Quadrupolar-fluctuation model for high-T_c superconductivity: A quantum Monte Carlo study

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We present results for quantum Monte Carlo simulations of the quadrupolar fluctuation model of high-temperature superconductivity. The simulations focused on measurement of the pairing susceptibility in various interesting pairing channels (on-site, nearest-neighbor, and second-nearest-neighbor s- and d-wave pairing). The lattice was 4×4 in the oxygen sites, with eight copper sites bearing quadrupole moments. Exchange of these quadrupolar fluctuations may lead to attraction between oxygen holes. As in weak-coupling theory, we find (i) favorable tendencies towards second-nearest-neighbor s- and d-wave filling, with larger doping favoring d-wave symmetry; (ii) a nonmonotonic dependence of the pairing tendencies upon the on-site quadrupole level splitting; and (iii) a strong suppression of all nearest-neighbor pairing.

I. INTRODUCTION

A promising mechanism proposed for the explanation of high-temperature superconductivity in the cuprate-based materials is based upon the quadrupolar fluctuation or intrasite d-d charge-transfer idea. In this picture, versions of which were first proposed by Weber[1,2] and independently by Gaidedey and Loktev,[3] itinerant holes nominally residing in oxygen orbitals in the Cu-O network are paired by the exchange of rather localized quadrupolar fluctuations on the copper sites. The key qualitative ideas are displayed in Fig. 1. The quadrupolar fluctuation is the virtual population of an excited $3d_{3z^2-r^2}$ state via excitation from the ground $3d_{x^2-y^2}$ state. Mechanistically, the in-plane interaction energy between holes on Cu and O sites may be lowered by this virtual population. Upon virtual population of the out-of-plane orbital, a relative negative excess of charge occurs in the plane (at least around certain oxygen sites) which leads to an effective hole-hole attraction.

We have argued elsewhere[4] that this mechanism enjoys some empirical support through (i) observed correlations of the energy splitting Δ_{dd} between the $3d_{x^2-y^2}$ and $3d_{3z^2-r^2}$ levels with T_c,[5] and (ii) the compound-dependent pressure dependence of T_c observed for the cuprates. It is thus prudent to examine the mechanism in some theoretical detail to determine its robustness as a candidate for high-temperature superconductivity.

In previous studies in which we have participated,[4,6] utilizing a more complete picture of the oxygen-hole–copper-quadrupole interaction than for Refs. 1–3 we have performed symmetry analyses of pair wave functions within weak-coupling BCS formalism utilizing lowest-order estimates of the pairing interaction. In this approach we find, dependent upon the density of carriers, either s-wave (low-density) or d-wave (high density) pair states. At sufficiently high density, the resulting critical temperatures are of plausibly high values to account for superconductivity in these materials.

In reality, the weak-coupling approach is flawed for a number of reasons, the foremost being (i) a neglect of high-order corrections to the (irreducible) pairing interaction, and (ii) a restriction to the parameter region where the excitation energy Δ_{dd} (which plays the role of the Debye energy in this theory) is small compared with the overall carrier bandwidth W. In fact, the strength of hole-quadrupole couplings, Δ_{dd}, and W may all be fairly comparable so that a full nonperturbative, non-weak-coupling treatment of the problem is appropriate. In other words, there is no "Migdal parameter" that affords confidence with weak-coupling or even Eliashberg theory

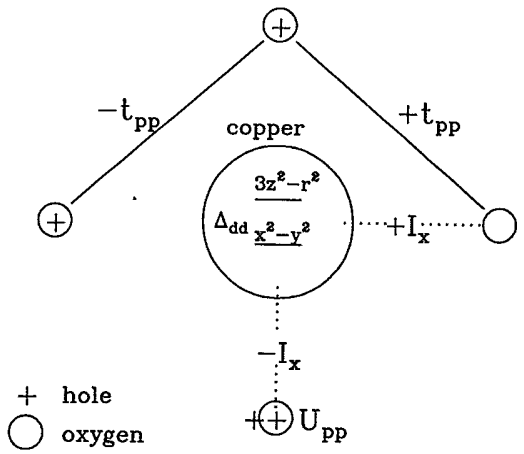

FIG. 1. Schematic model of the quadrupole fluctuation mechanism. Itinerant oxygen holes, which hop via matrix element t_{pp} with phasing as shown, and possess on-site Hubbard interaction U_{pp}, interact with copper-quadrupole moments at the center of every other oxygen plaquette via the phased interaction denoted by I_x. Physically, this interaction corresponds to dynamically induced mixing of the $3d(x^2-y^2)$ levels and $3d(3z^2-r^2)$ levels in the presence of an oxygen hole on a neighboring site. The transition energy is Δ_{dd}, and the Coulomb energy on the oxygen site is infinite, so the quadrupole degrees of freedom may be described by the pseudospin variables $\tau_z=n_{dx^2-y^2}-n_{d3z^2-r^2}$, and τ_x which flips the levels.

treatments of the problem.

