From $d$- to $p$-wave pairing in the $t$-$t'$ Hubbard model at zero temperature

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We develop a DCA(PQMC) algorithm which employs the projective quantum Monte Carlo (PQMC) method for solving the equations of the dynamical cluster approximation (DCA) at zero temperature, and apply it for studying pair susceptibilities of the two-dimensional Hubbard-model with next-nearest neighbor hopping. In particular, we identify which pairing symmetry is dominant in the $U$-$n$ parameter space ($U$: repulsive Coulomb interaction; $n$: electron density). We find that $p_{x+y}^\prime$ $(d_{x^2−y^2})$ wave is dominant among triplet (singlet) pairings at least for $0.3 < n < 0.8$ and $U \leq 4t$. The crossover between $d_{x^2−y^2}$-wave and $p_{x+y}$-wave occurs around $n \sim 0.4$.

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I. INTRODUCTION

Since the discovery of high-temperature superconductivity, the pursuit of identifying the microscopic mechanism for unconventional superconductivity such as $d$-wave in cuprates or $p$-wave in ruthenates has been a main driving force in condensed matter physics. Even now, 19 years after the discovery of high-temperature superconductivity, it is an issue of hot debate whether the one-band (two-dimensional) Hubbard model, the simplest model for electronic correlations, is becoming $d$-wave or $p$-wave superconducting at low temperatures.

There are indications that there is indeed $d_{x^2−y^2}$-wave superconductivity close to half-filling. For example, the functional renormalization group (fRG) predicts superconductivity for weak coupling. Also numerical quantum Monte Carlo (QMC) simulations for finite size systems observe an enhancement of the $d_{x^2−y^2}$-wave pairing. A promising method for addressing these questions is the dynamical cluster approximation (DCA), an extension of dynamical mean field theory (DMFT) which also takes non-local correlations and wave-vector dependences into account. This is essential for describing $p$- and $d$-wave superconductivity; DMFT itself only allows for $s$-wave superconductivity by construction. Such DCA calculations find $d_{x^2−y^2}$-wave superconductivity. However, when solving the DCA equations numerically by conventional Hirsch-Fye QMC simulations, one is restricted to rather high temperatures $T < t$. Hence, a difficult extrapolation to low $T$ is necessary which is further hampered since (numerically) exact statements also require an extrapolation cluster size $N_c \to \infty$.

Our paper will focus on a different parameter regime: Motivated by Sr$_2$RuO$_4$, many authors have recently addressed the possibility of triplet superconductivity in the two-dimensional one-band Hubbard model with finite next-nearest neighbor hopping $t'$ (the $t$-$t'$ Hubbard model) at intermediate electron densities. The results have been controversial as regards the dominant pairing symmetry: fRG calculations concludes that when $t' > 0.3t−0.4t$ and the Fermi level is at the van Hove (vH) singularity, the system becomes ferromagnetic at sufficiently low $T$. While a $d$-wave phase spreads next to the ferromagnetic phase in the $U$-$t'$ diagram for vH band fillings, the $p$-wave phase exists when going away from the vH band filling and for sufficiently large $t'$. Third-order perturbation theory showed that triplet superconductivity is realized even when ferromagnetic spin fluctuation are not dominant. On the other hand, QMC, FLEX and DCA calculations concluded that triplet pairing does not become dominant for intermediate filling even when $t'$ is as large as 0.4$t$.

It should be noted that fRG, third-order perturbation theory and the FLEX approximation are valid only for weak coupling; finite-size QMC is possible only for $U < 2t$ because of a serious negative sign problem and the DCA has been performed only for high $T$s. Thus, the question concerning $p$-wave (triplet) superconductivity in the Hubbard model is not conclusive yet.

In this paper, we introduce a new route to address this question, solving the DCA equations by an extended version of the projective QMC (PQMC) method. This DCA(PQMC) approach mitigates the $T$-extrapolation problem of DCA(QMC). We concentrate on the crossover between $d$- and $p$-wave instability in the intermediate electron density range $0.3 \lesssim n \lesssim 0.8$ and present results for the paramagnetic spectral function and the dominant pairing symmetry for $U \lesssim 4t$ and $t' = 0.4t$. On an equal footing with these pair susceptibilities, we also calculate the ferromagnetic and antiferromagnetic spin susceptibility of the DCA cluster.

