d-wave pairing in lightly doped Mott insulators

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We define a suitable quantity Z_c that measures the pairing strength of two electrons added to the ground-state wave function by means of the anomalous part of the one-particle Green's function. Z_c discriminates between systems described by one-electron states, like ordinary metals and band insulators, for which $Z_c=0$, and systems where the single particle picture does not hold, like superconductors and resonating valence bond insulators, for which $Z_c\neq 0$. By using a quantum Monte Carlo projection technique for the Hubbard model at $U/t=4$, a finite Z_c, with *d*-wave symmetry, is found at half filling and in the lightly doped regime, thus emphasizing a qualitatively new feature coming from electronic correlation.

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I. INTRODUCTION

Since the discovery of high-temperature superconductors, the question of whether a strongly correlated system, containing *only* repulsive interactions, may display a superconducting ground state has been intensively investigated and debated,[1] mainly because high-temperature superconductors are certainly strongly correlated materials and their properties, such as, for instance, their critical temperature and the linear-temperature behavior of the resistance at optimal doping, cannot be explained by the standard Eliashberg theory of the electron-phonon mechanism.[2]

On one side, any mean-field approximation of strongly correlated systems fails to explain superconductivity without an electron-electron attraction, which could be either explicit, as in the attractive Hubbard model,[3] or mediated by some boson, such as phonons in the BCS theory.[4] On the other hand, it is well known that correlated wave functions, obtained by applying a Gutzwiller projector that inhibits the expensive energy configurations, substantially improve the mean-field states and usually also enhance the superconducting correlations.[5–7] In particular, the fully projected wave function with a *d*-wave superconducting pairing has been proposed to be an excellent approximation of the exact ground state of the *t*-*J* model for the underdoped and optimally doped regimes.[5,7,8]

Moreover, the approach based on projected superconducting wave functions has been recently renewed, as it is possible to reproduce many important experimental aspects just by *assuming* that the ground state is described by a projected BCS wave function.[6,9] Within this scheme, the superconductivity is "hidden" in the undoped insulating state, where phase coherence is inhibited by the charge gap, and it is indeed stabilized by a small amount of doping. In this case, in the underdoped region, while the superconducting order parameter is proportional to the hole doping, the pairing strength, measured as the bare superconducting gap function of the unprojected wave function, decreases by adding holes to the undoped Mott insulator.[6] Unfortunately, the validity of this scenario for the actual ground state of a microscopic model remains a highly debated and controversial issue, despite a huge amount of numerical work.[7,10–13] In this paper, we present a suitable quantity that could be simply related to the pairing properties of the ground-state wave function and we present very accurate numerical calculations in favor of the above-mentioned picture for the simplest correlated systems, i.e., the single-band repulsive Hubbard model. Therefore, we give an explicit way to measure the pairing properties that does not depend upon the particular wave function, but, instead, is directly related to a true ground-state expectation value. Finally, we argue that the superconducting properties at finite doping naturally follow from the hidden pairing, which is also present in the undoped insulating state.

The outline of the paper is as follows: in Sec. II we present the model and the numerical technique and in Sec. III we show the results and draw the final remarks.

II. MODEL AND NUMERICAL TECHNIQUE

In the following, we consider the single-band Hubbard model on *L*-site clusters defined by the Hamiltonian:

$$H = -t\sum_{\langle i,j\rangle,\sigma} c^{\dagger}_{i,\sigma}c_{j,\sigma} + \text{H.c.} + U\sum_{i} n_{i,\uparrow}n_{i,\downarrow} - \mu N, \qquad (1)$$

where $c^{\dagger}_{i,\sigma}$ creates an electron with spin σ at the site i, $n_{i,\sigma}=c^{\dagger}_{i,\sigma}c_{i,\sigma}$ is the density operator at the site i, μ is the chemical potential, and $N=\Sigma_{i,\sigma}n_{i,\sigma}$ is the total number of particles. We use square lattices tilted by 45° with $L=2l^2$ and l odd with periodic boundary conditions, so that the half-filled case ($N=L$) has a nondegenerate ground state even at $U=0$. This condition strongly reduces the size effects, particularly important in two dimensions.

