Correlations in the two-dimensional Hubbard model

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Using Monte Carlo simulations, we have studied the question of phase separation and pairing in the doped two-dimensional Hubbard model. For a range of U/t values greater than as well as less than the bandwidth, we find no evidence for phase separation when the system is doped away from half filling. In agreement with previous work, we find that the d-wave and extended s-wave pairing correlations are enhanced by the interaction vertex but that none of the eight different pairing correlations that we studied increases as a function of lattice size. We have also examined the dependence of the kinetic energy, which determines the total optical spectral weight, on U/t and filling $\langle n \rangle$.

The two-dimensional Hubbard model on a square lattice with a nearest-neighbor hopping represents one of the most basic unsolved many-body problems. The nature of the dominant correlations depends on the band filling $\langle n \rangle = \langle n_{i\uparrow} + n_{i\downarrow} \rangle$ and the ratio of the on-site Coulomb interaction to the hopping U/t. Various types of correlations ranging from antiferromagnetic to ferromagnetic, from incommensurate and spiral spin-density-wave states to superconducting phases have been suggested.[1] In addition, the possibility of phase separation has recently been raised.[2] Here we discuss what has been learned from numerical simulations, presenting results which explore the question of phase separation and give further information regarding the apparent absence of long-range pairing correlations.[3-5] We also examine the pairing correlations when a next-nearest-neighbor hopping t' is present.[6,7]

The Hubbard model is defined by the Hamiltonian

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

where $c^{\dagger}_{i,\sigma}$ creates an electron at site i with spin projection σ, $n_{i,\sigma}$ is the number operator, and the sum $\langle ij \rangle$ is over pairs of nearest-neighbor lattice sites. Here, t is the hopping parameter and U the Coulombic repulsion, and we will add a chemical potential μ to fix the average value $\langle n \rangle$. Later we will also include a next-nearest-neighbor hopping along the diagonals t'.

At half filling $\langle n \rangle = 1$, Monte Carlo simulations have shown that the ground state has long-range antiferromagnetic correlations[3,8] for a range of U/t values, and it is believed that this is the case for all $U/t > 0$. For infinite U/t, when one electron is added or removed from the half-filled band, the ground state becomes ferromagnetic, as originally proposed by Nagaoka.[9] However, when a finite density of electrons or holes is added to systems with U less than several times the bandwidth, simulations give no indication of ferromagnetism. Now, as is well known, numerical simulations of systems doped away from half filling are presently limited in lattice size and inverse temperature β by fluctuations in the sign of the fermion determinant.[10] Thus while at half filling we have simulated lattices up to 16×16 with $\beta = 12$, in the interesting region near half filling, $0.7 < \langle n \rangle < 0.95$, it is very time consuming to go beyond 8×8 lattices with $\beta = 8/t$. However, within these constraints, one can explore the nature of the correlations on 4×4 and 6×6 lattices at temperatures of order $\frac{1}{50}$ of the bandwidth for various U/t and $\langle n \rangle$ values.

Previous work has shown that the $\langle n \rangle = 1$ antiferromagnetic correlations rapidly decrease with doping.[8,11] For weak ($U/t = 2$) to moderate ($U/t = 8$) values of U/t, where simulations have been carried out, it appears that the (π, π) peak at half filling splits into $(\pi - \delta, \pi)$ and $(\pi, \pi - \delta)$ peaks with doping.[8,12] However, over the accessible lattice size and temperature regime, there is no indication that the resulting spin-spin correlations scale with lattice size. Naturally, because of the commensurability problem posed by such correlations, the present limitations on lattice size represent a particularly serious obstacle, and we are unable to determine if an incommensurate spin-density-wave or spiral spin-density-wave phase may occur. At present, the simulations are consistent with a disordered spin system.