II. $t$-$t'$ HUBBARD MODEL

The $t$-$t'$ Hubbard model reads

$$H = -t \sum_{i,j,\sigma} c_{i\sigma}^\dagger c_{j\sigma} + t' \sum_{i,j,\sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (1)$$

Here, $c_{i\sigma}^\dagger$ and $c_{i\sigma}$ create and annihilate an electron with spin $\sigma$ on site $i$ of the two-dimensional lattice; the first and second sum are restricted to nearest neighbors (NN) and next-nearest neighbors (NNN), respectively. In the
following, all energies are given in units of $t$, corresponding to a bandwidth of $D = 8(t)$.

### III. DCA(PQMC) METHOD

In the DCA[5] the Brillouin zone is divided into $N_c$ patches, with a coarse-grained Green function $\tilde{G}(k_p, \omega)$ and self energy $\Sigma_c(k_p, \omega)$ for every patch $p$:

$$
\tilde{G}(k_p, \omega) = \frac{N_c}{N} \sum_k \left[ G_0^{-1}(k_p + \frac{1}{2}) - \Sigma_c(k_p, \omega) \right]^{-1}.
$$

(2)

Here, $G_0^{-1}$ is the non-interacting Green function and the $\k$ summation averages over all $k$-points of patch $p$ which is centered around $K_p$; $N$ is the total number of all $k$-points. $\tilde{G}$ and $\Sigma_c$ then define an effective cluster of Anderson impurities which can be described by the non-interacting Green function

$$
G_0^{-1}(k_p, \omega)^{-1} = \tilde{G}(k_p, \omega)^{-1} + \Sigma_c(k_p, \omega),
$$

(3)

or its Fourier transform $G_0(\omega)X_kX_{j\tau}$. This defines a cluster problem $H_c$ given by $G_0(\omega)X_kX_{j\tau}$ and a local Coulomb interaction on every cluster site $X_{i\tau}$. In the DCA, this cluster problem has to be solved self-consistently together with Eq. (2).

Here, we introduce a new cluster solver which is based on PQMC[15] and particularly constructed for zero temperature. Just as in Ref. 15, $T = 0$ expectation values of an arbitrary operator $\mathcal{O}$ are calculated as:

$$
\langle \mathcal{O} \rangle_0 = \lim_{\beta \to \infty} \lim_{\theta \to 0} \frac{\text{Tr} \left[ e^{-\beta H_T} e^{-\theta H_c/2} \mathcal{O} e^{-\theta H_c/2} \right]}{\text{Tr} \left[ e^{-\beta H_T} e^{-\theta H_c} \right]}.
$$

(4)

where $H_T$ is an auxiliary Hamiltonian for which we take the cluster defined by $G_0(\omega)X_kX_{j\tau}$ without Coulomb interaction ($U=0$). The local one-particle potential of $H_T$ is adjusted self-consistently to yield the same $n$ as the interacting cluster $H_c$. At least for $N_c = 1$, this yields the same asymptotic behavior of $G_0(\tau)$ and $\tilde{G}(\tau)$ for large $\tau$. Hence, the influence of breaking time translational symmetry at $\tau = 0$ is reduced. This gives a smoother Green function in the vicinity of $\tau = 0$, but does not affect the results after long enough projection, i.e., sufficiently away from $\tau = 0$.

As in Ref. 15, the limit $\beta \to \infty$ can be taken analytically for this $H_T$. Then, the interacting Green function $G$ is obtained via the same updating equations for the auxiliary Hubbard-Stratonovich fields as for finite-$T$ QMC. But the PQMC starting point is different: a $T = 0$ Green function with open boundary conditions defined for $0 \leq \tau, \tau' \leq \theta = 16t, 18t$, discretized into $L = 48, 64$ slices for $N_c = 4 \times 4 = 16$ cluster sites. For the measurement of physical quantities, $L = 8, 10, 12$ central time slices are taken, and the remaining $P$ time slices on the right and left side of the measuring interval are reserved for projection. Typically, we performed $10^5$ to $6 \times 10^5$ QMC sweeps. To obtain $G(\omega)$ from $G(\tau)$, the maximum entropy method (MEM) is employed, as in Ref. 15.

