d-wave superconductivity in the presence of nearest-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 nearest-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.

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I. INTRODUCTION

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 [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° 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 nonlocal contribution. For the cuprates, Sénéchal *et al.* [3] and Reymbaut *et al.* [4] estimated a nearest-neighbor Coulomb repulsion of ∼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 nonlocal 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 nonlocal 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 nonlocal repulsion.

Here we examine these questions in a two-dimensional extended Hubbard model. Its Hamiltonian,

$$H = -t \sum_{\langle ij\rangle,\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle ij\rangle,\sigma\sigma'} n_{i\sigma} n_{j\sigma'} \quad (1)$$

has the usual nearest-neighbor hopping t, on-site Coulomb repulsion U, and an additional nearest-neighbor Coulomb repulsion V. The question of whether the standard Hubbard model for $V = 0$ has a superconducting ground state or not remains open, and various numerical techniques have been used to address this question. Whereas quantum cluster approximations [5,6] generally find a superconducting instability at finite temperatures [5,7–9], other techniques, such as density-matrix renormalization-group [10] or determinantal quantum Monte Carlo [11] find inhomogeneous states with striped charge and/or magnetic order (for recent results see Refs. [12,13] and references therein).

Nevertheless, various studies have explored the effect of a finite V interaction on a possible superconducting instability. Weak-coupling studies [14,15] for $U \ll W$ of the model in Eq. (1), 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 $\sim U^2/W$. Variational Monte Carlo calculations with an additional nearest-neighbor exchange interaction J have found [16] 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 $V = 4J$. 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 nonlocal V can even lead to an enhancement of superconducting pair-field correlations by inducing transverse stripe fluctuations [17]. In a recent work using cellular dynamical mean-field theory (CDMFT) [3], Sénéchal *et al.* found that d-wave pairing at zero temperature is preserved at strong coupling even for $V \gg J$ as long as $V \lesssim U/2$. An extension of this paper to finite temperatures [4] found that at weak doping a finite V can even lead to an increase in T_c, whereas at large doping V reduces T_c. Based on a detailed analysis of the frequency dependence of the gap function, the authors argued that V gives rise to

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a low-frequency pairing contribution through an increase in the effective exchange interaction $J = 4t^2/(U - V)$, whereas at high frequencies, V suppresses pairing. These studies thus concluded that retardation plays an important role.

II. METHOD

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. In contrast to the previous CDMFT calculations, which were carried out inside the d-wave superconducting phase of model (1), our paper directly examines the dynamics of the pairing interaction in the normal state and thus provides different and complementary insight. In particular, we use the dynamical cluster approximation (DCA) [5,18] with a continuous-time auxiliary-field (CT-AUX) quantum Monte Carlo (QMC) cluster solver [19] 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 [5,18]. The intracluster contribution of the interaction V is treated exactly with QMC, whereas the intercluster terms may be treated with an additional bosonic dynamic mean field [8,20] similar to the extended dynamical mean-field theory [21]. Here, instead, we use a Hartree approximation [3], which reduces to a shift in the chemical potential in the absence of charge order [4]. Due to the neglect of dynamic intercluster effects of the interaction V, we do not coarse-grain V despite its nonlocality.

For the small 2×2 cluster we use, the sign problem of the underlying CT-AUX QMC solver [19,22] is manageable up to $V \sim U/2$ down to temperatures $T \sim T_c$. This cluster is too small to allow for the long-range (striped) magnetic and charge states that have been found in recent numerical calculations of the $V = 0$ model [12]. It does, however, allow us to study the effects of V on superconducting order for a large region in parameter space. We also note that the pairing dynamics, the issue of the primary focus of this paper, is expected to be well described already at the level of the 2×2 cluster 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 [23]. We use $t = 1$ as the unit of energy and set $U = 7$.

