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We examine the validity of the weak-coupling spin-susceptibility "glue" approximation (SSGA) in a two-dimensional Hubbard model for cuprates. For comparison, we employ the well-established dynamical cluster approximation (DCA) with a quantum Monte Carlo algorithm as a cluster solver. We compare the leading eigenvalues and corresponding eigenfunctions of the DCA and SSGA pairing matrices. For realistic model parameters, we find that the SSGA fails to capture the leading pairing symmetries seen in the DCA. Furthermore, when the SSGA is improved through the addition of a term with d-wave symmetry, the strength of this additional term is found to be larger than that of the glue approximation.

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I. INTRODUCTION

The pairing mechanism of cuprate superconductors has been a challenging problem since their discovery. To this day, among different scenarios, two stand out. First one is the Anderson's resonating valence bond scenario[1] in which superconductivity is pictured as a Mott liquid of pairs formed by the superexchange interaction.[2] This is a strong-coupling approach and can predict many features of the cuprate phase diagram.[3] Another is the body of weak-coupling approaches, including phenomenological models,[4] fluctuation exchange,[5,6] and random-phase approximation[7] in which the pairing interaction, i.e., the "glue," is mediated by the low-energy spin fluctuations.

Recently, much effort has been devoted, both in experimental and in theoretical fronts, to find more compelling evidence for the spin-fluctuation-mediated pairing. On the experimental side, neutron-scattering data show a prominent peak in the structure factor at the antiferromagnetic wave vector, relevant to d-wave pairing.[8] Using inelastic neutron-scattering data to parametrize the effective spin-susceptibility glue interaction, Dahm *et al.*[9] find an excellent agreement between the numerically calculated features of the spectral function and the angle-resolved photoemission spectroscopy data. Moreover, van Heumen *et al.*[10] find a correlation between the doping trends in the "glue spectra," derived from optical conductivity data and the superconducting critical temperature.

On the theoretical side, the dynamics of this type of pairing has been recently investigated by numerous authors. For instance, employing an extended Hubbard model, Markiewicz and Bansil[11] argue that while magnetic pairing mechanism is valid in cuprates, both high and low energies are relevant to pairing. Similar conclusion have been drawn using numerical calculations of the Hubbard model which often involve the dynamical mean-field treatments of the smallest system relevant to d-wave pairing, the cluster of four sites.[12,13] However, using similar techniques, others argue that only the low-frequency part of the pairing is important.[14,15]

In this work, we examine the validity of the spin-susceptibility glue approximation (SSGA), expressed in a form similar to that of random-phase approximation,[7,13,16–19]

$$\Gamma^{\mathrm{SSGA}}(K|K') = \frac{3}{2}\bar{U}^2\chi_s(K'-K) \tag{1}$$

by exploring the *momentum* dependence of pairing and comparing it to the results obtained from a dynamical cluster approximation (DCA)[20–22] simulation. Here, Γ is the particle-particle irreducible vertex function and χ_s is the fully dressed spin susceptibility. $K=(\mathbf{K},\omega_n)$ denotes both momentum and frequency and $\bar{U}$ is an effective Coulomb interaction. Unlike most previous calculations, we employ a relatively large cluster, the 16-site cluster, allowing for more pairing symmetries. Note that in our SSGA, χ_s is also obtained from the DCA simulation. This emulates the use of experiment to parametrize the glue approximation.[9,23]

We find that when a finite next-nearest-neighbor hopping, t', appropriate to describe the hole-doped cuprates[24–27] is considered, the SSGA form of the interaction leads to p-wave pairing[28] while for the same parameters the DCA yields robust d-wave pairing. We show that this is due to the predominant scattering with the antiferromagnetic wave vector, resulting from the momentum dependence of the spin susceptibility and the strong suppression of the density of states (DOS) at the antinodal points (strong pseudogap).[29] To re-establish the d-wave pairing symmetry and the agreement with the DCA, the SSGA can be improved by adding an additional term with d-wave functionality in the momentum space. However, we find that the strength of this additional term should be larger than that of the SSGA.