An alternative scenario, in which a phase separation occurs as the system is doped away from half filling, has been suggested.[2] In order to explore this possibility, we have calculated $\langle n \rangle$ versus μ. Phase separation would manifest itself as a discontinuity in $\langle n \rangle$ as a function of μ. This first-order phase transition indicates the separation between a phase poor in holes with $\langle n \rangle = 1$, and another one rich in holes with $\langle n \rangle = n_h$. Results for $U/t = 4$ on a 4×4, 6×6, and 8×8 lattice and $U/t = 10$ on a 4×4 lattice are presented in Figs. 1(a) and 1(b). In both cases $\langle n \rangle$ remains equal to 1 up to a finite value of μ due to the existence of the antiferromagnetic gap and then begins to change very smoothly, giving no indication of phase separation.[13]

It is also interesting to examine the dependence of the kinetic energy on the filling $\langle n \rangle$, Fig. 2. At $U/t = 0$, the kinetic energy $\langle K \rangle$ becomes more negative as electrons are added, until it reaches a minimum at half filling and then increases again as the number of holes begins to de-

crease. For finite values of U, the minimum in the kinetic energy curve shifts away from half filling. A particle-hole transformation of the Hamiltonian maps the kinetic energy at filling $\langle n \rangle$ below half filling, into the kinetic energy at filling $2-\langle n \rangle$. This means that at half filling the curve has a relative maximum. In Fig. 2 we have used particle-hole symmetry to obtain the kinetic energy for values of $\langle n \rangle$ larger than one. The existence of this symmetry allows us to use each Monte Carlo run to get two points on our plot. To check this, we made runs for $\langle n \rangle$ both below and above half filling and determined that the results were the same within error bars. The error bars are smaller than the points shown in the figure. Thus we find that the Monte Carlo program fulfills particle-hole symmetry with the degree of precision shown in the figure. The average kinetic energy $\langle K \rangle$ corresponds to the mean value of the hopping term in Eq. (1), and $-\langle K \rangle/N$ determines the total optical spectral weight[14] $(2/e^2\pi)\int_0^\infty \sigma(\omega)d\omega$. In Fig. 2(a) we show $\langle K \rangle$ as a function of the density $\langle n \rangle$ for different values of U/t at $\beta t=6$ on a 12×12 lattice. We were able to reach only intermediate values of U/t on these large lattices. To examine what happens for larger values of U/t, we show results including $U/t=10$ for a 4×4 lattice at $\beta t=6$ in Fig. 2(b). As U/t increases, the positions of the minima move further away from half filling. Finite-size effects are considerable for small U/t and decrease when the coupling increases. However, the qualitative behavior is similar to the one observed on larger lattices. We know that when $U/t=0$, the particles behave as electrons below half filling, where $\langle K \rangle$ is a decreasing function of $\langle n \rangle$, while they behave as holes beyond half filling where $\langle K \rangle$ is an increasing function of the filling. From this point of view, it would appear that for finite U/t the particles behave as holes (electrons) immediately below (above) half filling.

In order to investigate the possibility of superconducting pairing, here we examine various equal-time pair-field correlation functions

$$P_\alpha = \langle \Delta_\alpha^\dagger \Delta_\alpha \rangle \ , \tag{2}$$

obtained from the pair-field operators

$$\Delta_\alpha^\dagger = \frac{1}{2\sqrt{N}} \sum_{l,\nu} g_\alpha(\nu) c_{l\uparrow}^\dagger c_{l+\nu\downarrow}^\dagger \ . \tag{3}$$

Here, $\Delta_\alpha^\dagger$ adds a pair of electrons in a state whose structure is specified by $g_\alpha(\nu)$. N is the number of sites, ν runs over selected neighbors of site l, and $g_\alpha(\nu)$ is a function that determines the symmetry α of the pairs and takes values ±1. In Fig. 3 we show the different pairing symmetries that we have considered: local s (s); extended s (S); extended s along the diagonals (S_D), p_{xy}, and D; and extended D along the diagonals (D_D), p_y, and p_x.

To determine whether the interaction between particles is attractive or repulsive, we have compared P_α with the corresponding nonvertex correlation function

