Increasing *d*-Wave Superconductivity by On-Site Repulsion

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We study, through the variational Monte Carlo technique, an extended Hubbard model away from half filled band density which contains two competing nearest-neighbor interactions: a superexchange J favoring d-wave superconductivity and a repulsion V opposing it. We find that the on-site repulsion U effectively enhances the strength of J while suppressing that of V, thus favoring superconductivity. This result shows that attractions which do not involve charge fluctuations are very well equipped against strong electron-electron repulsion so much to get advantage from it.

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The interplay between strong correlation and superconductivity is one of the major problems raised by the discovery of cuprate high-T_c materials. Indeed, within the conventional BCS theory for phonon-mediated weak coupling superconductivity, a strong electron-electron short range repulsion, parametrized by a Hubbard U, can only depress T_c. Landau-Fermi liquid theory identifies two main sources for this reduction; namely, as U increases, the quasiparticle wave-function renormalization $Z \leq 1$ diminishes; meanwhile, the effective mass m_* increases. Thus, each interaction amplitude, including the phonon-mediated attraction g, acquires a renormalization factor Z^2 times a vertex renormalization. If the latter is negligible, the bare amplitude is reduced to $g_* = Z^2 g$. Therefore, as U increases, the dimensionless coupling which parametrizes the *bare* attraction, $\lambda_0 = \rho_0 |g|$, where ρ_0 is the uncorrelated density of states at the Fermi level, is renormalized into

$$\lambda_* = \rho_* |g_*| = Z^2 \frac{m_*}{m} \lambda_0 < \lambda_0,$$

where usually $Z \leq m/m_*$. On the other hand, the Coulomb pseudopotential μ_* increases, so that $\lambda_* - \mu_*$ diminishes even more, pushing T_c down.

By solving a model for alkali doped fullerenes within dynamical mean field theory, it has been recently argued [1] that there exist attractive channels for which vertex corrections may compensate the wave-function renormalization factor leading to

$$\lambda_0 \rightarrow \frac{m_*}{m} \lambda_0 > \lambda_0,$$

which may indeed lead to an enhancement of T_c by increasing U. The main ingredient was identified into a pairing mechanism not involving the charge-density operator, which is mostly subject to the renormalization induced by U, but other internal degrees of freedom, such as the spin (or the orbital index, if orbital degeneracy is present), unveiling a kind of spin-charge separation even within Landau-Fermi liquid theory.

This proposal is not far in spirit from the original resonating valence-bond (RVB) scenario for high-T_c superconductivity in the t-J model [2]. There, superconductivity occurs naturally upon doping since the parent insulating state is well described by an RVB state: the spin-singlet valence-bond pairs naturally evolve into Cooper pairs. They can propagate around the lattice only through the empty sites left behind by the holes. This constraint easily explains a superfluid density proportional to the hole doping. Moreover, although at small doping superconductivity is suppressed, the energy scale associated to the binding energy of the valence-bond pairs remains finite, which is advocated to explain the experimentally observed pseudogap phase of high-T_c materials [3,4].

Within the Fermi liquid framework, the constraint of no double occupancy appears to renormalize the quasiparticle hopping to a value $Zt \simeq 2\delta t$, δ being the doping, while leaving untouched the quasiparticle attraction, here provided by the superexchange J. The superconducting phase of the t-J model can be approached either from the half-filled antiferromagnetic Mott insulator upon increasing doping or at finite doping by decreasing temperature. In both cases, even though the $T = 0$ superconductor might still be described in terms of Landau-Bogoliubov quasiparticles, in the RVB language spinon-holon confined objects, the relevant excitations above T_c or in close vicinity to the half-filled antiferromagnet do not necessarily look like conventional quasiparticles.

For this reason, in this work we try to understand whether this strongly correlated d-wave superconductor can be approached at zero temperature starting from a weakly correlated regime, where standard many-body techniques and the well established Landau-Fermi liquid theory should apply.