Our purpose is to study the Gorkov's off-diagonal part of the equal-time Green's function at zero temperature

$$F^{BSP}_{k} = \langle\Psi_0|c^{\dagger}_{k,\uparrow}c^{\dagger}_{-k,\downarrow}|\Psi_0\rangle, \qquad (2)$$

where $|\Psi_0\rangle$ is the ground state of the Hamiltonian H. Obviously, F^{BSP}_{k} can be nonzero only in the thermodynamic limit, where, because of the broken symmetry phenomena, $|\Psi_0\rangle$ may not have a definite number of particles. On a finite system, broken symmetry phenomena do not occur and F^{BSP}_{k} is always zero, the ground state $|\Psi_0\rangle$ having always a definite number of particles N. In a finite system, F^{BSP}_{k} can be computed from[14]

$$F_k = \langle \Psi_0^{N+2} | c_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger | \Psi_0^N \rangle, \tag{3}$$

where $|\Psi_0^N\rangle$ is the ground state with N particles.

In order to evaluate F_k, we consider the auxiliary-field Monte Carlo technique, where the exact ground-state wave function is filtered out starting from a trial state.[15] Since we are interested in calculating F_k, we are forced to take as the initial wave function a BCS state $|\Psi_G\rangle$ containing only components with an even number of particles

$$|\Psi_G\rangle = \mathcal{J} \exp\left(\sum_k f_k c_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger \right) |0\rangle, \tag{4}$$

where $|0\rangle$ is the vacuum, $f_k = \Delta_k / (\epsilon_k - \mu_0 + E_k)$, $\epsilon_k = -2t(\cos k_x + \cos k_y)$ is the free-electron dispersion, μ_0 is a variational parameter of the initial state playing the role of the chemical potential of the underlying BCS Hamiltonian, Δ_k is the corresponding gap function chosen to have either a d-wave symmetry $\Delta_k = \Delta(\cos k_x - \cos k_y)$ or an s-wave symmetry $\Delta_k = \Delta$, and $E_k = \sqrt{(\epsilon_k - \mu_0)^2 + \Delta_k^2}$. The correlation factor $\mathcal{J} = e^{-g \Sigma_i n_{i,\uparrow} n_{i,\downarrow}}$, g being a variational parameter of the initial state, partially projects out expensive energy configurations with doubly occupied sites.

In the following, we assume that for an appropriate gap function symmetry, the N-particle ground state of H has a nonvanishing overlap with $|\Psi_G\rangle$, at least for $N = N^*$ and $N = N^* + 2$, where $N = N^*$ represents a closed shell density. This assumption has been verified on small clusters, where the exact diagonalization by Lanczos is possible.

Therefore, on each finite system, we compute for fixed imaginary time τ

$$F_k(\tau) = \frac{\langle \Psi_G | e^{-\tau H/2} c_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger e^{-\tau H/2} | \Psi_G \rangle}{\langle \Psi_G | e^{-\tau H} | \Psi_G \rangle}. \tag{5}$$

$F_k(\tau)$ will be finite even on a finite size, because the trial function $|\Psi_G\rangle$ contains sectors with different N, namely $|\Psi_G\rangle = \Sigma_N a_N |\Psi_G^N\rangle$. Then for large τ

$$F_k(\tau) = F_k \frac{b_{N^*+2}}{b_{N^*}} e^{-\tau \Delta_c / 2}, \tag{6}$$

where N^* is given by an appropriate choice of the true chemical potential μ, Δ_c is the energy gap between the states with N^* and $N^* + 2$, and

