Populated Domain Walls

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Several experiments suggest that the charge carriers in the normal state of certain cuprate superconductors reside on domain walls. In an earlier paper, we suggested that several aspects of the anomalous dynamical behavior of these materials could be explained, at least qualitatively, on this basis. Here, using results on the ground state energy of the one-dimensional Hubbard model (soluble by Bethe ansatz techniques) as a function of charge density, we argue that a nonzero charge density localized to domain walls is a very plausible consequence of strong short-range electron-electron repulsion. We also suggest a method to suppress meandering of the walls and thereby enhance their signature in neutron diffraction. [S0031-9007(97)02725-7]

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Recently, there has been great interest in the electronic structure of domain walls in effectively two-dimensional materials with antiferromagnetic order. Some materials in this class have empty walls, but there is mounting experimental evidence from neutron scattering that at least in some of the cuprate materials the length of the walls is a nontrivial multiple of the hole density [1,2]; indeed, the electron filling fraction on the wall appears to be approximately $1/4$—one electron per every two lattice sites—in a variety of circumstances. If correct, this is a very significant result because it implies the possibility of charge transport along the walls. Effectively, the populated walls would form a system of dynamical one-dimensional wires within the two-dimensional planes.

Even prior to the most recent experimental results the possibility that spatially inhomogeneous structures occur in the cuprates, and are important in understanding their markedly anomalous properties, was the subject of considerable theoretical work [3–8]. In a recent paper [9], written after [1] but just before [2], we suggested a particular hypothesis—the minimal domain wall hypothesis—which leads to domain walls having one hole per every two lattice sites. (It is interesting to note that this hypothesis might be rephrased as the existence of exclusion statistics [10] $g = 2$ for spinless holons on the wall.) Related ideas were suggested, independently, by Emery and Kivelson under the title topological doping [11]. We also suggested how several of the most striking anomalous features of the normal state of the cuprates could be understood, at least qualitatively, given the existence of one-dimensional walls supporting nontrivial charge transport.

Unfortunately, however, detailed studies of wall energetics in the Hartree-Fock approximation [3,4] have invariably suggested that empty walls are most favorable. This puts the existence of the suggested universality class open to doubt; more optimistically interpreted, it poses the challenge to find an alternative, appropriate approximation which makes it plausible that populated walls can be favorable.

Here we shall present an energetic argument, appropriate to electronic systems with very strong short-range repulsion (for which Hartree-Fock is unreliable) which suggests physically interesting conditions under which populated walls are energetically favored. Recall that in a Hartree-Fock calculation, an expectation value for the staggered magnetization is assumed, which leads to the opening of a gap at the boundary of the magnetic zone (which, in a model with only nearest-neighbor hopping, is the Fermi surface at half filling). In the presence of a domain wall, across which the staggered magnetization changes sign, there are, in addition, states which lie in the gap. Since their total length is smaller for a fixed number of holes, empty domain walls cause less disruption of the antiferromagnetic order than do domain walls with nonzero filling. As a result, they are energetically favored. Here, we consider the opposite limit of very large U in which a one-electron picture is not valid. The advantage of a domain wall with nonzero filling is that electrons on the wall can gain kinetic energy t which is much greater than J—but still much smaller than U, of course, which prevents them from escaping the wall. Said differently, in this limit, the states on the wall lie within the lower Hubbard band and therefore might be occupied. In a Hartree-Fock picture on the other hand, they lie between the lower and upper bands, which makes them energetically unfavorable.

Central to our argument is an old result of Lieb and Wu [12] on the ground state energy of the one-dimensional Hubbard model. The Hamiltonian of this classic model contains two parameters t and U, with the units of energy, which parametrize the amplitude for hopping and the

on-site repulsion, respectively. The general result is quite complicated, but in the limit $U \to \infty$ takes the following remarkably simple form:

$$E_{\text{kinetic}}/N_s = -t \sin 2\pi f , \tag{1}$$

where $f \equiv N_e/2N_s$ is the filling fraction, N_e and N_s being, respectively, the number of electrons and the number of sites along the wall. Note that this energetic effect of hopping remains finite as $U \to \infty$. One can crudely interpret the $U \to \infty$ result (1) as representing the energy of free *spinless* fermions: The exclusion constraint between different spins is satisfied, in the ground state, by enforcing complete antisymmetry. Remarkably, this energy is indeed minimized at $f = \frac{1}{4}$, the value suggested by the minimal domain wall hypothesis.