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We consider an extended Hubbard model in two dimensions for the average number of electrons per site $1 - \delta < 1$, namely, away from half filling,

$$\hat{H} = -t \sum_{\langle ij \rangle} \sum_{\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + \text{H.c.}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + J \sum_{\langle ij \rangle} \left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j \right) + V \sum_{\langle ij \rangle} n_i n_j, \qquad (1)$$

where, in addition to the on-site repulsion, we add a nearest-neighbor spin-exchange and a charge-repulsion term, with strengths J and V, respectively. These nearest-neighbor interactions compete, J favoring a d-wave singlet pairing away from half filling and V opposing it. For $V = 0$ and U strictly equal to ∞, (1) reduces to the standard t-J model, which also corresponds to the large U limit of the pure Hubbard model, in which case $J \rightarrow 4t^2/U$. However, contrary to the latter, model (1) for $J > V$ is undoubtedly a d-wave superconductor at weak coupling (U, V, and J all much smaller than t) also within the Hartree-Fock approximation. For this reason, model (1) is more suitable to address the issue of electron-electron correlation effects on d-wave superconductivity. Moreover, since V involves charge-density while J involves spin-density operators, the presence of both gives one the opportunity to test if U indeed induces different renormalization factors on charge with respect to spin vertices.

A variational approach which was shown to correctly reproduce both the weak [5] and the strong [6] coupling limits of the Hubbard model appears well suited for model (1) too. It consists in searching by the variational Monte Carlo (VMC) technique for the best wave function of the form

$$|\Psi\rangle = A \hat{P}_{\mathrm{N}} \hat{P}_{\mathrm{Jastrow}} \hat{P}_{\mathrm{G}} |\Psi_{\mathrm{BCS}}\rangle, \qquad (2)$$

where A is a normalization factor, $|\Psi_{\mathrm{BCS}}\rangle$ a BCS wave function [7] projected by $\hat{P}_{\mathrm{N}}$ onto a fixed number of particles, with a d-wave gap function $\Delta_k = \Delta_{\mathrm{var}}(\cos k_x - \cos k_y)$, Δ_{var} being a variational parameter. $\hat{P}_{\mathrm{G}}$ is a Gutzwiller projector:

$$\hat{P}_{\mathrm{G}} = \prod_{n} (1 - \alpha_0 n_{n,\uparrow} n_{n,\downarrow}), \qquad (3)$$

whereas $\hat{P}_{\mathrm{Jastrow}}$ a long-range Jastrow factor which enforces the correct long-wavelength behavior of the density structure factor:

$$\hat{P}_{\mathrm{Jastrow}} = e^{-\alpha_1 \sum_{\langle ij \rangle} n_i n_j - \alpha_2 \sum_{\langle\langle ij \rangle\rangle} n_i n_j - \dots}, \qquad (4)$$

where "..." stands for the summation over next, next-next, etc., nearest-neighbor sites (i.e., all those possible on a finite size sample).

The method is based on the stochastic reconfiguration technique [6], which allows one to minimize the energy of a variational wave function containing even a large number of parameters.

To get further insight from the numerics, we compare the results with those obtained by the Gutzwiller approximation (GA) [8,9] for the variational wave function without both the long-range Jastrow factors and the projector onto a fixed number of particles.

In Fig. 1 we plot the variational parameter Δ_{var} as a function of U for $J = 0.2t$, $\delta = 0.16$, and for different values of V. For $J > V$, Δ_{var} starts finite at $U = 0$ and increases with U. For $V > J$, $\Delta_{\mathrm{var}} = 0$ at small U, in agreement with the Hartree-Fock results. More remarkably, above a critical U_c a finite Δ_{var} appears. Namely, the normal metal at $V > J$ turns into a superconductor by increasing the on-site repulsion. Both results can be explained within the Fermi liquid picture provided by the Gutzwiller approximation, according to which the effective J_* acting between the quasiparticles stays essentially unrenormalized when U increases, contrary to the effective V_*, which is substantially suppressed with respect to its bare value V. Therefore, as U increases for $J > V$, the quasiparticle bandwidth gets reduced, the attraction staying unrenormalized, so that the dimensionless coupling λ_* increases, hence Δ_{var}. If $J < V$, a normal metal is stable until $V_* > J_* \simeq J$, after which superconductivity

