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Bond-centred, bond-ordered stripes in doped antiferromagnets

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Abstract

Motivated by recent inelastic neutron scattering experiments on cuprates, we discuss the formation of bond order in the stripe phase. We suggest that in this phase singlets are formed on some pairs of nearest neighbour (NN) sites in hole-rich domain walls (DWs) between hole-poor regions in which long-range antiferromagnetic (AF) correlations exist. These DWs take the form of two-leg ladders. The motion of a hole inside a bond-ordered ladder is in principle unconstrained while the hopping of a hole in AF domains is to some extent obscured by the fact that a moving hole destroys AF correlations. The propagation of a hole along a stripe is a combination of these two types of motion occurring in two different environments. By analysing the energy dispersion of a quasiparticle propagating in a stripe system with two-leg ladder-like bond-ordered DWs, and of a quasiparticle propagating in a stripe system with DWs in which intermediate bond order is not formed between AF domains, we conclude that the former structure is stable at and above the doping level 1/8. This conclusion seems to be relevant to the nature of the stripe phase in $La_{1.875}Ba_{0.125}CuO_4$.

1. Introduction

The phenomenon of high-temperature superconductivity (HTSC) in quasi-two-dimensional copper oxides and other aspects of unconventional behaviour observed in these systems are far from being understood. Nevertheless some evidence has been obtained that spin and charge ordering in these compounds influences their transport properties. For example, an anomalous suppression of the critical temperature in superconducting (SC) $La_{2-x}Ba_xCuO_4$ and $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$ at the doping parameter x in the vicinity of the commensurate level 1/8 [1] has been associated with the simultaneous formation of charge and spin order. Neutron-scattering studies suggest that the charge ordering in a copper–oxygen plane takes form of stripes which may be viewed as charge-filled DWs between AF regions [2]. The phase of the staggered magnetization in domains changes by π across each DW. It is not clear whether

stripe axes lead through sites occupied by copper atoms or through centres of bonds in the square lattice formed by these atoms. These two optional configurations are called site-centred and bond-centred stripes, respectively.

Some more recent results indicate that bond order may coexist with AF order in the stripe phase of cuprates. By bond order we mean the formation of singlets on some bonds. It seems that Tranquada and collaborators have found evidence of that order in the stripe phase of cuprates [3, 4] by observing that high-energy excitations observed in neutron-scattering studies of $La_{1.875}Ba_{0.125}CuO_4$ and $YBa_2Cu_3O_{6.6}$ are distinct from conventional spin waves which propagate in the AF and are similar to excitations which are measured in two-leg spin ladders. This suggestion has been supported by some recent calculations of magnetic excitation spectra in a system of weakly ferromagnetically coupled AF two-leg ladders which demonstrate that ladder physics may have some relevance to cuprates at the doping level for which stripes are formed [3, 5]. In the past, it has been shown that bond order determines the physics of excitations in undoped and doped AF two-leg ladders [6]. The relevance of that type of ordering to behaviour of doped two-dimensional (2D) AFs and cuprates in particular has also been suggested some time ago [7, 8]. A bond-ordered system may, in principle, fluctuate between different configurations of ordered bonds. The theory of strong fluctuations between many configurations with different patterns of bond singlets covering the whole lattice is even older, and is know as the resonating valence bond picture [9]. In this paper we concentrate on a scenario according to which fluctuations between different configurations are limited to small regions and a given pattern of bond ordering dominates. In particular, our aim is to analyse a unifying picture of coexisting AF ordered domains and bond-ordered DWs in the stripe phase of cuprates. We will try to check if the bond-centred, bond-ordered, hole-filled stripe is more stable than the narrow site-centred stripe. We will also analyse how doping and the formation of a stripe superlattice influence the outcome of the competition between these two types of structure. The possibility of the interplay between bond order and the AF order in the stripe phase has not been widely discussed in the past. Theories of stripes with purely AF order were being developed already in late 1980s [10]. Recently Sachdev *et al* presented some arguments which suggest the coexistence of the magnetically ordered Néel state with a bond-ordered state [11] in a minimal model for square lattice AFs. The scenario, which we analyse here, of the bond-ordered anti-phase domain wall is also motivated by results of a recent exact diagonalization which demonstrates the formation of a stripe and the existence of bond singlets in the t–J model ($t\,J$M) on a small cluster [12]. A subsequent analysis of the single-particle spectral function of such a system [13] additionally supports the idea of weakly hole-doped AF regions alternating with highly hole-doped bond-ordered stripes. Unfortunately, any exact diagonalization performed on a small cluster cannot take into account a key feature of the stripe phase, namely its spatial inhomogeneity. That inhomogeneity seems to be crucial for the formation of a rather conventional Fermi surface observed by means of angle-resolved photoemission spectroscopy (ARPES) from cuprates in the stripe phase [14]. Namely horizontal and vertical patches of the one-dimensional (1D) Fermi surface for ladders combined with a diagonal arc which is a part of the Fermi surface for the doped AF may form a conventional 2D-like Fermi surface. Motivated by this suggestion we will analyse the stability of bond-ordered stripes by means of the recursion method [15], which may be used to analyse larger systems than a finite cluster. That method has already been applied by Chernyshev *et al* [16] to discuss more conventional stripes in which bond order is not generated in DWs between AF regions. We will perform our analysis in the framework of the $t\,J$M on the square lattice. That model is widely used to describe the physics of a single copper–oxygen plane.