The purpose of the present work is to solve, essentially exactly, a restricted version of the quadrupolar fluctuation model to see whether the tendencies to pairing produced by weak coupling theory hold up in a better treatment. We have employed fermion Monte Carlo techniques to calculate the pair field susceptibilities of appropriate symmetry pair states on finite-sized lattices. Our main conclusion is that within this restricted model, the pairing tendencies exhibited in the weak-coupling theory are supported by the Monte Carlo calculations.

Our paper is organized as follows. In Sec. II, we outline the model, review the previous work using weak-coupling theory, give the details of our Monte Carlo algorithm, summarize our new results, and compare to the weak-coupling theory. In Sec. III we conclude and assess the limitations of the present study with an eye towards future work.

II. MODEL, METHOD, AND RESULTS

A. Model

The essential features of the model are illustrated in Fig. 1 (a more detailed description of the Hamiltonian may be found in Sec. III). Holes are presumed, for definiteness, to reside in planar nonbonding or π orbitals on the oxygen sites. These are described by next-nearest-neighbor tight-binding theory and assumed to possess an on-site Coulomb energy of U_{pp}. Only the quadrupolar degrees of freedom of the Cu ions are retained, and these are described conveniently in terms of a pseudospin variable σ, with pseudospin σ_z up (down) corresponding to the occupancy of the $3d_{x^2-y^2}$ ($3d_{3z^2-r^2}$) orbital. The holes couple to the quadrupolar transition operator σ_x through the interaction constants I_x which depend upon the site where the holes reside. For example, a hole on the $+x$ site of Fig. 1 has opposite quadrupolar interaction strength to a hole on the $+y$ site.

We restrict our model to include only the I_x coupling terms. Within this restricted model, we shall calculate to all orders in I_x. This restriction immediately throws out two key pieces of physics: (1) First, it omits Hartree-like renormalizations of the splitting Δ_{dd}. (2) Second, it omits the possibility of a Kondo effect which arises only when coupling of the itinerant holes to the σ_z pseudospin is included. We shall return to a discussion of these ideas in Section III.

To summarize this subsection, our model Hamiltonian may be written in form

$$H = H_{pp} + H_{dd} + H_{pd} \tag{2.1}$$

with

$$H_{pp} = \sum_{\langle ij \rangle \sigma} t_{\langle ij \rangle} (p^{\dagger}_{i\sigma} p_{j\sigma} + \text{H.c}) + \sum_{l} U_{pp} n_{pi\uparrow} n_{pi\downarrow} , \tag{2.2}$$

where $\langle ij \rangle$ represents a sum on nearest neighbors on the oxygen sublattice, $t_{\langle ij \rangle}$ represents the properly phased nearest-neighbor hopping of oxygen holes, $p^{\dagger}_{i\sigma}$ creates an oxygen hole of spin σ on site i, and $n_{pi\sigma}$ is the oxygen number operator for spin σ on site i;

$$H_{dd} = \sum_{l} \Delta_{dd} \sigma_{zl} + \bar{t} \sigma_{xl} , \tag{2.3}$$

where l indexes Cu sites, σ_{zl} represents the quadrupolar pseudospin on site l, the up (down) pseudospin is the $3d_{x^2-y^2}$ ($3d_{3z^2-r^2}$) level, and σ_{xi} represents the flipping component of the pseudospin. Note that $\bar{t}$, the mixing strength, vanishes in tetragonal symmetry;

$$H_{pd} = \sum_{\langle li \rangle} I_{xi} \sigma_{xl} n_{pi} , \tag{2.4}$$

where $\langle li \rangle$ sums over Cu sites l and those oxygens immediately neighboring, I_{xi} is the properly phased coupling strength between the total oxygen hole occupancy n_{pi} and the quadrupolar flip operator σ_{xi}.