II. FORMALISM

We consider a two-dimensional Hubbard Hamiltonian

$$H = -\sum_{ij\sigma} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + \mathrm{H.c.}) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}, \tag{2}$$

where t_{ij} is the hopping matrix, $c^{\dagger}_{i\sigma}(c_{i\sigma})$ is the creation (annihilation) operator for electrons on site i with spin σ, and

$n_{i\sigma}=c^{\dagger}_{i\sigma}c_{i\sigma}$. We show results for U equal to the bandwidth which is believed to be a realistic value for modeling cuprates[30–32] and at filling, $n=0.95$. Calculations at different hole dopings show that our conclusions are valid in the under-doped region ($n>0.85$), where the antiferromagnetic correlations are stronger while at larger dopings, the results are inconclusive since calculations are limited by the sign problem.

The DCA is a cluster mean-field theory that maps the original lattice model onto a periodic cluster of size $N_c=L_c^2$ embedded in a self-consistent host. Correlations up to a range L_c are treated explicitly using a quantum Monte Carlo (QMC) solver while those at longer length scales are described at the mean-field level. Previous DCA simulations have shown a robust d-wave superconductivity for the Hubbard model with U comparable to the bandwidth. The DCA has also established pseudogap and antiferromagnetic phases for this model which are in good qualitative agreement with experimental phase diagram of cuprates.[33,34]

To study the pairing, we calculate the eigenfunctions of the paring matrix, $\Gamma\chi_0$,[35]

$$\frac{T}{N_c}\sum_{K'}\Gamma(K|K')\chi_0(K')\phi(K')=\lambda\phi(K), \tag{3}$$

where T is temperature, $\chi_0[=-G(K)G(-K)]$ is the particle-particle bubble in the pairing channel and Γ can be either Γ^{SSGA} [Eq. (1)] or calculated in the DCA. For the latter, we measure the two-particle Green's function in the pairing channel (χ) in the QMC process. Then, using the Bethe-Salpeter equation, Γ is calculated by subtracting the inverse of χ from the inverse of the bare bubble in the same channel ($\Gamma=\chi_0^{-1}-\chi^{-1}$). The eigenfunction $\phi(K)$ represents the gap function and provides information about the symmetry and the frequency dependence of the pairing. The singularities in the two-particle Green's function, $\chi=\chi_0/(1-\Gamma\chi_0)$, which signal pairing instability, take place when the eigenvalue, λ, goes to unity. Therefore, one can explore the superconducting tendencies by studying the temperature dependence of the leading eigenvalues.

III. RESULTS

Unlike DCA calculations which yield d-wave pairing, when a finite next-nearest-neighbor hopping, appropriate to describe hole-doped cuprates, is considered the SSGA pairing vertex alone [Eq. (1)] does not result in pairing with d-wave symmetry. In Fig. 1, we compare the leading eigenvalues of the SSGA and DCA pairing matrices for zero and finite t'. When $t'=0$, the low-temperature DCA results have a d-wave leading eigenvalue, followed by s-wave and p-wave eigenvalues. Similar results are found with the SSGA pairing matrix, except that s-wave is not one of the leading eigenvalues. However, when $t'=-0.3t$, p-wave instead of d-wave becomes the dominant pairing symmetry for the SSGA while d-wave is still the leading eigenvalue in the DCA. Thus, the SSGA fails to capture the symmetry of the pairing obtained from the DCA calculation. Here, $\bar{U}$, which is shown for the two different values of t' in the inset of Fig. 1(b), is adjusted so that d-wave eigenvalue in SSGA is the same as its DCA counterpart.

