**$d$-wave superconductivity in the presence of a near neighbor Coulomb repulsion**

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Dynamic cluster quantum Monte Carlo calculations for a doped two-dimensional extended Hubbard model are used to study the stability and dynamics of $d$-wave pairing when a near neighbor Coulomb repulsion $V$ is present in addition to the on-site Coulomb repulsion $U$. We find that $d$-wave pairing and the superconducting transition temperature $T_c$ are only weakly suppressed as long as $V$ does not exceed $U/2$. This stability is traced to the strongly retarded nature of pairing that allows the $d$-wave pairs to minimize the repulsive effect of $V$. When $V$ approaches $U/2$, large momentum charge fluctuations are found to become important and to give rise to a more rapid suppression of $d$-wave pairing and $T_c$ than for smaller $V$.

In conventional superconductors, the retardation of the electron-phonon pairing interaction is essential to overcome the Coulomb repulsion between electrons and to give a net attractive interaction [1]. In strongly correlated superconductors, such as the cuprates, heavy fermion or iron-based materials, in contrast, it is a sign change in the pair wave function that allows the Cooper pairs to minimize the repulsive effect of the strong local Coulomb repulsion $U$ [2]. For example, the $d_{x^2−y^2}$-wave pair state in the cuprates completely avoids the local Coulomb repulsion because of the sign change under 90 degree rotation and the related lack of a local amplitude.

However, in realistic systems, the Coulomb repulsion is hardly screened to a completely local interaction, but has a short-ranged non-local contribution. For the cuprates, Sénéchal et al. [3] and Reymbaut et al. [4] estimated a near neighbor Coulomb repulsion of $\sim 400$ meV. If the Cooper pairs are made up of electrons sitting on neighboring sites, such as in the $d_{x^2−y^2}$-wave state, this non-local repulsion is expected to have detrimental effects on the pairing. This raises the important question of how much the superconducting transition temperature $T_c$ will be reduced by a non-local Coulomb repulsion and whether retardation effects, similar to the case of electron-phonon mediated pairing, can play a role in stabilizing superconductivity in the presence of a non-local repulsion.

Here we examine these questions in a 2D extended Hubbard model. Its Hamiltonian

\[
H = -t \sum_{\langle ij \rangle, \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle\langle ij\rangle\rangle, \sigma\sigma'} n_{i\sigma} n_{j\sigma'},
\]

has the usual near neighbor hopping $t$, on-site Coulomb repulsion $U$ and an additional near neighbor Coulomb repulsion $V$. Weak coupling studies for $U \ll W$ of this model, where $W = 8$ is the bandwidth, have found that $d$-wave pairing and $T_c$ are generally suppressed by $V$, but superconductivity survives provided that $V$ is not larger than $\sim U^2/W$ [5,6]. Variational Monte Carlo calculations of the model in Eq. (1) with an additional near neighbor exchange interaction $J$ have found that the on-site $U$ effectively enhances the $d$-wave pairing interaction $J$, while suppressing the opposing effects of $V$, so that for $U = 10$, $d$-wave pairing is preserved up to $V = 4J$ [7]. Density matrix renormalization group studies of a striped $t−J−V$ model, the strong coupling $U \gg W$ limit of Eq. (1), have demonstrated that a non-local $V$ can even lead to an enhancement of superconducting pair-field correlations by inducing transverse stripe fluctuations [8]. In recent work using cellular dynamical mean field theory (CDMFT), Sénéchal et al. found that $d$-wave pairing at zero temperature is preserved at strong coupling even for $V \gg J$ as long as $V \lesssim U/2$ [3]. An extension of this work to finite temperatures found that at weak doping a finite $V$ can even lead to an increase in $T_c$, while at large doping $V$ reduces $T_c$ [4]. Based on a detailed analysis of the frequency dependence of the gap function, the authors argued that $V$ gives rise to a low frequency pairing contribution through an increase in the effective exchange interaction $J = 4t^2/(U−V)$, while at high frequencies, $V$ suppresses pairing. These studies thus concluded that retardation plays an important role.

Here we use a similar cluster dynamical mean field treatment to examine the $V$-dependence of $T_c$ and the dynamics of the pairing interaction in this model. While the previous CDMFT calculations were carried out inside the $d$-wave superconducting phase of model (1), our work directly examines the dynamics of the pairing interaction in the normal state, and thus provides new and complementary insight. In particular, we use the dynamical cluster approximation (DCA) [9,10] with a continuous time auxiliary field (CT-AUX) quantum Monte Carlo (QMC) cluster solver [11] to perform numerical calculations of the model in Eq. (1).

The DCA maps the bulk lattice problem onto a finite
size cluster of size $N_c$ and uses coarse-graining to retain the remaining degrees of freedom as a mean-field that is coupled to the cluster degrees of freedom \[9, 10\]. The intra-cluster contribution of the interaction $V$ is treated exactly with QMC, while the inter-cluster terms may be treated with an additional bosonic dynamic mean-field \[12, 13\] similar to the extended dynamical mean-field theory \[14\]. Here, instead, we use a Hartree approximation \[3\], which reduces to a shift in the chemical potential in the absence of charge order \[3\]. Due to the neglect of dynamic inter-cluster effects of the interaction $V$, we do not coarse-grain $V$ despite its non-locality.

