Effects of strong correlations and disorder in *d*-wave superconductors

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We use exact diagonalization techniques to study the interplay between strong correlations, superconductivity, and disorder in a model system. We study an extension of the *t*-*J* model by adding an infinite-range *d*-wave superconductivity inducing term and disorder. Our work shows that in the clean case the magnitude of the order parameter is surprisingly small for low-hole filling, thus implying that mean-field theories might be least accurate in that important regime. We demonstrate that substantial disorder is required to destroy a *d*-wave superconducting state for low-hole doping. We provide the first bias free numerical results for the local density of states of a strongly correlated *d*-wave superconducting model, relevant for STM measurements at various fillings and disorders.

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The combination of strong correlations and reduced dimensionality makes the theoretical understanding of high-T_c superconductivity very difficult and consensus on its origin has not been reached.[1–3] Very recently, experiments using local probes, such as scanning tunneling spectroscopy (STS) and scanning tunneling microscopy (STM), have shown that the doped cuprates are highly inhomogeneous[4] (for a recent review, see Ref. 5). Specific aspects of high-T_c superconductivity, such as the robustness of the tunneling spectrum with respect to disorder,[6] emphasize its contrast with more conventional disorder sensitive[7] BCS-type superconductivity.

In this work, we probe the effects of strong correlations and disorder in *d*-wave superconductors derived from a Mott insulator. We introduce and study a generalized model derived from the *t*-*J* model[8] in which a superconducting (SC) ground state is argued to be inevitable. We consider a Hamiltonian $\mathcal{H}=\mathcal{H}_{tJ}+\mathcal{H}_d+\mathcal{H}_{\text{random}}$, with

$$\mathcal{H}_{tJ} = - t \sum_{\langle i,j\rangle\sigma} [\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{j\sigma} + \text{H.c.}] + J\sum_{\langle i,j\rangle}\left[\mathbf{S}_i\cdot\mathbf{S}_j - \frac{1}{4}n_i n_j\right], \quad (1)$$

where the sum $\langle i,j\rangle$ runs over nearest-neighbor sites, $\sigma=(\uparrow,\downarrow)$, and standard definitions for the projected creation and annihilation operators are employed.[8]

The *t*-*J* model is microscopically justified from either the one-band Hubbard model by a large U expansion or more generally from a reduction of the three-band copper oxide model to a single-band model,[9] with a greater freedom for the parameter ratio $J/|t|$. While a mean-field theory (MFT) for the doped *t*-*J* model[10,11] gives a *d*-wave SC ground state, it is an uncontrolled approximation. In the MFT, there are often states with other broken symmetries in the proximity of the superconductor that can be missed. Most importantly, in view of the very strong constraint of single occupancy in the model, we expect significant quantum fluctuations and the MFT cannot handle these precisely. Therefore it is not clear that the *t*-*J* model *does* have a SC ground state for the ranges of parameters studied. In order to precipitate a SC starting state, we add an attractive term

$$\mathcal{H}_d = -\frac{\lambda_d}{L}\sum_{i,j=1}^{L} D_i^{\dagger} D_j, \quad (2)$$

where $D_i=(\Delta_{i,i+\hat{x}}-\Delta_{i,i+\hat{y}})$, $\Delta_{ij}=\tilde{c}_{i\uparrow}\tilde{c}_{j\downarrow}+\tilde{c}_{j\uparrow}\tilde{c}_{i\downarrow}$, and L is the number of lattice sites. This is an infinite-range term of the type that BCS considered in their reduced Hamiltonian,[12] while building in the *d*-wave symmetry of SC order. We have also considered imposing an extended *s*-wave symmetry, where the results are qualitatively quite different and will be reported elsewhere. Within MFT, this model leads to the same *d*-wave state as found from the *t*-*J* model.[10,11] Our model is presumably a superconductor *for any* $\lambda_d \sim O(1)$ in the thermodynamic limit, and *for sufficiently large* λ_d, for any reasonable finite cluster. Notice that we have sidestepped the issue of the "mechanism" of superconductivity, which cannot be settled with studies of the kind undertaken here and focus instead on the nature of the state so produced. We argue below that despite the infinite-ranged nature of H_d, strong correlations produce a non-mean-field-like state; this state has an unexpectedly small order parameter (OP).