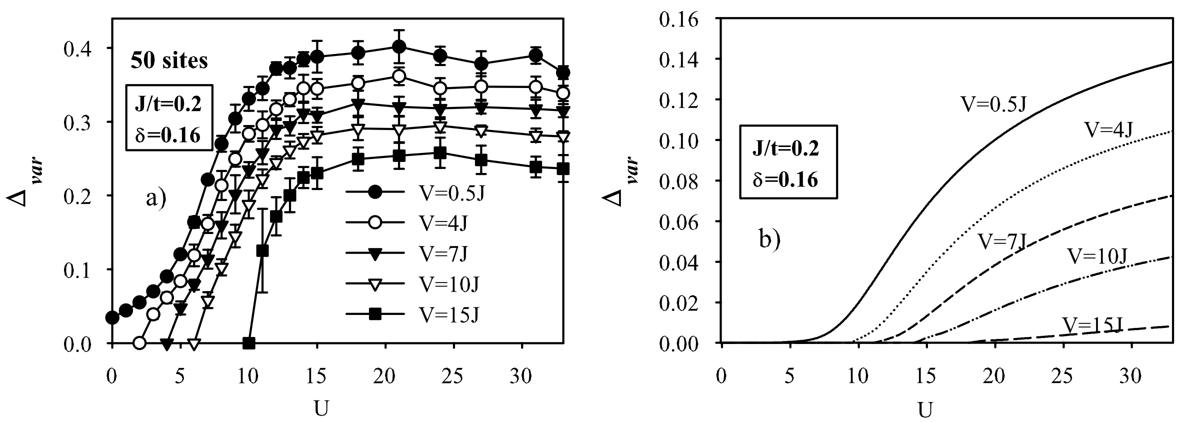

FIG. 1. Variational gap as a function of U for different values of V within (a) variational Monte Carlo and (b) GA.

gets in. In our numerical study we found that the inclusion of the long-range Jastrow factor (4) considerably improves the simpler Gutzwiller wave function and allows larger values of $\Delta_{\rm var}$. However, as shown in Fig. 1(b) the qualitative behavior of $\Delta_{\rm var}$ vs U is reproduced already by GA.

Within the GA it is possible to study explicitly the competing influence of both J and V on superconductivity. Let us consider the superconducting contributions to the uncorrelated expectation values for nearest-neighbor sites i and j,

$$\langle\Psi_{\rm BCS}|n_i n_j|\Psi_{\rm BCS}\rangle_{\rm SC} = 2\Delta_{\rm SC}^2, \tag{5}$$

$$\langle\Psi_{\rm BCS}|\vec{S}_i\cdot\vec{S}_j|\Psi_{\rm BCS}\rangle_{\rm SC} = -\tfrac{3}{2}\Delta_{\rm SC}^2, \tag{6}$$

where $\Delta_{\rm SC} = |\langle\Psi_{\rm BCS}|c_{i\sigma}^\dagger c_{j-\sigma}^\dagger|\Psi_{\rm BCS}\rangle|$ is the order parameter of the uncorrelated wave function. In the case of Eq. (5), this term derives from configurations in which i and j are both singly occupied, both doubly occupied, or one singly and the other doubly occupied, with weights δ^2, $(1-\delta)^2$, and $2\delta(1-\delta)$, respectively, where δ is the doping. On the contrary, Eq. (6) has contribution only by configurations where both sites are singly occupied. In the limit of very large U, the configurations with doubly occupied sites are projected out; hence, only the contributions from singly occupied sites survive in Eqs. (5) and (6). This implies that (5) gets a reduction factor δ^2 relative to (6), so that the actual condition for superconductivity at $U\to\infty$ reads approximately

$$\tfrac{3}{4}J > \delta^2(V - \tfrac{1}{4}J).$$

Since, in the same limit, the wave-function renormalization $Z \simeq 2\delta$, we indeed recover the desired Fermi liquid result that interactions involving the charge-density operators get renormalized down by a factor Z^2 with respect to those involving spin operators. The above discussion also shows that not all the pairing mechanisms are equally equipped against on-site repulsion. Indeed, a weak coupling d-wave superconductivity might be stabilized even by a negative V at $J = 0$: an explicit attraction between charges. However, for increasing U, the effective strength of this attraction would decrease as Z^2 so that $\lambda_* \sim Z\lambda_0$; hence, T_c would go down.