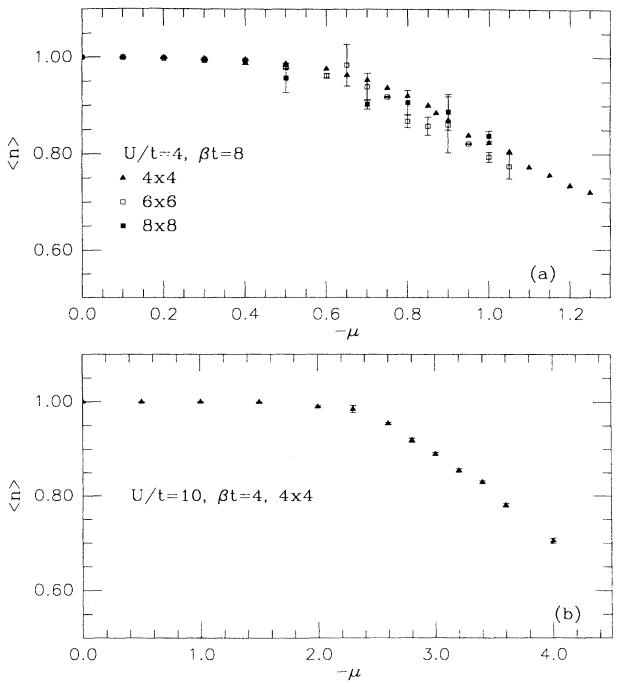

FIG. 1. The average site occupation $\langle n \rangle$ vs μ. (a) $U/t=4$, $\beta t=8$, on 4×4, 6×6, and 8×8 lattices, and (b) $U/t=10$, $\beta t=4$, on a 4×4 lattice.

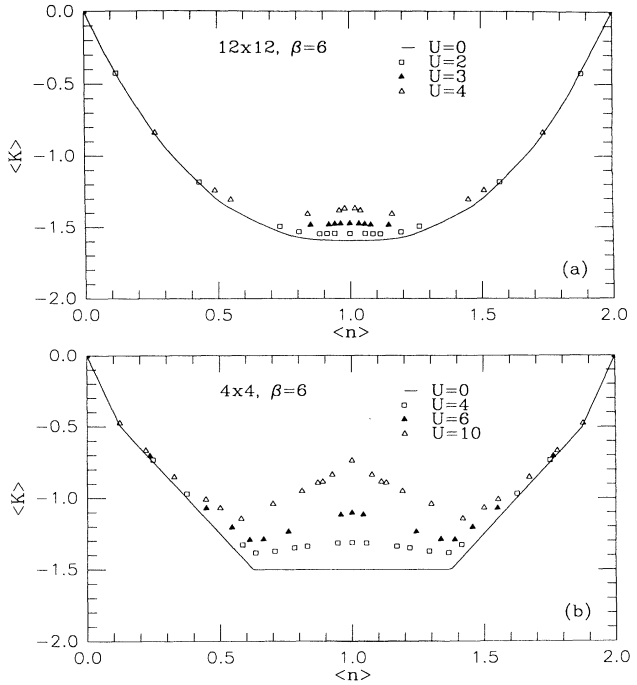

FIG. 2. (a) The kinetic energy $\langle K \rangle$ as a function of the filling $\langle n \rangle$ for different values of U/t on a 12×12 lattice. (b) The kinetic energy $\langle K \rangle$ as a function of the filling $\langle n \rangle$ for U/t values up to 10 on a 4×4 lattice.

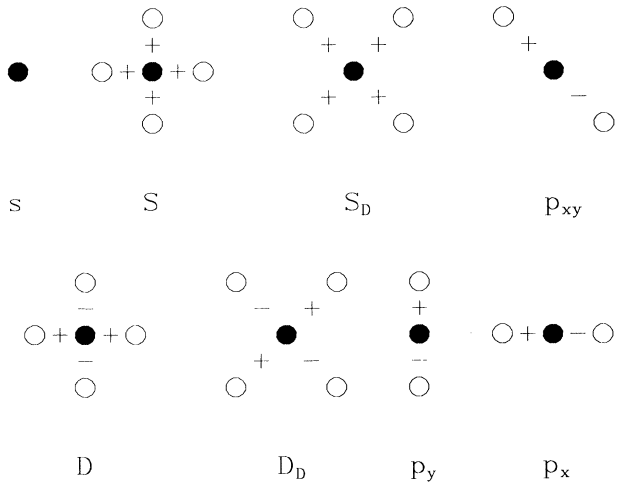

FIG. 3. Pairing symmetries considered in this work. The index α in Eq. (3) can take the values s, S, S_D, p_{xy}, D, D_D, p_y, and p_x. The + and − signs are placed on the links that connect site l (solid circle) with sites ν (open circles), and they represent the values of the function $g_\alpha(\nu)$.

$$\bar{P}_\alpha=\frac{1}{4N}\sum_{l,l'}\sum_{\nu,\nu'}\tilde{G}_\downarrow(l'+\nu',l+\nu)\times\tilde{G}_\uparrow(l',l)g_\alpha(\nu)g_\alpha(\nu')\ . \quad (4)$$

Here,

$$\tilde{G}_\sigma(l',l)=\langle c^\dagger_{l'\sigma}c_{l\sigma}\rangle\ , \quad (5)$$

is a dressed single-particle equal-time correlation function. If P_α is larger than $\bar{P}_\alpha$, then the effective particle-particle interaction enhances the pairing correlations.