$$b_N = \langle \Psi_G^N | \Psi_0^N \rangle a_N. \tag{7}$$

Therefore, in order to estimate F_k, the overall factor

$$\gamma = \frac{b_{N^*+2}}{b_{N^*}} e^{-\tau \Delta_c / 2} \tag{8}$$

must be computed by evaluating the average number of particles

$$\langle N \rangle = N^* + \frac{2\gamma^2}{(1+\gamma^2)}. \tag{9}$$

An efficient choice of $|\Psi_G\rangle$ is obtained by tuning μ_0 very close to the energy level $\bar{\epsilon}_k$ with $N^* + 2$ particles, and $\Delta \ll |\bar{\epsilon}_k - \mu_0|$, i.e., Δ much smaller than the free-electron finite-size energy gap. The last condition implies that $|\Psi_G^{N^*}\rangle$ and $|\Psi_G^{N^*+2}\rangle$ are free-electron wave functions in the thermodynamic limit. Therefore, $|\Psi_G\rangle$ essentially contains only two components in the sectors with $N = N^*$ and $N = N^* + 2$, and the imaginary time projection can be done without paying much attention to the chemical potential, the number of particles being conserved by H. It should be emphasized that, within this choice, the trial wave function is unbiased, apart from the choice of the symmetry of the gap function Δ_k, that is considered only to split the degeneracy of the noninteracting shells and to permit the calculation of the anomalous part of the Green's function Eq. (3).

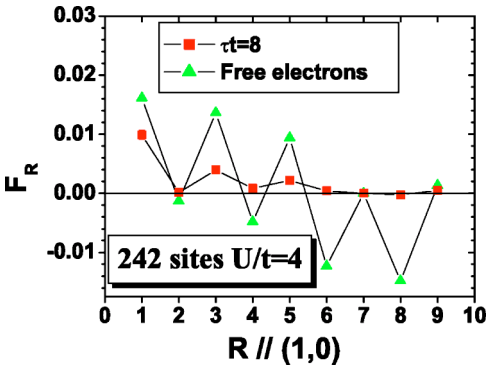

FIG. 1. (Color online) Anomalous part of the Green's function in real space at half filling for free electrons and for $U/t = 4$, obtained by the Monte Carlo projection technique described in Sec. II.

The superconducting order parameter P is related to the short-distance component of the Fourier transform

$$F_R = \langle \Psi_0^{N+2} | (c_{0,\uparrow}^\dagger c_{R,\downarrow}^\dagger + c_{R,\uparrow}^\dagger c_{0,\downarrow}^\dagger) | \Psi_0^N \rangle, \tag{10}$$

namely $P = 2F_\eta$, with $\eta = (\pm 1, 0)$ or $\eta = (0, \pm 1)$ for a d-wave superconductor, and $P = F_\eta$ with $\eta = (0,0)$ for an s-wave superconductor. A plot of F_R at half filling is shown in Fig. 1. Although the pairing function for $U/t = 4$ is smaller than the corresponding one for free electrons, which vanishes in the thermodynamic limit, the qualitative behavior is completely different. In the former case, F_R appears to have a coherence length as in a true superconductor, whereas in the latter a completely delocalized F_R is observed. Based on the resonating-valence bond (RVB) theory,[16] we want to define a quantity, closely related to F_k, that also makes sense when $P = 0$, as in the insulating case. Indeed, according to the RVB theory, the insulator already contains some sort of pairing, the electrons being paired in RVB singlets. Following this paradigm, we normalize the anomalous pairing function in real space and define the quantity

$$g_R = \frac{F_R}{\sqrt{\sum_{R'} F_{R'}^2}}, \tag{11}$$

where the sum is for all distances in the lattice, compatible with the symmetry of F_R. Notice that, also for an infinite system with a charge gap, though the anomalous average F_R is zero, a finite ratio g_R is still possible. In practice, g_R^2 may be interpreted as the probability function of two electrons added into a singlet state at a distance R and, therefore, determines the pair function, which is the true superconducting