In order to calculate T_c, we solve the Bethe-Salpeter equation (BSE) in the normal state [24],

$$-\frac{T}{N_c}\sum_{\mathbf{K}',\omega_{n'}} \Gamma^{pp}(\mathbf{K},\omega_n,\mathbf{K}',\omega_{n'})\bar{\chi}_0^{pp}(\mathbf{K}',\omega_{n'})\phi_\alpha(\mathbf{K}',\omega_{n'}) = \lambda_\alpha(T)\phi_\alpha(\mathbf{K},\omega_n). \quad (2)$$

Here $\Gamma^{pp}(\mathbf{K},\omega_n,\mathbf{K}',\omega_{n'})$ 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,

$$\bar{\chi}_0^{pp}(\mathbf{K},\omega_n) = \frac{N_c}{N}\sum_{\mathbf{k}'} G(\mathbf{K}+\mathbf{k}',\omega_n)G(-\mathbf{K}-\mathbf{k}',-\omega_n) \quad (3)$$

is calculated from the single-particle Green's function $G(\mathbf{k},\omega_n) = [i\omega_n + \mu - \varepsilon_{\mathbf{k}} - \Sigma(\mathbf{K},\omega_n)]^{-1}$ with μ as the chemical potential, $\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y)$ as the dispersion, and $\Sigma(\mathbf{K},\omega_n)$ as the cluster self-energy. Information about the bulk lattice is retained through the $\mathbf{k}'$ sum [25], 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 λ_d has a $d_{x^2-y^2}$-wave $\cos K_x - \cos K_y$ structure.

III. RESULTS

Figure 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 for a filling of $\langle n\rangle = 0.9$. As expected, the 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. Panel (b) in Fig. 1 shows that similar behavior is observed for all the fillings we have studied. However, one sees that the suppression of λ_d with V becomes more rapid as the system is doped away from half-filling.

From the data in Fig. 1(a) and $\lambda_d(T_c) = 1$, one can extract the V dependence of T_c shown in Fig. 1(c) for a filling of $\langle n\rangle = 0.9$. 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(c), 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 [3,4,14].

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 $\Gamma^{pp}(\mathbf{K},\omega_n,\mathbf{K}',\omega_{n'})$ and the leading d-wave eigenvector $\phi_d(\mathbf{K},\omega_n)$. Figure 2 shows a plot of the frequency dependence of the d-wave-projected pairing interaction,

$$\Gamma_d(\omega_m = \omega_n - \omega_{n'}) = \frac{\sum_{\mathbf{K},\mathbf{K}'} g_d(\mathbf{K})\Gamma^{pp}(\mathbf{K},\omega_n,\mathbf{K}',\omega_{n'})g_d(\mathbf{K}')}{\sum_{\mathbf{K}} g_d^2(\mathbf{K})} \quad (4)$$

for $\langle n\rangle = 0.9$. 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 ω_m. 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 $\Gamma^{pp}(\mathbf{K},\omega_n,\mathbf{K}',\omega_{n'}) \sim V(\mathbf{K}-\mathbf{K}')$, where $V(\mathbf{Q})$ is the Fourier transform of the nearest-neighbor interaction V. For the 2×2 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 [26], which is attractive at low frequencies due to the effective electron-phonon attraction, and repulsive at high frequencies due to the Coulomb repulsion.

