic limit. Rather, we argue that the ‘high density of states’ is necessitated in finite systems to make the situation closer to the thermodynamic limit, where $\Delta S/\Delta S^0$ diverges after all for any value of $D(E_F)$. On the other hand, by preferentially focusing on the scatterings between, e.g., $(0, \pi - \delta k)$ and $(\pi - \delta k, 0)$ as in Fig. 2, we may be mimicking the situation in many of the high $T_C$ cuprates for which the photoemission studies have revealed that $E_F$ lies very close to the extended van Hove singularity because the scatterings involving the $k$-points around $(0, \pi)$ and $(\pi, 0)$ would indeed be dominant due to the high density of states.

Present study is restricted to relatively small values of $U/t \sim 1$. For large $U/t$, the strategy of paying attention to the $U = 0$ energy levels can fail to detect the enhancement of the pairing correlation, if any, because free-electron levels may become irrelevant. Namely, some energy scale $\Delta S^0$ (possibly a kind of charge excitation energy), which vanishes in the thermodynamic limit with $\Delta S/\Delta S^0 \to \infty$, should still exist in finite systems even
for large $U/t$, but $\Delta \varepsilon_{\text{eff}}$ will not be dominated by $\Delta \varepsilon^0$. Then the problem will be how to tune $\Delta \varepsilon_{\text{eff}}$.

Our results suggest that the pair-tunneling processes are enhanced in the 2D Hubbard model, which possibly leads to superconductivity. Whether such an enhancement is due to, e.g., spin fluctuations remains to be an open question.

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27. We are not arguing that $t'$ always destroys $d_{x^2-y^2}$ pairing. In fact, $d_{x^2-y^2}$ pairing correlation is enhanced if $E_F$ lies between $(\delta k, \pi)$ and $(\pi - \delta k')$, regardless of the presence/absence of $t'$, as will be published elsewhere.
28. This is close to the parameter values for which the vertex part of the $d_{x^2-y^2}$ correlation was found to have a plateau-like behavior in ref. 8. Since we do not find an enhancement of the bare $d_{x^2-y^2}$ pairing correlation for this parameter set, our results should not be confused with those in ref. 8, where the behavior of the vertex part is used as the criterion for superconductivity.
29. Like in the ladders, the scatterings between exactly $(\pi, 0)$ and $(0, \pi)$ may not strongly favor superconductivity. We have numerical results suggesting such a possibility, which will be published elsewhere.
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