Detection of pairing correlation in the two-dimensional Hubbard model

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Quantum Monte Carlo method is used to re-examine superconductivity in the single-band Hubbard model in two dimensions. Instead of the conventional pairing, we consider a ‘correlated pairing’, $\langle \tilde{c}_{i\uparrow} \tilde{c}_{i\downarrow} \rangle$ with $\tilde{c}_{i\sigma} \equiv c_{i\sigma} (1 - n_{i\sigma})$, which is inferred from the $t$-$J$ model, the strong-coupling limit of the Hubbard model. The pairing in the $d$-wave channel is found to possess both a divergence like $1/T$ in the pairing susceptibility and a growth of the ground-state pairing correlation with sample size, indicating an off-diagonal long-range order near (but not exactly at) half-filling.

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Ever since the discovery of high-$T_c$ cuprate superconductors, there has been a controversy about its microscopic mechanism. Following a seminal proposal by Anderson [1] ascribing it to a purely electronic origin, extensive numerical and analytical studies have been done to explore a possibility of superconductivity in the Hubbard model in two dimensions (2D). Apart from possible relevance to the high-$T_c$ mechanism, it has been a longstanding problem to clarify whether the Hubbard model, a simplest possible model for correlated electrons, can indeed superconduct [5].

A number of studies suggest an effective attraction between electrons in the model. For example, two holes are found to be bound in some range of the on-site repulsion $U$ near half-filling from numerical calculations for finite systems [5,6]. Quantum Monte Carlo (QMC) results show that the pairing susceptibility is greater than the susceptibility calculated without the interaction vertex between quasi-particles near half-filling [6], indicating that the quasi-particles interact attractively.

However, it is not known whether these attractive interactions do indeed imply a superconducting off-diagonal long-range order (ODLRO). We can argue against the ODLRO by referring to the fact that the susceptibility itself for finite $U$ is suppressed from that for $U = 0$ [6]. In addition, the susceptibility diverges at most logarithmically with decreasing temperature $T$, which is exactly the $T$-dependence for the non-interacting case (inset of Fig. 3(a)). On top of these, the projector Monte Carlo (PMC) calculation for the ground state [6] does not show any sign of a growth with the system size in the equal-time superconducting correlation, indicating the absence of such an order at least for $U \leq 4t$, where $t$ is the hopping integral between nearest-neighbor sites.

Nevertheless, we can still raise two possibilities that the Hubbard model can indeed exhibit superconductivity that has eluded detection so far. One possibility is related to the view that the pairing should be composed of ‘quasi-particles’ rather than bare particles. Although this is the point proposed by White et al. [6], they have in fact calculated the conventional BCS pairing correlation $\langle \tilde{c}_{i\uparrow} \tilde{c}_{i\downarrow} c_{j\uparrow}' c_{j\downarrow}' \rangle$ with $\tilde{c}_{i\sigma}$ the spin-$\sigma$ electron creation operator at site $i$ by assuming implicitly that the bare electrons injected to the system will promptly turn into appropriately ‘dressed’ ones. However, as stressed recently by one of the present authors [9], the dressing may not take place so quickly and completely in a microscopically small system as usually encountered in numerical calculations. In such a situation, we should dress the electrons ‘by hand’ from the outset to detect superconductivity.

The other, more exotic, possibility is that correlated systems such as the Hubbard model may possess, in the thermodynamic limit, a new type of ODLRO that cannot be detected by $\langle \tilde{c}_{i\uparrow} \tilde{c}_{i\downarrow} c_{j\uparrow}' c_{j\downarrow}' \rangle$. In this case, we should characterize the condensate in terms of a certain operator $\tilde{O}$ distinct from $\tilde{c}_{i\uparrow} \tilde{c}_{i\downarrow}$ with an ODLRO in the sense that $\langle \tilde{O} \rangle \neq 0$ breaks the gauge symmetry.