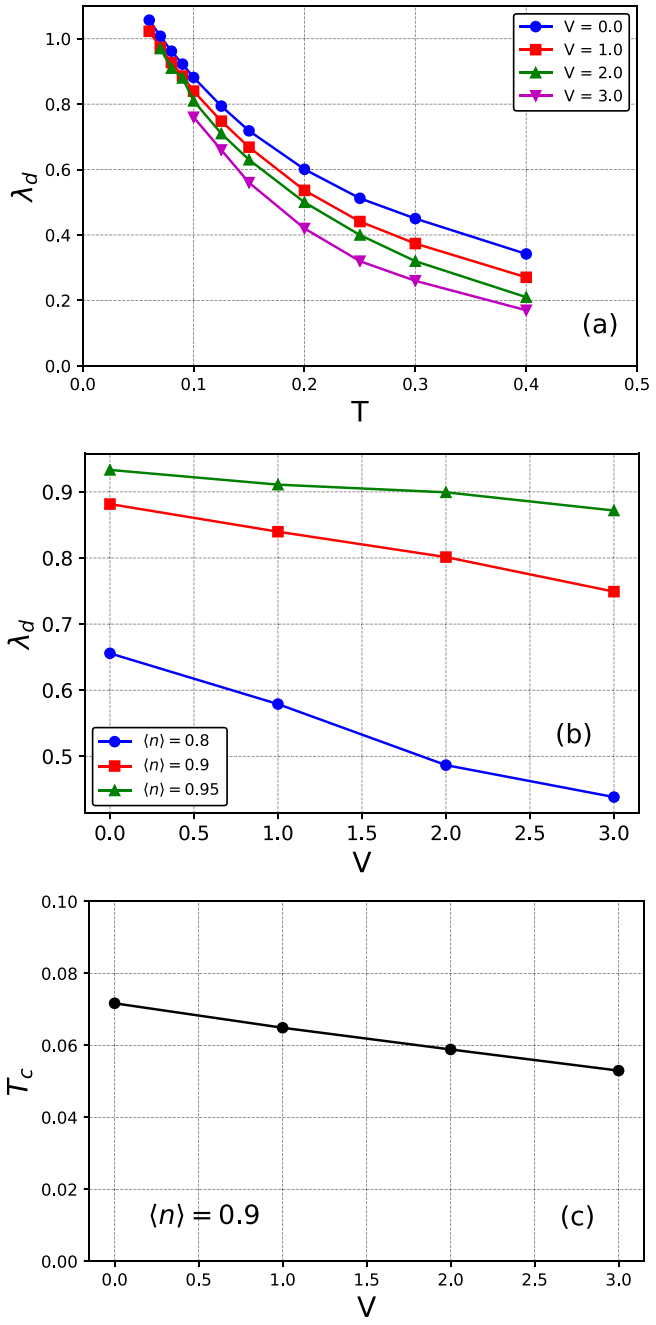

FIG. 1. (a) Temperature dependence of the leading ($d_{x^2-y^2}$-wave) eigenvalue $\lambda_d(T)$ of the Bethe-Salpeter equation in the particle-particle channel, Eq. (2) for the extended Hubbard model in Eq. (1) with $U = 7$ and $\langle n\rangle = 0.9$ for different magnitudes of the nearest-neighbor Coulomb repulsion V. (b) d-wave eigenvalue λ_d at a fixed temperature of $T = 0.1$ as a function of V for different fillings $\langle n\rangle$. (c) d-wave superconducting transition temperature T_c extracted from $\lambda_d(T_c) = 1$ as a function of V. d-wave pairing is only weakly suppressed by the interaction V as long as $V \lesssim U/2$.

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

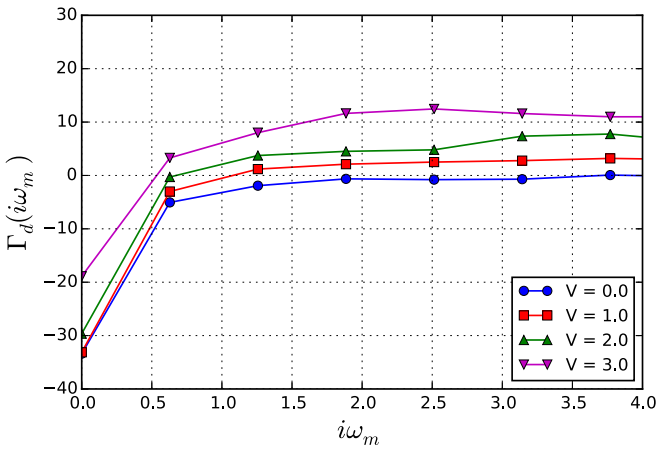

FIG. 2. The d-wave-projected irreducible particle-particle vertex $\Gamma_d(\omega_m)$ for different values of V for $\langle n\rangle = 0.9$. For finite V, Γ_d is attractive at low frequencies but then turns repulsive at higher frequencies where it approaches $4V$.

