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Quantum melting instability of a striped domain wall in the two-dimensional t–J model

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Abstract. We investigate the stability of a domain wall in the striped phase with simultaneous charge and spin ordering in doped planar antiferromagnets. The line defects gain magnetic energy but the localization of holes costs kinetic energy. A Hartree–Fock approximation is used to estimate the energy cost of a static kink in the domain wall. Such kinks can gain kinetic energy by delocalizing along the line. We find that for values of $t \gtrsim J$ this energy gain surpasses the cost in magnetic energy so that a quantum melting of the domain walls through the proliferation of kinks is predicted for this parameter regime.

1. Introduction

When holes are doped into a two-dimensional antiferromagnet a number of different broken symmetry phases may occur. One such phase is a so-called stripe phase characterized by simultaneous charge and spin ordering. In this phase there are regions of commensurate antiferromagnetic ordering separated by linear domain walls with the doped holes localized on these walls. Such structures have been found in Hartree–Fock calculations for the single-band Hubbard model for intermediate-to-strong coupling and in multiband Hubbard models for oxides [1–4]. In the single-band Hubbard model Inui and Littlewood [5] found that there was a critical value of the on-site repulsion, U, beyond which no stable Hartree–Fock solution could be found. In the closely related t–J model, Prelovšek and Zotos [6] have found evidence of such domain wall structures in the hole–hole correlation functions which evaluate exactly on finite clusters, when the ratio of J/t exceeds a critical value, which they estimate as $J_c \simeq 1.5t$. They estimate that true phase separation at low doping occurs only for a large value of the exchange coupling, $J > J_s(\simeq 2.5t)$. Prelovšek and Zotos [6] further made the interesting proposal that it is the existence of this striped or domain wall phase which accounts for the apparent large discrepancy between the criteria for phase separation at low doping in one and two dimensions. In the parameter regime $J < J_c$ but $J \gtrsim 0.3t$ they propose that the holes pair but do not form larger complexes so that a d-wave superconducting state follows. It is therefore of some interest to understand how and why such a linear domain wall becomes unstable at values $J < J_c$. Clearly some form of quantum melting process driven by the kinetic energy of the holes must occur. In this paper we will examine one way in which such a quantum melting process may occur, namely through the proliferation of kinks.

While such striped phases with simultaneous incommensurate charge and spin ordering have not been reported in the cuprates, they have, however, been observed in related

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compounds, namely doped La_2NiO_4 [7]. There are two differences between nickelates and cuprates. One is that the parent insulator is an $s = 1$ not a $s = 1/2$ antiferromagnetic. A second difference is the increased electron–phonon interaction in the nickelates [8] so that there is an enhanced tendency for holes to form localized polarons. We can crudely approximate these differences between the nickelates and cuprates through an increase in the value of J/t in the former compounds. The difference in physical behaviour between the two classes of materials could be ascribed to a change in the ratio of J/t through the critical value J_c/t.

These striped phases are conveniently described within a Hartree–Fock approximation. However the local constraint in the strongly correlated t–J model cannot be handled in this way. Therefore we consider a single-band model where we release the constraint but include a strong on-site repulsion, U, to mimic the constraint. We also include both nearest-neighbour (NN) and next-nearest-neighbour (NNN) hopping terms in the kinetic energy. This t–t'–J–U model is then examined within a Hartree–Fock scheme. First the energy of a kink in a (1, 1) domain wall is calculated and then the quantum delocalization energy gained by allowing the kink to move along the line defect. In this way we estimate the total energy to create a kink, and the stability criterion we use is that this energy should be positive.

2. Hartree–Fock approximation for simultaneous charge and spin ordering

We consider a modified t–J model described by the Hamiltonian

$$\begin{aligned} H = & -t \sum_{\langle i,j\rangle,\sigma} \left(c^+_{i\sigma} c_{j\sigma} + c^+_{j\sigma} c_{i\sigma} \right) + J \sum_{\langle i,j\rangle} \left(\boldsymbol{S}_i \cdot \boldsymbol{S}_j - \tfrac{1}{4} n_i n_j \right) \\ & + t' \sum_{\langle i,j,k\rangle} \left(c^+_{i\uparrow} c_{k\downarrow} c^+_{j\downarrow} c_{j\uparrow} + c^+_{k\uparrow} c_{i\downarrow} c^+_{j\downarrow} c_{j\uparrow} - c^+_{i\uparrow} c_{k\uparrow} n_{j\downarrow} - c^+_{i\downarrow} c_{k\downarrow} n_{j\uparrow} + \text{HC} \right) \\ & + U \sum_i n_{i\uparrow} n_{i\downarrow}. \end{aligned} \tag{1}$$