B. Summary of previous results from weak-coupling theory

In weak-coupling theory, one simply computes the effective hole-hole interaction to second order in I_x, giving it, in a local picture, a magnitude of I_x^2/Δ_{dd} between all holes surrounding a given Cu site. However, the sign of the interaction varies; nearest-neighbor oxygen holes feel a repulsion through this interaction, while on-site pairs and next-nearest-neighbor pairs feel an attraction. Because of the on-site Coulomb repulsion, on-site pairing is strongly disfavored, and we anticipate that next-nearest-neighbor s- or d-wave-like pairing should occur. The symmetry of the s (d) -wave pair is $\cos(k_x a) \pm \cos(k_y a)$.

Within the weak-coupling approach, we have solved the BCS gap equation for different pairing symmetries (the one with the largest transition temperature is most favored for superconductivity).[4] We have also accounted for the Coulombic energies within a pseudopotential approximation. We assume that the cutoff energy (given by Δ_{dd}) is small compared to the bandwidth. We have found that for all filling, if the tetragonal symmetry of the lattice is retained, the d-wave state is most stable. However, if the lattice is made orthorhombic, the nearest-neighbor repulsion is reduced sufficiently to allow s-wave pairing to stabilize at low filling. For low filling of the oxygen hole band, the next-nearest-neighbor s-wave state is possible, while for higher filling the d-wave-like state is favored. (In an orthorhombic crystal, the symmetry distinction between s- and d-wave states is lost, as is the distinction between the low-lying copper $3d$ states.) We also anticipate a nonmonotonic dependence of transition temperature upon Δ_{dd}, at least for sufficiently large filling. The transition temperature T_c should peak at some optimal filling.

Note that this is mean-field theory for a single copper oxide layer, which in reality should at most exhibit a Kosterlitz-Thouless transition. However, we expect, as do most workers, that the interlayer coupling restores the full three dimensionality but that the superconducting transition is driven by the intralayer physics. (Note that the absence of full three-dimensional cubic symmetry is important here: there Δ_{dd} would be zero, and in the absence of higher-order effects, T_c would vanish. Hence the two dimensionality enters in this sense.) Thus the most

stable symmetry should still exhibit a singular signature in the corresponding pair field susceptibility in the thermodynamic limit which would be measurable in Monte Carlo simulations in principle.

C. Monte Carlo method

We used the embedded method of Monte Carlo simulation described by Hirsch and Fye.[7] We chose this method as it is both stable at low temperatures and allows easy measurement of quantities off-diagonal in the imaginary time, such as the pair field susceptibility. In this simulation the problem is cast into a discrete path-integral formalism in imaginary time τ_l where $\tau_l = l\Delta\tau$, $\Delta\tau = \beta/L$, and L is the number of time slices. A discrete Hubbard-Stratonovich transformation on the oxygen correlation terms, which introduces an Ising field $s(\tau_l)$, is used to make the Hamiltonian quadratic in fermion operators. The fermion degrees of freedom are then integrated out, and one is left with an effective action which is a function of the $s(\tau_l)$ and the quadrupolar fields. The Monte Carlo algorithm is constructed to provide an importance sampling of these fields. We have taken $\Delta\tau = 0.25$ and studied β values as large as 6 in units where $t_{pp} = 1.0$. The systematic errors associated with the finite value of $\Delta\tau$ were estimated to be typically of order 2%.

D. New results of the Monte Carlo simulations

In the Monte Carlo simulations we have examined small lattices possessing at most 16 oxygen sites and 8 copper sites with periodic boundary conditions. We have measured the pair field susceptibilities for on-site s-wave, next-nearest-neighbor s- and d-wave pair symmetries, and second-nearest-neighbor pairing susceptibilities. The definition of the susceptibility P_α is, for a pair field operator Δ_α of symmetry α, given by

$$P_\alpha = \int_0^\beta d\tau \langle \Delta_\alpha^\dagger(\tau)\Delta_\alpha \rangle \ . \tag{2.5}$$

This susceptibility will diverge at the onset of a superconducting instability (even of the Kosterlitz-Thouless variety) to a state with pair symmetry α.

Working on the oxygen sublattice, indexed by positions i, i', say, the pair field operators of relevance are

$$\Delta_s = \sum_i p_{i\uparrow}^\dagger p_{i\downarrow}^\dagger \ , \tag{2.6}$$

$$\Delta_{xs} = \sum_{\langle ii' \rangle} (p_{i\uparrow}^\dagger p_{i'\downarrow}^\dagger - p_{i\downarrow}^\dagger p_{i'\uparrow}^\dagger) \ , \tag{2.7}$$

$$\Delta_{xd} = \sum_{\langle ii' \rangle} P_{ii'} (p_{i\uparrow}^\dagger p_{i'\downarrow}^\dagger) \ , \tag{2.8}$$

