Stripes and superconducting pairing in the *t*-*J* model with Coulomb interactions

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We study the competition between long- and short-range interactions among charge carriers in strongly-correlated electronic systems employing a method which combines the density-matrix renormalization-group technique with a self-consistent treatment of the long-range interactions. We apply the method to an extended *t*-*J* model which exhibits "stripe" order. The Coulomb interactions, while not destroying stripes, induce large transverse stripe fluctuations with associated charge delocalization. This leads to a substantial Coulomb-repulsion-induced *enhancement* of long-range superconducting pair-field correlations.

I. INTRODUCTION

Much of the interesting physics of the high-temperature superconductors, in particular that related to the "mechanism" of high-temperature superconductivity, is moderately local, involving physics on the length scale of the superconducting coherence length, ξ_0. Since ξ_0 is typically a few lattice constants, this would seem to indicate that numerical solutions of model problems on clusters with as few as 50–100 sites should be able to provide considerable insight concerning these problems, even though results in this range are manifestly sensitive to the choice of boundary conditions and other finite-size effects. Such studies can also serve as important tests of the *predictions* of analytic theories.

Studies of *t*-*J* systems have, indeed, provided strong evidence of a universal and robust *d*-wave character of local pairing correlations,[1] and of a strong clustering tendency of holes, which might either lead to "stripe" (i.e., unidirectional charge density order) formation,[2] or phase separation.[3] Both of these features were in fact anticipated by analytic theories.[4,5] However, these studies for the *t*-*J* and parent Hubbard models have failed to find compelling evidence of the strong superconducting correlations[6] needed to understand high-temperature superconductivity. Moreover, many features of the results, especially with regards to stripes, appear very sensitive to small changes in the model, e.g., the shape and size of the cluster,[7] whether or not a small second neighbor hopping *t'* is included or not,[2] etc.

All these calculations omit the long-range part of the Coulomb interaction because it is difficult to treat using any of the standard numerical methods. However, since in the high-T_c cuprates, where interactions are generally conceded to be strong, the (interband) screening is semiconductorlike and not metalliclike, so there is no *a priori* justification for neglecting the long-range part. In addition, in the case of stripes, charge inhomogeneities or phase separation, longer-range Coulomb interactions are clearly important, a point which has previously been addressed with various mean-field approximations.[5,8,9]

In this paper, we present a computational method for studying the ground-state properties of electrons with strong short- and long-range interactions on fairly large finite systems. The method, which may be termed a "density-functional DMRG," uses numerically very accurate DMRG methods to treat the short-range part of the interactions. The long-range piece is taken into account within the Hartree approximation, which becomes exact in the long-distance limit, and, as we show below and in the Appendix, turns out to work well already for short distances. An important point to note is that, through the self-consistency requirement, the Hartree potential accounts for screening effects in a similar spirit as density-functional theory.

We have studied $N \times 4$ *t*-*J* ladders and cylinders, with hole densities per site $n_h = 1/9$, 1/8, and 1/7, and $N = 27$, 18, 16, and 14. Our principal findings, as summarized in the figures, are (1) charge stripe formation is robust to the inclusion of Coulomb interactions of reasonable strength, although the associated charge density modulations have their magnitude somewhat reduced. However, "spin stripe" correlations (i.e., spin density modulations which suffer a π phase shift across the charge stripe resulting in a spatial period twice that of the charge modulations) are prominent on cylinders, but very weak on ladders; they are slightly enhanced by the Coulomb interactions. (2) The inclusion of Coulomb interactions strongly *enhances* the superconducting pair-field correlations at the longest distances accessible in these calculations. This is our most striking result. (3) We present evidence that stripe formation does not suppress *local* superconducting pairing. On the other hand, rigid stripe ordering competes with long-range phase ordering.[2,10] The enhanced superconducting correlations at long distances produced by Coulomb interactions are, thus, tentatively associated with the enhanced pair tunneling between stripes produced by the increased stripe fluctuations, in agreement with phenomenological arguments.[11]

This paper is organized as follows. In Sec. II we introduce our model and the combined DMRG-Hartree technique to deal with it. In Sec. III we present our results for the charge and spin densities as well as for the pairing susceptibility. Section IV discusses our conclusions. For the sake of completeness, a discussion of the validity of the Hartree approximation is given in the Appendix.