It consists of the standard t–J model, with three-site terms and an on-site Coulomb (U) term. In a Hartree–Fock theory, it is difficult to take into account the local constraint of no doubly occupied states, so the U term is included to approximate this restriction. The sums over the indices i and j are taken over NN $\langle i, j\rangle$ and the sums with i, j and k are over all triplets $\langle i, j, k\rangle$ where (i, j) and (j, k) are NN pairs. The Hartree–Fock approximation is obtained by introducing the position-dependent expectation values, $\langle n_{i\sigma}\rangle$ and $\langle c^+_{i\sigma} c_{j\sigma}\rangle$ ($\sigma = \uparrow, \downarrow$), which in turn are to be determined self-consistently. The numerical solution is facilitated by dividing the system into square supercells of N sites with periodic boundary conditions similar to [1]. Each cell contains $N_\uparrow$ electrons with spin up and $N_\downarrow$ electrons with spin down. Here we consider the hole-doped case with $N_\uparrow + N_\downarrow < N$. After factorizing the Hamiltonian we obtain a Hartree–Fock form which can be written as

$$H_{\text{HF}} = \sum_{i,j} H^{\uparrow}_{ij} c^+_{i\uparrow} c_{j\uparrow} + \sum_{i,j} H^{\downarrow}_{ij} c^+_{i\downarrow} c_{j\downarrow} + H_{\text{const}} \tag{2}$$

where the constant term H_{const} and the $N \times N$ matrices $H^\uparrow$ and $H^\downarrow$ depend on the expectation values $\langle c^+_{i\sigma} c_{j\sigma}\rangle$; more precisely, $H^\uparrow$ depends on the values of $\langle c^+_{i\downarrow} c_{j\downarrow}\rangle$ and $H^\downarrow$ on $\langle c^+_{i\uparrow} c_{j\uparrow}\rangle$. We diagonalize the Hamiltonian by making the linear transformation

$$\psi_{l\sigma} = \sum_R \sum_{j=1}^{N} \alpha^l_{j\sigma} \, c^+_{(R+r_j)\sigma} \tag{3}$$

with

$$(1/N)\sum_{j=1}^{N}\left|\alpha_{j\sigma}^{l}\right|^{2} = 1\,. \tag{4}$$

In the sums, j runs over the N sites of a supercell, while R runs over the positions r_1, in every supercell. After diagonalization, the Hamiltonian has the form

$$H_{\mathrm{HF}} = \sum_{l=1}^{N}\left(E_{l}^{\uparrow}\psi_{l\uparrow}^{+}\psi_{l\uparrow} + E_{l}^{\downarrow}\psi_{l\downarrow}^{+}\psi_{l\downarrow}\right) + H_{\mathrm{const}}\,. \tag{5}$$

The $2 \times N$ energy levels that result are populated up to the Fermi level, yielding an expectation value

$$\langle c_{i\sigma}^{+}c_{j\sigma}\rangle = \sum_{l,l'=1}^{N_\sigma}\left(\alpha_{i\sigma}^{l}\right)^{*}\alpha_{j\sigma}^{l'}\psi_{l\sigma}^{+}\psi_{l'\sigma} = \sum_{l=1}^{N_\sigma}\left(\alpha_{i\sigma}^{l}\right)^{*}\alpha_{j\sigma}^{l}\,. \tag{6}$$

The expectation values $\langle c_{i\sigma}^{+}c_{j\sigma}\rangle$ are to be solved for self-consistency. In practice, we started with some reasonable initial values, performed the diagonalization, inserted the expectation values resulting from (6) back into the Hamiltonian (2), and iterated the procedure until it converged to a self-consistent solution.