Finally, we consider a quenched random disorder term of the form

$$\mathcal{H}_{\text{random}} = \sum_i \varepsilon_i n_i, \quad (3)$$

where the ε_i's are taken randomly from a uniform distribution between $[-\Gamma,\Gamma]$. The full Hamiltonian Eqs. (1)–(3) thus describes an inhomogeneous strongly correlated superconductor. In our study, we use numerical diagonalization of clusters with 18 and 20 sites. The dimension of the largest Hilbert space diagonalized here is $\sim 10^8$.

In our model, we are interested in understanding how the evolution into the SC state occurs as λ_d is turned on. Toward this end, we show in Fig. 1 the derivative of the energy (main panels) and the energy itself (insets) as λ_d is increased, for different fillings of the 18 and 20 site clusters. For low fillings of electrons [Fig. 1(a)], we find that for certain cases of the number of particles, level crossings occur, as signaled by a jump in the energy derivative, indicating a change of the

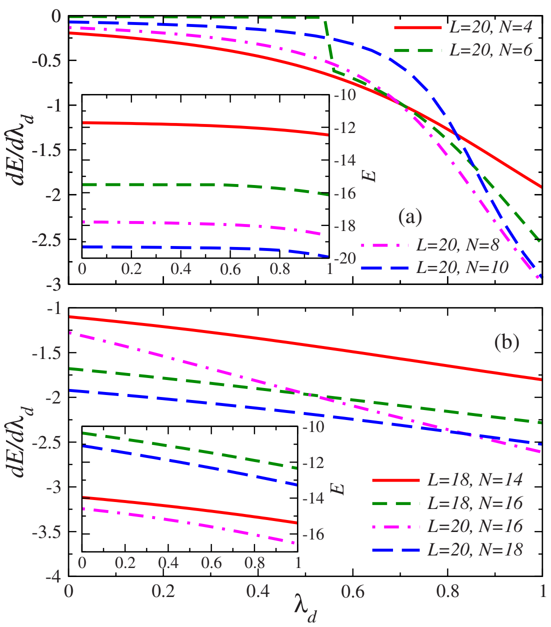

FIG. 1. (Color online) Energy (insets) and its derivative (main panels) vs λ_d. (a) Low density of particles (less correlated) and (b) low density of holes (strongly correlated). N is the number of electrons and $J=0.3$. All energies are in units of t.

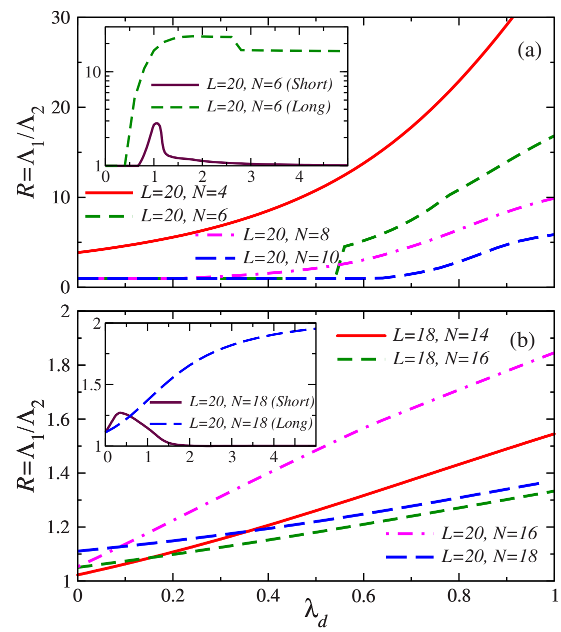

FIG. 2. (Color online) Ratio $R=\Lambda_1/\Lambda_2$ with increasing λ_d. (a) Low density of particles (less correlated) and (b) low density of holes (strongly correlated). In the insets, we compare the infinite-range model [Eq. (2)] with a short-range version of Eq. (2) (taking $i=j$ and dropping the L in the denominator) up to larger values of λ_d. N is the number of electrons and $J=0.3$.