II. MODEL AND TECHNIQUE

The Hamiltonian of the t-J model with nearest-neighbor hopping t and exchange interaction J plus long-range Coulomb interactions, which operates in the subspace of no doubly occupied sites, is given by

$$H = -t \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle \sigma} (c^{\dagger}_{\mathbf{r}\sigma} c_{\mathbf{r}'\sigma} + \text{H.c.})$$
$$+ J \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \left(\mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}'} - \frac{n_{\mathbf{r}} n_{\mathbf{r}'}}{4} \right) + \sum_{\mathbf{r}} V_{\text{Coul}}(\mathbf{r}) n_{\mathbf{r}}, \quad (1)$$

where $\langle \mathbf{r}, \mathbf{r}' \rangle$ are nearest-neighbor sites, σ is the spin index, $c^{\dagger}$ is the electron creation operator, $\mathbf{S}$ is the spin operator, and $n_{\mathbf{r}} = \Sigma_{\sigma} c^{\dagger}_{\mathbf{r}\sigma} c_{\mathbf{r}\sigma}$. The long-range part of the interaction[12]

$$V_{\text{Coul}}(\mathbf{r}) = V_0 \sum_{\mathbf{r}' \neq \mathbf{r}} \frac{n(\mathbf{r}') - \bar{n}}{|\mathbf{r} - \mathbf{r}'|} \quad (2)$$

is treated in the self-consistent Hartree approximation, whereby the density operator $n_{\mathbf{r}}$ is replaced with its ground-state expectation value $n(\mathbf{r}) \equiv \langle n_{\mathbf{r}} \rangle$ and $\bar{n}$ is the uniform positive background charge density. The Coulomb prefactor V_0 is given by $V_0 = e^2/[4\pi\varepsilon_0 \varepsilon a]$, where a is the lattice constant, and $\mathbf{r}$ is the coordinate of a lattice site in units of a. This long-range potential is screened by a background dielectric constant ε, given both by electronic interband and phonon contributions, which we take to be $\varepsilon = 8.5$, in reasonable accordance with cluster calculations for Coulomb matrix elements[10,13] and with quantum Monte Carlo simulations.[14] Thus, for $a \approx 3.4$ Å, the Coulomb prefactor in Eq. (2) is $V_0 \approx t$, being of the same order of magnitude as the kinetic energy.

Since V_{Coul} and the density $n(\mathbf{r})$ depend on each other, one needs a self-consistent solution of Eqs. (1)–(2). Our theoretical treatment is a combination of the DMRG technique,[15] which accurately accounts for short-range interactions, and a Hartree treatment of long-range interactions. In the spirit of "density-functional theory," we iteratively solve Eqs. (1) and (2) as follows: in the first step we set $V_{\text{Coul}} = 0$ and perform a DMRG calculation. This gives rise to a density profile $\{n(\mathbf{r})\}$ and, via Eq. (2), to a new potential V_{Coul}, which enters the next step DMRG calculation as an additional on-site potential. This procedure should be repeated iteratively up to convergence.[16] The fact that the Hartree approximation is appropriate for the long-range Coulomb part is discussed in detail in the Appendix.

Within a given loop, the goal of the DMRG simulation is to find iteratively an eigenstate of the Hamiltonian (1), using only a fraction of all the possible states of the system.[15] We have typically kept around 800–1000 states in the last iterations of the calculation, which results in a maximum discarded weight of the order 10^{-4}. We use systems with open (and cylindrical) boundary conditions chosen not to frustrate the domain walls.

III. RESULTS

In the end, we are able to compute ground-state energies for given quantum numbers and ground-state correlation functions. Because we do not have excited-state data, we are unable to compute dynamic susceptibilities. In the figures, we present representative results for various ground-state correlation functions. So as to make our principal findings clear, we have averaged these quantities over the transverse coordinate of the ladder. Thus, we define the average hole and spin density as a function of position along the ladder $0 < x \leq N$ as $\rho(x) \equiv \Sigma^4_{y=1}[1 - n(x,y)]/4$ and $S_z(x) \equiv \Sigma^4_{y=1}(-1)^{x+y}\langle S^z(x,y) \rangle/4$. Note that translational (in the x direction) and spin rotational symmetry are explicitly broken in these calculations by the ladder ends, themselves, and [following White and Scalapino (WS)[2]] by an applied staggered Zeeman field of magnitude $h = 0.1t$ on the ladder ends.[2,17]

