$d_{x^2-y^2}$ Pair Domain Walls

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(July 11, 2011)

Abstract

Using the density matrix renormalization group, we study domain wall structures in the t-J model at a hole doping of $x = \frac{1}{8}$. We find that the domain walls are composed of $d_{x^2-y^2}$ pairs and that the regions between the domain walls have antiferromagnetic correlations that are π phase shifted across a domain wall. At $x = \frac{1}{8}$, the hole filling corresponds to one hole per two domain wall unit cells. When the pairs in a domain wall are pinned by an external field, the $d_{x^2-y^2}$ pairing response is suppressed, but when the pinning is weakened, $d_{x^2-y^2}$ pair-field correlations can develop.

PACS Numbers: 74.20.Mn, 71.10.Fd, 71.10.Pm

In the low temperature tetragonal (LTT) phase of $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$, the tilt pattern of the CuO_6 octahedra form lines of displaced oxygens parallel to the Cu-O bond directions. These lines are rotated by 90° between adjacent layers. At a filling of $x = \frac{1}{8}$, superconductivity is suppressed and neutron scattering studies [1,2] reveal a striped domain wall ordering of holes and spins which is believed to be commensurately locked by the tilt distortion of the lattice. One model for this striped order [1,2] is illustrated in Fig. 1(a). Here the charge domain walls are shown running vertically and centered along the Cu-O-Cu legs, although the phase information required to determine whether the domains should be leg centered or bond centered (centered between two legs) is not known. As shown, the domains are separated by four Cu-O-Cu spacings and for $x = \frac{1}{8}$ contain one hole per two 4×1 domain wall unit cells. This latter feature is at odds with one-electron Hartree-Fock calculations [3–8] which predict a domain wall filling of one hole per domain wall unit cell. The spins in the regions between the walls are antiferromagnetically correlated with a π phase shift across a domain wall. When $x \neq \frac{1}{8}$, superconductivity is found to coexist with a weakened domain wall ordering, suggesting a close connection between the two.

Here we present results of numerical density matrix renormalization group calculations for a t-J model with a hole doping $x = \frac{1}{8}$. We find evidence for domain walls with π phase-shifted antiferromagnetic regions separating the walls, and with a filling of one hole per two 4×1 domain wall unit cells. In contrast to Fig. 1(a), however, the domain walls are bond centered, and are made up of $d_{x^2-y^2}$ pairs of holes. We find that just as for the two-leg and four-leg ladder problems, [9,10] there is a competition between a charge density wave (CDW) phase and a superconducting pair phase. The Coulomb interaction, arising from the 90° rotated domain walls on adjacent planes in the LTT phase [2,11], acts to pin the pairs within a domain wall for $x = \frac{1}{8}$. We show that when this pinning is weakened, $d_{x^2-y^2}$ pair field correlations develop.

The t-J Hamiltonian we will study is given by

$$H = -\sum_{\langle ij \rangle s} t\, P_G \left(c^\dagger_{i,s} c_{j,s} + c^\dagger_{j,s} c_{i,s} \right) P_G + \sum_{\langle ij \rangle} J \left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j \right). \tag{1}$$

Here $\langle ij \rangle$ are near-neighbor sites, s is a spin index, $\vec{S}_i = c^\dagger_{i,s}\sigma_{s,s'}c_{i,s'}$ and $n_i = c^\dagger_{i\uparrow}c_{i\uparrow} + c^\dagger_{i\downarrow}c_{i\downarrow}$, with $c^\dagger_{is}$ (c_{is}) an operator which creates (destroys) an electron at site i with spin s. The near-neighbor hopping interaction is t, the near-neighbor exchange interaction is J, and the Gutzwiller projection operator P_G excludes configurations with doubly occupied sites. We refer to the Cu-Cu lattice spacing as a and measure energies in units of t.

