Determinant quantum Monte Carlo study of the enhancement of *d*-wave pairing by charge inhomogeneity

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(Received 7 September 2012; published 7 November 2012)

Striped phases, in which spin, charge, and pairing correlations vary inhomogeneously in the CuO_2 planes, are a known experimental feature of cuprate superconductors, and are also found in a variety of numerical treatments of the two-dimensional Hubbard Hamiltonian. In this paper, we use determinant quantum Monte Carlo to show that if a stripe density pattern is imposed on the model, the d-wave pairing vertex is significantly enhanced. We attribute this enhancement to an increase in antiferromagnetic order which is caused by the appearance of more nearly half-filled regions when the doped holes are confined to the stripes. We also observe a π-phase shift in the magnetic order.

DOI: 10.1103/PhysRevB.86.184506   PACS number(s): 71.10.Fd, 02.70.Uu

I. INTRODUCTION

Cooper pairs in conventional BCS superconductors are typically envisioned to have a large spatial extent characterized by the coherence length ξ, which is many hundreds of lattice spacings in elemental, metallic superconductors. At the other extreme is the BEC regime, where much smaller Cooper pairs form into bosonic particles which subsequently can Bose-Einstein condense into a superfluid phase. The crossover between the BCS and BEC limits has been much explored.[1]

If real-space pairing on small length scales is favorable energetically, a natural question to ask is why more than two fermions do not bind together. Indeed, the competition of such "phase separation" with superconductivity was a central theme of investigation in early studies of Hamiltonians such as the two-dimensional (2D) fermion Hubbard[2–12] and t-J (Refs. 13–18) models in the context of cuprate superconductors, which have short coherence length. Upon doping away from one particle per site, a spatial division into half-filled antiferromagnetic (AF) regions and areas where the hole concentration is high occurs. The tendency to phase separation was found to be especially great in the t-J model, and somewhat less so in the Hubbard model. Roughly speaking, for small hole doping in the strong-coupling limit, such phase separation can be envisioned to arise because it minimizes the energy by preserving the largest number of antiferromagnetic bonds. On the other hand, when $t \gg J$ and the amount of holes is large, phase separation was shown to occur as to minimize the doped hole kinetic energy.[14]

A compromise between complete phase separation into distinct two-dimensional regions, and spatial homogeneity which would be favored by longer-range Coulomb interactions,[19,20] is the possibility that the doped particles form quasi-one-dimensional patterns in which hole-rich and hole-poor regions alternate. Magnetic domain lines were observed in inhomogeneous Hartree-Fock studies very early in the history of cuprate superconductivity. "Charge domain lines" were first reported in a multiband model which included both the copper d and oxygen p orbitals,[21] and subsequently in the single-band Hubbard Hamiltonian.[22,23]

Such striped patterns have also been observed experimentally.[24,25] In $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$, there is a suppression of superconductivity at $x = 1/8$ associated with a tilt pattern of oxygen tetrahedra and charge/spin domain walls. Away from $x = 1/8$, domain-wall ordering is weaker, with coexisting superconductivity.

The relation between pairing and stripes is still controversial. The formation of charge stripe order is related to an increase in the resistance perpendicular to the CuO planes, frustrating the formation of bulk superconductivity, as denoted by a sharp decrease of the critical temperature[26] T_c, resulting in values as low as 4 K. As stripes are perpendicularly stacked in each successive CuO plane, if the Josephson coupling between stripes in the same plane is negative, the coupling between stripes in different planes is destroyed.[27,28] In LaBaCuO, on the other hand, angle-resolved spectroscopy and transport measurements suggest a positive correlation between 2D pairing and stripes.[29,30]

There is an order-of-magnitude drop[26,30,31] in the in-plane resistivity ρ_{ab} when the spin order occurs at $T_{so} \sim 42$ K. Furthermore, there are indications of true 2D superconductivity for $T < T_{BKT} \approx 16$ K when ρ_{ab} goes to 0.[26,30]

A recent exciting development is the direct evidence of stripes in $YBa_2Cu_3O_y$. Nuclear magnetic resonance measurements show that high magnetic fields induce charge order,[32] with the same period of four lattice spacings as in LaBa-based cuprates.[33] Zero-field diffraction with resonant soft[34,35] and hard[36] x-ray scattering observed incommensurate charge order with a period around 3.2 lattice spacings. These experiments seem to indicate that stripes are an intrinsic phenomena in the cuprates, and that at least incipient charge ordering can be seen even in compounds with larger critical temperatures.

This has led to a large set of theoretical studies of charge-ordered patterns to refine and improve upon the initial mean-field treatment.[37–48] Given the complexity of the question of superconductivity even in the homogeneous model, it is not surprising that the details of the interplay with stripe formation should be challenging.

A recent calculation within the dynamical cluster approximation[49] (DCA) provided detailed information concerning pairing correlations amidst static stripes, and revealed a rich competition between an enhancement of the pairing interaction and a suppression of the noninteracting susceptibility. The latter effect occurs as a consequence of the formation of Mott regions away from the stripes, and a resulting suppression of quasiparticle weight. The two effects combine to give a nonmonotonic evolution of the transition temperature with the stripe modulation strength.

In this paper, we undertake determinant quantum Monte Carlo (DQMC) studies of stripe formation in the two-dimensional Hubbard model. The DQMC method complements the DCA approach, working in real space rather than momentum space. It is possible to study somewhat larger clusters with DQMC with, however, an off-setting greater restriction to the accessible temperatures. The key results of our work are an enhancement of antiferromagnetic order by charge modulation, and a π-phase shift above a critical threshold of the stripe potential. Accompanying this larger magnetic order is a stronger signal of d-wave pairing in the associated superconducting vertex, although we are not able to lower the temperature enough to cross below the transition temperature.