We have studied 4×4 and 6×6 lattices for $U/t=4$ and 10. We find that the only correlations for which P_α is enhanced relative to $\bar{P}_\alpha$ are the ones associated with D- and extended S-wave pairing. In Figs. 4(a) and 4(b), we show P_S and P_D as a function of the inverse temperature β. We observe the enhancement of both correlations relative to their nonvertex parts and we can see that in both cases the zero-temperature plateau is reached when $\beta\gtrsim6/t$. In Fig. 5 we show P_α and $\bar{P}_\alpha$ as a function of filling for $U/t=4$ at $\beta t=6$ on a 4×4 lattice. Naturally, at low filling P_α goes to zero. It appears that the only enhancement of P_D relative to its nonzero correlations occurs near half filling; however, P_S remains enhanced away from $\langle n\rangle=1$.

Under a particle-hole transformation, $\langle n\rangle$ goes to $2-\langle n\rangle$ and $P_\alpha=\langle\Delta^\dagger_\alpha\Delta_\alpha\rangle$ goes to $\langle\Delta_\alpha\Delta^\dagger_\alpha\rangle$. Note that since

$$\langle[\Delta^\dagger_\alpha,\Delta_\alpha]\rangle=\frac{1}{2N}\sum_p g^2_\alpha(p)\langle n_{p\uparrow}+n_{-p\downarrow}-1\rangle\ ,$$

the difference between $\langle\Delta^\dagger_\alpha\Delta_\alpha\rangle$ and $\langle\Delta_\alpha\Delta^\dagger_\alpha\rangle$ at a given filling simply reflects short-range correlations. From now on we will only give results for P_α in the region

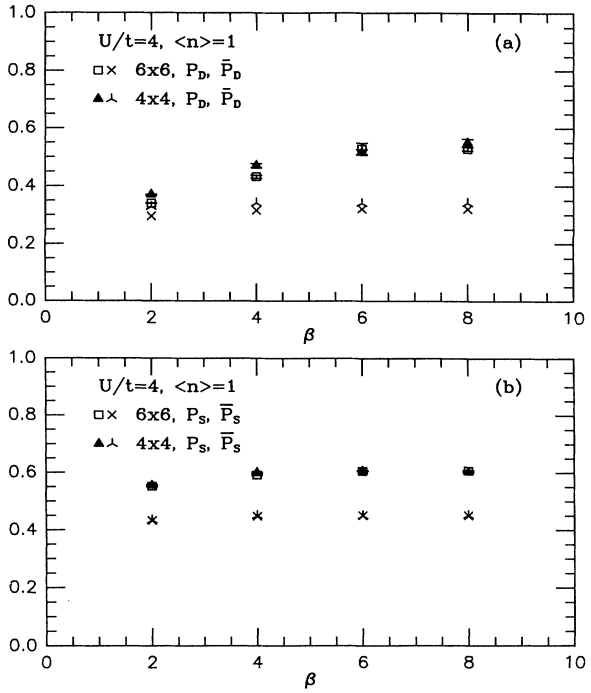

FIG. 4. (a) P_D with its nonvertex counterpart $\bar{P}_D$ as a function of the inverse temperature β, for $U=4$, $t=1$ on a 4×4 and 6×6 lattice at $\langle n\rangle=1$. (b) Same as above for P_S and $\bar{P}_S$.

