A consistent description of the pairing symmetry in hole and electron doped cuprates within the two dimensional Hubbard model

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Quantum Monte Carlo is used to calculate various pairing correlations of the 2D Hubbard model possessing band features experimentally observed in the cuprates. In the hole-doped case, where the Fermi level lies close to the van Hove singularities around \((0, \pi)\), the \(d_{x^2-y^2}\) pairing correlation is selectively enhanced, while in the electron-doped case, where the singularities are far below the Fermi level and the Fermi surface runs through \((\pm \pi/2, \pm \pi/2)\), both \(d_{x^2-y^2}\) and \(d_{xy}\) correlations are enhanced with the latter having a \(\sqrt{2} \times \sqrt{2}\) structure. The two pairing symmetries can mix to result in a nodeless gap.

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Since the seminal proposal by Anderson, great theoretical effort has been made to investigate the possibility of describing various aspects of the high \(T_C\) cuprates within the two dimensional (2D) Hubbard model. Those include the antiferromagnetic insulating phase in the undoped systems, the normal state above \(T_C\), and the superconducting state. Among all, it has been an open question whether the Hubbard model can actually account for the superconductivity, especially its pairing symmetry, in both hole and electron doped cuprates.

Many analytical calculations have supported the possibility of \(d_{x^2-y^2}\) pairing in the nearly half-filled 2D Hubbard model. While some previous numerical studies of pairing correlations in finite systems have given negative results for superconductivity, we have recently shown that an enhanced \(d_{x^2-y^2}\) pairing correlation is indeed detected numerically if we ensure that the highest occupied one-electron levels (HOL) and lowest unoccupied levels (LUL) at \(U = 0\) in finite systems are sufficiently close. This precaution, as motivated from the numerical studies on Hubbard ladders, has been necessitated because the energy scale of the superconductivity in the Hubbard model, if any, should be of the order of 0.01\(t\), while the discreteness of the energy levels in finite systems tractable in numerical calculation is much larger (\(\sim 0.1t\)) unless parameter values are tuned.

In the hole-doped cuprates such as YBCO and BSCCO there is now a body of accumulating evidence that the pairing symmetry is \(d_{x^2-y^2}\) (at least around the optimal doping), which is consistent with the previous Hubbard-model studies. On the other hand, experimental results for the electron-doped NCCO seems to indicate an s-wave, or more precisely, a symmetry with a nodeless superconducting gap. Experiments have also revealed further differences between hole-doped and electron-doped systems. Specifically, the angle-resolved photoemission spectroscopy (ARPES) has shown that the ‘extended’ van Hove singularity (VHS) around \(k = (0, \pi)\) and \((\pi, 0)\) lies very close to the Fermi level \(E_F\) in YBCO and BSCCO, while the VHS lies far below the Fermi level in NCCO.

The purpose of the present study is to explore whether the difference of the pairing symmetry between electron and hole doped systems can be explained within the 2D Hubbard model possessing the band features observed experimentally. The essential band features (namely, the shape of the Fermi surface and the relative position of the VHS to \(E_F\)) of YBCO, BSCCO, and NCCO can be reproduced by introducing a next-nearest neighbor (NNN) transfer about half the nearest neighbor (NN) one. Note that in our previous study mentioned above, such an electron-hole asymmetry was not taken into account since we considered the Hubbard model with only NN transfers.