symmetry of the ground state.[13] A similar jump is seen for *all fillings* between $N=4$ and $N=10$ in the 18-site cluster [not shown in Fig. 1(a)]. On the other hand, we find that for low-hole fillings in the 18 and 20 site clusters, the energy derivative is continuous with λ_d, suggesting a particular compatibility between the d-wave order and the t-J model. It is interesting that there is evidence of this compatibility from high-temperature expansions[14] and exact diagonalization studies,[15] which are also unbiased such as the present one.

One of our diagnostic tools for studying the nature of the SC state is the d-wave pair density matrix $P_{ij}=\langle D_i^\dagger D_j\rangle$.[16] Its largest ($\Lambda_1$) and next largest ($\Lambda_2$) eigenvalues are computed and their ratio $R(\geq 1)$ is monitored. This ratio is an effective probe of the order, both for clean and disordered superconductors. Taking the ratio eliminates uninteresting normalization effects related to the change in the particle density, etc. This procedure, for example, eliminates the expected diminishing of all the eigenvalues of P_{ij} as the hole doping decreases (due to Gutzwiller correlations). It is thus constructed as a pure number. For a SC ground state, it is expected to scale for large L like $R\sim\Psi^2 L+\Phi$, where Ψ is the dimensionless $O(1)$ OP (Ref. 16) and $\Phi\sim O(1)$ represents the depletion (i.e., spillover) from the condensate. This depletion occurs due to repulsive interactions, i.e., strong correlations. In the parallel case of a Bose system with N_b bosons,[17] we expect $\Lambda_1\sim O(N_b)$ while $\Lambda_2\sim O(1)$.

In Fig. 2, we show $R=\Lambda_1/\Lambda_2$ for different fillings of the 18 and 20 lattices as a function of λ_d. By comparing the low *electron* filling [Fig. 2(a)] to the low-*hole* doping case [Fig. 2(b)], one can gauge the effects of correlations for overdoped (a), and optimal or underdoped cuprates (b). For the lowest electron densities ($N=4$), R reaches very large values ($R>30$) and decreases as the density is increased, up to around $R\sim 6$ for ten electrons. We notice that sometimes for low electron filling one needs λ_d to exceed a critical value before R starts increasing, e.g., $N=6$ in Fig. 2(a). This is a signature of a quantum phase transition into a SC state and occurs in many but not all instances. The transition point coincides with the jump seen in the derivative of the energy in Fig. 1. Taken together, these confirm that the new ground state has a different symmetry than the ground state of the plain vanilla t-J model.

On the opposite end, for low-hole doping [two and four holes in 18 and 20 sites in Fig. 2(b)], one can see that R increases continuously with λ_d, i.e., no abrupt transition occurs. Figure 2(b) also shows that in that regime R increases very slowly with λ_d and does not exceed $R=2$ for $\lambda_d\leq 1$. We can interpret this as a small value of Ψ and a large value of Φ as defined above, implying a large depletion of the condensate. This shows that even in our infinite-range model, the SC OP at low doping is very strongly depleted. However by no means should we understand that *superconductivity* is weaker in that regime. From studies of purely bosonic systems, it is known that due to strong correlations, the superfluid (SC) fraction (i.e., ρ_s) can be much larger than the condensate fraction (i.e., the OP Ψ) (see, e.g., Ref. 18). Correlations also tend to make superfluidity (superconductivity) more stable against perturbations.