Our calculations were carried out using a density matrix renormalization group [12] (DMRG) algorithm in which transformation matrices were stored and used to construct the initial state for each superblock diagonalization [13]. We present results here for 8×8 and 4×18 doped systems. For the more difficult 8×8 system, typically 10 equilibration sweeps were made through the lattice, keeping of order 10^3 states per block on the final sweep. The transformation matrices were used to calculate the ground state expectation values of the desired operators at the end of the calculation. DMRG is extremely accurate for narrow systems, but its accuracy decreases rapidly as the width increases, and consequently, our 8×8 systems may represent the most ambitious DMRG calculations to date. Truncation errors were approximately 0.0003, which we consider to be at the limits of acceptability. In addition, the calculations sometimes got stuck in metastable hole configurations, in cases where two or more states had a very close separation in energy but corresponded to completely different hole configurations. In these cases it was necessary to perform several calculations, with the holes initially localized in different configurations, using the total energy to choose between different runs. (In contrast, the spin configuration equilibrated more readily.) Nevertheless, the domain wall configurations shown here were robust as long as the initial hole configurations were reasonably close to the final configurations displayed. In particular, three of the most robust features emerging from a variety of runs were that the domain walls are bond centered, composed of $d_{x^2-y^2}$ pairs, with π phase shifted antiferromagnetic regions separating the walls.

Figure 1(b) shows the charge and spin density in the ground state of the 8×8 system with $J/t = 0.35$ and 8 holes, corresponding to a filling $x = \frac{1}{8}$. Periodic boundary conditions

were used in the y-direction, and open boundary conditions in the x-direction. Along the left and right edges of the system a small staggered magnetic field of $0.05t$ was applied. The boundary conditions and the edge staggered field serve to orient and pin the domain walls in the configuration shown. In an LTT phase, the increased Cu-O bond length in one direction would act to orient the domain walls through an anisotropic hopping and exchange, $t_y = \gamma t_x$ and $J_y = \gamma^2 J_x$, with $\gamma \approx 1$, but for simplicity we have used $\gamma = 1$ throughout. The staggered edge field further acts to pick a direction for the spin order, which allows direct measurement of the spin configurations and reduces truncation errors in the DMRG calculation. The charge density in the x-direction shows a strong modulation with period $4a$, and the filling of the wall is consistent with that shown in Fig. 1(a). In addition, a small charge density modulation, also with period of $4a$, is present in the y direction [3]. This modulation is pinned in the y direction despite periodic boundary conditions by the truncation errors in the calculation. We cannot determine whether an exact calculation of the two-dimensional t-J lattice would have small pinned charge density modulations along the walls, but it seems clear that the system is near a CDW instability, with period $4a$, along the walls. The spin response $\langle S_i^z \rangle$ is also shown in Fig. 1(b) and corresponds to antiferromagnetic correlations which have a π phase shift across the bond domain wall. This π phase shift was purely the result of the simulation, not enhanced in any way by boundary or initial conditions.

In Fig. 1(c), the black circles show the most probable configuration of the eight holes obtained by maximizing the ground state expectation value of

$$P(\ell_1, \ell_2, \ldots, \ell_8) = \prod_i p(\ell_i), \tag{2}$$

with $p(\ell) = (1 - n_{\ell\uparrow})(1 - n_{\ell\downarrow})$ the hole projection operator for the ℓ^{th} lattice site. The thickness of the lines connecting various sites denotes the strength of the exchange field $\langle \vec{S}_i \cdot \vec{S}_j \rangle$ when the holes occupy the most probable configuration, consisting of four pairs. Note that the most probable configuration of a pair is a diagonal configuration, with a strong exchange bond running diagonally between the spins adjacent to the holes. This

configuration is the most likely configuration of a pair in a variety of t-J clusters [14,10].

From a strong coupling point of view, the pairing can be viewed as arising from a compromise in which two holes locally arrange themselves so as to minimize the disturbance of the background exchange energy while at the same time lowering their kinetic energy. In the unphysical regime of $J > t$, the holes would tend to be near neighbors to reduce the number of broken exchange bonds. In the physical region $J < t$, the kinetic energy plays an increasingly important role so that, as shown in Fig. 1(c), the most probable pair configuration has the holes sitting on diagonal sites with strong singlet correlations on the other diagonal. In this case, four of the eight one-electron hops leads to a configuration with a near-neighbor exchange bond which stabilizes the pair. As previously discussed, [15,14] the pair structure is such that it has an overlap with the undoped antiferromagnetic background through a hole pair field operator which has $d_{x^2-y^2}$ symmetry. Here we will see the $d_{x^2-y^2}$ structure of the pairs from the pair field response discussed below.