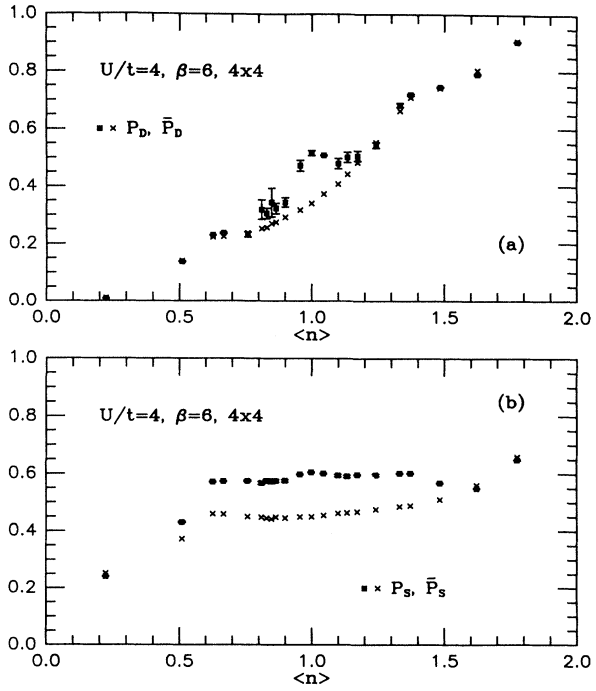

FIG. 5. (a) P_D with its nonvertex counterpart $\bar{P}_D$ as a function of the filling for $U=4$, $t=1$ and $\beta=6$ on a 4×4 lattice. (b) P_S with its nonvertex counterpart $\bar{P}_S$ as a function of the filling for $U=4$, $t=1$, and $\beta=6$ on a 4×4 lattice.

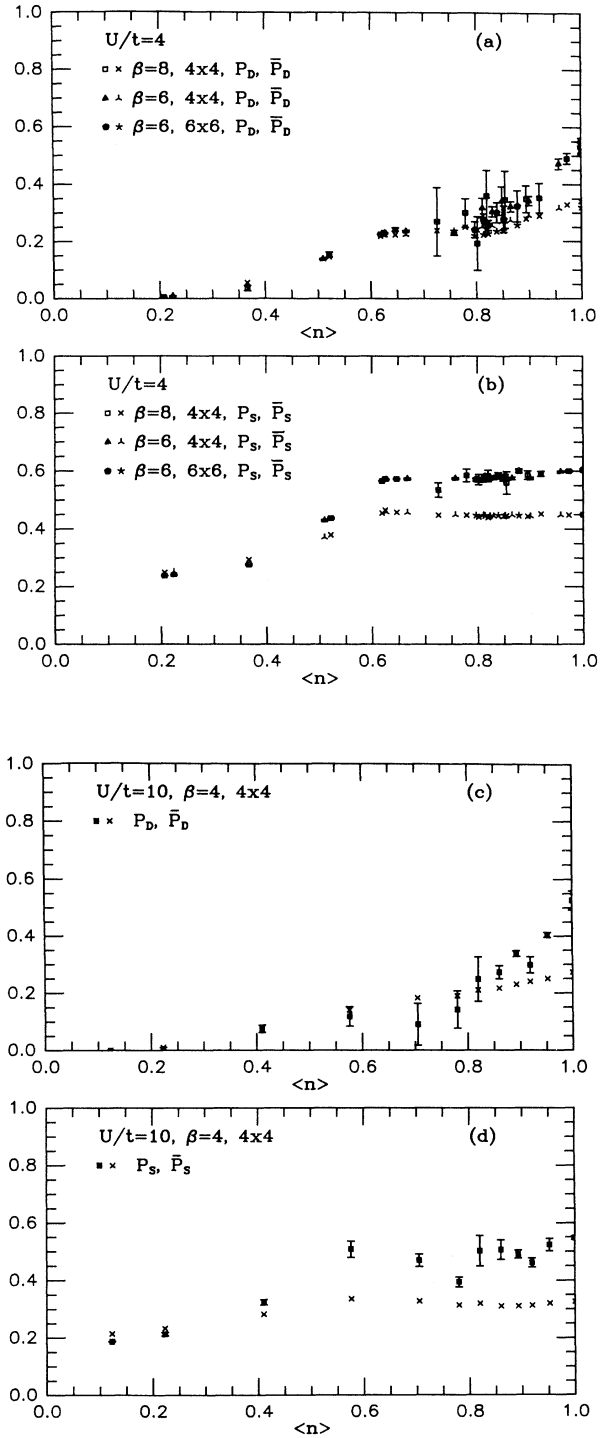

FIG. 6. (a) P_D and its nonvertex counterpart as a function of the filling for $U=4$ and $t=1$, for different values of β and lattice sizes. (b) P_S and its nonvertex counterpart as a function of the filling for $U=4$ and $t=1$, for different values of β and lattice sizes. (c) P_D and its nonvertex counterpart as a function of the filling for $U=10$, $\beta=4$, and $t=1$, on a 4×4 lattice. (d) P_S and its nonvertex counterpart as a function of the filling for $U=10$, $\beta=4$, and $t=1$, on a 4×4 lattice.