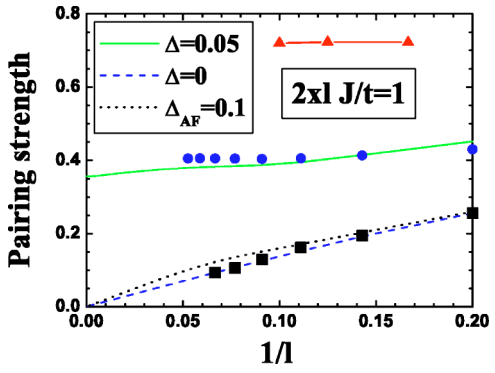

FIG. 2. (Color online) Size scaling of the *d*-wave pairing strength Z_c for different wave functions at half filling: the uncorrelated BCS wave function with $\Delta=0.05$, the free-electron wave function ($\Delta\to 0$), the wave function with a finite antiferromagnetic order parameter [obtained by adding to the $\Delta\to 0$ BCS Hamiltonian a further antiferromagnetic mean-field term $(-1)^i\Delta_{AF}(n_{i,\uparrow}-n_{i,\downarrow})$], the Gutzwiller wave function with $g=1$ (full squares) and the *fully* projected BCS wave function with $\Delta=0.05$ (full circles). The same quantity for the exact ground state of the two-chain *t*-*J* ladder at low doping is also shown (full triangles).

Cooper pair if $P>0$. For a BCS superconductor with a full gap (e.g., with *s*-wave symmetry) g_R is localized with a well-defined coherence length, whereas if the pairing function has nodes, such as in the *d*-wave case, g_R decays with a power law, but, nonetheless, a *finite* amplitude of the pairing function exists at short distance. In strong-coupling superconductivity, the coherence length is expected to be small, and the most important contribution to the pairing function is at the shortest distance η allowed by the symmetry of the pairing function. Therefore, we define the *pairing strength*, that we denote by

$$Z_c = |g_\eta|. \tag{12}$$

In Sec. III, we will show that Z_c is a fundamental quantity that is able to distinguish between simple nonpaired states, such as weakly interacting electron systems or standard band insulators, and states containing paired electrons, such as uncorrelated superconductors or Mott insulators, which cannot be adiabatically connected to band insulators.

III. RESULTS AND DISCUSSION

First of all, we present the results of the pairing strength for simple wave functions, whose properties are well established (see Fig. 2).

In the thermodynamic limit, Z_c is finite for an uncorrelated *d*-wave superconductor and, instead, it vanishes for free electrons, for a weakly correlated electron system, described by the Gutzwiller wave function, and for a spin-density wave insulating state with a finite antiferromagnetic order parameter. While in the former case the wave function obviously contains paired electrons, inducing a finite value of Z_c (and also of the superconducting order parameter P), in the latter cases the wave functions are clearly described within the single-particle picture and the electrons are not paired together, inducing a vanishing Z_c in the thermodynamic limit. Let us now consider much less trivial examples that clearly show that the pairing strength Z_c provides a general and quantitative definition of pairing, which holds not only for simple superconductor systems, but also for much more complicated systems. The first simple case is the *fully* projected *d*-wave superconducting wave function at half filling, where Z_c is finite (see Fig. 2) but the strong constraint of no double occupation, which does not allow us to destroy a pair and create it in a different position, rules out off-diagonal long-range order, i.e., $P=0$. Another striking example comes from the ground state of the *t*-*J* model on the two-leg ladder: in this case the off-diagonal long-range order is suppressed by one-dimensional quantum fluctuations, but, nevertheless, Z_c remains finite (see Fig. 2), showing that the pairing is well defined also in this system, as widely accepted.[17–19]

There is another important reason to study the pairing strength Z_c instead of the order parameter P: in a strongly correlated system the value of the quasiparticle weight Z_N, defined as $Z_N=|\langle\Psi_0^{N+1}|c_k^\dagger|\Psi_0^N\rangle|^2$, can be very small[20,21] and P, if finite, is expected to be at most of the same order. Therefore, whenever Z_N is very small, it is very difficult to detect a nonzero value of the anomalous average P. The suppression of the *d*-wave pairing obtained in previous calculations[11,12] can be explained by the fact that the quasiparticle weight decreases very rapidly with U (see below and Ref. 22). For this reason it is very difficult, at the present time, to detect pairing by studying directly the order parameter or the pairing correlations. The question of a finite anomalous average of order Z_N could be still compatible with the published numerical calculations[11,12] and it is beyond the scope of this paper. On the other hand, the pairing strength Z_c, being a ratio of two quantities of the same order, is not affected by the small quasiparticle weight Z_N and, therefore, represents a much more sensitive detector of pairing, a necessary but in principle not sufficient condition for superconductivity. In the following, we can safely discuss the *d*-wave pairing properties of the Hubbard model because a nonzero value of Z_c appears very clearly, and condensation of pairs is expected at finite doping in two dimensions.