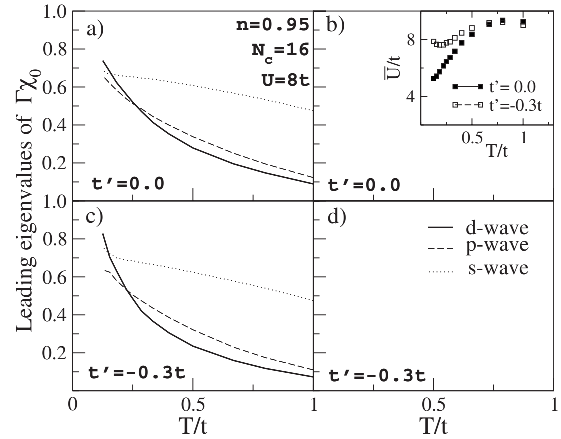

FIG. 1. Leading eigenvalues of the [(a) and (c)] DCA and [(b) and (d)] SSGA particle-particle pairing matrices versus temperature. Vertex function of Eq. (1) is used to form the SSGA pairing matrix. Top panels correspond to the Hubbard model with only nearest-neighbor hopping (t). In lower panels, a finite next-nearest-neighbor hopping is also taken into account. The inset of (b) shows the effective Coulomb interaction used in the SSGA vertex, which is adjusted so that d-wave eigenvalue in SSGA is the same as its DCA counterpart.

The momentum dependence of χ_s and the renormalization of particle-particle bubble due to finite t' are responsible for the disagreement between the symmetry of the leading eigenfunctions in the SSGA and the DCA. To better understand why the dominant pairing in the SSGA is not d-wave, we employ the following approximation: $\chi_s(K'-K)\approx\chi_s(\mathbf{Q},0)\delta_{\mathbf{K}'-\mathbf{K},\mathbf{Q}}\delta(\omega_{n'}-\omega_n)$. This is motivated by the fact that the spin susceptibility is considerable only at the antiferromagnetic wave vector, $\mathbf{Q}=\mathbf{K}'-\mathbf{K}=(\pi,\pi)$ and at small Matsubara frequency. In this approximation, Eq. (3) can be written as

$$\frac{3T}{2N_c}\bar{U}^2\chi_s(\mathbf{Q})\chi_0(\mathbf{K}+\mathbf{Q},\omega_n)\phi(\mathbf{K}+\mathbf{Q},\omega_n)\approx\lambda\phi(\mathbf{K},\omega_n). \tag{4}$$

Considering that

$$\frac{3T}{2N_c}\bar{U}^2\chi_s(\mathbf{Q})\chi_0(\mathbf{K},\omega_n)\phi(\mathbf{K},\omega_n)\approx\lambda\phi(\mathbf{K}+\mathbf{Q},\omega_n) \tag{5}$$

is also true, one gets

$$\lambda^2\propto\chi_s(\mathbf{Q})^2\chi_0(\mathbf{K},\omega_n)\chi_0(\mathbf{K}+\mathbf{Q},\omega_n). \tag{6}$$

This suggests that the leading eigenvalue of the SSGA pairing matrix corresponds to a momentum, $\mathbf{K}$, for which the quantity $\chi_0(\mathbf{K},\omega_n)\chi_0(\mathbf{K}+\mathbf{Q},\omega_n)$ has its largest value. Since the bubble $\chi_0(\mathbf{K},\omega_n)$ falls rapidly with frequency, only the lowest Matsubara frequencies are relevant for determining the leading eigenvalues. In the following, we will discuss the behavior of $\chi_0(\mathbf{K},\omega_n)\chi_0(\mathbf{K}+\mathbf{Q},\omega_n)$ at $\omega_n=\pm\pi T$.

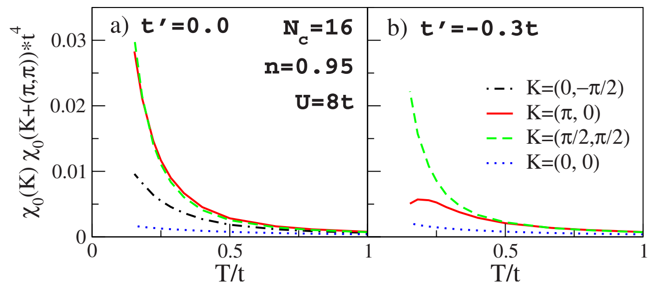

FIG. 2. (Color online) The product $\chi_0(\mathbf{K})\chi_0(\mathbf{K}+\mathbf{Q})$ with $\mathbf{Q}=(\pi,\pi)$ and $\omega_n=\omega_{n'}=\pi T$ at four different $\mathbf{K}$ points in the first Brillouin zone (1BZ) for (a) $t'=0$ and (b) $t'=-0.3t$ versus temperature. At low temperatures, the leading pairing symmetries in SSGA can be determined by the value of the product $\chi_0(\mathbf{K})\chi_0(\mathbf{K}+\mathbf{Q})$ at each $\mathbf{K}$ point. The one for $\mathbf{K}=(\pi,0)$ corresponds to the d-wave symmetry and shows a significant decrease with t' at low temperatures.