The behavior of the variational gap $\Delta_{\rm var}$ as shown in Fig. 1 suggests a crossover from weak to strong coupling superconductivity as U increases. This is manifested by comparing Fig. 2(a) with Fig. 2(b). In the latter the variational energy gap is displayed for several U's, while in the former we plot the true long-range order (LRO) parameter $\Delta_{\rm LRO}$ in the correlated wave function. $\Delta_{\rm LRO}$ is estimated on a finite cluster through the pair-pair correlation function f as follows:

$$\Delta_{\rm LRO} = \tfrac{1}{2}\sqrt{f - f_{\rm norm}},$$

where

$$f \equiv \sum_{\sigma,\sigma'}\langle c_{\vec{x},\sigma}^\dagger c_{\vec{x}\pm\vec{1},-\sigma}^\dagger c_{\vec{y}\pm\vec{1},-\sigma'} c_{\vec{y},\sigma'}\rangle, \tag{7}$$

being evaluated around the maximum distance $|\vec{x}-\vec{y}|$ available on a given size. Notice that f includes normal contributions $f_{\rm norm}$, which nevertheless vanish in the infinite size limit. In order to improve the quality of any finite size analysis, one should estimate $f_{\rm norm}$ to get a meaningful value of the true long-range order parameter. We decided to approximate $f_{\rm norm}$ by the value of f calculated with the optimized wave function having the same form (2) with the variational parameter $\Delta_{\rm var}$ equal to zero [see inset in Fig. 2(a)]. After this subtraction, size effects are acceptable, at least for our qualitative analysis [see Fig. 2(a)].

The crossover region where the gap $\Delta_{\rm var}$ rapidly moves from small BCS-like values to much larger values corresponds to a maximum of the true order parameter, as one would expect in the intermediate region between weak to

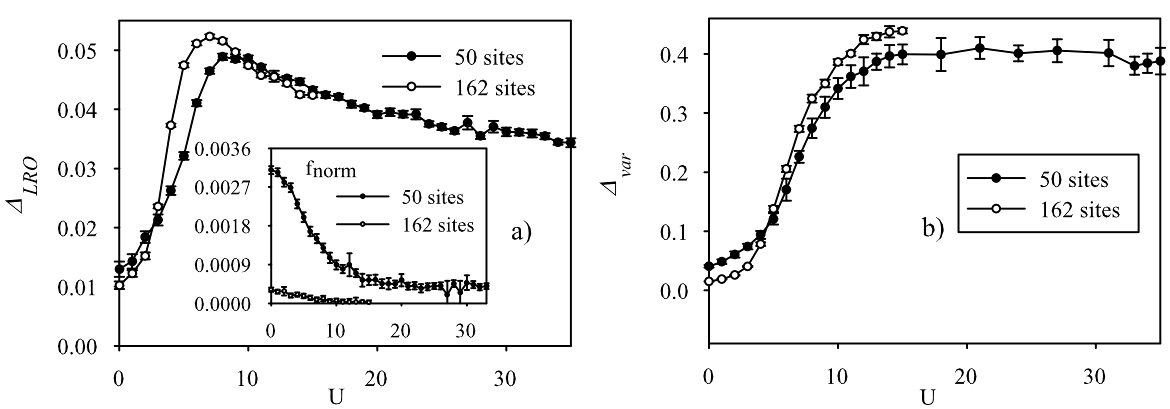

FIG. 2. (a) Superconducting order parameter $\Delta_{\rm LRO}$ and (b) the variational gap $\Delta_{\rm var}$ as a function of U at $V = 0$, $J/t = 0.2$, $\delta = 0.16$. The inset in (a) shows the long distance pairing correlations for the nonsuperconducting state (see text).