Before considering the quantum Monte Carlo results, we show the results for a small lattice of $L=18$ sites, where it is possible to perform exact diagonalization by the Lanczos algorithm. In Fig. 3, we report the results for Z_c, P, and Z_N as a function of U/t. The comparison between P and Z_N clearly supports our picture: P is small in the strong-coupling Hubbard model because Z_N is small. On the other hand, a much higher signal of paired electrons can be obtained by studying the pairing strength Z_c, which shows a broad maximum $Z_c\simeq 0.5$ for $U/t\simeq 16$, decreasing to the minimum value $Z_c\simeq 0.16$ for $U\to\infty$. At this point, it is useful to compare our exact results with the ones obtained by the simple variational wave function of Eq. (4) with the optimized *d* wave Δ_k and g.[23] Although the value of the anomalous average P and the quasiparticle weight are highly overestimated at strong coupling, this variational wave function provides an excellent estimate of Z_c for all values of $U/t\lesssim 20$, thus capturing the correct feature of pairing.

We now turn to larger systems and calculate the pairing strength by using the zero-temperature Monte Carlo projec-

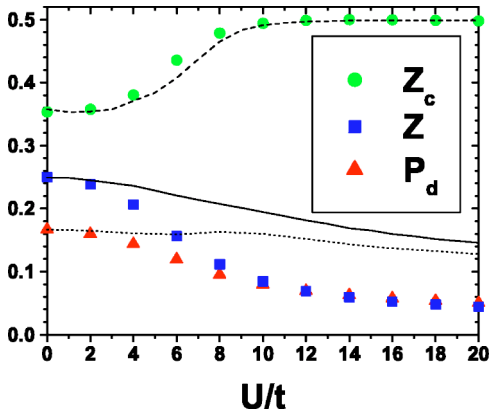

FIG. 3. (Color online) The d-wave pairing strength Z_c (circles) as a function of U in an $L=18$ site cluster with $N^*=L$. The quasiparticle weight Z_N for $N=16$ (squares) at the momentum $(2\pi/3,0)$ and the short-distance anomalous average P (triangles) are also shown. Continuous (Z_N), long dashed (Z_c), and dotted (P) lines correspond to the variational calculation with the variational wave function of Eq. (4) with an optimized Δ_k and projected onto the subspaces with 16 and 18 electrons.

tion technique based on auxiliary fields.[15] The inclusion of the simple Gutzwiller factor $\mathcal{J}$, which improves substantially the convergence in imaginary time τ, is particularly important because, at finite doping, the sign problem prevents us from working with arbitrary large imaginary time.

Firstly, we consider the half-filled case. Remarkably, for large systems, Z_c increases with the projection time τ (see Fig. 4). In this case, in order to reduce the size effects, we have performed the finite-size scaling of $Z_c - Z_c^G$, where Z_c^G is the value corresponding to the Gutzwiller wave function $|\Psi_G\rangle$ with $\Delta \to 0$ [$Z_c^G \to 0$ in the thermodynamic limit (see Fig. 2)]. Already for $L=50$ sites, the evaluation of the pairing strength is rather accurate and close to larger sizes. As shown in Fig. 4, Z_c increases monotonically with τ, and the value for $\tau=6$ should safely represent, for all sizes considered, a rather accurate lower bound for the $\tau \to \infty$ limit. The thermodynamic limit of Z_c appears therefore clearly finite, considering also that for $\tau=6$, $Z_c - Z_c^G$ *increases* with the system size (see the inset of Fig. 4). Our extrapolation is consistent

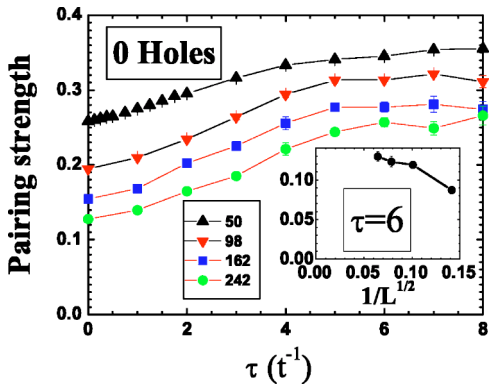

FIG. 4. (Color online) The d-wave pairing strength Z_c as a function of the projection time τ for different clusters at half filling. The inset shows the finite size scaling of $Z_c - Z_c^G$ for $\tau=6$.