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 and $\langle n\rangle = 0.9$. For $V = 0$, $\phi_d[(\pi,0),\omega_n]$ falls to zero on a characteristic frequency scale. As previously found in Refs. [24,27], 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 $\mathbf{K}$ space reflecting the repulsive nature of the pairing interaction at large momentum transfer [2,24], $\phi_d(\mathbf{K},\omega_n)$ 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

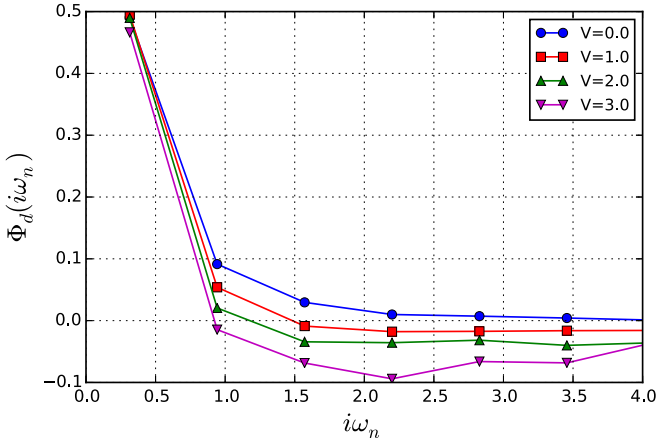

FIG. 3. The frequency dependence of the leading d-wave eigenvector $\phi_d(\mathbf{K},\omega_n)$ of the Bethe-Salpeter Eq. (2) for $\mathbf{K} = (\pi,0)$ and $T/t = 0.1$ for different values of V and $\langle n\rangle = 0.9$. The sign change in $\phi_d(\mathbf{K},\omega_n)$ as a function of frequency for finite V minimizes the repulsive effect of V.

important in preserving the attractive nature of the pairing interaction in the presence of V.

We have also calculated the zero-frequency cluster spin (s) and charge (c) susceptibilities,

$$\chi_{s/c}(\mathbf{Q},\omega_m=0)=\frac{1}{2N_c}\sum_{ij}e^{i\mathbf{Q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\int_0^\beta d\tau\langle[n_{i\uparrow}(\tau) \mp n_{i\downarrow}(\tau)][n_{j\uparrow}(0)\mp n_{j\downarrow}(0)]\rangle. \quad (5)$$