To probe superconductivity, we have computed the ground-state pair-field correlation function

$$D(x) = \left\langle \Delta\left(\frac{N}{2} + \frac{x}{2}\right) \Delta^{\dagger}\left(\frac{N}{2} - \frac{x}{2}\right) \right\rangle. \quad (3)$$

Here $\Delta^{\dagger}(x)$ creates a $d_{x^2-y^2}$-like pair around the $(x,2)$ site.[18] We have explored the dependence of our results on parameters to some extent, but in all the figures have adopted a conventional value $J/t = 0.35$.

Consider first the results of the DMRG calculations without the long-range Coulomb potential. Results for the spin and charge density are shown as the dashed lines in Figs. 1 and 2 and for the pairing susceptibility $D(x)$ by the dashed line in Fig. 3(a).

In the low-doping case ($n_h = 1/9$) depicted in Fig. 1, charge stripe order is clearly seen. Stripes form in the t-J model so as to satisfy the competing requirements of minimizing the kinetic energy of the doped holes and minimizing the disturbance of the background exchange interactions.[2,4] In order to distinguish between stripes and ordinary Friedel oscillations, we have compared the hole-density profile for different length ladders (18×4 and 27×4) at the same doping. As one can see from Figs. 1(c) and Figs. 1(d) for the cases with and without Coulomb interaction, respectively, the amplitude in the center of the system is essentially independent of the system size, while Friedel oscillations should decay as a function of the distance from the boundary.[7,19] As seen in Fig. 1(b), any π phase shift in the AF order (spin stripes) is quite weak in the present calculation, although it is slightly enhanced by the Coulomb interaction. In accordance with Ref. 2 for the bare t-J model, spin stripe order is stronger in the case of cylindrical boundary conditions. There is roughly one hole per two stripe unit cells, which was taken by WS (Ref. 2) as evidence that the t-J model favors stripes with a minimum energy for a linear charge density of $\lambda \sim 0.5$. This is in agreement with experiments,[20–22] which find stripes with $\lambda \approx 0.5$ at hole dopings smaller than $n_{h,c} \approx 1/8$.[23–26] For $n_h \geq 1/8$ the density-wave structure seen in Fig. 2 is less clear. Were the stripes to retain their integrity at these higher hole concentrations, they would be forced very closer together, at considerable cost in energy. However,
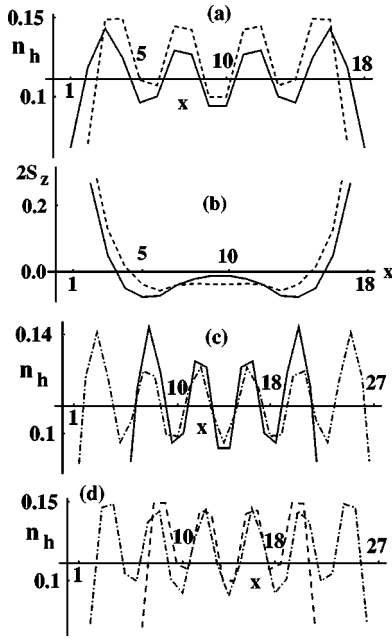
FIG. 1. (a) Hole density $\rho(x)$ and (b) staggered spin density $S_z(x)$ as a function of position x along a 18×4 ladder (i.e., with open boundary conditions in the y direction) (Ref. 12) with eight holes ($n_h = 1/9$). The results with nonvanishing Coulomb prefactor ($V_0 = t$, solid lines) are compared with those without Coulomb interaction ($V_0 = 0$, dashed lines). A comparison of $\rho(x)$ in a longer system (12 holes in 27×4) with the same $n_h = 1/9$ (dashed-dotted line in both cases) is shown in (c) and (d) respectively with and without Coulomb interactions.

the clustering tendency of holes is still apparent in the ground-state charge distribution, which is suggestive of two hole-rich puddles, each with four holes.