where $P_{ii'} = \mathrm{sgn}(R_{i'x} - R_{ix})\mathrm{sgn}(R_{i'y} - R_{ij})$,

$$\Delta_{xxs} = \sum_{i,\delta} (p_{i\uparrow}^\dagger p_{i+\delta\downarrow} - p_{i\downarrow}^\dagger p_{i+\delta\uparrow}^\dagger) \ , \tag{2.9}$$

with δ indexing nearest-neighbor vectors for the copper sublattice, and

$$\Delta_{xxd} = \sum_{i,\delta} P_\delta (p_{i\uparrow}^\dagger p_{i+\delta\downarrow}^\dagger - p_{i\downarrow}^\dagger p_{i+\delta\uparrow}^\dagger) \ , \tag{2.10}$$

where P_δ is a phase factor that is negative for δ along the y direction, and positive for δ along the x direction. Clearly Δ_s denotes the conventional on-site pair field, Δ_{xd} the d-wave pair field of nearest-neighbor holes, Δ_{xs} the s-wave pair field of nearest-neighbor holes, xxs the s-wave pair field of second-nearest-neighbor holes (on the oxygen sublattice) and xxd the second-nearest-neighbor d-wave pair field.

The raw pair field susceptibility is of little value in determining any pairing tendencies, for two well-known reasons: (i) the noninteracting susceptibility already diverges at zero temperature due to the singular energy denominators in a spectral representation, and (ii) strict comparison to the noninteracting susceptibility is misleading since it is quasiparticles that pair and "uninteresting" wave function and vertex renormalization effects may suppress the pair field susceptibility at a given temperature relative to the noninteracting limit.

We have therefore followed the convention of White *et al.*[8] by measuring the reduced susceptibility defined by

$$p_\alpha = (P_\alpha - P_{\alpha 0})/P_{\alpha 0} \ , \tag{2.11}$$

where $P_{\alpha 0}$ corresponds to the bubble diagram containing renormalized oxygen hole Green's functions but no interaction lines (see Fig. 2). Since the tendency towards pairing will be exhibited in the interaction-induced contributions to the pair field susceptibility, this reduced susceptibility should unambiguously exhibit enhanced pairing correlations. Put another way, it will determine the sign of the pairing interactions in the relevant channel. On the other hand, this comparison compensates for renormalization factors omitted in a straight comparison to the noninteracting pair field susceptibility.

Our results are displayed in Figs. 3–10. We denote the pairing symmetries considered in this paper as s for on-site s-wave pairing, xxd for next-nearest-neighbor d-wave pairing, and xxs for next-nearest-neighbor s-wave pairing. We have measured the pair field susceptibilities at the lowest accessible and meaningful temperatures as functions of band filling ρ, d-level splitting Δ_{dd}, hole-quadrupole–moment coupling I_x, and on-site oxygen Coulomb energy U_{pp}. Note that the xs and xd susceptibilities are uniformly suppressed by I_x, and so are not included in Figs. 3–8.

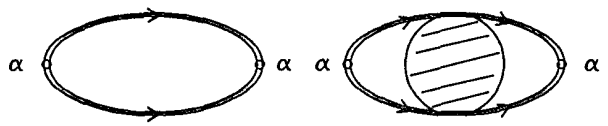

FIG. 2. Reduced pairing susceptibility diagrams. Following Ref. 8 we measure the reduced susceptibility as follows: compute the bubble diagram at left for the fully renormalized oxygen-hole Green's function and compute the full pair susceptibility (bubble plus diagram at right). If the interaction dressed diagram at right is positive, the pairing interaction is attractive and the susceptibility is enhanced. The reduced susceptibility is the full susceptibility minus the bubble contribution divided by the bubble contribution.