The plan of the paper is as follows. Our main goal is to discuss in the framework of the $t\,J$M on the square lattice the coexistence of AF order with bond order in the stripe phase of

cuprates. We begin with the description of mechanisms which govern the propagation of a hole in the bond-ordered background and in the AF spin background and use the insight which we have gained from that discussion to analyse the stripe which is formed when a bond-ordered anti-phase DW between AF domains is filled with holes. We calculate the energy of a band which is formed in this way. We consider not only some optional structures of bond order in the DW, but the narrow DW without an intermediate magnetic structure and the homogeneous AF spin background in which holes may propagate as well. Next, in order to find the total energy and the reference level for the band energy we calculate the energy of the empty bond-ordered DW. Finally we discuss the stability dependence of different stripe structures and their arrays on doping.

2. Composite motion of a hole along a ladder-like stripe with bond order on rungs

The most obvious possible form, which can be analysed, of a stripe viewed as a hole-filled DW is a single chain of sites with a higher density of holes. It is expected that the behaviour of charge and spin excitations in the stripe of that kind resembles the physics of the 1D tJM in which the separation of spin and charge takes place [17, 18]. We analyse a different scenario of a stripe system consisting of DWs which take form of two-leg ladders. We discuss the formation of bond-order in ladder-like DWs either on rungs or on legs. An isolated two-leg ladder is already an interesting object to analyse both experimentally and theoretically [6, 19–21]. For example, it is known that the motion of a hole in the tJM on the two-leg ladder is completely different in character than the motion of a hole in the tJM on the square lattice, in which at least short-range AF correlations exist. In the two-leg ladder, the exchange interaction gives rise to the formation of singlets on rungs. The hopping of the single hole between two sites along a rung favours an even bonding state of the hole on that rung. The bonding even state represents a single fermion with a well-defined spin. The propagation of the hole along the ladder is related to a process during which the bonding fermion and the singlet on two nearest rungs exchange their positions. Therefore, the motion of the hole in the ladder may be represented to lowest order by a tight binding model of spin-$\frac{1}{2}$ fermions [6]. The hopping parameter related to the propagation of the bonding fermionic state is reduced by a factor of 2 relative to the value t of the bare hopping parameter.

The motion of a hole in AF domains between ladder-like DWs in a stripe system is related to a different energy scale $\sim J$ which is lower than t or $t/2$. The hopping hole shifts spins and creates defects in the AF ordered state. The presence of defects brings about an increase of energy and confinement of the hole [22]. That confinement is not perfect because the defects may be annihilated by the exchange term in the Hamiltonian which flips antiparallel spins on NN sites. In our calculation we will predominantly analyse how partial confinement of a hole which enters and leaves AF domains influences its motion along the stripe.