That is not by any means the full story, however. We are really more interested in the minimum energy per hole, not per wall site. Furthermore, the energy involved in creating the walls must be taken into account.

Let us step back a moment to roughly survey the problem of energetics for holes doped into an antiferromagnetic background, with large short-range (say, for simplicity, on-site) repulsion. If one sprinkles isolated holes into such a background, simply by emptying sites, then each hole removes four potential $J\mathbf{S}_i \cdot \mathbf{S}_j$ spin-spin alignment terms, so that there is a penalty $4\lambda J$ in energy. (Breaking a singlet bond costs energy $-\frac{3}{4}J$. In an antiferromagnet, one cannot have singlets throughout, the energy per bond is reduced, $\lambda < \frac{3}{4}$.) One can cut this down by allowing the holes to form connected patches; then the energy cost is $2\lambda J$ per hole. Alternatively, one can put the holes on walls; the cost of this is $3\lambda J$ per wall site. The question then becomes whether the energy gained by allowing for hopping, as extracted above, can allow the walls to compete successfully against the patches, and if so, at what filling fractions.

The total energy per hole, if they are localized to walls at electron filling fraction f, is

$$\frac{E_{\text{T}}}{N_h} = \frac{3\lambda J}{2f'} - \frac{t \sin 2\pi f'}{\pi f'} , \tag{2}$$

where $f' \equiv \frac{1}{2} - f$ is the hole filling fraction. Defining $r \equiv 3\pi\lambda J/2t$, and $x \equiv 2\pi f'$, we are led to minimize the function

$$h(x) = \frac{r}{x} - \frac{\sin x}{x} \tag{3}$$

in the interval $0 \le x \le \pi$. A short analysis shows that to insure favorability against the patch configuration we must require $\sin x \ge 1/3$. For very small r the minimum occurs at $x \approx (3r)^{1/3}$, a nearly filled wall; for $r = 1$ it occurs at $x = \pi/2$, the "minimal domain wall" value; for $r \ge \pi$, the minimum occurs at $x = \pi$, an empty wall. Using Newton's method, one readily calculates that near this value the filling fraction changes with r as

$$\left(\frac{df}{dr}\right)_{|r=1} = \frac{1}{\pi^2} . \tag{4}$$

Populated domain walls remain favorable compared to patches up to $r \approx 1.4$, corresponding to $f' \approx 0.43$. Because of the simple form of the energy function h, there is never any advantage to having coexisting walls and patches.

The calculation presented above is far from rigorous, primarily because the antiferromagnetic background is regarded as given and inert, while it properly should be regarded as composed of dynamical electrons on the same footing as those in the walls. It could easily be formulated as a variational calculation, though again with no firm control on the errors. In its defense, we can fairly claim the virtue of simplicity, and that the terms retained plausibly represent basic effects having clear physical interpretations. Taken at face value, its result certainly suggests that the ground state of an antiferromagnetic system with strong short-range repulsion will generically contain populated domain walls.

Within this framework there is as yet no clear sign that $f = \frac{1}{4}$ is especially favored. It is worth noting, however, that for effective spinless fermions, which as mentioned above we seem to have at least in some approximate sense, $f = \frac{1}{4}$ corresponds to half filling; and when phonon interactions are taken into account there is a favorable commensuration energy near this value, due to the possibility of a Peierls distortion, as pointed out by Zaanen and Oles [6]. One can model this by using a modified dispersion relation for the electrons; but we leave that (and other refinements) for future work.

A few other comments are in order. First, we have neglected the effects of the long-range part of the Coulomb interaction. As has been emphasized by Emery and Kivelson [7], this interaction strongly disfavors large clusters of holes; but walls with nonzero electron filling are less affected [1]. Second, formally, one could both gain in hopping energy and break fewer bonds by merging two (or more) populated walls. Each wall site would then break $2\frac{1}{2}$ sites instead of 3, and at $1/4$ filling a short calculation shows that one gains about 10% in hopping energy per electron, in so far as the electrons are effectively free spinless fermions. However, one would pay a heavy price in Coulomb energy; one sign of this is that the electrostatic force between separated walls is certainly repulsive, so that a configuration with uniformly spaced walls of unit thickness is at least locally stable. Entropic considerations also favor the separated walls. Third, although we have been using the term domain wall, at no point did we require the staggered magnetization to change sign across the wall (unlike in a Hartree-Fock calculation). If it did not change sign, however, there would be an effective staggered magnetic field at the wall and electrons on the