When $t'=0$, $\chi_0(\mathbf{K})\chi_0(\mathbf{K}+\mathbf{Q})$ is the largest for $\mathbf{K}=(\pi,0)$ and $\mathbf{K}=(\pi/2,\pi/2)$ at low temperature, as can be seen in Fig. 2(a). The former situation favors d-wave pairing whereas the latter favors p-wave pairing. The close values of $\chi_0(\mathbf{K})\chi_0(\mathbf{K}+\mathbf{Q})$ at these momenta explain the competition between d-wave and p-wave symmetries in SSGA. Note that for a small 2×2 cluster, the resolution in momentum space is poor [e.g., $\mathbf{K}=(\pi/2,\pi/2)$ is not represented in the Brillouin zone] and the scattering between the nodal points which favors p-wave pairing is suppressed. Thus, a larger cluster with good momentum resolution is important in capturing symmetries other than d-wave in the pairing channel. The 16-site cluster provides four independent values for $\chi_0(\mathbf{K})\chi_0(\mathbf{K}+\mathbf{Q})$. This is illustrate in Fig. 3 where each arrow represents a $\mathbf{Q}=(\pi,\pi)$ scattering between $\mathbf{K}$ and $\mathbf{K}+\mathbf{Q}$.

A finite t' strongly suppresses $\chi_0(\mathbf{K})\chi_0(\mathbf{K}+\mathbf{Q})$ at the antinodal points while it has a small effect at other k points [see Fig. 2(b)]. Therefore, according to Eq. (6), the d-wave eigenvalue will also be suppressed relative to the p-wave eigenvalue. Consequently, the p-wave pairing will be dominant in the SSGA, which explains the results discussed in Fig. 1. The renormalization of the bare bubble at the antinodal points can be understood from the changes in the DOS. At low temperatures, the low-energy DOS at $\mathbf{K}=(0,\pi)$ is strongly suppressed (i.e., the pseudogap is enhanced) with t' for the hole-doped systems while this effect is negligible at other k points.[29] This indicates that in the over-doped region, where pseudogap is less pronounced, SSGA might be a good approximation.

We find that the spin-susceptibility representation of the pairing interaction, which is appreciable only at $\mathbf{K}'-\mathbf{K}=(\pi,\pi)$, does not always yield d-wave as the leading pairing symmetry. This seems to be especially true when realistic parameters for cuprates such as next-nearest-neighbor hopping are considered. We show that despite the inherent correspondence between the $\mathbf{Q}=(\pi,\pi)$ wave vector, at which the SSGA interaction is large, and the d-wave symmetry, other pairing symmetries which also associate with the (π,π) wave vector can be dominant. On the other hand, the DCA exhibits a robust d-wave pairing for the same physical parameters of the Hubbard model.

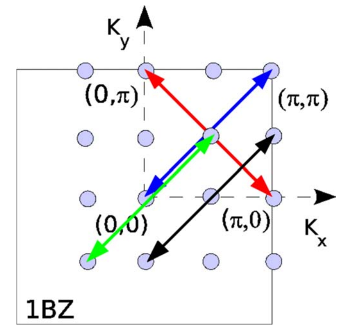

FIG. 3. (Color online) The 1BZ for $N_c=16$. Arrows show the four independent (π,π) scatterings between $\mathbf{K}$ and $\mathbf{K}'$ on this cluster. The one that connects $(\pi,0)$ to $(0,\pi)$ is associated with the d-wave symmetry.