### IV. SPECTRAL PROPERTIES OF THE PARAMAGNETIC PHASE

Now, let us turn to the DCA(PQMC) results. We performed calculations for $n = 0.3, 0.4, 0.6, 0.8$ and $U = 2t, 3.5t, 4t$. Throughout the study, we took $t' = 0.4t$ and $N_c = 4 \times 4 = 16$ DCA patches. In the upper panel of Fig. 11 we present the one-particle spectral function $A(k_p, \omega) = -1/\pi \text{Im} G(k_p, \omega)$, i.e., the averaged spectrum over the six irreducible patches $p$ of the Brillouin zone, as indicated in the inset. Patches 2, 3, and 4 have contributions at the Fermi surface and hence a contribution at $\omega = 0$. Thereby, $A(k_3, \omega)$ has a particular sharp peak because the $vH$ singularity is located at $(\pi, 0)$ and $(0, \pi)$. This sharp peak also reflects in the fully $k$-integrated $A(\omega) = \sum_p A(k_p, \omega)$, shown in the bottom panel of Fig. 11. Let us note that the quantitative and qualitative features are very similar to those of DMFT (dashed line); there is no pseudo gap for $t' = 0.4, n = 0.8, U = 4t$ in our $T = 0$ DCA(PQMC) calculation.

### V. CALCULATION OF CLUSTER SUSCEPTIBILITIES

To discuss the magnetic and pairing instabilities, we first calculate the corresponding susceptibilities

$$
\chi^{\text{spin}}(Q, \tau_1 - \tau_2) = \sum_{X_1, X_2} \langle \mathcal{O}(X_1 - X_2) \rangle_0
$$

$$
\langle T_{\tau_1 - \tau_2} \langle c_{X_1 \uparrow}^\dagger(\tau_1) c_{X_2 \downarrow}^\dagger(\tau_1) c_{X_2 \uparrow}^\dagger(\tau_2) c_{X_1 \downarrow}(\tau_2) \rangle \rangle,
$$

(5)

$$
\chi^{\text{pair}}(\tau_1 - \tau_2) = \sum_{X_1, X_2} g(K_1)g(K_2)
$$

$$
\langle T_{\tau_1 - \tau_2} c_{K_1 \uparrow}^\dagger(\tau_1) c_{-K_1 \downarrow}^\dagger(\tau_1) c_{-K_2 \downarrow}^\dagger(\tau_2) c_{K_2 \uparrow}(\tau_2) \rangle
$$

(6)

for the $4 \times 4$ cluster at self-consistency. Here, $c_{K\sigma} = \sum_{\chi_\sigma} \chi_{K\sigma} \exp(iKX) \text{ and } g(K)$ is the form factor, i.e.,

$$
g(K) = \begin{cases} 1 & \text{for } s\text{-wave}, \\ \sqrt{2} \sin(K_x) & \text{for } p_x \text{ wave}, \\ \sqrt{2} \sin(K_x + K_y) & \text{for } p_{x+y} \text{ wave}, \\ \cos(K_x) - \cos(K_y) & \text{for } d_{x^2-y^2} \text{ wave} \end{cases}
$$

(7)

Second, we calculate $\text{Im} \chi(\omega)$ from $\chi(\tau)$ by MEM and from this obtain the static susceptibility via the Kramers-Kronig relation

$$
\chi(\omega = 0) = \int \frac{\text{Im} \chi(\omega)}{\omega} d\omega.
$$

(8)

In DCA, the susceptibilities of the Hubbard model are calculated from the above cluster $\chi$ by solving the Bethe-Salpeter equation[13]. However, to this end it would be necessary to calculate susceptibilities for two $\tau$’s instead of
Eqs. (5) and (6) which would tremendously increase the numerical effort. Hence, we look at the cluster susceptibilities Eqs. (5) and (6) for simplicity. We can expect that this quantity already captures the essential features of the competition between ferromagnetic and antiferromagnetic spin fluctuation, or that between superconductivity with different symmetries.

Let us mention one more technical point: The decay of χ in τ-space can be underestimated because of a finite number of projection time slices P. In this case, the MEM calculation of Imχ(ω) depends on up to which τc value the MEM input χ(τ) is considered, see Fig. 2. Whenever we encounter a strong cutoff (τc-dependent) like in Fig. 2 (right inset) we take a short cutoff τc (only four τ points). With such a short cutoff τc which is very close to the asymptotical behavior τc → 0, we certainly do not overestimate χ(0). However, if the weak decay of χ in τ-space is not due to the finite P but due to physics, we underestimate χ(0) this way. In Figs. 3 and 4 these more problematic data points, where we possibly underestimate χ(0), are indicated by an arrow.