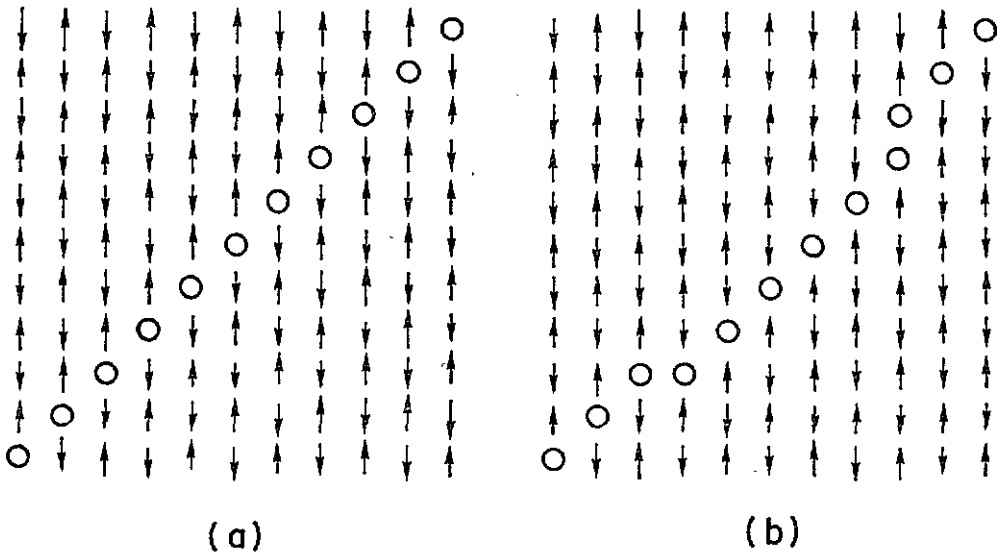

Figure 1. The spin and charge ordering patterns showing diagonal solitons with no kinks (a) and a double kink (b) for the (11×11) supercell with periodic boundary conditions used here.

We investigated first the situation where the Hartree–Fock ground state has a domain wall with a line of holes (soliton) on the diagonal of a square supercell. The form of the solution is illustrated in figure 1. We started with the parameter set: $t = 1$, $J = 1/2$, $t' = 1/8$ and $U = 16$. The values of t, J and t' correspond to an intrinsic ratio of $U/t = 8$ when we use the relationship for the large-U limit of the Hubbard model, that the Heisenberg exchange $J_{\mathrm{H}} = 4t^2/U$. The large additional value $U = 16$ was included to restrict the states with doubly occupied sites. We used supercells with 11×11 sites and the numbers of $\uparrow$-spin and $\downarrow$-spin electrons $N_\uparrow = N_\downarrow = 55$. This leaves a single diagonal

soliton with a hole number $N_h = 11$ (with respect to half-filling). We checked that with these parameter values, the diagonal soliton is lower in energy than either the vertical or horizontal solitons and also stable with respect to removing or adding holes to the soliton line. Note that the holes are not localized on a single site but for these parameter values the holes tend to spread over two sites, the width of the domain wall however does not vary rapidly in the Hartree–Fock calculations. In table 1 we list the total energy per site that we obtained for the diagonal soliton with no kinks as E_{nK}. Also listed is the total energy per site of the Hartree–Fock solution at half-filling, E_{HF}. The average energy per hole in the no-kink solution is $E^h_{nK} = (2)(E_{nK} - E_{HF})/11$. We then reduced the value of the t parameter in steps to the value of $t = 0.6$ keeping the other parameter values fixed. This reduces the kinetic energy of the holes without changing the values of the exchange coupling introduced by the virtual processes.

Table 1. The values of the total energy per site of the Hartree–Fock solution with a double kink (E_K), with no kink (E_{nK}) and at half-filling E_{HF}. ΔE^* is the energy of a static double kink. $\langle \Psi_1 \mid \Psi_2 \rangle$ is the overlap upon translation of the double kink as described in the text. E_c is the creation energy of the double kink including the kinetic energy of localization.

