Metallic stripe in two dimensions: stability and spin-charge separation

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The problems of charge stripe formation, spin-charge separation, and stability of the antiphase domain wall (ADW) associated with a stripe are addressed using an analytical approach to the $t$-$J_z$ model. We show that a metallic stripe together with its ADW is the ground state of the problem in the low doping regime. The stripe is described as a system of spinons and magnetically confined holons strongly coupled to the two dimensional (2D) spin environment filling holon-spin-polaron elementary excitations filling a one-dimensional band.

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In a light of experimental evidence for incommensurate spin and charge order in high-$T_c$ superconductors the concept of stripes, i.e., one-dimensional spatial structures of holes condensed at an antiphase domain wall (ADW) of antiferromagnetic (AF) spins, has been discussed extensively in the literature. In the physics of high-$T_c$ superconductors magnetism plays an important role and it is believed that stripe formation is due to the strong interplay between the charge and spin degrees of freedom. Various proposals for the driving mechanism of such a stripe phase have been made. A large body of them emphasize the importance of the so called topological doping, i.e., the breaking of the symmetry of the ground state in order to lower the total energy of the system when the charge carriers are introduced into it. For the cuprates the symmetry breaking corresponds to the formation of a superconducting state of holes condensed at an antiphase domain wall (ADW). In this context the importance of the kinetic energy of holes, both along the domain wall and transverse to it, has been noted in the studies of the Hubbard and the $t$-$J$ models. The role played by the long-range Coulomb field in the ordering of the stripes has been also discussed. Numerical studies of the $t$-$J$ model indicate that the (dynamic) stripe phase may be the ground state of the system but there is still no consensus on this issue. However, the actual picture of such topological doping is far from being complete mainly due to the lack of microscopic insight into the problem. There is no clear understanding of the stabilization mechanism of the stripe as well as of the nature of low-energy excitations of the system. Thus it is important to study a model of AF spins and mobile holes within an approximation which is not subject to the limitations of mean field theories or numerical studies.

In this paper we study analytically the problem of the stability of an ADW in the anisotropic $t$-$J_z$ model. We calculate the Green’s function of a charge excitation at the ADW in a well controlled procedure. We show that although an empty ADW (no holes) is a highly excited state it is stabilized even at low doping concentrations due to the gain in hole kinetic energy. As a consequence the doped holes become spatially confined in the direction transverse to the ADW and exhibit spin-charge separation features. Namely, the holes behave like holons (charge-1, spin-0 fermions) at the ADW and they are spin polarons (charge-1, spin-1/2 fermions) outside of the ADW. The confining potential in the transverse direction leads to quantized states whose energy grows roughly $\sim J_z^2/3$. We argue that due to the 1D nature of an ADW holon even Trugman loops are energetically costly. We also compare some of our results to recent DMRG calculations for the isotropic $t$-$J$ model and find very good agreement.

Our starting point is the $t$-$J_z$ model which is given by:

$$
\mathcal{H} = -t \sum_{(ij)\sigma} (c^\dagger_{i\sigma} \tilde{c}_{j\sigma} + \text{H.c.}) + J \sum_{(ij)} [S_i^z S_j^z - \frac{1}{4} N_i N_j],
$$

where $t$ is the kinetic energy, $J$ is the AF exchange, and $N_i = n_i^\uparrow + n_i^\downarrow$. All operators are defined in the space without double-occupancy of the sites. The natural source of exchange anisotropy in real systems is the spin-orbit coupling. Although the $t$-$J_z$ model is the strongly anisotropic limit of the more realistic $SU(2)$ $t$-$J$ model, it is known from numerical and analytical studies that the low-energy physics of holes is very similar in both models. Therefore, as long as the hole dynamics is concerned, it should be instructive to study the $t$-$J_z$ model which captures general properties of the doped AFs and allows an analytical treatment of the problem.

According to the idea of topological doping a single charge carrier must benefit energetically from breaking the symmetry of the ground state. Thus, it is natural to consider the problem of one hole at the ADW, in order to obtain the low-energy excitations which then can be used for description of many-hole system. The single-hole problem in a homogeneous AF background is very well studied with analytical results and numerical data being in a very good agreement. The charge quasiparticle is understood as a spin polaron, i.e., a hole dressed by strings of spin excitations. In other words, the hole movement in a regular AF is frustrated because...
of the tail of misaligned spins following the hole. The idea that an ADW can be more favorable configuration for holes relies on the fact that such a frustration of the hole’s kinetic energy can be avoided for movement inside the wall, such that the hole is essentially free in the 1D structure. Then, holes populating this 1D band can compensate the cost of magnetic energy (≈ \( J \cdot \text{length} \)) of the wall. However, this 1D energy alone (≈ \(-2t\)) cannot overcome the energy of the spin polaron in the bulk \( E_p \approx -2\sqrt{3}t \) (at \( t \gg J \)), especially if the energy cost for creating an ADW is taken into account. Therefore, the “transverse” hole movement away from the domain boundary must be equally important. Moreover, it is evident that such a movement is very similar to the hole movement in a homogeneous AF, i.e. it also generates strings of misplaced spins. It is easy to see that such strings are also weaker, i.e. cost less energy near the ADW than in the bulk. Then, the coupling of the longitudinal and transverse hole movements for this many-body problem gives a true low-energy elementary excitation, which unifies the features of the 1D charge carrier with the properties of the spin polaron.