To investigate the possibility of a missing term, we propose to add an extra term to Γ^{SSGA} which enhances the scattering between the antinodal points. Such approximation for the interaction vertex can be written as

$$\Gamma'(K|K')=\frac{3}{2}\bar{U}^2\chi_s(K'-K)-\alpha\phi_d(K')\quad{}_d(K). \tag{7}$$

Here, $\;_d$ is the d-wave eigenfunction of the DCA pairing matrix, and $\bar{U}$ and α are temperature-dependent fitting parameters which are adjusted to reproduce both the d-wave and the p-wave leading eigenvalues of the DCA pairing matrix. It is worth mentioning that Maier *et al.*[13] proposed a similar term, $-\bar{J}g(\mathbf{K})g(\mathbf{K}')$, to be added to the SSGA form in which $g(\mathbf{K})\quad(\cos K_x-\cos K_y)$ is the d-wave form factor and $\bar{J}$ is an effective exchange interaction. However, their motivation for the necessity of this extra term is quite different from ours. Since they did not consider a finite t', the SSGA gave a d-wave pairing. So, this term was suggested only to restore the large frequency behavior of the pairing gap found in the DCA. Our focus, on the other hand, is to examine the relevance of an additional term based on a momentum space argument. Note that because our calculations are done using QMC on the imaginary frequency axis, generally comments about the frequency dependence of the pairing interaction cannot be made. However, if relevant, the additional term may be responsible for the instantaneous part of the interaction, as described in Ref. 13. We also find that using $\;_d(K)$ instead of $g(\mathbf{K})$ in our approximation provides a better fit to the DCA results while imposing the d-wave symmetry.

For a finite t', the second term in Eq. (7) (α term) has a prominent role in capturing the correct leading symmetries in this new form of the interaction. In Fig. 4, we show the fractional values of α and the d-wave component of the SSGA term,[18,36]

$$V_d^{\mathrm{SSGA}}=-\sum_{K,K'}\quad{}_d(K')\frac{3}{2}\bar{U}^2\chi_s(K'-K)\quad{}_d(K), \tag{8}$$

for the two values of t'. We define $V_d=V_d^{\mathrm{SSGA}}+\alpha$ as the total d-wave projected interaction. When $t'=0$, the contribution of the α term to the d-wave interaction is insignificant. However, when $t'=-0.3t$, this term has a dominant role in the

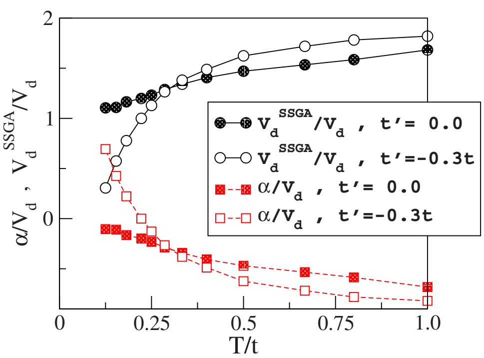

FIG. 4. (Color online) Fractions of the d-wave pairing interaction for the SSGA term (first term) and the α term (second term) of Eq. (7) for zero and finite t' versus temperature. $V_d = V_d^{\mathrm{SSGA}} + \alpha$ is the total d-wave projected interaction of Eq. (7). For $t'=0$, the contribution of the α term to the d-wave interaction is insignificant while for $t'=-0.3t$, it becomes more important than the SSGA term at low temperatures.

d-wave pairing at low temperatures. So, although the additional term enhances d-wave pairing, its contribution overshadows the contribution of the main part of the interaction, i.e., the term proportional to the spin susceptibility. This suggests that the SSGA may not be improved by simply adding terms that enhance d-wave scattering.

IV. CONCLUSIONS

We study the validity of the SSGA representation of the pairing interaction in the Hubbard model. By comparing the leading pairing symmetries of this interaction with the pairing symmetries produced by the DCA, we find that this approximation alone does not capture the correct pairing symmetry in the under-doped and optimally doped regions, particularly when a finite t' is considered. We do not dismiss the possibility that SSGA can be valid in the over-doped region, where the pseudogap phenomenon is less relevant. We show that this form of the interaction, which is large only at the antiferromagnetic wave vector, requires an additional term with d-wave symmetry to yield d-wave pairing at low temperatures. However, in case of finite t', the additional term dominates the interaction as the temperature is lowered.

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