For the small $2 \times 2$ cluster we use, the sign problem of the underlying CT-AUX QMC solver \[11, 15\] is manageable up to $V \sim U/2$ down to temperatures $T \sim T_c$. While the results obtained from this $2 \times 2$ cluster should be regarded as mean-field results for the $d$-wave $T_c$, the pairing dynamics is expected to be well described since temporal fluctuations are fully retained through the inclusion of the dynamic mean field. Larger clusters were recently considered in a DCA study of the half-filled model, which does not have a sign problem \[10\]. We use $t = 1$ as the unit of energy and set $U = 7$. All results are for a filling $\langle n \rangle = 0.9$.

In order to calculate $T_c$, we solve the Bethe-Salpeter equation (BSE) in the normal state \[17\]

$$-\frac{T}{N_c} \sum_{\mathbf{k}, \omega_n} \Gamma_{\mathbf{k}, \omega_n}(\mathbf{K}, \omega_n, \mathbf{K}', \omega_{n'}) \phi_{\mathbf{k}}^{\mathbf{k}'}(\mathbf{K}, \omega_n) = \lambda_\alpha(T) \phi_{\mathbf{k}}(\mathbf{K}, \omega_n).$$

(2)

Here $\Gamma\mathbf{pp}(\mathbf{K}, \omega_n, \mathbf{K}', \omega_{n'})$ is the irreducible particle-particle vertex of the effective cluster problem with the cluster momenta $\mathbf{K}$ and Matsubara frequencies $\omega_n = (2n + 1)\pi T$. The coarse-grained bare particle-particle susceptibility

$$\chi\mathbf{pp}(\mathbf{K}, \omega_n) = \frac{N_c}{N} \sum_{\mathbf{k}'} G\mathbf{pp}(\mathbf{k} + \mathbf{k}', \omega_n) G\mathbf{pp}(-\mathbf{K} - \mathbf{k}', -\omega_n)$$

(3)

is calculated from the single-particle Green’s function $G\mathbf{k}(\omega_n) = [i\omega_n + \mu - \varepsilon_k - \Sigma(\mathbf{k}, \omega_n)]^{-1}$ with $\mu$ the chemical potential, $\varepsilon_k = -2t(\cos k_x + \cos k_y)$ the dispersion and $\Sigma\mathbf{k}(\omega_n)$ the cluster self-energy. Information about the bulk lattice is retained through the $\mathbf{k}'$ sum \[15\], which runs over the $N/N_c$ momenta within a square patch with $k_{x/y} \in [-\pi/2, \pi/2]$. At $T = T_c$ the leading eigenvalue of Eq. (2) becomes 1 and the symmetry of the superconducting state is given by the momentum and frequency dependence of $\phi\mathbf{k}(\omega_n)$. For all values of $V$ we consider, we find that the eigenvector corresponding to the leading eigenvalue $\lambda_d$ has $d_{x^2-y^2}$-wave $\cos K_x - \cos K_y$ structure.

Fig. 1(a) shows the temperature dependence of the leading $d$-wave eigenvalue $\lambda_d(T)$ of the BSE \[2\] for different magnitudes of the nearest-neighbor repulsion $V$. As expected, finite $V$ leads to a reduction of $\lambda_d(T)$ showing that $d$-wave pairing is weakened in the presence of a nearest-neighbor repulsion.

From $\lambda_d(T_c) = 1$ we can extract the $V$-dependence of $T_c$. For $V = 3$, where the QMC sign problem inhibits calculations down to $T_c$, we use a polynomial fit of $\lambda_d(T)$ to extract $T_c$ from extrapolating to $\lambda_d(T_c) = 1$. As one sees from Fig. 1(b), the $d$-wave $T_c$ is almost unchanged for $V = 1$ and only slightly reduced by about 15% for $V = 2$. The reduction becomes stronger for $V = 3$ when $V$ approaches $U/2$. This robustness of the $d$-wave pairing against a finite nearest-neighbor repulsion is consistent with previous studies \[3, 5\].

In order to understand this resilience of $d$-wave pairing with respect to the nearest neighbor Coulomb repulsion, we examine the dynamics of the pairing interaction $\Gamma\mathbf{pp}(\mathbf{k}, \omega_n, \mathbf{k}', \omega_{n'})$ and the leading $d$-wave eigenvector $\phi_d\mathbf{k}(\omega_n)$. Fig. 2 shows a plot of the frequency
dependence of the d-wave projected pairing interaction
\[ \Gamma_d(\omega_m = \omega_n - \omega_n') = \sum_{\mathbf{K},\mathbf{K}'} g_d(\mathbf{K}) \Gamma^{pp}(\mathbf{K}, i\omega_n, \mathbf{K}', i\omega_n') g_d(\mathbf{K}') \]
(4)