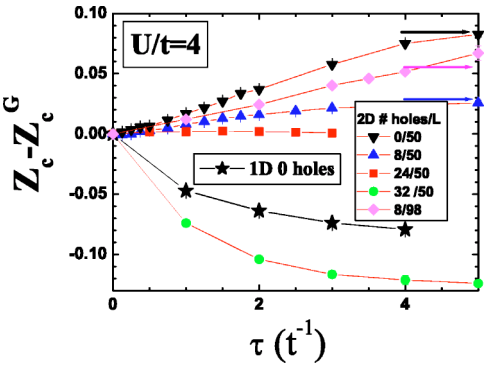

FIG. 5. (Color online) The d-wave pairing strength $Z_c - Z_c^G$ as a function of the projection time τ for different dopings. The arrows indicate the value of Z_c corresponding to the variational wave function of Eq. (4) with an optimized Δ_k for zero and eight holes. Z_c for the s-wave pairing in one dimension is also shown. In this case, the value of the pairing F_R at the nearest-neighbor distance is smaller than the corresponding on-site value, despite the repulsive interaction U.

with a *finite* $Z_c \gtrsim 0.1$ in the thermodynamic limit. It is important to stress that this is a purely ground-state property, since the initial state does not contain a sizable pairing and the imaginary time projection unambiguously increase the pairing strength. It is worth noting that, in this case, a finite value of Z_c does not mean that the ground state is superconducting, but only that two added electrons in the half-filled Hubbard model are paired together in a d-wave singlet.

In the doped case, the limitation of the sign problem and the strong dependence upon hole doping prevent us from performing an accurate finite-size scaling, but, as shown in Fig. 5, the effect remains rather clear, and $Z_c - Z_c^G$ increases immediately as soon as the projection time is turned on. On the other hand, at large enough doping, we have found the opposite effect, clearly against d-wave pairing. Interestingly, also the s-wave pairing strength, obtained by using an initial wave function $|\Psi_G\rangle$ with s-wave symmetry, is not enhanced by the imaginary time projection (not shown). However, we have not checked other symmetry sectors such as p or d_{xy} and, therefore, at large doping there maybe other types of pairing instabilities.[24] It is remarkable that also for large clusters the simple Gutzwiller wave function with a finite, and optimized, d-wave gap function (stabilized in the underdoped region) describes accurately the enhanced pairing strength Z_c, as shown by the arrows in Fig. 5.

Finally, it is important to emphasize that a finite Z_c is a peculiar aspect of purely two-dimensional systems, as, for instance, in one dimension no evidence of a finite pairing strength is found even at half filling (see Fig. 5).

To conclude, it turns out that the pairing is a robust property of two-dimensional lightly doped Mott insulators and appears already in small size calculations. The pairing strength Z_c increases with decreasing doping and has its maximum at half filling, where phase coherence is inhibited by the charge gap. We argue that a finite pairing strength for an insulator is just the *qualitative* feature that discriminates a band insulator, for which a single-particle description holds, from RVB insulator, which is defined in terms of singlet

pairs, as in a fully projected BCS wave function of Eq. (4). Within this framework, determined by the measurable quantity Z_c and *independent of the variational ansatz*, we discover the possibility of having a RVB-like insulator when the existence of a finite pairing strength is accompanied by the antiferromagnetic long-range order, as in the half-filled Hubbard model.[25] In this simple model, the insulator is somehow prepared to become a superconductor (with *d*-wave symmetry) and a small amount of doping allows the propagation of the RVB pairs.[16] This scenario offers a simple and natural explanation of the ultimate mechanism of the high-temperature superconductivity.

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