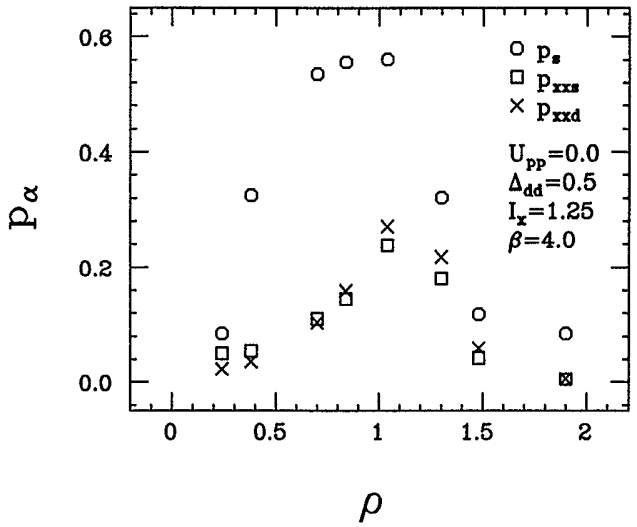

FIG. 3. Reduced pairing susceptibility vs filling ($U_{pp}=0$). All energies and temperatures are measured in units of the oxygen hopping t_{pp}. $\beta=4$ is the largest inverse temperature reasonable for this lattice size (4×4 on the oxygen sublattice). For these calculations, the oxygen Coulomb energy U_{pp} was turned off, which explains the pronounced enhancement of on-site s-wave pairing. Note the nonmonotonic dependence of second-neighbor s- and d-wave pairing upon filling. The dropoff at larger fillings is due to the onset of a charge-density wave corresponding to intracell transfer of oxygen charge (e.g., $p_x \rightarrow p_y$) which is suppressed by U_{pp}. Namely, one would have an array of bipolarons bound by the quadrupole-mediated attraction along either the x or y direction. Note that for this figure and Figs. 4–8, the nearest-neighbor pairing susceptibilities are now shown, as they are uniformly suppressed when I_x is finite.

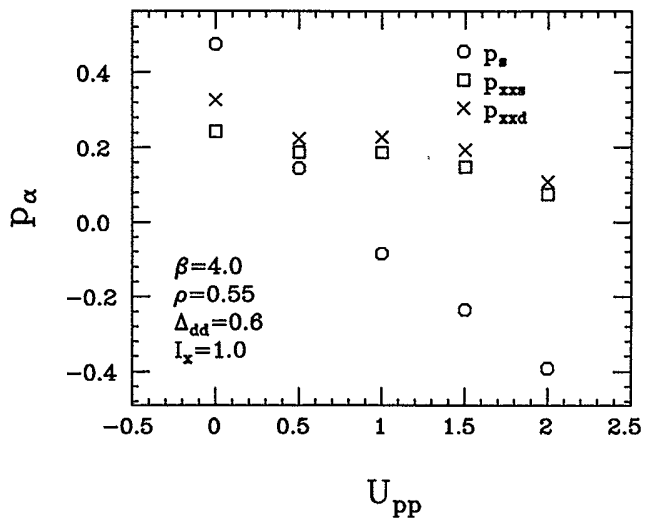

FIG. 4. Reduced pairing susceptibility vs oxygen Coulomb energy U_{pp} at fixed filling. Turning on a moderate U_{pp} value immediately renders the on-site pairing tendencies unfavorable. In contrast, the second-neighbor s and d-wave pairing susceptibilities are less severely affected.

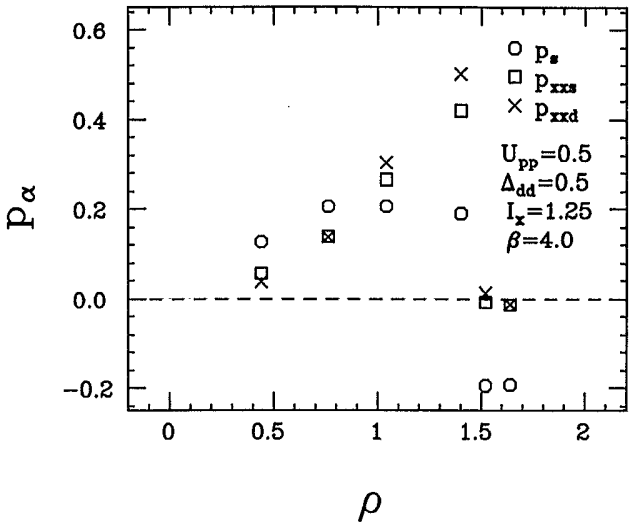

FIG. 5. Reduced pairing susceptibility vs filling for a moderate U_{pp} value. Note now that the on-site s-wave pairing tendency is favored only for low fillings, while second-neighbor pairing becomes more favored at higher filling, and the tendency towards second-neighbor d pairing is marginally favored over that of second-neighbor s pairing. The charge-density-wave formation tendency is suppressed to higher band fillings.

We note several basic features which energy from our results.

First, there is a general tendency for the pairing correlations to increase with filling (see Fig. 3). In fact, as we shall discuss in somewhat more detail later, the rapid drop in the reduced pairing susceptibilities as the filling ρ approaches 2 is due to a charge-density-wave instability corresponding to double occupancy of one oxygen atom per cell.