t	E_K	E_{nK}	E_{HF}	ΔE^*	$\langle \Psi_1 \mid \Psi_2 \rangle$	E_c
0.6	− 0.5715	− 0.5731	− 0.5862	0.0568	0.0117	0.043
0.7	− 0.6146	− 0.6152	− 0.6170	0.0522	0.0148	0.034
0.8	− 0.6621	− 0.6617	− 0.6525	0.0490	0.0185	0.024
0.85	− 0.6876	− 0.6866	− 0.6719	0.0478	0.0242	0.015
0.9	− 0.7141	− 0.7127	− 0.6924	0.0467	0.0570	−0.035
0.925	− 0.7278	− 0.7261	− 0.7031	0.0462	0.0601	−0.041
0.95	− 0.7418	− 0.7398	− 0.7141	0.0456	0.0613	−0.045
0.975	− 0.7560	− 0.7538	− 0.7253	0.0450	0.0657	−0.054
1.0	− 0.7704	− 0.7680	− 0.7368	0.0446	0.0691	−0.062

3. Kinks in the diagonal soliton line

For computational convenience, we introduce a double kink consisting of a separated kink and an anti kink as illustrated in figure 1(b). (For one kink only, a combination of periodic and antiperiodic boundary conditions would have been required. As a result, $H^{\uparrow}_{ij}$ would have depended not only on the expectation values $\langle c^+_{i\downarrow} c_{j\downarrow} \rangle$ but also on $\langle c^+_{i\uparrow} c_{j\uparrow} \rangle$, leading to a linear equation system of size $2N \times 2N$ instead of $N \times N$.) Again we calculated the total energy per site, E_K for the solution with a double kink. Note in the presence of the double kink an extra hole is introduced so that the supercell in figure 1(b) has $N_h = 12$ and $N_\uparrow = 55$, $N_\downarrow = 54$. The extra hole and spin is shared between the kink and antikink. The unequal numbers of $\uparrow$- and $\downarrow$-spin electrons cause no problems in the calculation, but one has to check separately that the Fermi energies of the $\uparrow$- and $\downarrow$-bands are consistent with a minimization of the total energy of the system.

To investigate the dynamics of a moving double kink, we consider a Hamiltonian

$$\mathcal{H} = \tau \sum_{\langle m,n \rangle} \left(a^+_m a_n + \text{HC} \right) + E_0 \tag{7}$$

where the indices m, n mark the location of a double kink along the diagonal soliton line and the summation $\langle m, n \rangle$ is taken over NN locations. The operator $a^+_m a_n$ moves the double kink from location n to m. This can be achieved by moving the whole electron pattern

in figure 1(b) along the diagonal. The kinetic energy associated with Hamiltonian (7) is $E_{\text{kin}} = 2\tau = 2\langle\Psi_1 \mid \mathcal{H} \mid \Psi_2\rangle$, where $\mid \Psi_1\rangle$ and $\mid \Psi_2\rangle$ are the states corresponding to adjacent locations of the double kink. To evaluate E_{kin}, we take $\mid \Psi_1\rangle$ and $\mid \Psi_2\rangle$ to be the Hartree–Fock ground states

$$\left|\Psi_\mu\right\rangle = \left[\psi_{1\uparrow}^{+(\mu)} \cdots \psi_{N_\uparrow\uparrow}^{+(\mu)}\right]\left[\psi_{1\downarrow}^{+(\mu)} \cdots \psi_{N_\downarrow\downarrow}^{+(\mu)}\right]\left|0\right\rangle \tag{8}$$

and make the approximation $\langle\Psi_1 \mid \mathcal{H} \mid \Psi_2\rangle \simeq \widetilde{E}_{\text{HF}}\langle\Psi_1 \mid \Psi_2\rangle$ where $\widetilde{E}_{\text{HF}}$ is the Hartree–Fock energy eigenvalue corresponding to states $\mid \Psi_1\rangle$ and $\mid \Psi_3\rangle$.