II. HAMILTONIAN AND METHODOLOGY

We study a two-dimensional repulsive Hubbard Hamiltonian in which stripes are introduced externally via a raised site energy V_0 on a set of rows of period $\mathcal{P}$:

$$\hat{\mathcal{H}} = -t\sum_{\langle \mathbf{i}\,\mathbf{j}\rangle\,\sigma}(c^{\dagger}_{\mathbf{i}\sigma}c_{\mathbf{j}\sigma}+c^{\dagger}_{\mathbf{j}\sigma}c_{\mathbf{i}\sigma}) + U\sum_{\mathbf{i}} n_{\mathbf{i}\uparrow}n_{\mathbf{i}\downarrow} - \mu\sum_{\mathbf{i}}(n_{\mathbf{i}\uparrow}+n_{\mathbf{i}\downarrow}) + V_0\sum_{i_y\in\mathcal{P}}(n_{\mathbf{i}\uparrow}+n_{\mathbf{i}\downarrow}). \quad (1)$$

Here, $t = 1$ is the intersite fermion hopping between near-neighbor sites $\mathbf{i}$, $\mathbf{j}$ on a square lattice, U is an onsite repulsion, μ is a global chemical potential, and V_0 is an additional onsite energy imposed on a set of rows $\mathbf{i} = (i_x,i_y)$ with $\mathrm{mod}(i_y,\mathcal{P}) = 0$. When $\mathcal{P} = 4$, this choice produces the spin and charge patterns postulated based on neutron scattering studies[24,25] and shown to arise in density-matrix renormalization group (DMRG) studies on the t-J Hamiltonian.[50]

This Hamiltonian does not, of course, address the issue of *spontaneous* stripe formation in a translationally invariant system, nor does it acknowledge the tendency of charge domain walls to fluctuate. Nevertheless, it allows us to examine the nature of spin and pairing correlations in the presence of a set of preformed lines of reduced charge density, and is an appropriate approximate model in the limit where the energy scale of stripe formation is considerably greater than that of pairing.

Most of our results will be for 16×16 lattices with $\mathcal{P} = 4$, so that each stripe (row with V_0 term active, blue filled circles in Fig. 1) is separated by three rows where the V_0 term is not present (empty circles in Fig. 1). The entire 16×16 site system accommodates four stripes for this $\mathcal{P} = 4$ case. We will also analyze finite-size effects and present a smaller amount of data for pairing correlations at other periodicities $\mathcal{P}$. Most of our results will be for a total density $\rho = 0.774$ averaged

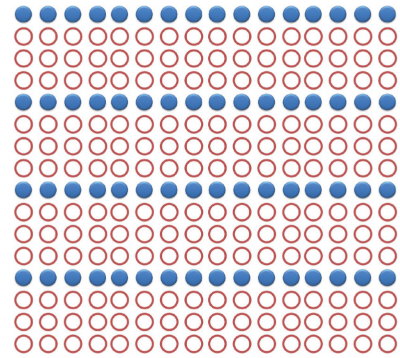

FIG. 1. (Color online) 16×16 lattice with period $\mathcal{P} = 4$, sites with V_0 active are depicted in blue (filled circles), whereas the interstripe sites are red (empty circles).

over the entire lattice. This value was chosen because it allows for the exploration of a broad range of densities on the stripe and between stripes, and also because certain experimentally observed characteristics of the striped phase, such as the "π-phase shift" of the spin correlations when traversing a stripe, are absent at some other fillings.

In this $\mathcal{P} = 4$ case, we expect the charge order to be modulated along the y direction with the same period four, and the spin order has a period twice as large as a result of the π-phase shift (see below), also observed in experiments. Therefore, x-ray and neutron diffraction experiments are expected to show peaks at $\mathbf{Q}_{\mathrm{CO}} = \frac{2\pi}{a}(0;\pm 2\delta)$ and $\mathbf{Q}_{\mathrm{SO}} = \frac{2\pi}{a}(0.5;0.5\pm\delta)$.[24,31,51] respectively. The value of δ is doping dependent in the $La_{2-x}Ba_xCuO_4$ family[31] and is assumed to be 1/8 for doping higher than 0.125,[52,53] in agreement with the stripe sketch in Fig. 1. Some experiments, however, displayed incommensurate charge stripes with δ smaller than expected.[31,54]

Our methodology is determinant quantum Monte Carlo (DQMC).[55,56] In this approach, the quartic interaction term is replaced by a coupling of the local z component of spin to an auxiliary field.[57] The fermion degrees of freedom are integrated out analytically, leaving a Monte Carlo over the auxiliary field. In the process of eliminating the interaction term, the inverse temperature β is discretized. We choose the discretization mesh $\Delta\tau = 1/8t$. The resulting Trotter errors are typically only a few percent, and their elimination is of consequence only if subtle changes in short-range correlation functions are of interest.[58,59] In DQMC, the Trotter errors are typically smaller than accessible statistical errors on long-range spin, charge, and pairing correlations at the lowest temperatures.

The stripe potential V_0 breaks particle-hole symmetry so that there is a sign problem[60] for all fillings. Thus, we can not obtain ground-state properties as can be accessed, for example, in the half-filled homogeneous system or the attractive Hubbard Hamiltonian at any filling. A contour plot of the sign for $\rho = 0.774$ and $U = 4$ for a 16×16 lattice is shown in Fig. 2. It can be seen that the sign problem is no worse than in the doped, homogeneous case where one can already discern significant trends concerning the superconducting correlations.[61]

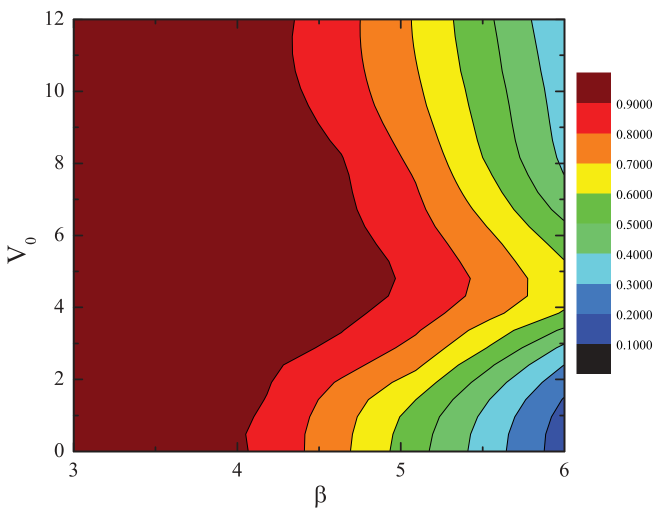

FIG. 2. (Color online) Contour plot of the sign as a function of V_0 and β for a 16×16 lattice with $U = 4$ and $\rho = 0.774$. The contours are basically vertical, indicating that the sign problem is independent of V_0. However, for $V_0 \sim 4$, there is a modest improvement in the sign. This is the potential for which the interstripe density goes through half-filling.