In the LTT phase, the CuO_6 tilt structure causes the domain walls to be perpendicular in adjacent planes [1]. This gives rise to an electrostatic potential, with a period of $4a$, along the domain wall [11]. For $x = 1/8$, this corresponds to the CDW instability of the $d_{x^2-y^2}$ domain wall and can lead to a pinning of the pairs along the wall. Here we have modeled this effect by adding a spatially varying site potential $\Delta V = 0.1t$ on the 8×8 lattice shown in Fig. 2. The sites with the extra potential ΔV are shown by the shaded rectangles, which also indicate the domain walls in the adjacent planes. The potential pins the pairs, forming a CDW lattice of pairs.

The charge and spin structure factors

$$S_c(\mathbf{q}) = \frac{1}{64} \sum_{\ell} e^{i\mathbf{q}\cdot\vec{\ell}} \langle n_{\vec{l}\uparrow} + n_{\vec{l}\downarrow} \rangle \tag{3}$$

and

$$S_\sigma(\mathbf{q}) = \frac{1}{64} \sum_{\ell} e^{i\mathbf{q}\cdot\vec{\ell}} \langle n_{\vec{l}\uparrow} - n_{\vec{l}\downarrow} \rangle \tag{4}$$

for this lattice are also shown in Fig. 2. The intensity in $S_c(\mathbf{q})$ at $(\frac{\pi}{2a}, 0)$ is expected for vertical charged domain walls. The intensity at $(\frac{\pi}{2a}, \frac{\pi}{2a})$ and $(0, \frac{\pi}{2a})$ reflect the pair correlations

along the domain walls. With the 90° rotations of the domain walls from layer to layer, it is the $(\frac{\pi}{2a}, \frac{\pi}{2a})$ peak that would be important to observe. The spin structure factor at $(\frac{3\pi}{4a}, \frac{\pi}{a})$ reflects structure of the π-phase shifted antiferromagnetic regions. The amplitude of the third harmonic intensities is much weaker.

At dopings away from $x = 1/8$, the $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$ system becomes superconducting, and the size of the tilt modulation as well as the intensity of the magnetic Bragg peaks decreases [2]. This suggests that when the pinning is weakened, either through a reduced pinning potential or through a mismatch in the periods of the pinning potential and the CDW instability, stripe order and superconducting pairing can coexist. As a test of this, we have used a 4×18 cluster to model a single, longer domain wall, with a variable pinning potential ΔV which acts on the sites in the shaded regions shown in Fig. 3(a). This cluster has open boundary conditions on all sides with a staggered magnetic field of magnitude $0.05t$ applied along the top and bottom edges. The magnetic field has a π phase shift between the edges in order to mimic the single domain wall structure shown in Fig. 2(a). In order to measure the tendency for superconductivity, a weak pair field proximity effect term

$$H_1 = d \sum_i (\Delta^\dagger_{i,i+\hat{y}} + \Delta_{i,i+\hat{y}}) \tag{5}$$

was added to the Hamiltonian. Here

$$\Delta^\dagger_{i,i+\hat{y}} = c^\dagger_{i,\uparrow} c^\dagger_{i+\hat{y},\downarrow} + c^\dagger_{i+\hat{y},\uparrow} c^\dagger_{i,\downarrow} \tag{6}$$

adds a singlet electron pair to sites i and $i+\hat{y}$. Note that the interaction H_1 couples equally to $d_{x^2-y^2}$-like and extended s-wave-like pairs. That is, it does not distinguish whether the internal structure of the pair field has a change in sign for the singlet components in the y-direction relative to those in the x-direction. In order to include this term, rather than use the number of electrons N as a good quantum number to break up the Hilbert space, N modulo 2 was used. (Total S_z was conserved in the usual fashion.) We then measured the strength of the pair fields in the ground state in both the x and y directions, $\langle \Delta_{i,i+\hat{x}} \rangle$ and $\langle \Delta_{i,i+\hat{y}} \rangle$ for all sites i. The charge and spin structure of the 4×18 cluster with 8 holes