The states $\mid \Psi_1\rangle$ and $\mid \Psi_2\rangle$ correspond to different Hartree–Fock Hamiltonians, so in order to compute the transfer matrix element we must express both states in the original basis set defined by the electron number operators $c_{i\sigma}^{+}c_{i\sigma}$:

$$\begin{aligned}\langle\Psi_1 \mid \Psi_2\rangle = \sum_{\substack{\{i_{1\uparrow},\cdots,i_{N_\uparrow\uparrow},i_{1\downarrow},\cdots,i_{N_\downarrow\downarrow}\}=1 \\ \{j_{1\uparrow},\cdots,j_{N_\uparrow\uparrow},j_{1\downarrow},\cdots,j_{N_\downarrow\downarrow}\}=1}}^{N} & \left[\left(\alpha_{iN_\uparrow\uparrow}^{N_\uparrow}\right)^* \cdots \left(\alpha_{i_1\uparrow}^{1}\right)^*\right]\left[\left(\alpha_{iN_\downarrow\downarrow}^{N_\downarrow}\right)^* \cdots \left(\alpha_{i_1\downarrow}^{1}\right)^*\right] \\ & \times \left[\beta_{i_1\downarrow}^{1} \cdots \beta_{iN_\downarrow\downarrow}^{N_\downarrow}\right]\left[\beta_{i_1\uparrow}^{1} \cdots \beta_{iN_\uparrow\uparrow}^{N_\uparrow}\right] \\ & \times \left\langle 0\left|c_{N_\uparrow\uparrow} \cdots c_{i_1\uparrow} \mid c_{N_\downarrow\downarrow} \cdots c_{i_1\downarrow}\right| c_{i_1\downarrow}^{+} \cdots c_{N_\downarrow\downarrow}^{+}\left|c_{i_1\uparrow}^{+} \cdots c_{N_\uparrow\uparrow}^{+}\right|0\right\rangle .\end{aligned} \tag{9}$$

The transformation coefficients for the states Ψ_1 and Ψ_2 are noted by $\alpha_{i\sigma}^{\nu}$ and $\beta_{i\sigma}^{\nu}$, respectively.

Once the coefficients $\alpha_{i\sigma}^{\nu}$ have been computed by iteration of the Hartree–Fock equations, the coefficcients $\beta_{i\sigma}^{\nu}$ can be easily deduced by using the fact that $\mid \Psi_2\rangle = T \mid \Psi_1\rangle$ where T is a translation operator moving all electrons by a vector d onto an adjacent lattice site along the diagonal direction, so that

$$\beta_{r,\sigma}^{\nu} = \alpha_{(r_i-d)\sigma}^{\nu} . \tag{10}$$

The overlap (9) can be evaluated as the determinant of an $(N_\uparrow + N_\downarrow) \times (N_\uparrow + N_\downarrow)$ matrix A, the elements of which are defined by

$$A_{\mu\nu} = \begin{cases} \displaystyle\sum_{i=1}^{L}\left(\alpha_{i\downarrow}^{\mu}\right)^* \beta_{i\uparrow}^{\nu} & \text{for } 1 \leqslant \mu \text{ and } \nu \leqslant N_\uparrow \quad (11) \\ \displaystyle\sum_{i=1}^{L}\left(\alpha_{i\uparrow}^{\mu-N_\uparrow}\right)^* \beta_{i\downarrow}^{\nu-N_\uparrow} & \text{for } N_\uparrow + 1 \leqslant \mu \text{ and } \nu \leqslant N_\uparrow + N_\downarrow \quad (12) \\ 0 & \text{otherwise.} \quad (13) \end{cases}$$

The results for $\langle\Psi_1 \mid \Psi_2\rangle$ and for the lowest kinetic energy E_{kin} are listed in table 1. Note that τ is larger with increasing values of t and the increase near $t \simeq 0.85$ may already point towards an instability of the Hartree–Fock solution.

The physical system we have in mind consists of a fixed (large) number of lattice sites with fixed doping. The task is to determine the minimum energy configuration of a fixed number of extra holes in an antiferromagnetic background. The average Hartree–Fock energy of a hole in the solution with the double kink is $E_{\text{K}}^{\text{h}} = (11 \times 11)(E_{\text{K}} - E_{\text{HF}})/12$. Therefore the extra energy associated with moving an extra hole onto the diagonal soliton and creating a static double kink is

$$\Delta E^* = 12\left(E_{\text{K}}^{\text{h}} - E_{\text{nK}}^{\text{h}}\right) = (11 \times 11)\left(E_{\text{K}} - (12/11)\,E_{\text{nK}} + (1/11)E_{\text{HF}}\right) . \tag{14}$$

This is the self-energy part of the total energy to create the double kink. Note that an increase in domain wall width through the formation of double kinks will lead to a reduction in the number of walls.