We will show results for the spin and (d-wave) pair correlations

$$c_{\rm spin}(\mathbf{i}) = \langle S^-_{\mathbf{j}+\mathbf{i}} S^+_{\mathbf{j}} \rangle, \quad S^+_{\mathbf{j}} = c^\dagger_{\mathbf{j}\uparrow} c_{\mathbf{j}\downarrow}$$
$$c_{d\,\rm pair}(\mathbf{i}) = \langle \Delta_{d\,\mathbf{j}+\mathbf{i}} \Delta^\dagger_{d\,\mathbf{j}} \rangle, \tag{2}$$
$$\Delta^\dagger_{d\,\mathbf{j}} = c^\dagger_{\mathbf{j}\uparrow}(c^\dagger_{\mathbf{j}+\hat{x}\downarrow} - c^\dagger_{\mathbf{j}+\hat{y}\downarrow} + c^\dagger_{\mathbf{j}-\hat{x}\downarrow} - c^\dagger_{\mathbf{j}-\hat{y}\downarrow}).$$

The quantities $c_{\rm spin}(\mathbf{i})$ and $c_{d\,\rm pair}(\mathbf{i})$ do not have complete translation invariance owing to the presence of the stripes. They will depend on the row index i_y, for example, whether $\mathrm{mod}(i_y,\mathcal{P}) = 0$ so the row has a reduced density or for $\mathrm{mod}(i_y,\mathcal{P}) \neq 0$ on the distance from the reduced density stripe.

In a phase with long-range spin or pairing order, the appropriate correlation function would approach a constant value asymptotically as $|\mathbf{i}| \to \infty$. Indeed, precisely this is seen in the ground state of the half-filled Hubbard model which has long-range antiferromagnetic order[56,62] and the attractive Hubbard model at a range of fillings.[63] It is still an open issue as to whether $c_{d\,\rm pair}(\mathbf{i})$ is nonzero at long distances when the homogeneous Hubbard model is doped away from half-filling because the sign problem prevents attaining the ground state in the doped case.

Given this limitation on the simulations, it is important to develop methods which extract the maximal useful information about the tendency to order at temperatures above the putative superconducting phase transition. To this end, one introduces a somewhat more sensitive measure of pairing by considering the pair-field susceptibility P_d and its associated vertex. To define P_d, we first extend the definition of the equal time pair correlation function $c_{d\,\rm pair}(\mathbf{i})$ to allow the insertion and removal of the Cooper pair to be separated in imaginary time. P_d is the sum over all spatial sites $\mathbf{i}$ and integral over all imaginary-time τ separations of $c_{d\,\rm pair}(\mathbf{i},\tau)$:

$$c_{d\,\rm pair}(\mathbf{i},\tau) = \langle \Delta_{d\,\mathbf{j}+\mathbf{i}}(\tau) \Delta^\dagger_{d\,\mathbf{j}}(0) \rangle,$$
$$\Delta^\dagger_{d\,\mathbf{j}}(\tau) = e^{\tau H} \Delta^\dagger_{d\,\mathbf{j}}(0) e^{-\tau H}, \tag{3}$$
$$P_d = \sum_{\mathbf{i}} \int_0^\beta c_{d\,\rm pair}(\mathbf{i},\tau)\, d\tau.$$

We also define the uncorrelated pair field susceptibility $\overline{P}_d$ which instead computes the expectation values of pairs of operators *prior* to taking the product, with expressions such as $\langle c_{\mathbf{i}+\mathbf{j}\downarrow}(\tau) c_{\mathbf{i}+\mathbf{j}\uparrow}(\tau) c^\dagger_{\mathbf{j}\uparrow}(0) c^\dagger_{\mathbf{j}\downarrow}(0) \rangle$ which appear in evaluating the P_d in Eq. (3) being replaced by $\langle c_{\mathbf{i}+\mathbf{j}\downarrow}(\tau) c^\dagger_{\mathbf{j}\downarrow}(0) \rangle \langle c_{\mathbf{i}+\mathbf{j}\uparrow}(\tau) c^\dagger_{\mathbf{j}\uparrow}(0) \rangle$.

P_d includes both the renormalization of the propagation of the individual fermions as well as the interaction vertex between them, whereas $\overline{P}_d$ includes only the former effect. In short, in DQMC, the averaging over the Hubbard-Stratonovich field replaces the interaction with the one-body potential by the original electron-electron interactions, so that the order of averaging and multiplying the operators can be used to control which many-body effects are included.

By evaluating both P_d and $\overline{P}_d$, we are able to extract[61] the interaction vertex Γ_d:

$$\Gamma_d = \frac{1}{P_d} - \frac{1}{\overline{P}_d}. \tag{4}$$

If $\Gamma_d \overline{P}_d < 0$, the associated pairing interaction is attractive. In fact, rewriting Eq. (4) as

$$P_d = \frac{\overline{P}_d}{1 + \Gamma_d \overline{P}_d} \tag{5}$$

suggests that $\Gamma_d \overline{P}_d \to -1$ signals a superconducting instability. This is the analog of the familiar Stoner criterion $U\chi_0 = 1$, which arises from the random phase approximation expression $\chi = \chi_0/(1 - U\chi_0)$ for the interacting magnetic susceptibility χ in terms of the noninteracting χ_0. We will discuss this criterion in more detail in the coming sections.

III. RESULTS

When the total density, averaged over the entire lattice, is fixed, the densities on and in-between the stripes depend on V_0 as shown in Fig. 3 for $\rho = 0.774$ and 0.875. $V_0 = 0$ corresponds to the homogeneous lattice, and the stripe and interstripe densities are equal there. As V_0 increases, charge is driven off the stripes until, ultimately, for $V_0 > 10$, the stripes are nearly empty. The fermions flow into the interstripe regions. Their density rises, going through half-filling at $V_0 \approx 6$, and asymptotically increasing to a bit over unity for large V_0 for $\rho = 0.774$. If the average density on the entire lattice were $\rho = 3/4$, then, for $\mathcal{P} = 4$, the interstripe regions would be precisely half-filled when the stripes are completely empty. For $\rho = 0.875$, the interstripe density crosses half-filling at $V_0 \approx 3$ and approaches $\rho \simeq 1.2$ as V_0 increases.