In either possibility, a search for the pertinent correlation function deserves investigation. We propose in the present Letter to look at $\langle \tilde{c}_{i\uparrow} \tilde{c}_{i\downarrow} c_{j\uparrow}' c_{j\downarrow}' \rangle$ as a candidate with $\tilde{c}_{i\sigma} \equiv c_{i\sigma} (1 - n_{i\sigma})$ and $n_{i\sigma} \equiv c_{i\sigma}^\dagger c_{i\sigma}$. In the strong-coupling limit, the Hubbard model can be reduced into the $t$-$J$ model in which the electrons move with excluded double occupancies as represented explicitly by the operator $\tilde{c}_{i\sigma}$. Thus, in this limit, the conventional pairing correlation automatically turns precisely into $\langle \tilde{c}_{i\uparrow} \tilde{c}_{i\downarrow} c_{j\uparrow}' c_{j\downarrow}' \rangle$ [3]. Our proposal amounts that even for the Hubbard model with a moderate $U$, this can be a proper quantity, for which we have implemented QMC to obtain the correlation functions for the ‘correlated pairing’. The results indeed turn out to exhibit an evidence for superconductivity in the 2D single-band Hubbard model.

The Hamiltonian $\mathcal{H}$ for the model is written as

$$\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} \langle c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} \rangle + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (1)$$

Through a large-scale QMC study, we have evaluated both the equal-time correlated pairing correlation in real
As for the pairing symmetries we consider $d$ as a function of $\beta \lesssim \sim$ the total sign to the total number of samples degrades to $T$ and/or decreased liable results for large interactions, we have increased the negative-sign problem prevents us from obtaining re-
INAL algorithm used by several authors to investigate state pairing correlation. We have adopted the stabi-
fty with each temperature. For $\beta$ is kept to 0.74 by adjusting the chemical potential for $\times$ is performed for an 8 lattice, where the band filling $\beta$ increases with $\sqrt{|U|}$ when we increase the repulsion to $U$ when we increase the repulsion to $U$.

The logarithmic behavior is similar to that for the con-
INAL susceptibility of the single-band Hubbard
showing much weaker dependence on either $\beta$ or $U$ (Fig. 2(a)). There the $\beta$ dependence is so small that we cannot even decide whether it is linear or logarithmic within the error bars. If we increase the band filling to the
DE of the QMC algorithm are the follow-
ing. We have used both the finite-temperature and the
CERAL algorithm used by several authors to investigate ground-state PMC formalisms. In both cases, we have
EMPLOYED the discrete Hubbard-Stratonovich transformation introduced by Hirsch. In the Trotter decomposi-
tion, the imaginary time increment [\Delta \tau = \tau/\text{number of Trotter slices}] is taken to be either $\lesssim 0.03$ for finite-
temperature susceptibilities or $\lesssim 0.03$ in the ground-
state pairing correlation. We have adopted the stabil-
ization algorithm used by several authors to investigate ground-state and low-temperature properties. Since
THE negative-sign problem prevents us from obtaining re-
iable results for large interactions, we have increased $\beta$ and/or decreased $T$ up to the point where the ratio of the total sign to the total number of samples degrades to $\sim 0.3$.

We first show the results for the finite-temperature $d$-
wave pairing susceptibility, $\bar{S}_d$, in Fig. 1(a). Calculation is performed for an $8 \times 8$ lattice, where the band filling $n$ is kept to 0.74 by adjusting the chemical potential for each temperature. For $U = 0$ and $U = 1$ (in units where $t = 1$), $\bar{S}_d$ increases only logarithmically with $\beta=1/T$. The logarithmic behavior is similar to that for the con-
ventional susceptibility $S_d$ shown in the inset. However, when we increase the repulsion to $U = 3$, $\bar{S}_d$ starts to increase more rapidly and can no longer be fitted to a logarithmic form within the error bars. Strikingly, the behavior fits rather well to a linear $(1/T)$ dependence for $\beta \geq 5$. The $1/T$ behavior is indicative of a long-range order, as exemplified by the $1/T$ divergence of the staggered magnetic susceptibility of the single-band Hubbard model at half-filling $\frac{1}{4}$. By contrast, $\bar{S}_d$ in Fig. 1(b) is strongly suppressed when $U$ is switched on, and barely increases with $\beta$.