Quantum Monte Carlo (QMC) method is used to calculate correlation functions of \(d_{xy}\), NN and NNN extended s as well as \(d_{x^2-y^2}\) pairings. To look into such diverse symmetries has been motivated from the following physical consideration. Namely, the pair-tunneling processes between \((k_1 \uparrow, -k_1 \downarrow)\) and \((k_2 \uparrow, -k_2 \downarrow)\) favors the pairing order parameter \(\Delta\) that satisfies \(\Delta(k_1) = -\Delta(k_2)\), which is a picture known to be at work in the two-leg and three-leg Hubbard ladders. In this picture, the pair-tunneling between the \(k\)-points around \((0, \pi)\) and \((\pi, 0)\) favors \(d_{x^2-y^2}\) pairing. Such processes should indeed be pronounced in the hole-doped cuprates because \(E_F\) lies close to \((0, \pi)\) and \((\pi, 0)\), and the density of states around these points is large. Thus, in this case, \(d_{x^2-y^2}\) pairing should be dominant with possibly other symmetries mixing slightly. By contrast, in the electron doped case, other pair-tunneling processes may set in on a nearly equal footing in determining the pairing symmetry, because VHS lies far below \(E_F\). Then, not only \(d_{x^2-y^2}\) but also \(d_{xy}\) pairing or extended s pairing (with gap functions that have nodes on the Fermi surface, but do not change sign by a 90 degree rotation) will become eligible, so that some of these symmetries may mix with comparable weights.
In fact, we find here that the $d_{x^2-y^2}$ correlation is dominant in the hole-doped case, while in the electron-doped case both $d_{x^2-y^2}$ and $d_{xy}$ correlations are enhanced, with the latter having a $\sqrt{2} \times \sqrt{2}$ structure. These two pairing symmetries can in fact mix ending up with a nodeless gap without breaking the time reversal symmetry, unlike in $d_{x^2-y^2} + id_{xy}$ pairing [24], where the symmetry is broken. Correlation of the extended $s$-wave pairings is found to be suppressed in all the cases investigated.

We consider the 2D Hubbard model on a square lattice with NN ($t$), NNN ($t'$), and third NN ($t''$) hoppings,

$$
\mathcal{H} = -\sum_{x,y,\sigma} \left[ t_x (c_{x,y,\sigma}^\dagger c_{x+1,y,\sigma} + c_{x,y,\sigma}^\dagger c_{x+1,y+1,\sigma}) + t_y (c_{x,y,\sigma}^\dagger c_{x,y+1,\sigma} + c_{x,y,\sigma}^\dagger c_{x+1,y+1,\sigma}) + t'_x (c_{x,y,\sigma}^\dagger c_{x+1,y+1,\sigma}) + t'_y (c_{x,y,\sigma}^\dagger c_{x+1,y,\sigma} + c_{x,y,\sigma}^\dagger c_{x+1,y,\sigma}) + t'' (c_{x,y,\sigma}^\dagger c_{x+1,y,\sigma} + c_{x,y,\sigma}^\dagger c_{x+1,y,\sigma}) + \text{h.c.} \right] + U \sum_{x,y} n_{x,y}^\dagger n_{x,y}.
$$

Here, $(x, y)$ is the coordinate of the sites, and the lattice constant is taken as unity. Periodic boundary condition is assumed, and we set $t_x = 1$ hereafter.

As mentioned above [10], it is necessary to put $E_F$ at $U = 0$ between the HOL’s and LUL’s separated by an energy of $\Delta c^0$ less than $O(0.01)$ in order to detect a symptom of superconductivity having an energy scale of $O(100 K)$. On the other hand, QMC is unstable for exactly $\Delta c^0 = 0$, namely for open shell configurations. Thus, we accomplish $\Delta c^0 \sim O(0.01)$ by making $t_x$ and $t_y$, and/or $t'_x$ and $t'_y$ slightly different, where $t_x \neq t_y$ lifts the degeneracy between $(\pm k_1, \pm k_2)$ and $(\pm k_2, \pm k_1)$ for $|k_1| \neq |k_2|$, while $t'_x \neq t'_y$ lifts the degeneracy between $(k_1, k_1)$ and $(\pm k_1, \mp k_1)$.

We have employed the ground-state, canonical-ensemble QMC, where we have implemented the stabilization algorithm adopted by several authors. [28] We adopt the free Fermi sea as the trial state, and take the projection imaginary time $\tau$ up to $\sim 40$ to ensure the convergence. Small $\Delta c^0$ makes the negative sign problem serious, but by taking a relatively small value of $U(=1)$, we can check the convergence with respect to $\tau$ without running into serious sign problem.

We have calculated the pairing correlation functions,

$$
P(r) = \sum_{|\Delta x|+|\Delta y|=r} \langle O^\dagger(x + \Delta x, y + \Delta y) O(x, y) \rangle \quad \text{with} \quad O_{NN}(x, y) = \sum_{\delta, \sigma} \sigma (c_{x,y,\sigma} c_{x+\delta,y,-\sigma} \pm c_{x,y,\sigma} c_{x,y+\delta,-\sigma})
$$

$$
O_{NNN}(x, y) = \sum_{\delta, \sigma} \sigma (c_{x,y,\sigma} c_{x+\delta,y+\delta,-\sigma} \pm c_{x,y,\sigma} c_{x-\delta,y+\delta,-\sigma}),
$$

where $\delta = \pm 1$. The plus (minus) sign in $O_{NN}$ corresponds to NN $s$ ($d_{x^2-y^2}$) symmetries, while the plus (minus) in $O_{NNN}$ to NNN $s$ ($d_{xy}$) symmetries.