is shown in Fig. 3(a) for $\Delta V = 0.05t$. In Fig. 3(b), the pair field strength is shown by the width of the lines, and the sign of the field is indicated by the type of line, dashed or solid. A relative sign difference between the x and y directions indicates $d_{x^2-y^2}$ pairing. In Fig. 3(b) we see a significant $d_{x^2-y^2}$ pair response coexisting with a modest charge density wave. In Fig. 3(c), we show the pair field $\langle \Delta_{\rm mid} \rangle$ averaged over all the y-bonds in the middle four rungs as a function of ΔV. The suppression of pairing by the CDW is evident. We expect that a larger, two dimensional array of domain walls would show a more enhanced response versus ΔV.

These calculations show that holes doped into a t-J lattice can form domain walls of pairs. For a filling $x = \frac{1}{8}$, these walls have an average filling of one hole per two domain wall unit cells, and there is a tendency for the pairs to form a pinned CDW structure. If the pinning is weakened, the pairs fluctuate, developing phase coherence, and $d_{x^2-y^2}$ superconducting correlations appear. The idea that the domain walls are made up of pairs provides a natural explanation of the special filling $x = \frac{1}{8}$ and the intimate relationship between the stripes and superconductivity. The pairs give rise to a bond centered charge density periodicity of $4a$ along a wall which should give a Bragg peak at $(\frac{\pi}{2a}, \frac{\pi}{2a})$. Other evidence of the pair structure of the domain wall should be seen in NMR measurements.

The structure we have discussed differs from the one-electron mean field domain walls found in Hartree-Fock [3–8] and Gutzwiller variational calculations [16] in both its filling and its relationship to pairing. It also differs from the one-dimensional large U/t Hubbard model of a domain wall recently discussed by Nayak and Wilczek [17]. At $J/t = 0.35$, our system is well away from the phase separation regime, and we have no long-range intraplanar Coulomb interaction as in the frustrated phase separation domain wall model of Kivelson and Emery [11]. The singlet stripe phases discussed by Tsunetsugu [18,19] and the competing CDW-pairing phases in the 2- and 4-leg ladder systems recently discussed [9,10] have some of the features found in this present study. In particular, they have the interplay of $d_{x^2-y^2}$ superconducting pairing and charge density wave order. Clearly, it will be important to understand if this is the behavior that underlies the structure of the domain

walls in $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$.

ACKNOWLEDGEMENTS

We would like to thank J. Tranquada for discussions of his experimental results, and J. Lawrence for helpful discussions. SRW acknowledges support from the NSF under Grant No. DMR-9509945, and DJS acknowledges support from the Department of Energy under grand DE-FG03-85ER45197, and from the Program on Correlated Electrons at the Center for Material Science at Los Alamos National Laboratory.

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[19] The region between the walls in our system appears to be a low energy two-leg mostly-undoped ladder of the typed discussed previously [18,14]. However, in the system we have discussed here, there is a significant π phase shifted exchange coupling between ladders, mediated by the domain walls. This exchange coupling reduces, and may eliminate, the spin gap.

FIGURES

FIG. 1. (a) Spin and hole structure suggested in Ref. [1] to account for neutron scattering experiments. (b) Hole density and spin moments for an 8×8 t-J model. The diameter of the gray holes is proportional to the hole density $1 - \langle n_i \rangle$, and the length of the arrows is proportional to $\langle S_i^z \rangle$, according to the scales shown. (c) For the same system, the exchange field strength $-\langle \vec{S}_i \cdot \vec{S}_j \rangle$ is given by the width of the lines according to the scale shown, when the holes (black dots) occupy their most probable configuration. In addition to showing all nearest neighbor exchange bonds, we show next nearest neighbor correlations about each hole if those correlations are antiferromagnetic, $\langle \vec{S}_i \cdot \vec{S}_j \rangle < 0$.