In Fig. 4, the spin-spin correlation $c_{\rm spin}(\mathbf{i})$ is shown along the center of the interstripe region (i.e., parallel to the stripes, see arrows in the inset), at $\rho = 0.774$ for $V_0 = 4$ [Fig. 4(a)] and $V_0 = 10$ [Fig. 4(b)]. As seen in Fig. 3, these values

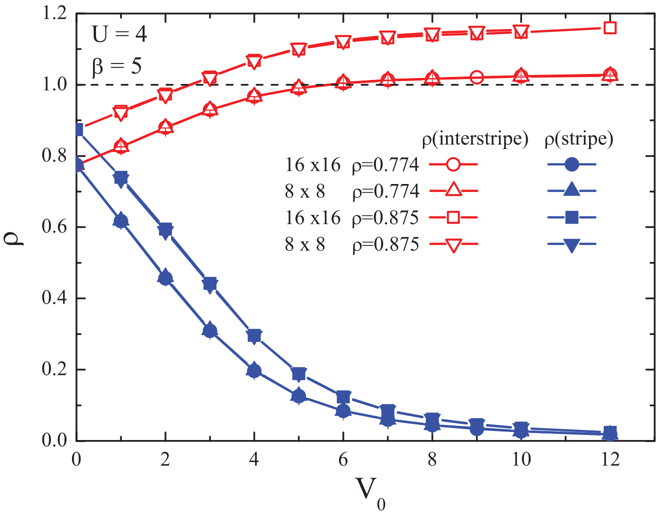

FIG. 3. (Color online) The density of particles is shown on the striped rows where V_0 acts (closed symbols) and on the unstriped rows (open symbols). The total density of the system is fixed at $\rho = 0.774$ (circles for 16×16 and up triangles for 8×8 lattices) and $\rho = 0.875$ (squares for 16×16 and down triangles for 8×8 lattices). There is only a very small variation of density on the unstriped rows with different distance from the stripes, so only the average is shown. Data for 8×8 and 16×16 lattices are essentially indistinguishable.

correspond to densities slightly below and slightly above half-filling, respectively. Despite the doping, there is a fairly robust antiferromagnetic pattern as T is lowered.

In contrast, in the absence of stripes $V_0 = 0$, the doped holes are spread uniformly throughout the lattice, and for the same density as exhibited in Fig. 4, antiferromagnetic order is very short ranged, as seen in Fig. 5. In the absence of any sort of charge inhomogeneity, it would be very unlikely that these weak magnetic correlations could provide the "pairing glue"

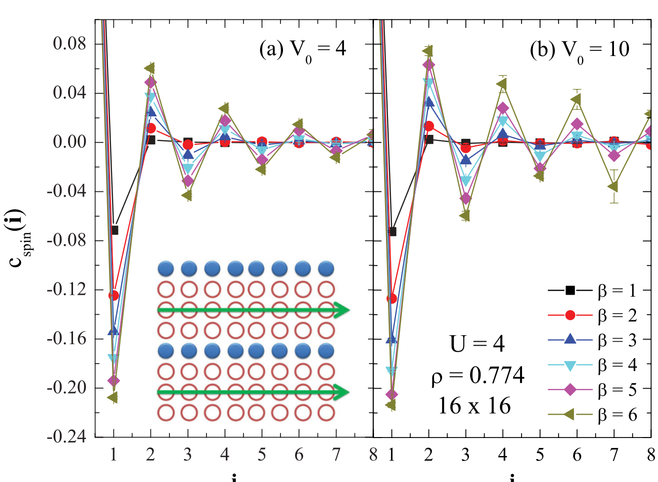

FIG. 4. (Color online) The spin correlation function $c_{\mathrm{spin}}(\mathbf{i})$ along the center of one of the (three-site-wide) interstripe regions. Here, $U = 4$, and the average density $\rho = 0.774$ over the whole lattice, for $V_0 = 4$ (a) and $V_0 = 10$ (b). The interstripe region is fairly close to half-filling and so, as the temperature T is lowered, $c_{\mathrm{spin}}(\mathbf{i})$ oscillates over fairly large distances. The arrows indicate the sites along which the spin-spin correlations are calculated.

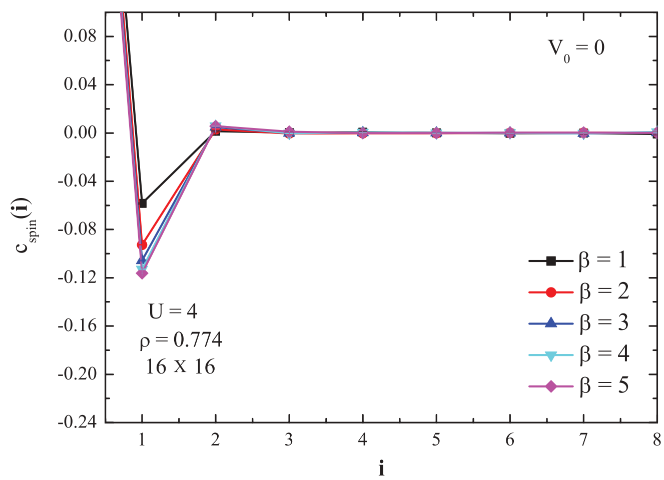

FIG. 5. (Color online) Same as Fig. 4 except for $V_0 = 0$ so that the lattice is at homogeneous density. When there are no stripes, the spin correlations die out very rapidly for this doping of the uniform Hubbard Hamiltonian. They would be unlikely to be able to supply the "glue" for Cooper pairing.

for high-temperature superconductivity. Thus, the results of Figs. 4 and 5 suggest that domain formation is a prerequisite for any superconductivity which is postulated to arise from robust magnetism at this density.

The presence of stripes alone is not enough to guarantee the presence of antiferromagnetic correlations. Figure 6 shows the same spin-spin correlations as in Figs. 4 and 5, but for $\rho = 0.875$. Although spin-spin correlations are slightly higher at $V_0 = 3$, where the interstripe density is close to one, antiferromagnetic correlations are very short ranged for all V_0.