Let us consider a bond-centered domain wall with one hole injected in it. If the hole is allowed to move along the wall it will create a spin defect (a spinon - charge-0, spin-1/2 fermion, which is massive in our case because of the anisotropy) and then propagate freely as a holon. The structure shown in Fig.1a is the natural starting point for the consideration of a hole whose movement along the stripe is free from the beginning. Fig.1b shows the same configuration schematically. It is clear that the domain wall not only corresponds to an antiphase shift of the staggered magnetization across the stripe, but also ensures that the hole moves as a holon in the longitudinal direction. Fig.1c shows an example of a string generated by the transverse hole movement. Notably, the first element of such a string is a spinon. These strings lead to an effective confinement of the hole in the direction perpendicular to the stripe and to the formation of a spin-polaron-like cloud of spin excitations around the holon. This can be viewed as a generalization of 1D physics to higher dimensions in the presence of an ADW.

The bare Green’s function for longitudinal hole movement in Fig.1a is given by

\[
G^0_{x_0}(k_y, \omega) = \left[ \omega - 2t \cos(k_y) + i0 \right]^{-1},
\]

so the holon band minimum is located at \( k_y = \pi \), where the index \( x_0 \) corresponds to the \( x \)-coordinate of the stripe. Then the renormalization of the Green’s function, as in the case of the spin polaron, is coming from the retraceable path movements of the hole away from ADW and back. The retraceable path approximation is equivalent to the self-consistent Born approximation for the self energy. Corrections due to terms beyond this approximation are very small and will be omitted. The full Green’s function is then given by

\[
G_{x_0}(k_y, \omega) = \left[ \omega - 2t \cos(k_y) - \Sigma_{x_0}(\omega) + i0 \right]^{-1},
\]

where \( \Sigma_{x_0}(\omega) \) takes the form of a continued fraction

\[
\Sigma_{x_0}(\omega) = \frac{2t^2}{\omega - \omega_1 - \frac{2t^2}{\omega - \omega_1 - \omega_2 - \ldots}},
\]

where \( \omega_i \) is the energy of the \( i \)-th segment of the string, which is equal to the number of broken AF bonds (\( J/2 \) each) associated with the segment. In the retraceable path approximation \( \Sigma_{x_0}(\omega) \) has no \( k_y \) dependence. Since the energy spectrum of the elementary excitations is given by the poles of the Green’s function Eq. (3) with the self energy Eq. (4), one needs to calculate \( \Sigma(\omega) \) and seek solutions of \( E(k_y) - 2t \cos(k_y) - \Sigma(E(k_y)) = 0 \). A standard simplification is to assume that the energy of the string is independent of the path of a hole and is simply proportional to the length of the path. For the spin polaron this is plausible because only very few strings do not follow this rule. Then an analytical solution for the self energy is given by the ratio of Bessel functions. If we assume that \( \omega_1 = J/2, \omega_{i+1} = J \) (two broken bonds per segment of string, see Fig.1c), Eq. (4) transforms to

\[
\Sigma(\omega) = \frac{2t^2}{\omega - J/2 + \sqrt{3} t \Upsilon(\omega - J/2)},
\]

with \( \Upsilon(\omega) = \sum_{l} J_{-l}(\nu)/J_{-l}(\nu-1) \), \( J_{\nu}(r) \) the Bessel function, and \( r = 2\sqrt{3}/J \). The energy of the lowest pole of \( G(k_y, \omega) \) Eq. (3) at \( J/t = 0.4 \) with \( \Sigma(\omega) \) from (4) versus \( k_y \) is plotted in Fig.2 (dotted line). The zero energy level is chosen to be equal to the energy of a static hole in the configuration in Fig.1a. This reference to the \( t = 0 \) limit is natural to show which of the magnetic configurations is best for optimizing the kinetic energy.