In the first part of our analysis we will concentrate on the anisotropic version of the tJM which is the t–J_z model (tJ_zM) defined by the Hamiltonian H_z,

$$H_z = -t\sum_{\langle i,j\rangle}(c^{\dagger}_{i,\sigma}c_{j,\sigma} + \text{H.c.}) + J\sum_{\langle i,j\rangle} S^z_i S^z_j, \tag{1}$$

where $\langle i, j\rangle$ denotes a pair of NN sites. Namely, we will first calculate the energy of different hole and spin configurations for the isotropic exchange interaction. Later we will analyse how the energy of states which we consider is modified by the additional term,

$$H - H_z = J/2\sum_{\langle i,j\rangle}(S^+_i S^-_j + S^-_i S^+_j), \tag{2}$$

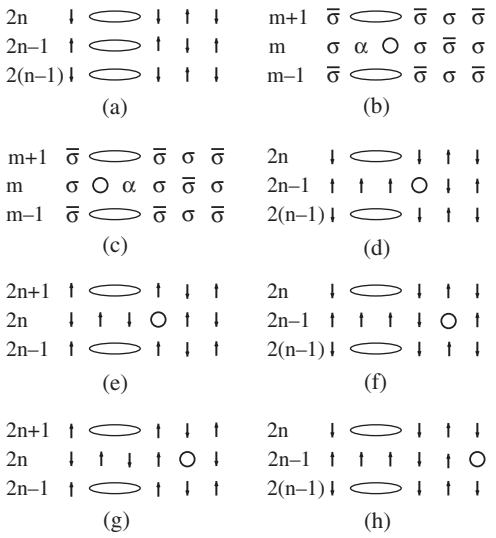

Figure 1. Graphical representation of some string states created by the hopping inside AF domains of a hole created at the ladder-like DW with bond order on rungs. $\bar{\sigma}$ is equivalent to $-\sigma$.

which is present in the fully isotropic $t\,J$M. For completeness it is necessary to mention that the Hilbert space in which the $t\,J$M acts is restricted to states representing configurations without doubly occupied sites.

We start the analysis of charge propagation along a stripe with the discussion of single-hole motion inside the ladder-like DW with bond order on rungs. The physics of this motion is different in one aspect from the propagation of a hole in the ladder. The exchange interaction with the AF ordered domains acts on the DW as an effective staggered magnetic field. We may assume, for convenience, that spins up occupy sites in domains on both sides of odd numbered rungs in the DW, as has been presented in figure 1(a), where numbers which label rungs are explicitly shown. An oval represents a bond singlet. The bonding state representing a single hole on a rung is even with respect to the reflection in the stripe axis

$$|\Psi^{(1)}_{m,\alpha}\rangle = \frac{1}{\sqrt{2}}\left(|\Psi^{(1)}_{m,\alpha,L}\rangle + |\Psi^{(1)}_{m,\alpha,R}\rangle\right) \tag{3}$$

of states $|\Psi^{(1)}_{m,\alpha,L}\rangle$ and $|\Psi^{(1)}_{m,\alpha,R}\rangle$ representing a single fermion with spin α on the left site and on the right site in the mth rung respectively; see figures 1(b) and (c). Equation (3) minimizes the energy of hopping between two sites on the opposite sides of the stripe axis. In the states $|\Psi^{(1)}_{m,\alpha,L}\rangle$ and $|\Psi^{(1)}_{m,\alpha,R}\rangle$, apart from the mth rung all rungs are occupied by singlets. Since the problem of hole motion along the ladder-like stripe with bond order on rungs possesses axial symmetry, without any loss of generality we will later use in our considerations an even combination of reflected states representing holes residing on both sides of the stripe axis. The bonding state (3) is an example of such an even state. The meaning of the label '(1)' in equation (3) will become clear later. Greek letters in figure 1 represent spins, $\bar{\sigma} \equiv -\sigma$, and a circle denotes a hole (an empty site). For the matrix elements of the hopping term H_t in the $t\,J$M or the $t\,J_z$M we have

$$\langle\Psi^{(1)}_{m,\alpha,L}|H_t|\Psi^{(1)}_{m,\alpha,R}\rangle = -t, \tag{4}$$

$$\langle\Psi^{(1)}_{m,\alpha}|H_t|\Psi^{(1)}_{m,\alpha}\rangle = -t. \tag{5}$$

The contribution to energy from the magnetic part of the tJ_zM in the states $|\Psi^{(1)}_{m,\alpha,L}\rangle$ or $|\Psi^{(1)}_{m,\alpha,R}\rangle$, figures 1(b) and (c), is higher if spins σ and α are parallel and has a lower value if they are antiparallel. For parallel spins that contribution is higher by $J/2$ relative to the energy of the empty DW; see figure 1(a). For antiparallel spins σ and α, the magnetic contribution to energy from the single fermion on a rung, figures 1(b) or (c), does not increase relative to the energy of the state in which the rung is occupied by the singlet.