If the lattice is traversed perpendicular to the stripes, we expect the spin correlations to be significantly reduced: the low density on the stripes does not support a very large moment. In Fig. 7, we show $c_{\mathrm{spin}}(\mathbf{i} = 2\hat{y})$, corresponding to a pair of sites on a line parallel to the $\hat{y}$ axis and traversing a stripe (see inset for a sketch). The scale of $c_{\mathrm{spin}}(\mathbf{i} = 2\hat{y})$ is roughly an order of magnitude smaller than $c_{\mathrm{spin}}(\mathbf{i} = 2\hat{x})$, as suggested should be the case by the preceding argument. Apart from the size of the correlation, there is another feature of crucial interest. For

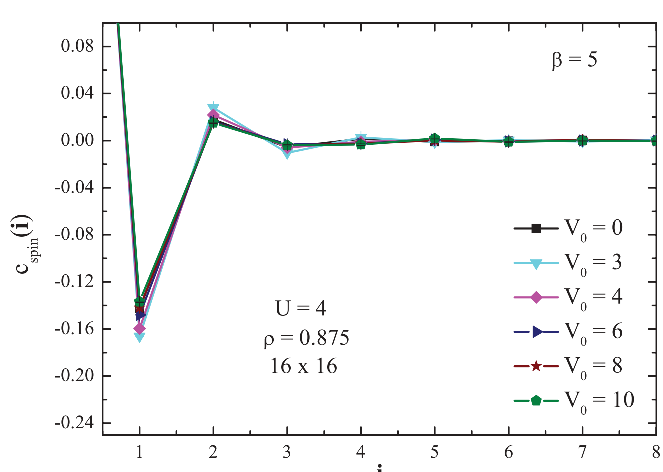

FIG. 6. (Color online) Same as Fig. 4 except for $\rho = 0.875$ at fixed $\beta = 5$ and different values of V_0.

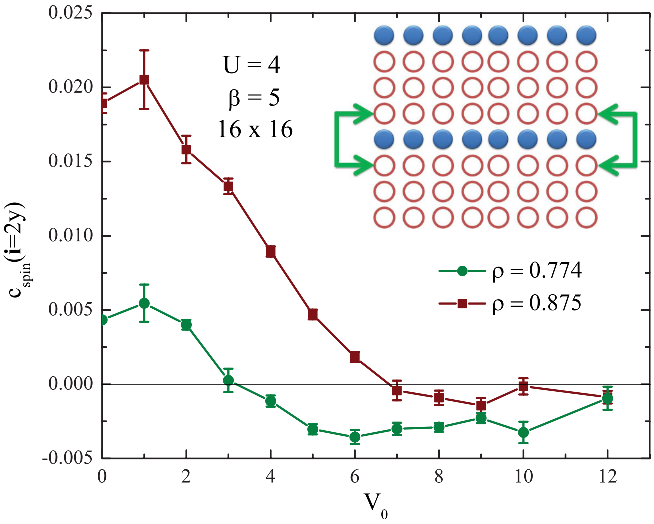

FIG. 7. (Color online) Spin correlations are shown perpendicular to the stripe and, specifically, for fixed distance $\mathbf{i} = 2\hat{y}$ which crosses a stripe and varying V_0. For V_0 small (the nearly homogeneous limit), $c_{\rm spin}(\mathbf{i} = 2\hat{y})$ is positive, as would arise in an up-down-up- . . . staggered magnetic pattern. However, as stripes are introduced, $c_{\rm spin}(\mathbf{i} = 2\hat{y})$ flips sign. The magnetic order exhibits a π-phase shift and the sublattices of the (bipartite) square lattice on which the up-spin electrons sit are reversed upon crossing a stripe. Arrows in the inset show pairs of sites traversing the stripe, where the spin-spin correlation functions are calculated.

$\rho = 0.774$ and small V_0, i.e., close to the homogeneous limit, the spin correlation two sites away $c_{\rm spin}(\mathbf{i} = 2\hat{y})$ is positive, as expected for an antiferromagnet. However, for $V_0 > 3$, the sign flips and $c_{\rm spin}(\mathbf{i} = 2\hat{y})$ becomes negative. This effect is strongly reduced for $\rho = 0.875$, where the negative values of $c_{\rm spin}(\mathbf{i} = 2\hat{y})$ are smaller in magnitude than those for $\rho = 0.774$ and only occur for $V_0 \gtrsim 7$.

This π-phase shift is a prominent experimental feature of stripe physics in the cuprates.[24,25] These results show that this shift in the sublattice order across a stripe is also a characteristic of the doped 2D fermion Hubbard model, at least in the case considered here in which the stripes are created through an externally imposed potential.

We turn now to the pairing correlations. Figure 8 shows the d-wave pairing correlation function along a stripe. As we will see in the following, the lowest temperatures achieved are well above the superconducting transition and therefore the superconducting correlations are short ranged. Figure 9 shows the pairing correlations between two neighboring sites within a stripe as a function of V_0. It is clear that the presence of stripes enhances pairing, and it is interesting to note that for both $\rho = 0.774$ and 0.875, $c_{d\,\rm pair}(\mathbf{i})$ stabilizes for V_0 close to the value for which the π-phase shift takes place, namely, $V_0 \sim 4$ and $V_0 \gtrsim 7$, respectively.

Figure 10 shows the key result of this paper. As charge domains are introduced into the square-lattice Hubbard model, the d-wave pairing vertex becomes considerably more attractive. Indeed, not only is its magnitude increased by a factor of 3 relative to the homogeneous system, the temperature evolution becomes increasingly steep. As in all existing DQMC studies of the repulsive Hubbard Hamiltonian, the sign problem

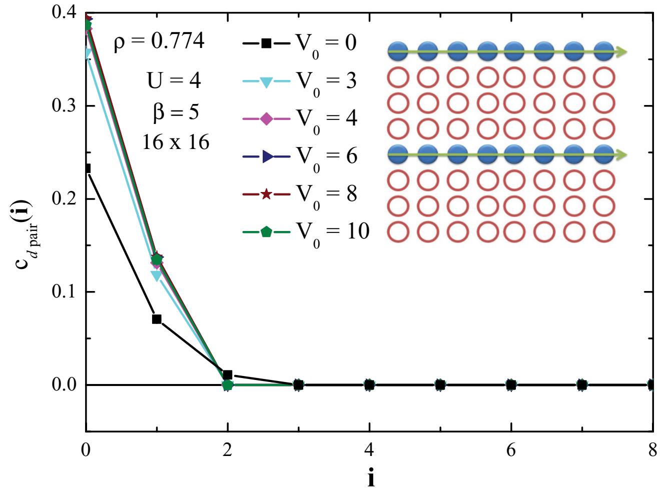

FIG. 8. (Color online) d-wave pair-pair correlation functions along the stripes for $\beta = 5$, $\rho = 0.774$, and different V_0. Pairing correlations are shown to be short ranged.

prevents accessing low enough temperatures to establish a critical T_c where $\Gamma \overline{P}_d = -1$, if such a superconducting transition does indeed occur in this model. Nevertheless, the results of Fig. 10 are suggestive that charge domains considerably enhance the d-wave pairing.