We have looked into various values of $n$, $t'$, and $t''$ including other than the ones described below, and found NN and NNN $s$-wave pairing correlations to be strongly suppressed with $U$ at large distances. At first this may seem odd because these pairings do not have any on-site amplitude. This might be because the extended $s$-wave pairings always couple, at least at the mean-field level, with the on-site $s$ pairing, [29] which is directly suppressed with $U > 0$. Thus, we show only $d_{x^2-y^2}$ and $d_{xy}$ pairing correlations in the following.

We first look at the hole-doped case. We consider a 12 x 12 lattice with 118 electrons (band filling $n = 0.82$) with $t_y = 0.999$, $t'_y = -0.429$, $t'_x = -0.43$, $t'' = 0.07$, and $U = 1$ ($\bigcirc$). The dashed lines represent the $U = 0$ result. The inset shows the HOL’s and LUL’s within 0.01 to $E_F$.

![FIG. 1. QMC result for $d_{x^2-y^2}$ (a) and $d_{xy}$ (b) pairing correlations for a hole-doped system (12 x 12 system with 118 electrons with $n = 0.82$). $t_y = 0.999$, $t'_y = -0.429$, $t'_x = -0.43$, $t'' = 0.07$, and $U = 1$ ($\bigcirc$). The dashed lines represent the $U = 0$ result. The inset shows the HOL’s and LUL’s within 0.01 to $E_F$.](image_url)
of the d-states are smaller than that in the hole-doped case. The correlation is enhanced at even distances (\(\Delta x, \Delta y\)) component is enhanced with \((\pi, -\pi/3), (-\pi/3, \pi/3), (-\pi/3, -\pi/3/2\) lie within 0.01 in energy at \(U = 0\). The Fermi surface, represented by these HOL’s and LUL’s is displayed as an inset in Fig. 3(a). There, reflecting the high density of states around VHS, many \(k\)-points around \((0, \pi)\) and \((\pi, 0)\) appear, while the points around \(|k_x| = |k_y|\) appear, although fewer, also exist.

In Fig. 3(a), we show the \(d_{x^2-y^2}\) correlation as a function of real space distance \(r = |\Delta x| + |\Delta y|\). It can be seen that the correlation is enhanced for \(U = 1\) over that for \(U = 0\), especially at large distances. By contrast, the \(d_{xy}\) correlation shown in (b) is not enhanced within the error bars. The dominant \(d_{x^2-y^2}\) pairing is consistent with the expectation from the pair-tunneling picture given above. On the other hand, we cannot rule out the possibility of a small \(d_{xy}\) mixing, since if more \(k\)-points exist in the vicinity of \(E_F\), not only the \(d_{x^2-y^2}\) correlation would be more enhanced, but also the \(d_{xy}\) might be enhanced, which would imply their mixture. Further, \(d_{xy}\) may mix in a time-reversal broken form, \(d_{x^2-y^2} + id_{xy}\), especially in magnetic fields, which is of interest from the viewpoint of the recent experimental observations suggesting such a possibility at low temperatures.

Let us now turn to the case of electron doping. This time, we take 190 electrons /12 \times 12 (\(n = 1.32\)) with \(t_y = 0.999, t'_y = -0.499, t'_t = -0.5, \) and \(t''_t = 0\). (In the actual calculation we have employed the electron-hole transformation to consider a 98 electron system with \(t'_t > 0\)). Here, HOL’s reside at \((\pi, \pi/3, \pi), (\pi/2, -\pi/2), (-\pi/2, \pi/2), (\pi/2, \pi/2), (-\pi/2, -\pi/2)\) for \(U = 0\) (inset of Fig. 3(a)). Note that \((\pi/2, \pi/2)\) lies right on the Fermi surface, a feature seen in the ARPES data of NCCO.