One can consider the problem more rigorously taking into account the energy of each string exactly up to a certain length \( l_c \) and applying the path-independent assumption only for \( l \gg l_c \). The lowest-pole energy versus \( k_y \) for such calculations with \( l_c = 4 \) is shown in Fig.2 (solid line). Because of the ADW, there is less energy required to create a spin flip near it and therefore there is a subset of strings having lower energy than the string of the same length in the bulk. It is worth mentioning that the energy of this ADW elementary excitation relative to the energy of the magnetic background is lower than the energy of the spin polaron in the bulk at all \( k_y \) (Fig.2). For \( J/t = 0.4 \) the gain of the energy of the holon at the bottom of the band over the spin polaron is about 1.5\( J \), that is the energy of three broken AF bonds. Another informative quantity, the residue of the Green’s function \( Z(k_y) \), is shown in Fig.2 (inset). It gives a measure of the amount of “bare” holon in the wave function of the elementary excitations. One can see that a significant part of the initial holon at \( k_y = \pi \) resides inside the wall and almost all its weight is transferred to strings at \( k_y < \pi/2 \).
Because the band is very flat at the same $k_y < \pi/2$, the velocity of the elementary excitations is much slower than the bare Fermi velocity $v_F = 2t \sin(k_F)/\hbar$. It is easy to show that the velocity at the Fermi level for our 1D band is $v_F = v_F^0 Z(k_F)$. For realistic values of $J$, $t$, and $k_F$ around $\pi/2$ one finds $h v_F \sim 50 - 100$ meVÅ, which is close to the velocity of the slow mode ($\sim 35$ meVÅ) deduced from experimental data in Ref. [7] for the cuprates.

The next step is to fill the obtained 1D band up to some Fermi momentum $k_F$ and study the stability of the whole system as a function of the 1D hole concentration $n_\parallel$. Obviously, the rigid band filling neglects all effects of interaction between the carriers except Fermi repulsion. Such interactions would include attractive as well as repulsive terms coming from the nearest-neighbor hole-hole interaction, crossing of the strings, spin-flip exchange, and kink-kink or kink-antikink scattering of holons. However, as a first step towards the microscopic study of the metallic stripe, the rigid-band approximations should help to establish the energy scale underpinning the stripe ground state. The total energy of the stripe must include the magnetic energy paid for the domain wall $E_{ew} = (L_y - N_h)J/2$ and kinetic energy of holes $E_{kin} = \sum_{k < k_F} E(k_y)$. Here, $L_y$ is the number of sites in the $y$-direction, $N_h$ is the number of holes, $k_F = \pi n_\parallel$ is the Fermi momentum relative to $\pi$ (band minimum), and $n_\parallel = N_h/L_y$. Thus, the total energy per hole is

$$E_{tot}/N_h = J/2 \left( \frac{1}{n_\parallel} - 1 \right) + \frac{1}{2\pi n_\parallel} \int_{\pi - k_p}^{\pi + k_p} E(k_y) dk_y.$$

Results for $E_{tot}/t$ versus $n_\parallel$ at $J/t = 0.4$ are shown in Fig. 3. The stripe wins over the homogeneous phase when $n_\parallel$ is as low as $1/4$ and then it has significantly lower energy. Another feature of the data is that from the Fermi momentum relative to $\pi$ (band minimum), and $n_\parallel = N_h/L_y$. Thus, the total energy per hole is

$$E_{tot}/N_h = J/2 \left( \frac{1}{n_\parallel} - 1 \right) + \frac{1}{2\pi n_\parallel} \int_{\pi - k_p}^{\pi + k_p} E(k_y) dk_y.$$

In the case of a hole in a pure Ising background it is known that the hole can escape from the confinement potential via some high energy processes [12] remaining beyond the retraceable path approximation (Trugman loops). However, in the case of the hole at the ADW the holon in the stripe has no spin, whereas the hole in the bulk has both spin and charge. Therefore, to leave the stripe and acquire a spin the hole must create a spinon which costs energy $\sim J$. In other words, a holon can only virtually decay into a spin-polaron and a spinon.

In the more realistic $t$ - $J$ model spins are dynamic, which would renormalize the energies of the magnetic background and the holes in our picture. We believe, however, that the essential physics of the system will remain the same.

In conclusion, we have presented an analytical study of a stripe of holes at an ADW of AF spins. Longitudinal as well as transverse kinetic energy of holes are explicitly taken into account in our approach, and their role in stabilization of the stripe as a ground state of the system is revealed. We have provided a description of the charge carriers building the stripe as a system of 1D elementary excitations, unifying the features of holons, spinons, and AF spin polarons. This represents a new level of understanding of the structure of the stripe phase in cuprates.

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FIG. 1. Single hole at an ADW separating AF domains. Broken AF bonds are marked by strings. (b) Same as (a). Pluses and minuses represent staggered magnetization. (c) String of spin flips generated by the hole.

FIG. 2. Energy of elementary excitation $E(k_y)$ v.s. $k_y$, residue of the Green’s function versus $k_y$ (inset). Dotted lines are for path-independent string calculations, solid lines are the results of more rigorous calculations described in the text. Solid straight line is the energy of a spin polaron in the bulk. All energies are relative to the energy of a static hole in a corresponding magnetic background.

FIG. 3. Total energy of the system per hole versus $n_\parallel$. Horizontal line is the energy of free spin polarons in the homogeneous AF. Dotted and solid lines are the same as in Fig. 2. $J/t = 0.4$. Inset: spatial density of holes (diamonds) and modulus of the staggered magnetization (circles) across the stripe at $n_\parallel = 2/3$, $J/t = 0.35$. Lines are guide to the eye. Empty diamonds are numerical data from Ref. 9.