We can study these same data as a function of V_0 at constant temperature. Figure 11 shows results for our canonical parameters, 16×16 lattices, $U = 4$, and $\rho = 0.774$. We find that the pairing vertex becomes more and more robust with increasing V_0. This is not completely intuitive. One might expect that a maximum pairing would occur for $V_0 \approx 6$ where, according to Fig. 3, the interstripe regions are most close to half-filling and hence antiferromagnetic correlations are most strong. Alternately, as V_0 becomes very large, the particle density within the stripes drops to zero. If the physical picture is that of pairing of mobile carriers in the doped region driven by spin correlations in the half-filled domains, at large V_0 the

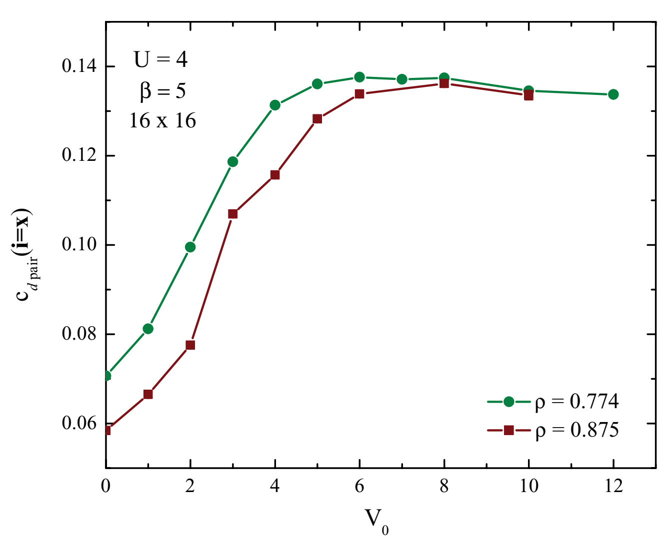

FIG. 9. (Color online) d-wave pair correlations on neighboring sites, along the stripe, as a function of V_0. It is clear that as V_0 is increased, the d-wave pairing is enhanced along the stripes.

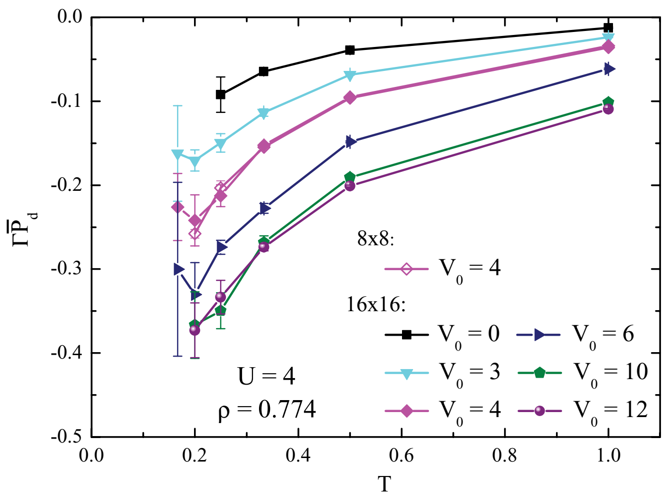

FIG. 10. (Color online) The d-wave pairing vertex is shown as a function of temperature for $U = 4$, $\rho = 0.774$, and different values of the externally imposed stripe potential V_0. For the homogeneous system $V_0 = 0$, and small V_0 generally, $|\Gamma\overline{P}_d| \lesssim 0.10$. For larger V_0, $|\Gamma\overline{P}_d|$ exceeds 0.3 in magnitude. A superconducting instability is signaled by $\Gamma\overline{P}_d \rightarrow -1$. Data for 8×8 lattice ($V_0 = 4$, open symbols) show finite-size effects are negligible.

density of these carriers becomes small, and one would again expect $\Gamma\overline{P}_d$ to turn over.

Recent DCA calculations[49] indeed reveal an initial enhancement of pairing with the introduction of stripes, followed by a falloff as the above physical arguments suggest. However, this nonmonotonicity is observed only at very low temperatures $T \sim 0.05$ quite close to T_c. For higher T, closer to the range studied here, there is no sign of the d-wave eigenvalue coming down at large V_0. Although the lower-temperature scales are the most likely explanation for the DCA nonmonotonicity, it is also possible that, in the work presented here, the decline of pairing correlations in the doped stripes is

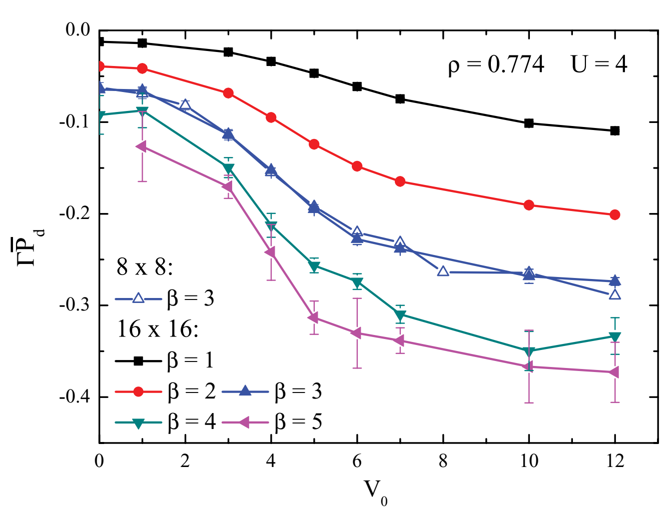

FIG. 11. (Color online) The data of Fig. 10 are replotted to show the d-wave pairing vertex as a function of V_0 for fixed inverse temperature β. $\Gamma\overline{P}_d$ becomes monotonically more attractive. Data for 16×16 lattices (closed symbols) and 8×8 lattice (open symbols) show finite-size effects are smaller than statistical fluctuations.