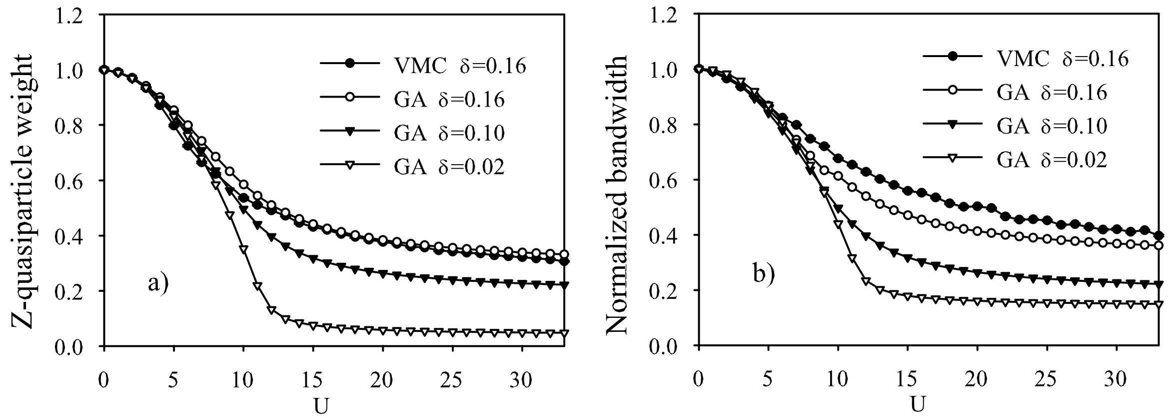

FIG. 3. (a) Wave-function renormalization Z as calculated through the jump in the momentum distribution along the nodal direction. Finite size scaling from 50 to 162 is used to evaluate the jump Z in the thermodynamic limit for the VMC. (b) Quasiparticle bandwidth normalized to its uncorrelated value. The VMC refers to the 50-site cluster, as finite size effects are small. $V = 0$ and $J/t = 0.2$ for both figures.

strong coupling superconductivity. The notable difference with the latter is that in our model the crossover does not occur by varying the bare attraction λ, but by increasing the repulsion U.

The different behavior of the variational gap with respect to the true order parameter, which has been associated with the behavior of the pseudogap versus T_c in the cuprates [3,4], has a clear explanation within the GA, where $\Delta_{\rm LRO}$ is suppressed by the factor Z with respect to the uncorrelated $\Delta_{\rm SC}$. Indeed, as shown in Fig. 3(a), the quasiparticle residue Z, defined as the jump in the momentum distribution function along the nodal directions, is a decreasing function of U tending to $Z \sim 2\delta$ as $U \to \infty$.

However, as shown in Fig. 3(b), Z is not the reduction factor of the full quasiparticle bandwidth, which gets contributions also from J and V. Again, this is an obvious result in the GA where the Hartree-Fock decoupling of the nearest-neighbor interactions effectively generate hopping terms. In spite of that, the charge current vertex is still determined by the true hopping t, and hence gets suppressed by a factor $Z \simeq 2\delta$. On the contrary, spin current vertex does include a contribution from J and survives against the strong wave-function renormalization Z.

In conclusion, we have shown that strong short range correlations enhance or suppress pairing correlations if they primarily involve spin or charge degrees of freedom, respectively. This behavior is manifested at strong U, in agreement with slave boson approaches [10] and numerical calculations [3,4,11], but starts to appear already at weak coupling. Indeed, a recent calculation within the random phase approximation [12] shows that the d-wave superconducting phase of model (1) at $V = 0$ gains more exchange-correlation energy than a normal metal, thus supporting the results here obtained by the variational Monte Carlo technique.

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Note added.—When this work was completed, we became aware of a preprint by Zhang [13] which considers the Hamiltonian (1) with $V = 0$ within the GA, in the context of the gossamer superconductivity scenario recently proposed by Laughlin [14]. The results of Ref. [13] qualitatively agree with our VMC data.

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