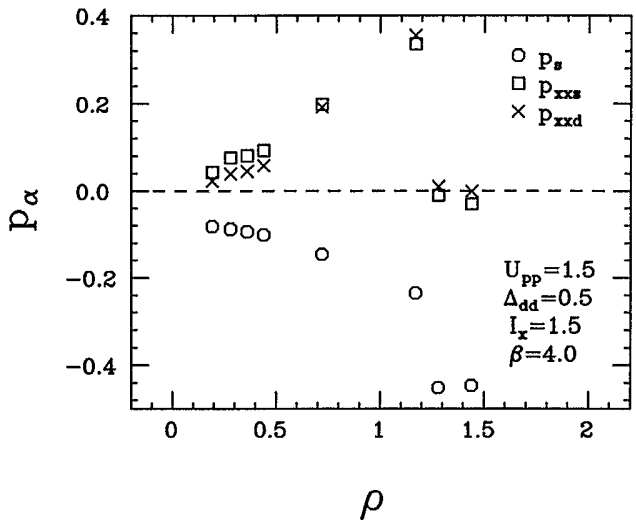

FIG. 6. Reduced pairing susceptibility vs filling for a large U_{pp} value. The main feature of note relative to the previous figure is the complete suppression of on-site s-pairing tendencies. The charge-density-wave effects are similar here as in Fig. 5 because of a compensating increase in the coupling I_x.

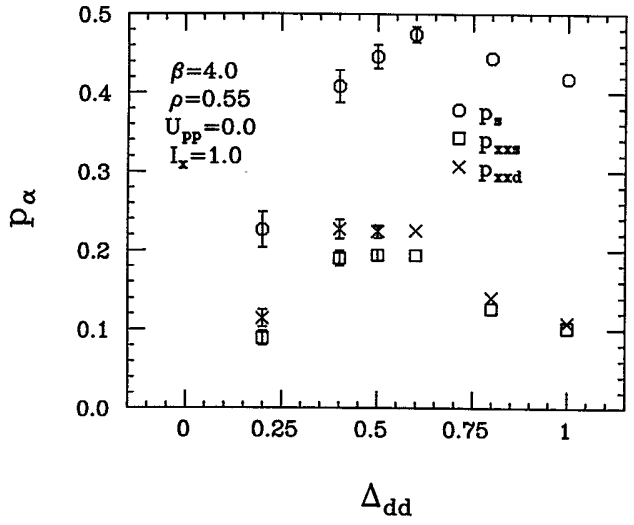

FIG. 7. Reduced pairing susceptibility vs on-site d-d splitting Δ_{dd} at fixed filling. Turning on appreciable U_{pp} immediately suppresses the on-site s-wave pairing tendencies, so the focus is to be placed on the second-neighbor pairing. The pairing tendency is nonmonotonic with Δ_{dd} as anticipated from weak-coupling theory, and in this case optimized with $\Delta_{dd} \approx 0.5 t_{pp}$, which in realistic units would be of the order of 0.3 eV. Note that this filling (0.55 holes per cell) is of the order of that anticipated for $YBa_2Cu_3O_7$.

Second, as expected, Coulomb correlations strongly suppress the tendency towards on-site s-wave pairing while having a less pronounced effect on the xxs and xxd pairing channels (Figs. 4 and 5). Coulomb correlations strongly reduce the tendency towards the charge-density-wave formation mentioned above (compare Fig. 3 and Figs. 5 and 6).

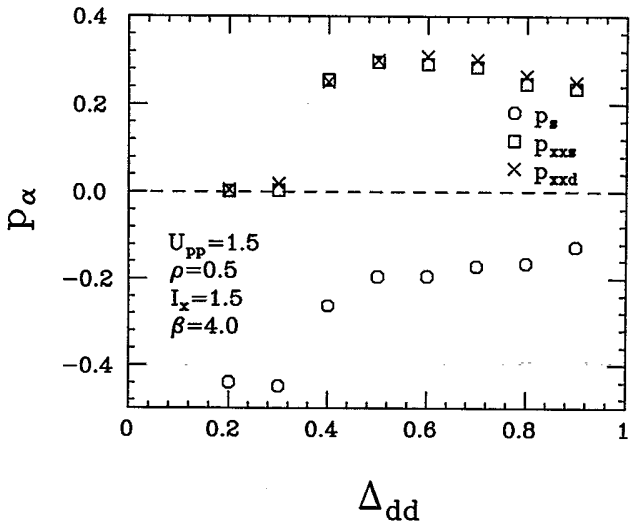

FIG. 8. Reduced pairing susceptibility vs on-site d-d splitting Δ_{dd} at fixed filling and finite U_{pp}. As anticipated, the on-site pairing tendencies are strongly suppressed, while the shape and strength of second-nearest-neighbor pairing susceptibility curves are little affected by turning on U_{pp}.