The QMC result in Fig. 3(a) shows that, although the Fermi surface is now shifted away from \((\pi, 0), (0, \pi)\) down to \((\pi, \pi/3, \pi), (\pi/3, \pi, \pi), \) we still have an enhancement of the \(d_{xy}\) correlation, although the enhancement is smaller than that in the hole-doped case.

Now, more striking is the behavior of the \(d_{xy}\) correlation shown in Fig. 2(b). At large distances, the \(d_{xy}\) correlation is enhanced at even distances (\(\Delta x + \Delta y = \) even), while suppressed at odd distances, which means that it has a \(\sqrt{2} \times \sqrt{2}\) superstructure. A Fourier transform of the correlation function indeed shows that its \((\pi, \pi)\) component is enhanced with \(U\).

The result suggests a coexistence of the \(d_{x^2-y^2}\) and the \(\sqrt{2} \times \sqrt{2}\) \(d_{xy}\) pairings, whose order parameters are \(c_{k+Q}c_{-k} (\cos k_x - \cos k_y)\) and \(c_{k+Q}c_{-k} (\sin k_x \sin k_y)\), respectively, with \(Q = (\pi, \pi)\). If they both have long-range orders, we should take \((c_{k+Q}^\dagger, c_{k+Q})\) and \((c_{-k+Q}^\dagger, c_{-k+Q})\) as basis to diagonalize the \(2 \times 2\) order parameter matrix to have

\[
\Delta_\pm (k) = \pm \sqrt{A (\cos k_x - \cos k_y)^2 + B (\sin k_x \sin k_y)^2},
\]

where \(A, B > 0\). This form, which is nodeless, is similar to the energy spectrum of the chiral spin state proposed by Wen, Wilczek, and Zee. The order parameter of the chiral spin state is defined for \(\langle c^\dagger c \rangle\), the hopping amplitude, while we are here talking about \(\langle cc \rangle\), the pairing amplitude. The corresponding superconducting gap coincides with that of the \(d_{x^2-y^2} + id_{xy}\) pairing, but we must stress that the present order parameter is real and hence does not break the time reversal symmetry as in \(d_{x^2-y^2} + id_{xy}\). Thus we end up with a fully-gapped, time-reversal-symmetric mixture of \(d_{x^2-y^2}\) and \(d_{xy}\) pairings.

As seen in Fig. 3(b), the \(\sqrt{2} \times \sqrt{2}\) structure of the \(d_{xy}\) correlation is not observed in the hole-doped case. In fact, we have considered a wide variety of cases, some of

FIG. 2. A plot similar to Fig. 1 for an electron-doped system (190 electrons /12 \times 12 with \(n = 1.32\)) for \(t_y = 0.999, t'_y = -0.499, t'_t = -0.5, t''_t = 0, \) and \(U = 1\).
which will be published elsewhere, and found that the $\sqrt{2} \times \sqrt{2}$ structure in the $d_{xy}$ pairing emerges only when $(\pm \pi / 2, \pm \pi / 2)$ lies on the Fermi surface. Then, the difference in the pairing symmetry between the hole-doped and electron-doped cases may be not only due to the relative position of the VHS against $E_F$, but may also come from the fact that $(\pm \pi / 2, \pm \pi / 2)$ lies very close to the Fermi surface in NCCO.

The relation of $(\pm \pi / 2, \pm \pi / 2)$ to the pairing having a superstructure has also been suggested for the $t$-$J$ model by Ogata quite recently [36]. Using a variational approach to the $t$-$J$ model, he showed that the energy of $d_{x^2-y^2}$ pairing state is lowered with a full gap when mixed with NN extended-$s$ pairing having finite momentum of $(\pi, 0)$ or $(0, \pi)$, if the system is lightly doped, so that $(\pm \pi / 2, \pm \pi / 2)$ is close to the Fermi surface. [37] The difference with the present result is obtained for the Hubbard model and Ogata’s result for the $t$-$J$ model.

In summary, we have shown that the 2D Hubbard model possessing band features experimentally observed in the cuprates can account for both the $d_{x^2-y^2}$ pairing for hole doping and a nodeless pairing for electron doping. The fact that the present result is obtained for rather small values of $U(\sim t)$ suggests that large interactions ($U \gg t$) may not be essential to the occurrence of superconductivity, although the strength of the interaction will certainly dominate the absolute magnitude of the gap or $T_C$.

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