As discussed by WS, the hole clusters locally share a number of features with the two-hole pair state, which accounts for the fact that the energy per hole for a domain wall is close to the energy per hole for a pair.[2] This is suggestive of a competition between stripe stability and superconductivity.[10] Such a competition has already been demonstrated in a model which includes next-nearest-neighbor hoppings t' by WS. For large enough $|t'|$, the domain walls "evaporate" into quasiparticles ($t' < 0$) without significant pairing correlations or into pairs ($t' > 0$).[2] It has long been clear that stripe formation suppresses long-range
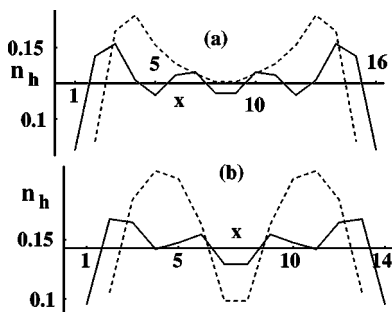

FIG. 2. Hole density $\rho(x)$ for eight holes in a 16×4 (a) and a 14×4 (b) ladder. Conventions are as in Fig. 1.
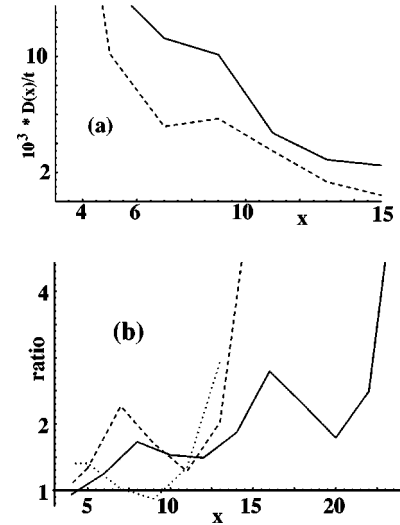

FIG. 3. (a) The long-distance part of the pair-field correlation $D(x)$ for 8 holes in a 18×4 ladder without V_{Coul} (dashed line) and with V_{Coul} (solid line). (b) The ratio between $D(x)$ with V_{Coul} and without V_{Coul} for $N \times 4$ ladders with 8 holes and $N = 18$ (dashed) $N = 16$ (dotted), and $N = 27$ with 12 holes (solid) (Ref. 18).

superconducting phase coherence,[11] as is clear from the rapid falloff with distance of the pair-field correlator in Fig. 3(a) (dashed line).

We now turn to our results in the presence of the Coulomb interactions. Unscreened Coulomb interactions ($\varepsilon = 1$, i.e., $V_0 \simeq 8.5t$) are so strong that they entirely dominate the physics, destroying all clustering or pairing tendencies of the system. However, for the physically relevant case, $\varepsilon \sim 8.5$, the results are much more interesting.

In the lightly doped case, $n_h = 1/9$, shown in Fig. 1, the stripe structure is essentially unchanged by Coulomb interactions, although the amplitude of the charge modulations is suppressed (by roughly a factor of 1.5), and the anti-phase character of the spin correlations is slightly enhanced. We interpret this as meaning that the stripe order is robust, but that the Coulomb interactions enhance the transverse stripe fluctuations. The most dramatic effect of the Coulomb interactions is the strong enhancement of the pair-field correlations shown in Fig. 3. From Fig. 3 (in which the short-distance data is off scale) one might conclude that the Coulomb interactions primarily increase the *overall* magnitude of the pair correlations. On the other hand, from the ratio between the two functions, which is displayed in Fig. 3(b) over the whole range of x, one can see that it is only the *long-distance* part that is enhanced. In order to sort out boundary effects, which are probably responsible for part of the strong increase of the ratio at the longest distances available, we have also treated a larger (27×4) ladder. Although the calculation of $D(x)$ is less accurate for this system,[18] we can still draw some conclusions. As one can see from the figure, the ratio of $D(x)$ shows oscillations with twice the stripe periodicity, whose envelope is clearly increasing with distance, even far away from the boundaries.