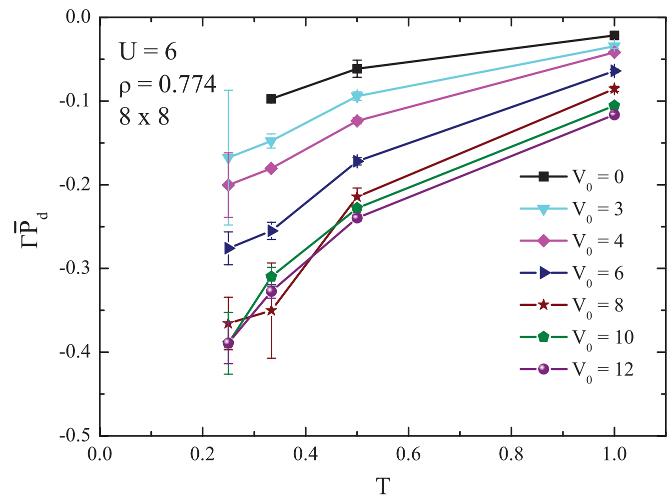

FIG. 12. (Color online) The pairing vertex is shown as a function of temperature for the same parameters as Fig. 10, except for a larger onsite repulsion $U = 6$ rather than $U = 4$, and 8×8 lattices. The behavior is similar: charge inhomogeneities make the d-wave vertex more attractive.

compensated by an increase in the interstripe domains, which are shifted away from half-filling at large V_0. It seems clear that for large V_0 and density $\rho = 0.750$, where the interstripe regions are precisely half-filled, the pairing signal would be forced to be small, and hence that a turnover such as is seen in DCA calculations should occur.

The physics of the half-filled homogeneous Hubbard model on a square lattice is believed not to be highly sensitive to the interaction strength U. That is, the ground state is an antiferromagnetic insulator for all U, although the precise nature of the phase evolves from a weak-coupling regime described by spin density wave physics to a strong-coupling Mott insulator. In order to assess whether the enhancement of d-wave pairing due to striped formation is similarly generic to different U or specific to $U = 4$, we show data for $\Gamma\overline{P}_d$ as a function of temperature T in Fig. 12 for $U = 6$. The same basic evolution is observed as in Fig. 10, with the vertex being enhanced by V_0 both in magnitude and also in the steepness of its evolution as T is lowered. A comparison of the data ranges of Figs. 10 and 12 also reveals some of the limitations of DQMC. As U gets larger, the sign problem grows, as do the fluctuations (error bars). For $U = 6$, the lowest accessible temperature is $T \sim 0.3$ ($\beta = 3$), compared to $T \sim 0.2$ ($\beta = 5$) at $U = 4$. Smaller interaction strengths, e.g., $U \sim 2$, can readily be simulated, but tend to harbor large finite-size effects which are the remnants of high degeneracies in the noninteracting energy levels on a square lattice.

We next explore a different lattice periodicity $\mathcal{P} = 2$. Unlike the case of different interaction strengths, where the qualitative physics remains unchanged, $\mathcal{P} = 2$ behaves in a very different manner from $\mathcal{P} = 4$, as seen in Fig. 13. In this case, increasing V_0 reduces the magnitude of $\Gamma\overline{P}_d$, and by the time $V_0 = 3$, the vertex has even changed sign and become repulsive. It should be noted that because for $\mathcal{P} = 2$ there are fewer sites which do not feel the V_0 potential to absorb the fermions as V_0 increases, their density is increased above $\rho = 1$, where AF correlations are most evident, far more easily

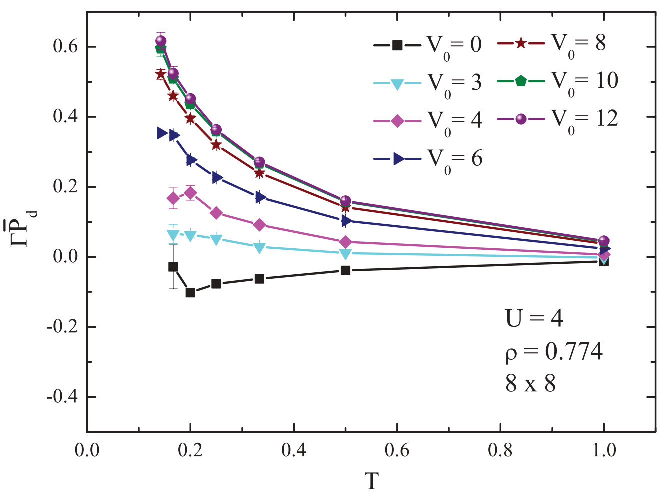

FIG. 13. (Color online) Pairing vertex for the $\mathcal{P} = 2$ case, where the stripes are separated by a single interstripe row. Unlike the $\mathcal{P} = 4$ case where a three-site-wide interstripe region separates the stripes, increasing charge inhomogeneity is detrimental to pairing. In fact, the d-wave vertex becomes repulsive for $V_0 > 2$.

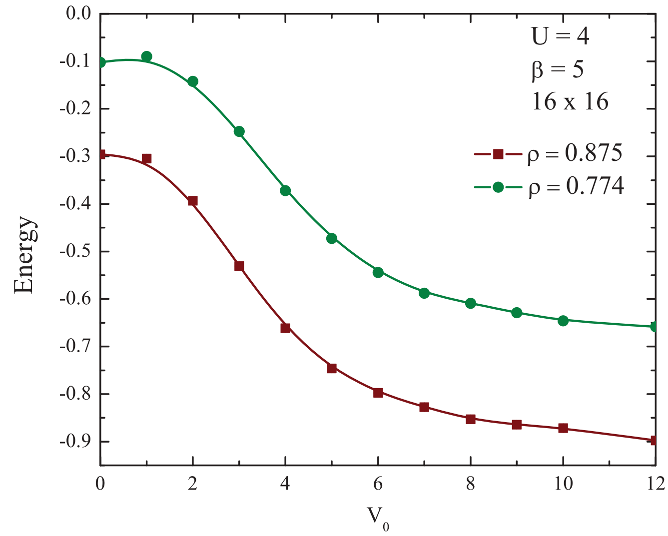

FIG. 15. (Color online) The total energy as a function of V_0 for 16×16 lattices with $U = 4$, $\beta = 5$, $\mathcal{P} = 4$, and $\rho = 0.875$ (squares) and $\rho = 0.774$ (circles).

than in the $\mathcal{P} = 4$ case shown in Fig. 3. This is the probable cause for the decrease in d-wave pairing correlations.

Our final check of the robustness of the enhancement of pairing by stripes is to explore a different density $\rho = 0.875$, which is optimal for pairing in the absence of stripes. Figure 14 indicates that the temperature evolution for nonzero V_0 is essentially unchanged from the homogeneous case. Thus, even though at $V_0 = 0$ the product $\Gamma\overline{P}_d$ is larger for $\rho = 0.875$ than for $\rho = 0.774$, this is no longer the case for nonzero V_0. Indeed, stripes can ultimately make the pairing vertex substantially larger for the lower density. The strong antiferromagnetic correlations induced by the stripes at $\mathcal{P} = 4$ provide the "glue" for pairing at $\rho = 0.774$, whereas at $\rho = 0.875$ this "glue" is not present.