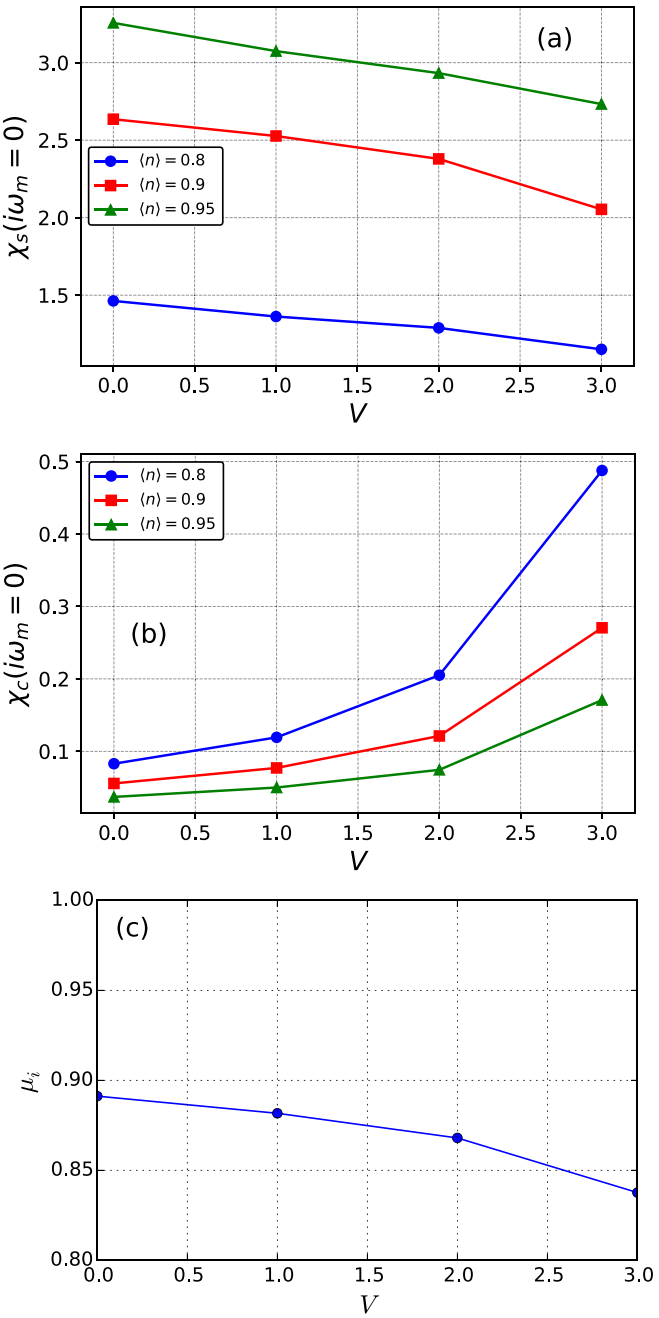

FIG. 4. Frequency dependence of the spin and charge susceptibilities, $\chi_s(i\omega_m=0)$ in (a) and $\chi_c(i\omega_m=0)$ in (b), respectively, for $\mathbf{Q}=(\pi,\pi)$ and $T=0.1$ as a function of V for different values of the filling $\langle n\rangle$. (c) Local magnetic moment $\mu=\sqrt{\langle(n_{i\uparrow}-n_{i\downarrow})^2\rangle}$ for $T=0.1$ as a function of V for different $\langle n\rangle$'s. With increasing V, charge fluctuations become stronger, whereas spin fluctuations are weakened through a reduction of the local magnetic moment.

The V dependence of $\chi_s(\mathbf{Q},0)$ and $\chi_c(\mathbf{Q},0)$ is shown in Figs. 4(a) and 4(b), respectively, for $\mathbf{Q}=(\pi,\pi)$ and different $\langle n\rangle$'s. As V increases, $\chi_s(\mathbf{Q},0)$ decreases, whereas $\chi_c(\mathbf{Q},0)$ increases. The rise in the charge susceptibility reflects the increasing tendency of the system to form a (π,π) charge-density wave-ordered state [14]. Although this rise is consistently observed for all the fillings we have studied, it does become more pronounced as the system is doped away from half-filling.

The V dependence of the spin susceptibility is more difficult to understand. Based on a strong-coupling picture, Reymbout *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 $\chi_s[(\pi,\pi),0]$, however, are not in line with this picture since one would expect $\chi_s[(\pi,\pi),0]$ 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 $\mu_i=\sqrt{\langle(n_{i\uparrow}-n_{i\downarrow})^2\rangle}$, which leads to a suppression of the spin fluctuations.

The destructive effects of the increasing charge fluctuations are thus twofold: As shown previously, d-wave pairing in the Hubbard model is mediated by a repulsive (positive) pairing interaction in momentum space that increases with momentum transfer and which reflects the momentum structure and dynamics of the spin susceptibility [24,27]. Since charge fluctuations contribute negatively to $\Gamma^{pp}(\mathbf{K},\omega_n,\mathbf{K}',\omega_{n'})$ [24], large momentum charge fluctuations weaken the d-wave pairing interaction. In addition, through their suppression of the local magnetic moment, they further weaken the large momentum spin fluctuations as seen in Fig. 4(a). Moreover, the fact that the charge fluctuations increase in strength with V more rapidly when the doping increases as seen in Fig. 4(b) explains that the destructive effect of V on the d-wave pairing strength becomes more pronounced as the doping increases, as seen in Fig. 1(b).

IV. SUMMARY

To summarize, we have used dynamic cluster quantum Monte Carlo calculations of an extended Hubbard model to study d-wave superconductivity when a nearest-neighbor Coulomb repulsion V is present in addition to the on-site Coulomb repulsion U. Consistent with previous studies, we find that d-wave pairing and T_c are only weakly suppressed by V and remain stable as long as V does not exceed $U/2$. The d-wave pairing interaction is attractive at low frequencies and repulsive at high frequencies due to the repulsive effect of V on d-wave pairing. Reflecting this sign change, the d-wave eigenfunction of the particle-particle Bethe-Salpeter equation $\phi_d(\mathbf{K},\omega_n)$ also changes sign as a function of frequency, similar to the case of electron-phonon-mediated pairing thus reducing the repulsive effect of the Coulomb interaction V. This demonstrates that retardation plays an important role in stabilizing d-wave pairing in the presence of V. A further analysis of the spin and charge susceptibilities shows that (π,π) charge fluctuations become strong when V approaches $U/2$. This leads to a more rapid suppression of d-wave pairing and T_c through both a reduction of the (π,π) spin fluctuations

and a direct negative contribution to the *d*-wave pairing interaction.

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