A state representing a single spin-up bonding fermion which propagates inside the ladder-like DW with bond order on the rungs is given by the coherent sum,

$$|\Psi^{(1)}_{\uparrow}(k_{\|})\rangle = \frac{1}{\sqrt{L/2}} \sum_{n} \mathrm{e}^{\mathrm{i}2nk_{\|}} (\beta_{\mathrm{o},\uparrow}(k_{\|})|\Psi^{(1)}_{2n-1,\uparrow}\rangle + \beta_{\mathrm{e},\uparrow}(k_{\|})|\Psi^{(1)}_{2n,\uparrow}\rangle), \tag{6}$$

where $k_{\|}$ is the momentum in the direction parallel to the stripe and L denotes the total length of the stripe. The hole motion which is described by (6) is restricted by definition to the interior of the DW modelled by the two-leg ladder. Two different parameters $\beta_{\mathrm{o},\uparrow}(k_{\|})$ and $\beta_{\mathrm{e},\uparrow}(k_{\|})$ have been introduced for odd and even numbers labelling the rungs, because the energy of the spin–spin interaction between the fermion in the DW and spins in the domains is different for fermions occupying even and odd rungs. We will determine the value of these parameters by looking for the minimum of the quasiparticle energy. The non-vanishing matrix element of H_t between bonding states which appear in (6) is [6]

$$\langle \Psi^{(1)}_{m,\alpha}|H_t|\Psi^{(1)}_{m\pm1,\alpha}\rangle = t/2. \tag{7}$$

After having analysed hole hopping inside the DW we proceed to discuss the motion of the hole outside it. A hole which enters an AF domain leaves a sequence of defects on its way. It must retreat to the stripe along the line formed by these defects, in order to repair them. Thus the basis of states which may be used to describe the hole motion along the stripe consists of wavefunctions obtained during consecutive hopping in the domain, without retreats, of the hole which has started from an arbitrary site in the DW [17]. The creation of a next state belonging to this basis is mediated by the hopping term in the Hamiltonian. The recursion method is an approach that is useful for analysing a Hamiltonian H acting in a basis which consists of states created by applying consecutively that Hamiltonian to a given initial state $|1\rangle$ [15]. This method has been already applied to discuss the hole motion in the Ising AF [23] and to discuss the hole propagation along the narrow DW [17, 16]. Before we use that approach to the analysis of the complex hole-motion along the ladder-like DW we will briefly review the basic principles of the recursion method. In general, any Hamiltonian generates a basis of orthogonal states according to the following set of rules,

$$|2\rangle = H|1\rangle - \frac{\langle 1|H|1\rangle}{\langle 1|1\rangle}|1\rangle, \tag{8}$$

$$|n+1\rangle = H|n\rangle - \frac{\langle n|H|n\rangle}{\langle n|n\rangle}|n\rangle - \frac{\langle n-1|H|n\rangle}{\langle n-1|n-1\rangle}|n-1\rangle, \tag{9}$$

where $n \geqslant 2$. The Hamiltonian H is tridiagonal in the basis formed by states $|n\rangle$ and its eigenenergies may be found by analysing the poles of the diagonal Green's function $g_{11}(\omega) = \langle 1|\frac{1}{\omega - H}|1\rangle$ which takes the form of a continued fraction,

$$g_{11}(\omega) = \cfrac{\langle 1|1\rangle}{\omega - \frac{\langle 1|H|1\rangle}{\langle 1|1\rangle} - \cfrac{\langle 2|2\rangle}{\langle 1|1\rangle\left(\omega - \frac{\langle 2|H|2\rangle}{\langle 2|2\rangle} - \frac{\langle 3|3\rangle}{\langle 2|2\rangle(\omega - \ldots)}\right)}}. \tag{10}$$