The dependence of $D(x)$ on distance, seen in Fig. 3(a), is altered from rapidly decreasing in the absence of Coulomb

interactions, to much slower distance dependence in the presence of Coulomb interactions. This result supports the idea that while the longer-range phase coherence (or, in other words, pair delocalization) is inhibited by rigid stripe order, as obtained in the pure t-J model, stripe fluctuations, induced by the Coulomb interaction, permit the pairs to tunnel from stripe to stripe. It should be pointed out that this conclusion may not be generic and may depend on the stripes stiffness. If stripes are intrinsically weak, we expect their fluctuations to be strong *without* the need of Coulomb interaction. In this case, the pair-breaking effects of the Coulomb interaction would probably obtain the opposite effect and suppress pairing correlations. It could also be the case that in our relatively narrow systems stripes are particularly stiff, due to the fact that they cannot meander effectively.

To further corroborate this interpretation, we have computed the (finite-size) spin gap with and without Coulomb interactions for the $N=14$ system (with $h=0$). This is $\Delta_s \sim 0.16t$ without Coulomb interaction, and $\Delta_s \sim 0.12t$ with $V_0=t$. Since we know from the work of WS,[2] that the local stripe energetics is essentially dominated by the short-range pair binding (which sets a scale for the spin gap as an $S=1$ excitation of the pair) and since we find Δ_s only slightly reduced in the presence of Coulomb interaction, it is reasonable to assume that the local pairing itself is still due to the short-range t-J physics.

The effects of Coulomb interactions on the charge-density profile are even stronger (and more complex) in the more heavily doped systems as shown for $N=16$ ($n_h=1/8$) and $N=14$ ($n_h=1/7$) in Fig. 2. In these systems, even the period of the stripe array is altered by the Coulomb interactions. In particular, the two hole puddles seen as minima in the electronic density in the absence of Coulomb interactions are broken apart into structures that look somewhat more similar to the four-stripe pattern seen in the $N=18$ ladder. This result is an example of a period selection caused by a Coulomb-frustrated tendency to clustering, or phase separation.[5] In this case, we expect particularly large fluctuations between the competing configurations to enhance the delocalization of pairs between stripes.

IV. CONCLUSIONS

In summary, in this paper we present a new approach capable of bridging the gap between work[5,10] arguing that stripes are due to a delicate balance between kinetic and long-range Coulomb interaction energy, and work[2] supporting the idea that short-range interactions alone can lead to stripe formation. Based on the "density-functional" DMRG, we present numerical results, supporting the view that—while short-range "t-J-like" interactions locally bind holes into pairs—it is the long-range Coulomb interaction which induces their delocalization accompanied with substantial enhancement of superconducting pairing correlations. Moreover, the Coulomb-induced stripe fluctuations suppress the magnitude of charge-density wave order, but can actually slightly enhance the ("antiphase") spin-density wave correlations with twice the wavelength.

APPENDIX:

VALIDITY OF THE HARTREE APPROXIMATION

The Coulomb interaction part of the Hamiltonian reads

$$W = \frac{1}{2} \sum_{\mathbf{r} \neq \mathbf{r}'} \frac{V_0}{|\mathbf{r} - \mathbf{r}'|} n_{\mathbf{r}} n_{\mathbf{r}'}, \quad (A1)$$

where $n_{\mathbf{r}}$ is the density operator. This can be rewritten as

$$W = \sum_{\mathbf{r} \neq \mathbf{r}'} \frac{V_0}{|\mathbf{r} - \mathbf{r}'|} \langle n_{\mathbf{r}} \rangle n_{\mathbf{r}'} + \frac{1}{2} \sum_{\mathbf{r} \neq \mathbf{r}'} \frac{V_0}{|\mathbf{r} - \mathbf{r}'|} (n_{\mathbf{r}} - \langle n_{\mathbf{r}} \rangle)$$
$$\times (n_{\mathbf{r}'} - \langle n_{\mathbf{r}'} \rangle) + \text{const}, \quad (A2)$$

where $\langle n_{\mathbf{r}} \rangle$ is the ground-state expectation value of $n_{\mathbf{r}}$. Here, the first term on the right hand side of Eq. (A2) (let us us call it W_H) corresponds to the Hartree approximation, while the second (W_c) gives its correction. Of course, when the expectation value of W_c vanishes, the Hartree approximation becomes exact (for ground-state properties). Since, by definition, $g(\mathbf{r}, \mathbf{r}') \equiv \langle n_{\mathbf{r}} n_{\mathbf{r}'} \rangle / \langle n_{\mathbf{r}} \rangle \langle n_{\mathbf{r}'} \rangle$, $\langle W_c \rangle$ can be also written as

$$\langle W_c \rangle = \frac{1}{2} \sum_{\mathbf{r} \neq \mathbf{r}'} \frac{V_0}{|\mathbf{r} - \mathbf{r}'|} \langle n_{\mathbf{r}} \rangle \langle n_{\mathbf{r}'} \rangle [g(\mathbf{r}, \mathbf{r}') - 1], \quad (A3)$$

and, thus, the correction to Hartree vanishes when $g(\mathbf{r}, \mathbf{r}') = 1$.