VI. INSTABILITIES OF THE PARAMAGNETIC PHASE

Let us finally turn to the physical results, starting with the (inverse) ferromagnetic and antiferromagnetic susceptibilities plotted in Fig. 3 as a function of T for three exemplary parameter values; finite-T data have been obtained by conventional DCA(PQMC). First of all, let us emphasize the obvious: DCA(PQMC) directly provides well for the T = 0 susceptibilities without extrapolation-in very contrast to the finite-T DCA(QMC) for which it is difficult to forecast/extrapolate the low-T behavior. Turning to the physical results, we see that the ferromagnetic spin susceptibility becomes larger than the antiferromagnetic one for n ≤ 0.6. Note that the vH filling is at ∼ 0.6 for t' = 0.4. In fact, the fRG studies found a strong ferromagnetic instability for t' > 0.3 ∼ 0.4 at

![Image](image_url)
On the other hand, third ordered perturbation model, accord with QMC calculations for a finite-size Hubbard for far away from half-filling. These findings are also in reports also a ferromagnetic phase for those data points where $\chi > U$ (middle), and $U = 2t, n = 0.8$ (right). The arrows indicate those data points where $\chi$ is possibly underestimated ($1/\chi$ overestimated), as discussed in Fig. 2.

Next, let us discuss superconductivity. Fig. 3 shows the inverse static pair susceptibilities as a function of $T$. First of all, we find that $d_{x^2-y^2}$-wave ($p_{x+y}$-wave) is dominant among singlet (triplet) pairings for all $(U, n)$’s considered. For $n = 0.8$, $d_{x^2-y^2}$-wave dominates over triplet pairings as expected. When we reduce $n$ to 0.6, antiferromagnetic spin fluctuation become weak, see Fig. 3. Nonetheless, the $d_{x^2-y^2}$-wave instability is still larger than those for triplet pairings. This is consistent with finite-temperature DCA calculation of Ref. 8 for $U = 3t, n = 0.67$, and suggests $d_{x^2-y^2}$-wave ordering for low enough $T$ -even for far away from half-filling. These findings are also in accord with QMC calculations for a finite-size Hubbard model showing a dominant $d_{x^2-y^2}$-wave instability for $t' \sim 0.4, n \sim 0.67$, and $U = 2t$. The fRG study Ref. 12 reports also a ferromagnetic phase for $t' = 0.4, n \sim 0.6$, and $U > t$, while there is possibly a $d$-wave phase for $U < t$. On the other hand, third ordered perturbation calculations have shown that triplet superconductivity becomes dominant even for weak coupling. We find such triplet pairing only for smaller $n$’s, while the detailed structure of $k$-dependence of the vertex corrections may be essential which is possibly smeared out by the coarse-graining of DCA.

VII. DISCUSSION AND OUTLOOK

Fig. 5 summarizes our main finding, i.e., the dominant superconducting susceptibility on the cluster. We find that $d_{x^2-y^2}$-wave pairing is dominant in an unexpectedly broad range of fillings $n$, whereas $p_{x+y}$-wave prevails only for small $n$. The transition between $p_{x+y}$-wave and $d_{x^2-y^2}$-wave is at about $n \sim 0.4$.

The $t$-$t'$ Hubbard model with $t' \sim 0.4$ and $n \sim 2/3$ has been considered to be a good model for the $\gamma$-band of Sr$_2$RuO$_4$. Our DCA(PQMC) results indicate however that there is no triplet superconductivity for these $n$ and $t'$ values, at least for the moderately strong values of $U$ we studied and which are e.g. considered in local density approximation (LDA)+DMFT calculations.

Hence our results suggest that a nearest-neighbor Coulomb interaction $V$, as suggested in Ref. 2, or a multi-orbital model is necessary for an appropriate description of triplet pairing in Sr$_2$RuO$_4$. Below $T_c \sim 1$ K. In contrast to the standard finite-$T$ DCA(QMC), we can expect that DCA(PQMC) will open the door to such low temperatures -even for calculations with orbital realism. Similarly, we can hope that DCA(PQMC) will allow for more definite statements concerning superconductivity in the two-dimensional Hubbard model in the future. To this end, still a $N_c \rightarrow \infty$ extrapolation and the calculation of lattice susceptibilities is necessary. But at least the problematic extrapolation to low temperatures is mitigated.

FIG. 3: (Color online) Inverse magnetic susceptibilities as a function of $T$ for $U = 2t, n = 0.3$ (left), $U = 4t, n = 0.6$ (middle), and $U = 2t, n = 0.8$ (right). The arrows indicate those data points where $\chi$ is possibly underestimated ($1/\chi$ overestimated), as discussed in Fig. 2.

FIG. 4: (Color online) Same as Fig. 3 but now for $p_x$, $p_{x+y}$, and $d_{x^2-y^2}$-wave pairing as indicated in the right panel.

FIG. 5: (Color online) $U$-$n$ diagram showing the dominant pairing symmetry; for $n = 0.4$, $U = 2t$ it is too close to call which instability is strongest.
PQMC is the direct route to $T=0$.

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