We choose a coherent sum of states representing the bonding state and the singlets on the rest of rungs (6) for the state $|1\rangle \equiv |\Psi^{(1)}_{\uparrow}(k_{\|})\rangle$ which we will apply in the recurrence method. This choice is based on the assumption that the motion of the hole along the ladder-like stripe has

two components. The motion inside the DW is analogous to the propagation between rungs of the bonding state, while the motion of the hole which has left the DW and has entered a domain is governed by processes related to the formation of defects in the AF background [17, 22]. By acting successively with the kinetic part of the tJ_zM on the state which represents the hole created in the DW one creates string-like states, $|2\rangle \equiv |\Psi_{\uparrow}^{(2)}(k_{\parallel})\rangle$, $|3\rangle \equiv |\Psi_{\uparrow}^{(3)}(k_{\parallel})\rangle, \ldots$, representing the hole that enters the domain from a given rung in the ladder-like DW. Here, by a string is meant a line consisting of defects created in the domain by the hopping hole which has started from a given site in the DW. A combination of states obtained in this way may be viewed as a spin polaron pinned to the ladder at the rung from which the hole has commenced its motion.

The first matrix element $\langle 1|H|1\rangle$ in the continued fraction (10) is related to states which represent holes which occupy sites inside the DW from which they start the excursions into domains. $\langle 1|H|1\rangle$ can be deduced by summing up contributions from the hopping term, equations (5) and (7), and from the Ising term,

$$\langle \Psi_{\uparrow}^{(1)}(k_{\parallel})|H_{tJ_z}|\Psi_{\uparrow}^{(1)}(k_{\parallel})\rangle = -t + t[\beta_{\mathrm{o},\uparrow}^{*}(k_{\parallel})\beta_{\mathrm{e},\uparrow}(k_{\parallel})\cos(2k_{\parallel})\mathrm{e}^{-\mathrm{i}k_{\parallel}} + \mathrm{H.c.}] + \frac{J}{2}|\beta_{\mathrm{o},\uparrow}(k_{\parallel})|^2. \tag{11}$$

We found their values when we were analysing the hole motion inside the DW. The Ising contribution to energy from the Hamiltonian H_z of tJ_zM in the previous expression is measured relative to the energy of the empty DW.

Now, after a necessary detour, we come back to the issue of hole motion outside the DW. The hopping term moves the hole deeply into the domains. States obtained after the nth hop of the hole contribute to the $(n+1)$th state in the sequence $|1\rangle, |2\rangle, |3\rangle, \cdots$ which is created when the recurrence method is applied in the analysis of string-like excitations in the ladder-type stripe. States depicted in figures 1(d) and (e) contribute to the vector $|2\rangle = |\Psi_{\uparrow}^{(2)}(k_{\parallel})\rangle$ which appears in the definition of the Green's function (10). The contribution to the Ising energy in the tJ_zM from a state obtained by one hop of the hole into the domains from a rung occupied by a single fermion is higher if the spin direction of the rung fermion and the direction of the nearest spin in this domains are parallel in the initial state. This remark concerns the state depicted in figure 1(d). If these directions are antiparallel that contribution is lower because more bonds are occupied by antiparallel spins in the state created after a single hop of the hole; see figure 1(e). The hole which enters deeper into domains frustrates more AF bonds and its energy increases; see figures 1(f)–(h). After the first hop the hole has several choices between different directions of the next move inside the domain. There are exactly $(z-1)$ possible directions of the next hop during which the hole does not return to the site occupied by it before the previous hop. $z = 4$ is the coordination number. Thus, each next move may in general give rise to $(z-1)$ new states, examples of which have been depicted in figures 1(f)–(h). The scalar products which appear in (10) are given by

$$\langle \Psi_{\uparrow}^{(1)}(k_{\parallel})|\Psi_{\uparrow}^{(1)}(k_{\parallel})\rangle = 1, \tag{12}$$

$$\langle \Psi_{\uparrow}^{(n)}(k_{\parallel})|\Psi_{\uparrow}^{(n)}(k_{\parallel})\rangle = (z-1)^{n-2}t^{2(n-1)}, \tag{13}$$