In order to measure the accuracy of a mean-field approximation for a generic operator $\hat{O}(\mathbf{r}) \hat{O}(\mathbf{r}')$ in the Hamiltonian, one should evaluate its fluctuations

$$\Delta_O(\mathbf{r}, \mathbf{r}') \equiv \langle [\hat{O}(\mathbf{r}) - \langle \hat{O}(\mathbf{r}) \rangle][\hat{O}(\mathbf{r}') - \langle \hat{O}(\mathbf{r}') \rangle] \rangle. \quad (A4)$$

Since these terms give the corrections to the mean-field approximation [see Eq. (A3)], a small value for Δ_O means that the mean-field approximation for O is accurate.

In our calculations, the density fluctuations $\Delta_n(\mathbf{r}, \mathbf{r}')$ are typically about $20-30$ times smaller than the spin fluctuations $\Delta_{\mathbf{S}}(\mathbf{r}, \mathbf{r}')$, for nearest-neighbor $\mathbf{r}$ and $\mathbf{r}'$, where both fluctuations are largest (for $\mathbf{r} \neq \mathbf{r}'$). This is the reason for using the Hartree approximation for the Coulomb part and to treat the "J" part exactly. Similarly, on the same lattice site, $\Delta_n(\mathbf{r}, \mathbf{r}) \approx 0.1$, which is of the same order as $\Delta_{\mathbf{S}}(\mathbf{r}, \mathbf{r}')$, which, in turn, justifies an exact treatment of the *on-site* interaction.

Notice that the inhomogeneous state brought about by the

open boundary conditions is decisive in making the Hartree approximation work better. Indeed, in a homogeneous system (obtained by periodic b.c.) $\langle n_{\mathbf{r}} \rangle$ would be constant, and the oscillations in the charge will be all shifted to the fluc-

tuations $n_{\mathbf{r}} - \langle n_{\mathbf{r}} \rangle$, making the correction $\Delta_n(\mathbf{r},\mathbf{r}')$ large. On the other hand, for open boundary conditions, part of the charge oscillations are taken care of by the mean values $\langle n_{\mathbf{r}} \rangle$ making $n_{\mathbf{r}} - \langle n_{\mathbf{r}} \rangle$ [and thus $\Delta_n(\mathbf{r},\mathbf{r}')$] smaller.

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[16] In practice, the self-consistent procedure has been speeded up by using a variant of the Newton method.

[17] The introduction of h improves the convergence of the DMRG procedure, although it also substantially modifies the charge and spin distributions. However, *once h is switched on*, and provided

h is not too large ($h \lesssim 0.2t$), these distributions turn out to be weakly field dependent.

[18] The accuracy of the pair-field correlations is especially slowly converging with the number of states kept in the DMRG procedure (see also Ref. 2). In our case, by keeping a moderate number of states ($m \sim 900$) in each block, we can estimate for the 18×4 system (where the convergence is worst) a maximum error of $\sim 40\%$ in the pair correlation at the largest accessible distance. In the 27×4 system the error in $D(l \geq 12)$ is probably larger than 50%. However, we have checked that the ratio at large distances plotted in Fig. 3 *increases* with increasing m, i.e., with increasing accuracy. One can, thus, expect that in a more accurate calculation (i.e., with larger m) the Coulomb enhancement effect shown in Fig. 3 would be even more dramatic.

[19] Obviously, our calculation, limited to small system sizes especially in the stripe direction, does not allow us to make strong conclusions about whether we have true charge-density-wave long-range order or not. In fact, physically, this is probably not the case for dynamic stripes. Nevertheless, our calculation *does* show that charge fluctuations are strong and extend to many lattice sites.

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