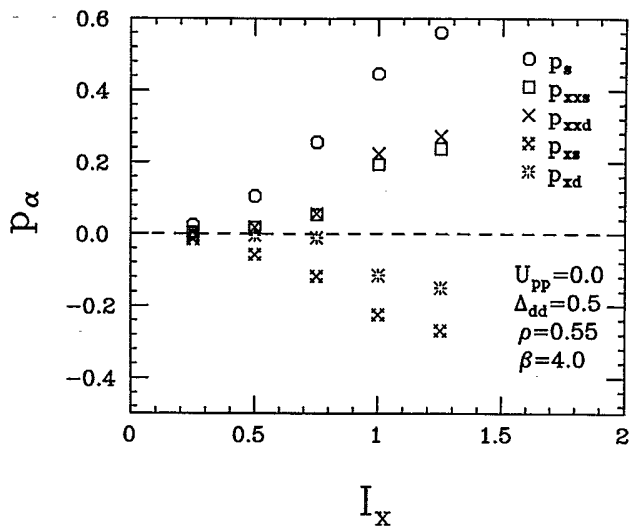

FIG. 9. Reduced pairing susceptibility vs quadrupole coupling I_x. As expected, the enhancement of second-neighbor pairing tendencies increases monotonically with the coupling strength I_x, and the suppression of nearest-neighbor pairing tendencies also increases monotonically.

Third, the reduced pair field susceptibilities display nonmonotonic behavior as a function of Δ_{dd} (Figs. 7 and 8) in agreement with the results from weak-coupling theory discussed above.

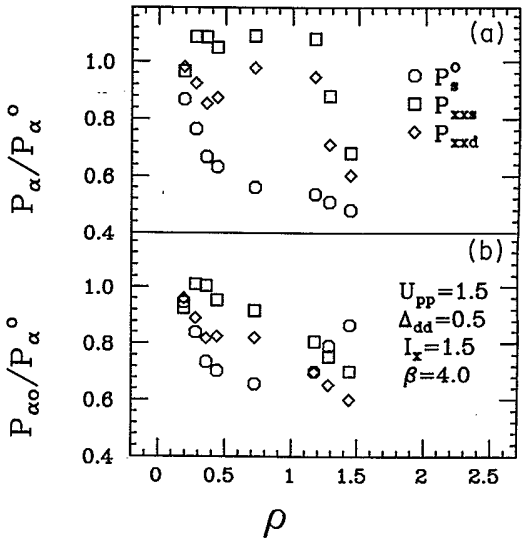

FIG. 10. Comparison of pair field susceptibilities in the interacting and noninteracting limit as a function of filling for fixed U_{pp}, I_x, and Δ_{dd}. In (a) the ratio of the full pair field susceptibility to the noninteracting limit (I_x, $U_{pp}=0$) result P_α^0 is displayed for s, xxs, and xxd symmetries. In (b), the ratio of the bubble contribution $P_{\alpha 0}$ to the full interacting susceptibility to the noninteracting susceptibility is displayed.

Fourth, the *xxd* channel wins over the *xxs* channel at high fillings, but not at low fillings (Figs. 3–6) as anticipated by the weak-coupling treatment. This statement is stronger than apparent from Fig. 8 for reasons we shall discuss later.

Fifth, an increase in the coupling strength I_x with all other parameters held fixed produces a monotonic increase in the pairing tendencies of the *s*, *xxs*, and *xxd* symmetries, while strongly reducing the pairing tendencies of nearest-neighbor *s*- and *d*-wave states (noted as *xs* and *xd* in Fig. 9). This is fully consistent with the simple perturbative estimate of the effective hole-hole interaction induced by the quadrupolar fluctuations.

Thus, despite the severe approximations made within the weak-coupling treatment (as well as the neglect of intersite correlations between copper ions induced by the oxygen holes) the qualitative picture of quadrupole-fluctuation-induced pairing presented there appears to hold up when treated by the essentially exact Monte Carlo technique. However, it should be noted that the Monte Carlo results, being limited to a finite-size cluster, do not prove the existence of a superconducting transition. The results presented herein support the picture obtained within weak-coupling theory.