We have focused thus far on the density, spin, and pairing correlations. Figure 15 examines the total energy as a function of V_0 on 16×16 lattices. Although we have imposed V_0 in our Hamiltonian, this computation of the energy provides a crude measure of the tendency for spontaneous stripe formation. The monotonically decreasing behavior of the energy with V_0 suggests that a maximization of charge imbalance is favored. When we study the effect of the periodicity of the stripes, as shown in Fig. 16 on a 12×12 lattice, we see that $\mathcal{P} = 3, 4$ have much lower energies, suggesting their formation might be favored. These periodicities have densities on the lines which are not subject to the additional potential V_0 relatively close to half-filling, and hence they have the largest antiferromagnetic correlations.

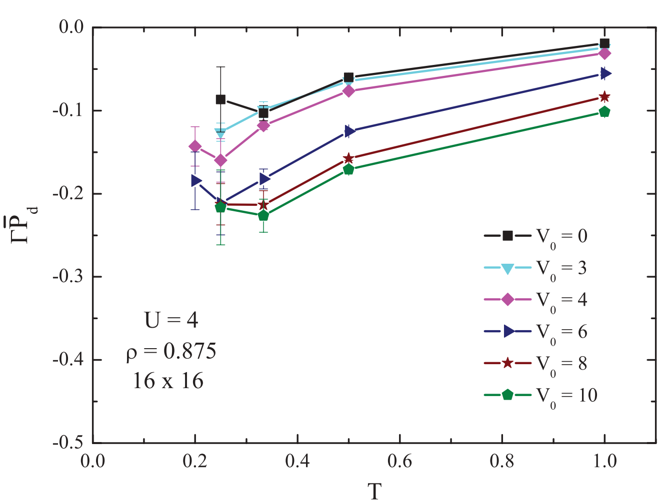

FIG. 14. (Color online) For a total density corresponding to close to the "optimal" doping of the cuprate superconductors, $\rho = 0.875$, the pairing vertex, while remaining attractive, shows somewhat less enhancement as V_0 is turned on.

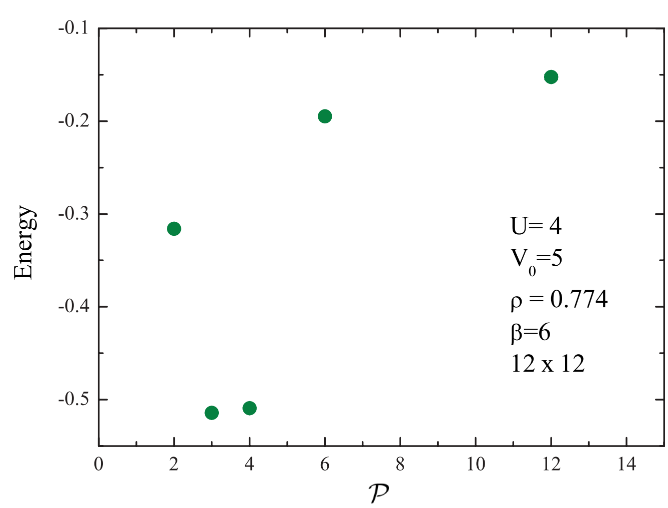

FIG. 16. (Color online) The total energy for different distances between stripes. The minimum for $\mathcal{P} = 3, 4$ is associated with the fact that the density of the $V_0 = 0$ rows is close to half-filling for total density $\rho = 0.774$.

IV. CONCLUSIONS

The external imposition of stripes via the introduction of a linear pattern of reduced chemical potential has been shown to result in a significant enhancement of the d-wave pairing vertex of the two-dimensional Hubbard Hamiltonian. When the overall density and periodicity of the stripes are such that the density in the interstripe region is close to one, antiferromagnetic correlations are also made larger, and exhibit a π-phase shift across the stripes. Both the π-phase shift and the growth in the superconducting response occur only when the charge inhomogeneity is sufficiently large, specifically when the additional inhomogeneous site potential V_0 exceeds roughly three times the hopping.

This enhancement of superconductivity has previously been observed in the closely related dynamical cluster approximation treatment of the two-dimensional Hubbard Hamiltonian, again in the case when a site potential V_0 was introduced externally. In this situation, the modulation was chosen to be broader than the purely one-dimensional pattern explored here. The observation of an optimal stripe potential in the DCA calculations might be associated with this difference. It is also interesting to note the possible differences between pinned and fluctuating stripes. There are suggestions[25,64–66] that the motion of charge/spin domain walls is important to the enhancement of superconductivity, whereas frozen stripes, such as created by Nd doping, is inimical to pairing. The studies in this paper, as well as the earlier DCA work of Maier *et al.*,[49] indicate that the situation may not be quite so straightforward and that, in fact, the stripes produced by an external potential might also be able to enhance superconductivity.

We have motivated our form for the externally imposed stripe potential at $\mathcal{P} = 4$ as producing the charge/spin patterns suggested by neutron scattering[24] and DMRG calculations.[50] Our pattern contains equal Fourier components for all wave vectors $Q_n = 2\pi n/\mathcal{P}$. In the DCA work,[49] the effect of different Fourier components $Q = \pi/2$ and $\pi/4$ was explicitly isolated, with the former showing little effect on pairing and the latter driving significant enhancement.

Spontaneous stripe formation in the doped Hubbard model, if it occurs, takes place at temperatures below those accessible to DQMC simulations, which are limited by the sign problem[60] to temperatures greater than roughly 1/40 of the noninteracting bandwidth. It would be interesting also to explore the possible enhancement of pairing at these temperature scales by other types of charge inhomogeneities such as checkerboard patterns[67] and in the presence of nonmagnetic disorder.[68,69]

ACKNOWLEDGMENTS

T.Y. was supported by a fellowship from the China Scholarship Council. Support from CNPq and FAPERJ (T.P. and R.M.) is greatly acknowledged. This work is supported by NSF-PIF-1005503 and DOE SSAAP DE-FG52-09NA29464. We thank B. Brummels for useful input and S. A. Kivelson for invaluable comments on the manuscript.

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