Here \( g_d(\mathbf{K}) = \cos K_x - \cos K_y \) and we have set \( \omega_n' = \pi T \) and \( T = 0.1 \). For \( V = 0 \), \( \Gamma_d(\omega_m) \) is negative (attractive) for all frequencies and falls to zero at large \( \omega_n \). For finite \( V \), \( \Gamma_d(\omega_m) \) remains attractive at low frequencies, but then turns positive (repulsive) at higher frequencies. This reflects the fact that at high frequencies \( \Gamma^{pp}(\mathbf{K}, i\omega_n, \mathbf{K}', i\omega_n') \sim V(\mathbf{K} - \mathbf{K}') \), where \( V(\mathbf{Q}) \) is the Fourier-transform of the nearest neighbor interaction \( V \). For the 2x2 cluster we have used here, one obtains \( \sum_{\mathbf{K},\mathbf{K}'} g_d(\mathbf{K}) V(\mathbf{K} - \mathbf{K}') g_d(\mathbf{K}') / \sum_{\mathbf{K}} g_d^2(\mathbf{K}) = 4V \) consistent with the results in Fig. 2. The dynamics of \( \Gamma_d(\omega_m) \) is reminiscent of the dynamics of the conventional electron-phonon pairing interaction \([19]\), which is attractive at low frequencies due to the effective electron-phonon attraction, and repulsive at high frequencies due to the Coulomb repulsion. One also sees that \( \Gamma_d(\omega_m) \) becomes less attractive at low frequencies with increasing \( V \). This reduction even exceeds the frequency independent 4V repulsive contribution, indicating that there is another repulsive and dynamic contribution that further weakens the d-wave pairing interaction. We come back to this point later when we examine the spin and charge susceptibilities.

The dynamics of the pairing interaction is reflected in the frequency dependence of the d-wave eigenvector \( \phi_d(\mathbf{K}, \omega_n) \). This quantity is plotted in Fig. 3 for \( \mathbf{K} = \pi,0 \) and \( T = 0.1 \) for different values of \( V \). For \( V = 0 \), \( \phi_d(\pi,0,\omega_n) \) falls to zero on a characteristic frequency scale. As previously found in Refs. \([17][20]\], this scale is determined by the spin \( S = 1 \) particle-hole continuum which for large \( U \) is several times \( J = 4t^2/U \). For finite \( V \), the eigenvector changes sign and becomes negative at higher frequencies. This sign change mirrors the sign change in \( \Gamma_d(\omega_n) \). Just as \( \phi_d(\mathbf{K}, \omega_n) \) changes sign in K-space reflecting the repulsive nature of the pairing interaction at large momentum transfer \([2][17]\), \( \phi_d(\mathbf{K}, \omega_n) \) also changes sign in frequency to adapt to the repulsive tail of the pairing interaction due to the Coulomb \( V \) at high frequencies. Thus, just as in the electron-phonon case, retardation is important in preserving the attractive nature of the pairing interaction in the presence of \( V \).

We have also calculated the cluster dynamic spin \( (s) \) and charge \( (c) \) susceptibilities
\[
\chi_{s/c}(\mathbf{Q}, \omega_m) = \frac{1}{N_c} \sum_{ij} e^{i\mathbf{Q}(\mathbf{R}_i - \mathbf{R}_j)} e^{-i\omega_m \tau} \int_0^\beta d\tau [n_{i\uparrow}(\tau) \mp n_{i\downarrow}(\tau)] [n_{j\uparrow}(0) \mp n_{j\downarrow}(0)].
\]
(5)

Here \( \omega_m = 2m\pi T \) are the bosonic Matsubara frequencies. The frequency dependence of the spin- and charge-susceptibilities is shown in Figs. 4(a) and (b) for \( \mathbf{Q} = (\pi,\pi) \). As \( V \) increases, \( \chi_s(\mathbf{Q}, \omega_m) \) decreases at low frequencies, while \( \chi_c(\mathbf{Q}, \omega_m) \) increases. The rise in the charge susceptibility reflects the increasing tendency of the system to form a \( (\pi, \pi) \) charge density wave ordered state \([5]\).

The \( V \)-dependence of the spin susceptibility is more difficult to understand. Based on a strong-coupling picture, Reymundt et al. \([4]\) have argued that a finite \( V \) increases the exchange coupling \( J = 4t^2/(U - V) \) and thus the magnetic pairing mechanism. Our results for \( \chi_s((\pi, \pi), \omega_m) \), however, are not in line with this picture, since one would would expect \( \chi_s((\pi, \pi), \omega_m = 0) \) to increase with \( J \) and thus \( V \). Rather, the decrease we observe can be understood from the increase in the charge fluctuations. As shown in Fig. 4(c), these
give rise to a decrease in the local magnetic moment
\[ \mu_i = \sqrt{\langle (n_{i\uparrow} - n_{i\downarrow})^2 \rangle} \]
for \( T = 0.1 \) as a function of \( V \). With increasing \( V \),
charge fluctuations become stronger while spin fluctuations are weakened through a reduction of the local magnetic moment.

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