$0\leq\langle n\rangle\leq1$.

In Fig. 6(a) we show the behavior of P_D for $U/t=4$. Note that its enhancement is maximum at half filling and decreases toward lower filling. Data points for $\beta t=6$ and 8 fall on top of each other, showing that the system has reached its low-temperature plateau. However, the values of P_D do not increase when the lattice size is increased from 4×4 to 6×6. This suggests, in agreement with previous work,[3–5] that there is no long-range order (LRO). In Fig. 6(b) we have plotted P_S. While the enhancement is smaller than for D-wave at half filling, it actually becomes larger when the filling is reduced.[15] To see how the behavior of the pairing correlations changes with U/t, we studied the case $U/t=10$. Since the factorization of the exponential operator involves errors of order $(\Delta\tau)^2U/t$, in going from $U/t=4$ to 10 we had to reduce $\Delta\tau$ by 50% to get accurate results. In Figs. 6(c) and 6(d), we present P_α for D and extended s waves for $U/t=10$ and $\beta t=4$. (For this large value of U/t, $\beta t=4$ is already in the zero-temperature plateau.) In this case again the D-wave correlation is more enhanced than the extended s at half filling but falls more rapidly away from half filling, while the extended s remains enhanced over a larger region of doping. We were able to run some points on a 6×6 lattice, and in spite of large error bars, we did not observe indications of a growth of P_α with the lattice size. On the other hand, long-range order in the extended s-wave channel would be very unlikely in the Hubbard model, due to the fact[16] that

$$\langle[H,\Delta_s]\rangle=0=\langle\Delta_S\rangle+f(U,t,\mu)\langle\Delta_s\rangle\ , \tag{6}$$

where H has been defined in Eq. (1), Δ_s (Δ_S) is the operator that destroys a pair of electrons with on-site (extended) s-wave symmetry, and f is a known function of U, t, and μ. Equation (6) tells us that to have long-range extended s-wave order in the Hubbard model we need to observe on-site s-wave order as well, which is very unlikely, due to the on-site Coulombic repulsion among electrons. Numerically we observed that the on-site s pairing is never enhanced as a function of the filling.

Our results show that away from half filling there is more attraction in the extended s-wave channel than in the D wave. However, symmetries associated with the Hubbard Hamiltonian are preventing extended S LRO. The addition of a new term to the Hubbard Hamiltonian may fix the problem. We decided to add a hopping term with intensity t' along the diagonals. The Hubbard model becomes now the U-t-t' model. This model has been proposed as a reduced CuO_2 model[17] and was previously studied[6,7] to examine the effect of moving the Van Hove singularity away from half filling. Following similar steps to those of Ref. 16, we found that

$$\langle[H,\Delta_s]\rangle=0=\langle\Delta_S\rangle+f(U,t,\mu)\langle\Delta_s\rangle+h(t,t')\langle\Delta_{S_D}\rangle\ . \tag{7}$$

Here, $\langle\Delta_{S_D}\rangle$ is the operator that destroys a pair of electrons with extended S symmetry along the diagonals (see Fig. 3), and h is a function of t and t'. This means that the extended S channel may have LRO even if the local S