Finally, we note in Fig. 10 a comparison of the total pairing susceptibilities P_α [Fig. 10(a)] and the bubble contributions $P_{\alpha 0}$ [Fig. 10(b)] to the noninteracting $(I_x, U_{pp}=0)$ pair field susceptibilities P_α^0 for the *s*, *xxs*, and *xxd* symmetries. While the comparison is in some sense meaningless, as discussed above, it is nevertheless interesting to observe that the noninteracting *xxs* and *xxd* susceptibilities are very close to the full pair field susceptibilities for nonzero I_x, U_{pp} at least until the onset of the charge-density-wave instability.

III. SUMMARY AND CONCLUSIONS

In summary, we have carried out a quantum Monte Carlo study of the pairing susceptibilities in the quadrupole fluctuation model of high-temperature superconductivity for finite lattices. While the Monte Carlo–based calculations cannot prove the existence of pairing instabilities for our model system, they can produce qualitative information about the pairing tendencies of the system. An advantage of the Monte Carlo analysis over the weak-coupling analysis we have performed previously is that (at least for a restricted form of the model) the oxygen-hole-copper-quadrupole interactions are treated essentially exactly to all orders, and retardation effects are automatically included and treated exactly.

Consistent with our previous weak-coupling analysis,[4] when significant repulsion between oxygen holes is turned on, we find enhancement of next-nearest-neighbor (oxygen sublattice) *s*- and *d*-wave pairing, in a filling-dependent fashion—the reduced pair field susceptibilities increase with the filling until the onset of a charge-density-wave instability. We believe the latter instability to be an unphysical feature of the model. The *d*-wave pairing is slightly favored as the filling is raised, through the crossover between next-nearest *s*- and *d*-wave susceptibilities is parameter dependent. Realistic oxygen repulsion values almost completely suppress on-site (isotropic in **k** space) pairing. Also consistent with the weak-coupling analysis also are the suppression of nearest-neighbor *s*- and *d*-wave pairing, and the nonmonotonic dependence of the next-nearest-neighbor pairing tendency upon the on-site quadrupole splitting Δ_{dd}.

We now turn to discuss some important features which the calculation does not include, and which should be examined in further studies of the model.

First, the measurement of "diagonal" pair field susceptibilities is insufficient for a discussion of pairing instabilities. The reason is easily illustrated by a discussion of on-site, nearest-neighbor, and next-nearest-neighbor oxygen-hole *s*-wave pairing in the weak-coupling context. While the corresponding pair field harmonics 1 (on site), $|\cos(k_x a/2)\cos(k_y a)/2|$ (nearest neighbor), and $\cos(k_x a)+\cos(k_y a)$ (next nearest neighbor) are linearly independent, they are not orthogonal with respect to the properly defined inner product of the weak-coupling theory. On the other hand, the on-site and nearest-neighbor hole-hole repulsion do not enter the diagonal pair field susceptibility of the next-nearest-neighbor pairing. Proper inclusion of the mixing of next-nearest-neighbor pair fields with on-site and nearest-neighbor pair fields will lead to suppression of the next-nearest-neighbor pairing: only that part orthogonal to the on-site and nearest-neighbor fields may go unstable. It is not yet clear how to include this kind of mixing in the Monte Carlo procedure. (Note that in tetragonal symmetry, at least, there can be no mixing of *s*- and *d*-channel susceptibilities.)

Next, we note that retaining only the coupling of oxygen holes to the quadrupole flip operator σ_z omits the possibility of a nonmagnetic Kondo effect between the itinerant holes and the copper-quadrupole moments.[9,10] A scaling analysis with a coupling to the copper σ_z operator included suggests that significant renormalizations of the effective coupling strengths are possible. In particular, the next-nearest-neighbor *d*-wave channel should be significantly enhanced if Δ_{dd} is not too large compared with the Kondo scale estimate T_0. We have attempted to generalize the current algorithm to include this coupling of the oxygen holes to the σ_z operator of the copper sites, but the average sign of the effective probability density for the Ising fields is too close to zero to allow meaningful Monte Carlo measurements.

A corollary to the above omission is the neglect of Hartree shifts of the on-site splitting Δ_{dd} in the presence of finite-hole concentrations. This could significantly modify the dependence upon doping of the pair field susceptibilities. Finally, and perhaps most serious, is the omission of the copper magnetic moments in the calculation. The magnetic fluctuations of the Cu sites are still clearly present in the real materials, and it is prudent to ask what effect they have on the present picture. For example, the magnetic fluctuations will surely induce pair breaking of the oxygen-hole superconducting state. We acknowledge this deficiency of the current work, and reserve resolution of the question for future studies.

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