When we delocalize the double kink along the diagonal soliton we gain the kinetic energy E_{kin} and thus we obtain a minimum creation energy for a double kink as $E_c = \Delta E^* + E_{kin}$. This value is listed in table 1 also and plotted in figure 2 for varying values of the hopping parameter, t, keeping the other parameters fixed. We see that the creation energy E_c is positive only for values of $t < t_{c,d}$ with $t_{c,d} = 0.87$. A positive value for E_c is necessary to insure the stability of the no-kink solution. When the creation energy E_c is negative in the parameter region $t > t_{c,d}$, then the no-kink solution is unstable against the creation of double kinks due to their quantum mechanical delocalization and a breakdown of the no-kink solution ensues through the proliferation of double kinks.

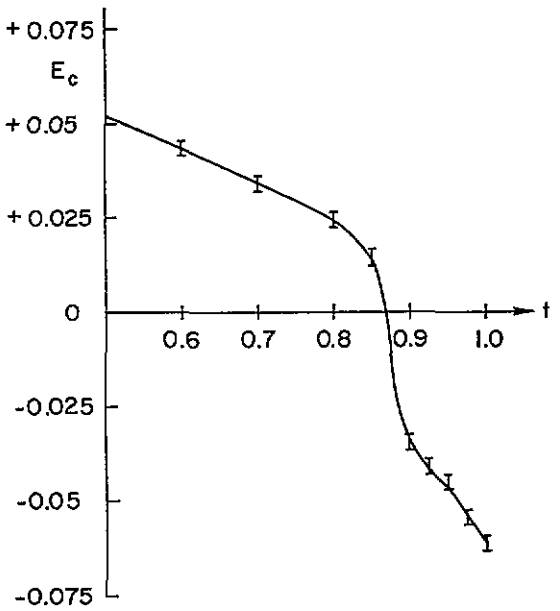

Figure 2. The creation energy of a delocalized double kink, E_c, including the self-energy and kinetic energy contributions. Positive values of E_c are required for stability of the soliton solution displayed in figure 1(a). The other parameters are fixed at $J = 0.5$, $t' = 0.125$ and $U = 16$.

The critical value that we obtain corresponds to a critical ratio $J/t_{c,d} = 0.575$. For values of $J/t > 0.575$, the soliton Hartree–Fock solution is stable against the proliferation of double kinks. This value of $J/t_{c,d}$ is substantially lower than the critical value estimated by Prelovšek and Zotos [6] by examining exact diagonalization results on small clusters, namely $J_c/t \simeq 1.5$. Thus a wider range of stability for the striped phase with simultaneous spin and charge ordering is obtained when we use the criterion of a positive creation energy for double kink creation.

There are two effects which act to reduce this discrepancy. First if we add the induced exchange through the large but finite value of the Hubbard on-site Coulomb energy U we arrive at the total exchange value $J_{tot} = J + 4^2/U$. This effect enhances the critical ratio to $J_{tot}/t = 0.79$. A second effect is the underestimation of the kinetic energy. For

computational convenience we calculated the kinetic energy of the rigid translation of a double kink consisting of a separated kink and antikink. If we allow both the kink and antikink to move separately so we can expect to double the gain in kinetic energy. This effect shifts the critical value of t to $t_{c,s} = 0.8$ and gives a critical ratio $J_{tot}/t = 0.825$ which is somewhat larger but still substantially lower than the value estimated by Prelovšek and Zotos [6] ($J_c/t = 1.5$).

4. Conclusions

In this paper we examined the stability of the striped Hartree–Fock solutions with simultaneous spin and charge ordering against the proliferation of kinks and the antikink. The method yields no information about the nature of the state after the instability occurs but we note that Prelovšek and Zotos [6] found evidence of hole pairing in this parameter region, which points towards a superconducting ground state with $d_{x^2-y^2}$ symmetry. The stability criterion that we obtained with a critical ratio $J/t_{c,s} \simeq 0.8$ is qualitatively similar to that obtained by Prelovšek and Zotos although a substantial quantitative discrepancy remains. In view of the neglect of fluctuations in any Hartree–Fock calculation, it is perhaps reasonable that we overestimate the region of stability of the Hartree–Fock solution.

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