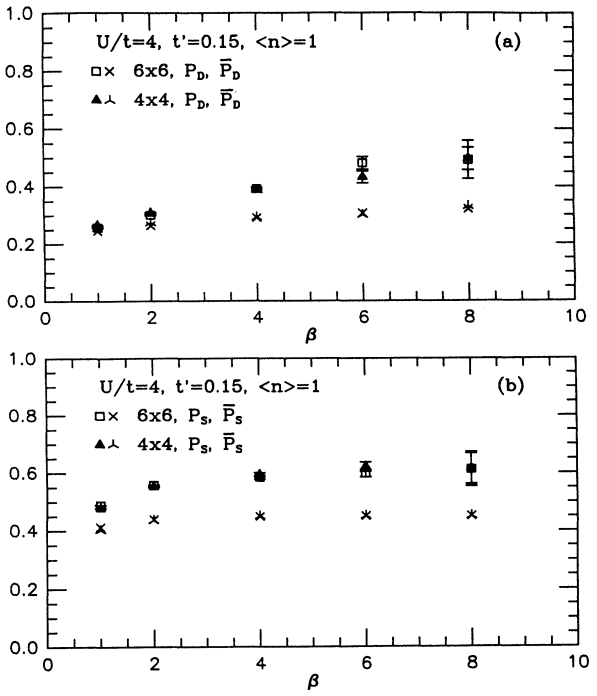

FIG. 7. (a) P_D with its nonvertex counterpart as a function of β for $t=1$, $t'=0.15$, $U=4$, and $\langle n \rangle = 1$ on a 4×4 and 6×6 lattice. (b) Same as above for P_S.

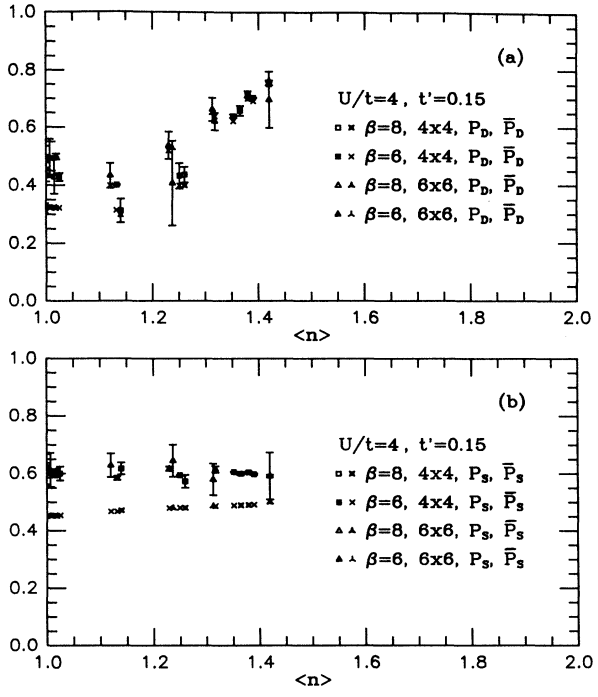

FIG. 8. (a) P_D and its nonvertex counterpart as a function of the filling for $U=4$, $t=1$, and $t'=0.15$ for different values of β and lattice sizes. (b) P_S and its nonvertex counterpart as a function of the filling for $U=4$, $t=1$, and $t'=0.15$ for different values of β and lattice sizes.

does not. But if this happens, one has to observe LRO in the S_D channel as well.

In Fig. 7 we show results with $U/t=4$, $t'/t=0.15$ obtained on 4×4 and 6×6 lattices with $\langle n \rangle = 1.0$. In this case, the extended S- and D-wave pair fields appear to reach their low-temperature plateaus by $\beta t=6$. In Fig. 8 we fix βt at 6 and 8 and plot P_α versus $\langle n \rangle$ in the regime where the Van Hove singularity in the density of states occurs. As for the previous case in which $t'=0$, both the D- and extended S-wave pairing are attractive with the S-wave pairing showing a wider doping region over which it is enhanced. However, as before, we do not observe the pairing correlations to increase with the lattice size, and S_D correlations do not show any attraction. We found similar results for $t'/t=+0.3$ and -0.15.

In this paper we have continued a numerical study of the Hubbard model. From calculations of $\langle n \rangle$ versus μ for $U/t=4$ and 10, we found no evidence for phase separation. The kinetic energy shows an interesting variation with doping and U/t, exhibiting a double-well structure with minima which move out from $\langle n \rangle = 1$ as U/t increases. We made a detailed study of equal-time pairing correlations with different symmetries for both the Hubbard and the U-t-t' model. For the Hubbard model we examined values of $U/t=10$ larger than the bandwidth $8t$ as well as $U/t=4$. Although we observed enhancement of the pair correlations relative to the nonvertex pair correlations indicating an attractive interaction in both the D- and extended S-wave channels, we did not find evidence for scaling in going from 4×4 to 6×6 lattices. Since it appeared that we were able to reach the low-temperature plateaus for these correlations, our results suggest that there are only short-range pairing correlations.

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