FIG. 2. (a) Hole density and spin moments for an 8×8 t-J model with a static potential $\Delta V = 0.05t$ applied to the sites in the shaded rectangles. (b) Charge structure factor $S_c(\mathbf{q})$ expected for a 2D system, obtained by periodically repeating the pattern shown in (a). (c) Spin structure factor $S_\sigma(\mathbf{q})$. Here we have measured ℓ from the center of a domain wall. In both (b) and (c), the area of the circle is proportional to the structure factor, open circles denote negative values, and the axes are labeled in units of $1/a$.

FIG. 3. A single domain wall, modeled by a 4×18 system with left and right edge π-phase shifted antiferromagnetic fields $h = 0.05t$, with a static potential $\Delta V = 0.05t$, and with an applied proximity affect field $d = 0.03t$. (a) Hole density and spin moments. (b) Pair field strengths on each nearest neighbor link. (c) The average pairing strength on the y links for the central 4 rungs, as a function of ΔV.

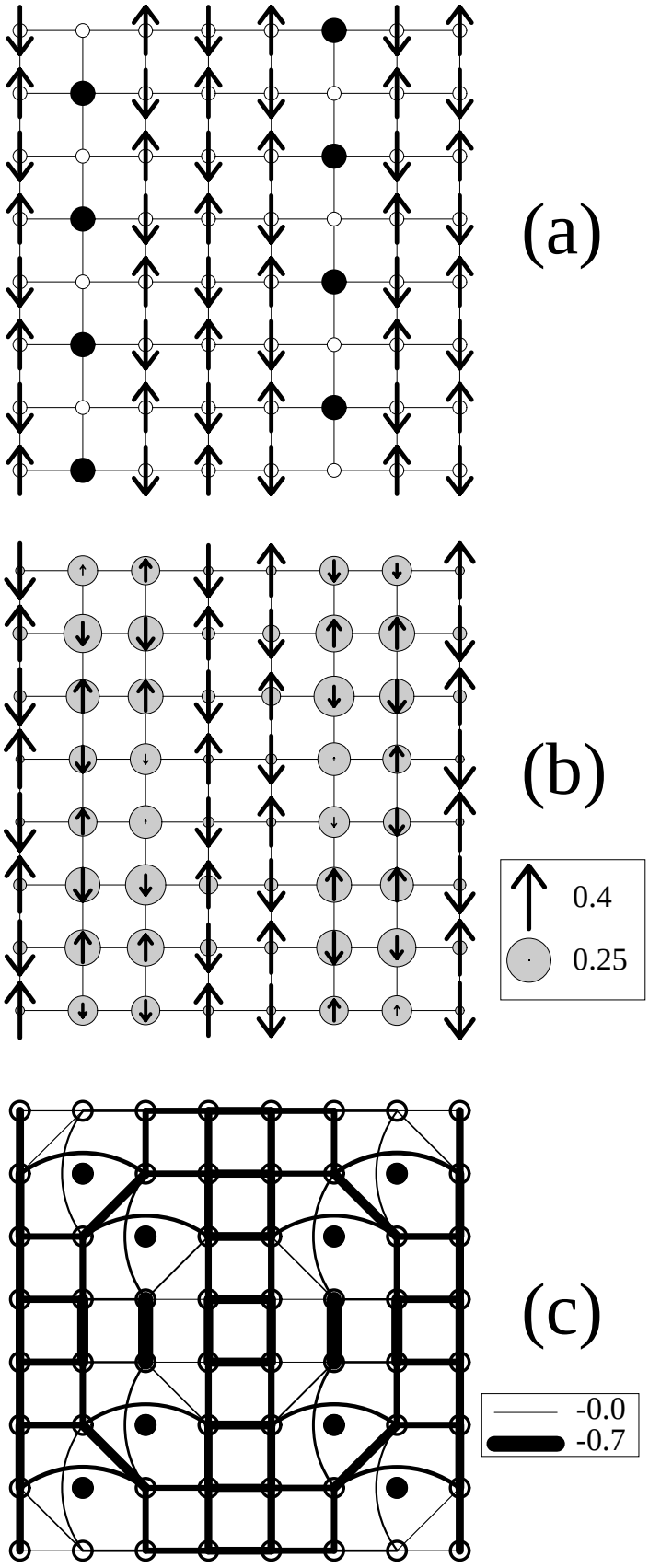

Fig. 1
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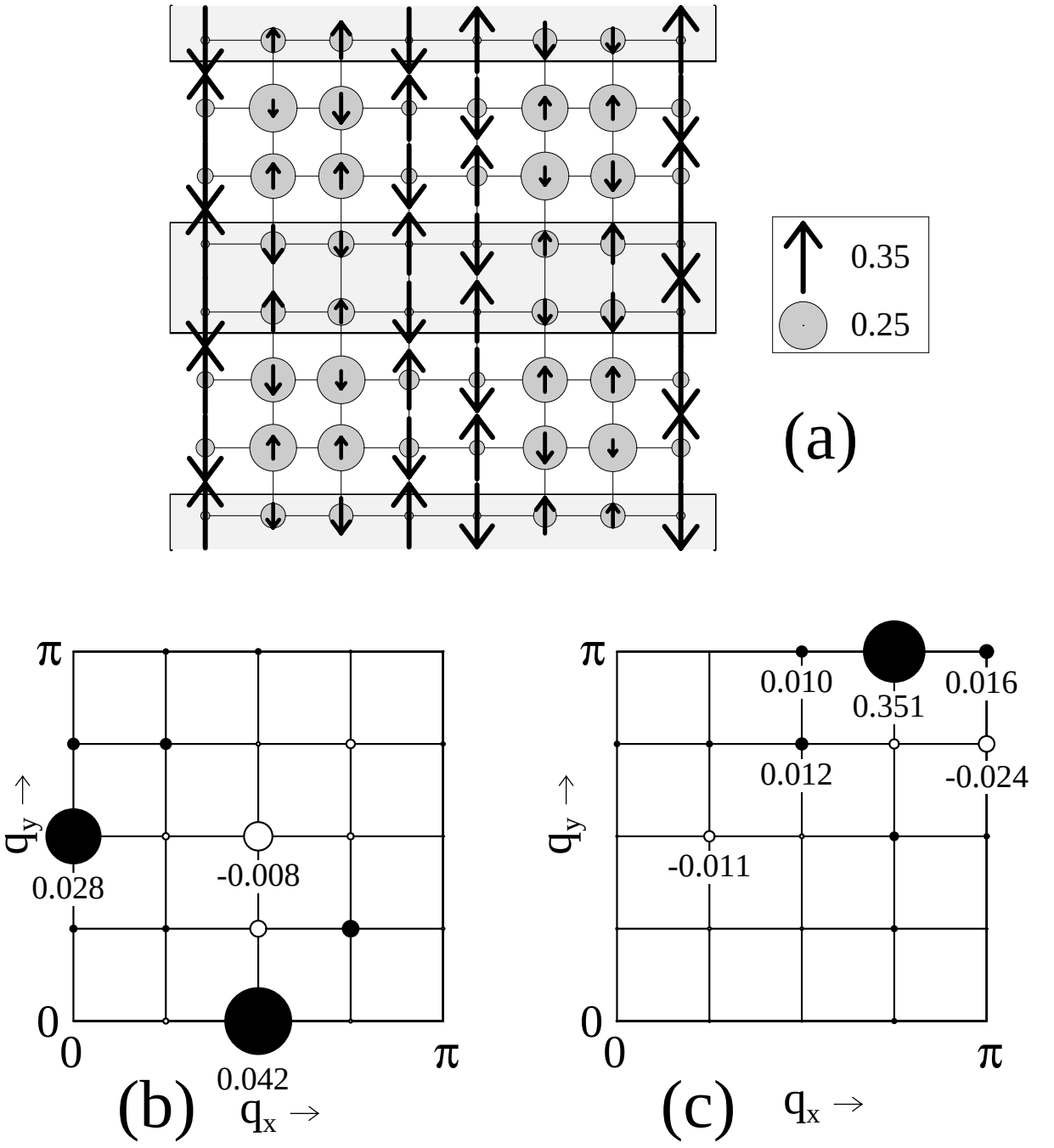
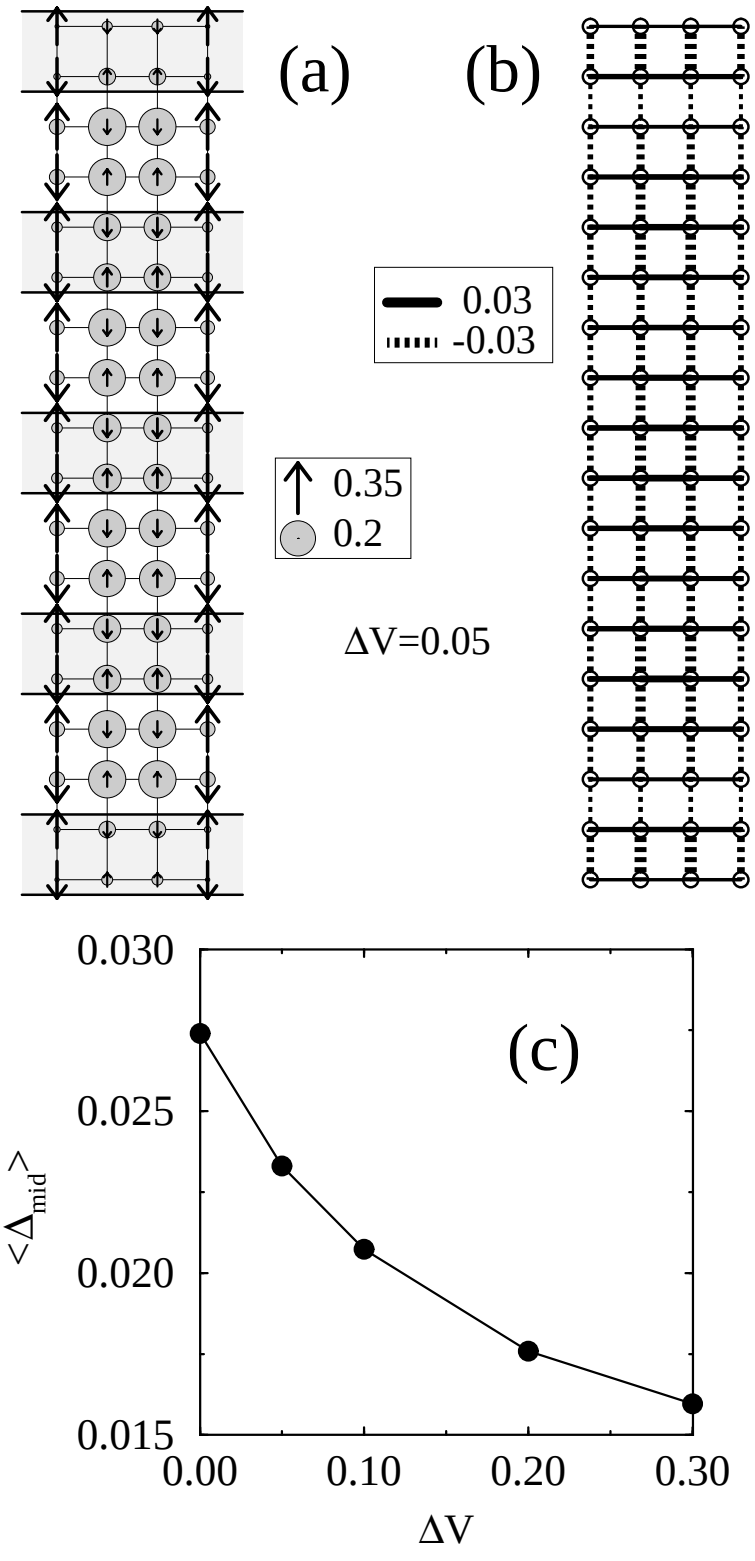


Fig. 2
White and Scalapino


(a)
(b)
0.03
-0.03
0.35
0.2
ΔV=0.05
(c)
0.030
0.025
0.020
0.015
0.00
0.10
0.20
0.30
ΔV
<Δmid>
Fig. 3
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