wall would tend to form a spin-ordered state. The principal effects of the interaction between the wall and the antiferromagnetic regions which surround it would be a renormalization of the hopping amplitude and fluctuation in the position of the wall (see below); both effects are important quantitatively, but do not affect our qualitative conclusion. Finally, there is some numerical evidence, from simulations of the t-J model on small lattices, that can be interpreted as indicating the existence of populated domain walls [13,14]. The latter study suggests that the walls two lattice spacings thick might be most favorable, which is not inconsistent with our general picture. We plan to investigate these more delicate aspects of the energetics analytically in the near future; again, our main point here is that what is presumably the dominant energetic effect, namely the short-range repulsion, seems strongly to favor populated domain walls in some form.

It is interesting now to apply these considerations to actual materials, using the parameters of t-J models as extracted from phenomenological models fitted to their low-energy behavior [15]. They find $J/t \approx 1/4$. Numerical estimates of the energy per bond of a 2D Heisenberg antiferromagnet give $\lambda \approx 0.5$. Formally, these estimates lead us to an electron filling fraction $f = 0.29$ on the wall, which is significantly (though not grossly) larger than $1/4$; clearly, however, our approximations have been too crude to support close numerical comparison with experiment. Systems with substantially larger values of J/t, such as doped La_2NiO_4 studied experimentally by Tranquada *et al.* [16] and theoretically by Zaanen and Littlewood [17], are predicted to have small or vanishing wall occupation.

All this certainly encourages us to take the possibility that populated domain walls, generally curved and fluctuating in space and time, can be important dynamical objects. A direct experimental signature for inhomogeneous structures could come from neutron scattering, but in practice it requires that these structures be at least quasistatic and fairly regularly arrayed. One would expect that running currents through the walls (possible if they contain the charge carriers!) would tend to straighten them out and suppress fluctuations, just as a garden hose straightens out when water runs through it.

To make this intuition quantitative, let us consider the energy governing the fluctuations. Since it is proportional to the number of broken antiferromagnetic bonds, it is of the form

$$E_{\text{curv.}} = \int dx\, \alpha \sqrt{1 + \left(\frac{dy}{dx}\right)^2} = \text{const} + \int dx\, \alpha \left(\frac{dy}{dx}\right)^2, \tag{5}$$

for a wall in the x direction. Here the tension α is proportional to J/a, where J is the effective antiferromagnetic (super)exchange interaction and a the lattice spacing; in the second equation we have assumed the wall is nearly straight. If we think of x as a mock time variable, then the wall executes a random walk in the y direction; such fluctuations will disorder an array of walls. A very similar problem was considered in the context of krypton adsorbed on graphite in [18] and for antiferromagnetic domain walls (as here) in [5]. The domain walls form a fluid at high temperatures, but at low temperatures undergo a Kosterlitz-Thouless transition to an ordered phase. The neutron scattering data alluded to above, interpreted in this way, require that the structural phase transition stabilizes the ordered phase in $La_{1.48}Nd_{0.4}Sr_{0.12}CuO_4$, while $La_{2-x}Sr_xCuO_4$ is in the fluid phase.

Now let us consider the current-carrying state. The voltage produces an electrostatic energy of the form

$$E_{\text{estat.}} = \int dx\, \lambda E x \sqrt{1 + \left(\frac{dy}{dx}\right)^2}, \tag{6}$$

where λ is the charge density along the wall; while the force exerted on a current i by a wall that bends through angle θ is $\hbar k_F \theta i/e$, corresponding to an energy functional

$$E_{\text{current}} = \int dx\, \hbar k_F i/e \left(\frac{dy}{dx}\right)^2. \tag{7}$$

The latter contribution the energy dominates and will be significant when it becomes comparable to the temperature. An order-of-magnitude calculation indicates that a current per domain wall of 10^{-7} A, corresponding to a current density $\approx 10^7$ A/cm^2, which is very large but perhaps not prohibitive, suffices.

Finally, we note that by applying pressure it should be possible to vary the effective t and thereby, modify the favored wall filling factor.

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