When the band filling is decreased to $n \sim 0.6$, $\bar{S}_d$ shows much weaker dependence on either $\beta$ or $U$ (Fig. 2(a)). There the $\beta$ dependence is so small that we cannot even decide whether it is linear or logarithmic within the error bars. If we increase the band filling to the
HALF-filling ($n = 1$), on the other hand, $\bar{S}_d$ is suppressed when $U$ is switched on, where the susceptibility seems to assume a logarithmic $\beta$-dependence as indicated in Fig. 2(b). These results suggest that the strong divergence of $\bar{S}_d$ with $\beta$ occurs only in a limited region of $n$ near half-filling.

Now we turn to the equal-time pairing correlation, $\bar{P}_d(i, j)$ (Eq. 3), in the ground state. We represent its real-space behavior by the quantity $\bar{P}_d(R)$, defined by the sum of $\bar{P}_d(r, r + \Delta r)$ on a square at a distance $|\Delta r_s| = R$ or $|\Delta r_y| = R$. This sum is intended to reduce statis-
tical errors. In Fig. 3, we show the ratio of $\bar{P}_d(R)$ for $U = 3$ to that for $U = 0$ for both $d_{x^2-y^2}$ and extended $s$ channels for a $10 \times 10$ system with $n = 0.82$. For the $d$-
wave ($\bar{P}_d(R)$), the pairing correlation at large distances is indeed enhanced by $U$, while the correlation is strongly suppressed for the extended $s$. There we should note that the results at $R = \text{half} = \text{sample size}$ suffer from an effect of periodic boundary condition.

An increase of the correlation function with $U$ does not necessarily signify the occurrence of ODLRO as stressed by various authors. An appropriate quantity for this purpose is the $k = 0$ Fourier component, i.e., $\sum_R \bar{P}_d(0, j) = \sum_R \bar{P}_d(0, j)$ of the real-space correlation, and its system-size dependence in particular. This quantity should grow with the system size when a long-range order sets in.

The QMC calculation is done for this quantity in two different sizes: a $10 \times 10$ lattice with 74 electrons ($n = 0.740$), and a $14 \times 14$ lattice with 146 electrons ($n = 0.745$). The choice of these sizes is made due partly to the fact that the band fillings are almost the same, but we also have paid special attention to the fillings satisfying the closed-shell condition, i.e., band fillings for which the non-interacting Fermi sea is non-degenerate. The pairing correlation at open-shell fillings is inherently smaller, so that a mixture of results for close- and open-shell fillings would obscure the conclusion. The closed-shell condition also reduces greatly the difficulty arising from the negative-sign problem in the PMC calculation. The above two fillings are the closest closed-shell ones within the system sizes tractable in the QMC. Even for such close fillings, $\bar{P}_d(R)$ at very short distances ($R = 0$ or 1) has a considerable filling dependence due primarily to the filling dependence of density (diagonal) correlations contained inherently in the pair-
ing correlation. In order to focus on the longer-range (off-diagonal) part, we have evaluated $\bar{P}_d$ by the sum of $\bar{P}_d(R)$ for $R \geq 2$. The values for $\bar{P}_d$'s thus obtained for the two system sizes almost coincide (with the difference being less than 0.0008) for $U = 0$. The same is true as long as $U$ is smaller than 1.5.