We now compare our results for the infinite-range model of Eq. (2) to those produced by the more standard short-range case [Eq. (2), for $i=j$ and no normalization by L in the denominator] used in the literature dealing with the Hubbard model. The insets in Fig. 2 show that while in the infinite-range model R saturates with increasing λ_d, in the short-range model R attains a maximum value for $\lambda_d\sim 1$ and then decreases toward unity. The latter occurs because for $\lambda_d\gg 1$

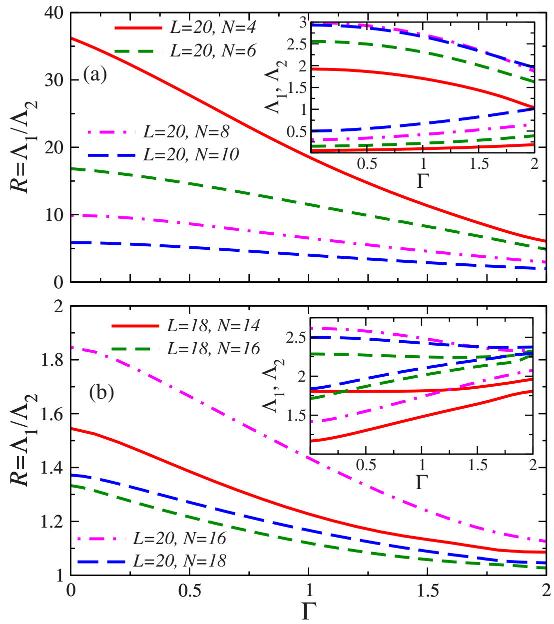

FIG. 3. (Color online) Ratio $R=\Lambda_1/\Lambda_2$ with increasing disorder (Γ). (a) Low density of particles (less correlated) and (b) low density of holes (strongly correlated). In the insets, we show the separate values of Λ_1 (upper plots) and Λ_2 (lower plots), corresponding to the results shown in the main panels. Here $J=0.3$ and $\lambda_d=1$. These results were obtained averaging over ten different disorder realizations.

one produces localized pairs, i.e., there is no long-range coherence.

Turning to disorder, in the main panel in Fig. 3, we show how R evolves with increasing disorder for $\lambda_d=1$. (Those results were obtained averaging over ten different disorder realizations.) Here one can see that disorder produces a very large reduction of Λ_1/Λ_2 for low electron filling, i.e., disorder has a very large impact on the SC OP. For the case of low-hole density, the relative reduction of Λ_1/Λ_2 is much smaller, i.e., as λ_d had a small effect in increasing R, so is Γ having a smaller effect in reducing it.

From the main panels in Fig. 3 we see that the effect of disorder in the SC state is always to make R decrease. It is of considerable interests to understand what happens to Λ_1 and Λ_2 separately as Γ is increased. Results for these quantities are presented in the insets in Fig. 3. There one can see that Λ_1 behaves qualitatively very differently between low-electron fillings and low-hole fillings. In the first case Λ_1 exhibits a very large reduction, which points toward the destruction of superconductivity. On the other hand, for low-hole doping, Λ_1 is almost unaffected by the increase of disorder and can even be enhanced, as shown for 14 particles in 18 sites. Unexpectedly, the reduction of R in this case is related to an increase of Λ_2. This increases points toward a slower decay of P_{ij} when disorder is increased. This suggests the possibility of an emerging algebraic long-range order, producing a different signature in the density matrix than the case of standard LRO. For example, in the 2D *XY* model below T_c, or in the 1D Heisenberg antiferromagnetic ground state, there is no true LRO, but several of the largest density-matrix eigenvalues scale as L^{η}, with $\eta<1$. The system sizes

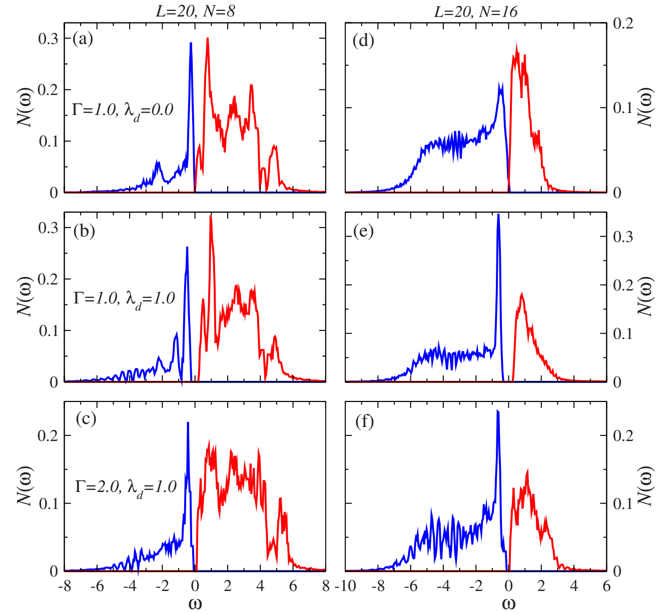

FIG. 4. (Color online) Averaged density of states $[N(\omega)]$ for two different fillings ($N=8$ and $N=16$) of the 20-site cluster. We show results for [(a) and (d)] $\Gamma=1$ and $\lambda_d=0$, [(b) and (e)] $\Gamma=1$ and $\lambda_d=1$, and [(c) and (f)] $\Gamma=2$ and $\lambda_d=1$. $N(\omega)$ was computed as the average over different lattice sites and over two different disorder realizations.

we treat here are too small to make definitive statements. However, it is interesting to note that for low-hole doping the behavior is qualitatively different from the low electron filling, in which the largest eigenvalue exhibits a large decrease with increasing disorder. An analysis of the data for the *s*-wave superconductor studied in Ref. 19 exhibits exactly the latter behavior, in contrast to the one we see for the SC *t-J* model in the low-hole doping regime. Our results therefore suggest unusual power-law type superconductivity in the presence of disorder close to half filling.

In order to make connection with experimentally measurable STM curves, we show in Fig. 4 the local density of states of the $L=20$ site cluster for two different fillings in the presence of disorder and λ_d. Figures 4(a) and 4(d) correspond to fillings where the ground state of the plain *t-J* model ($\lambda_d=0$) is adiabatically connected to the SC ground state at finite λ_d. In the presence of disorder, the density of states is similar to the one reported previously for the translational invariant *t-J* model with $L=16$ sites.[20] These curves display a striking asymmetry between adding a particle and taking out a particle, and the evolution of this asymmetry with doping is similar to that of the clean *t-J* model.

Adding the SC term ($\lambda_d>0$) to the disordered system opens a gap. This can be clearly seen in Figs. 4(b) and 4(e). Our system sizes are too small to see the V shape expected for a *d*-wave superconductor, i.e., we see a real gap. As disorder is increased, Figs. 4(c) and 4(f) show the reduction of the gap. From the results shown in Fig. 4, we see that the SC gap closes only for a substantial disorder ($\Gamma \gtrsim 2\lambda_d$). Our calculations therefore also shed light on this aspect of the STM spectra, namely, the robustness against disorder.

In conclusion, we have presented and studied a variant of the *t-J* model, with an infinite-range *d*-wave superconducting term. We have shown how the energy, its derivative, and the *d*-wave superconducting order parameter evolve with increasing the strength of the superconducting term. In addition to discontinuities in all the above quantities for low electron densities, we find a severe reduction of the magnitude of the order parameter at low-hole filling. This is a signature of strong quantum fluctuations near the Mott insulator. In relation to current STM experiments, we find that superconductivity survives considerable disorder close to half filling. The local density-of-states curves yield bias free (i.e., nonvariational) results for a strongly correlated *d*-wave superconductor in the presence of disorder and provide a picture of the large energy scale structure of this important object.

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