When $U$ is further increased, the long-range part of the correlation grows with $U$, where $\bar{P}_d$ does concomitantly start to increase with the sample size as seen in Fig. 4.
To be more precise, the amount of this increase exceeds the error bar for $U$ larger than about 2. Although there still remains, to be rigorous, a possibility that this size-dependence contains an effect of the slight discrepancy in the filling, the result for the correlation may be taken as an indication toward the ODLRO, which reinforces the conclusion drawn from the $T$-dependence of the susceptibility.

We expect that the long-range behavior of $\tilde{P}_d$ and $\tilde{S}_d$ continues to grow for larger $U$, in which the present correlated pairing correlation will eventually tend to the conventional one. We can then envisage a consistent picture that encompasses a recent result \cite{14} for the Mott-Hubbard regime of Emery’s three-band Hubbard model \cite{15}, where an indication of a long-range order in the conventional $d$-wave pairing is detected for $U_d$ comparable to the one-electron (anti-bonding $d$-$p$) bandwidth.

As for the nature of superconductivity for moderate $U$, further investigation is necessary in the following two respects. First, we cannot at the present stage decide whether the correlated pairing either represents just a de-vice for detection of superconductivity in small systems or indicates a new ODLRO. Second, extensive studies for the $t$-$J$ model in 1D \cite{13} and 2D \cite{14} suggest that superconductivity appears for a large enough superexchange interaction $J/t$ with apparently the same form of pairing as ours. However, these studies focus on a parameter region distinct from the present study. Remember that if the $t$-$J$ model is regarded as an effective Hamiltonian for the Hubbard model for $U \to \infty$, we end up with a perturbatively small $J/t$. Thus whether the mechanism for superconductivity in the $t$-$J$ model with a large $J/t$ is similar to the present case remains to be another future problem.

In summary, we have shown from the results of the pairing susceptibility and the correlation function obtained in the QMC method that the ‘correlated pairing’ with a $d_{x^2-y^2}$ symmetry can become long-ranged in the 2D Hubbard model with moderate $U$ near half-filling.

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\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{(a) The correlated $d$-wave pairing susceptibility, $\tilde{S}_d$, for a fixed band filling $n \simeq 0.74$ is plotted against $\beta(=1/T)$ for $U = 3 (\bigcirc)$ or $U = 1 (\triangle)$, while the solid curve represents the non-interacting case. The dashed curve is a logarithmic least-squares fit for $U = 3$ (for $4 \leq \beta \leq 6$), the dash-dotted line a linear fit for $U = 3$ (for $5 \leq \beta \leq 10$), and the dotted curve a logarithmic fit for $U = 1$ (for $4 \leq \beta \leq 10$). The inset depicts the conventional $d$-wave pairing susceptibility, $S_d$, for comparison, where $\bigcirc$ represents the result for $U = 3$ with a logarithmic fit for $4 \leq \beta \leq 10$, while the solid curve indicates the non-interacting case. (b) The correlated extended $s$-wave pairing susceptibility, $\tilde{S}_s$, for $U = 3 (\bigcirc)$ with a logarithmic fit for $4 \leq \beta \leq 10$ (dashed line), or for $U = 0$ (solid line).}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig2.png}
\caption{(a) $\tilde{S}_d$ as a function of $\beta$ for a fixed $n \simeq 0.6$ with $U = 3 (\bigcirc)$ and the non-interacting case (solid curve). (b) A similar plot for $n = 1$, where the dashed curve is a logarithmic fit for $U = 3$.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig3.png}
\caption{The ratio of the correlation function $\tilde{P}_d(R)$ for $U = 3$ to that for $U = 0$ is plotted against $R$ for the $d$ (\bigcirc) or extended-$s$ (\triangle) pairing. The system size is $10 \times 10$ with 82 electrons ($n = 0.82$).}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig4.png}
\caption{$\tilde{P}_d$ is plotted against $U$. Number of electrons and system size are 146 electrons/14 $\times$ 14 (\bigcirc), $n = 0.745$ and 74 electrons/10 $\times$ 10 (\bigcirc, $n = 0.740$).}
\end{figure}