where $n \geqslant 2$. The formula (12) is merely the normalization condition for the amplitudes $\beta_{\mathrm{o},\uparrow}$ and $\beta_{\mathrm{e},\uparrow}$. The factor $(z-1)^{n-2}$ in (13) represents the number of different paths along which the hole can move without retreats, while the factor $t^{2(n-1)}$ appears there because the hopping term transforms the state $|n\rangle$ into the state $|n+1\rangle$. The diagonal matrix elements of the Hamiltonian for the tJ_zM, between states $|\Psi_{\uparrow}^{(n)}(k_{\parallel})\rangle = |n\rangle$ representing holes, which have left the DW and have entered domains have their origin in the Ising term in that Hamiltonian, and are given by

$$\langle \Psi_{\uparrow}^{(n)}(k_{\parallel})|H_{tJ_z}|\Psi_{\uparrow}^{(n)}(k_{\parallel})\rangle = (z-1)^{n-2}t^{2(n-1)}J\left(n - \tfrac{3}{2} + |\beta_{\mathrm{o},\uparrow}(k_{\parallel})|^2\right), \tag{14}$$

where $n \geqslant 2$. The formula (14) has been obtained by counting the number of frustrated AF bonds in string states, as depicted in figures 1(d)–(h). The energy of the propagating quasiparticle in the ladder-like stripe, $\epsilon_1(k_\parallel)$, measured relative to the energy of the empty DW, may be found within the recurrence procedure by looking for the lowest pole in (10) and by minimizing its value with respect to the parameters $\beta_{e,\uparrow}(k_\parallel)$ and $\beta_{o,\uparrow}(k_\parallel)$ under an additional condition that they are normalized according to the relation

$$|\beta_{o,\uparrow}(k_\parallel)|^2 + |\beta_{e,\uparrow}(k_\parallel)|^2 = 1, \tag{15}$$

which follows from the normalization condition (12) for $|1\rangle = |\Psi^{(1)}_{\uparrow}(k_\parallel)\rangle$.

Strings formed by defects which have been created by the moving hole may be shortened in the isotropic system by the transverse part of the Heisenberg model. This term swaps antiparallel spins on NN sites. Such a process effectively shifts the hole or, to be more precise, such a process shifts the spin polaron to a second or a third NN site. Finite mobility of holes in an AF may bring about their evaporation from the single DW and it is likely that the single stripe is not stable in the doped isotropic AF described by the tJM. On the other hand, when stripes form an array, holes cannot escape to infinity. In addition, it is clear that the system of stripes will be additionally stabilized by the tunnelling of holes between them. The full quantitative analysis of hole tunnelling between stripes is beyond the scope of this paper. Here we concentrate on energy changes related to the internal structure of the single stripe. The energy scale of these changes is higher than the energy scale related to tunnelling between stripes. Thus it is sufficient to consider the motion along the single stripe to draw some conclusions about the stability of the whole stripe system. We will now give some more arguments to justify this statement. The motion of the hole inside the DW does not bring about any persistent changes in the magnetic structure, apart from some triplet excitations. It has been demonstrated that triplets play a minor role and may be neglected [6]. It turns out that triplet excitations merely contribute to the incoherent background. Their presence does not substantially influence the form of the quasiparticle dispersion and therefore to lowest order it does not change the energy of the system. The longitudinal component of the quasiparticle propagating along the stripe resembles a moving free fermion. That component which is related to the motion in the ladder of the bonding state on a rung, is crucial for lowering the energy of the stripe relative to the energy of the doped homogeneous AF. Since the energy scale for the polaron propagation in the AF is $\sim J$, while the energy scale for the propagation in the DW (figure 1(a)) of the bonding fermion is $\sim t$, in the lowest approximation we may neglect, in the analysis of the stripe stability, the processes which give rise to coherent propagation of polarons inside domains and tunnelling between stripes. On the other hand, we consider the motion inside domains of holes which start from a given rung in the DW, retrace their steps and return to the initial site. That motion brings about a considerable change in the energy of the quasiparticle propagating in the stripe relative to the energy of the bonding fermion propagating in the ladder. This change is of order $\sim t$. The reduction of the distance between stripes may bring about an energy change which is also of order $\sim t$, because the length of strings is effectively limited by the width of domains. We will take into account in our calculation the effect which the domain width has on the energy.

The translational invariance of the stripe in the direction parallel to its axis is broken by the interaction with the AF ordered domains. Thus the energy band formed by holes propagating along the stripe becomes split and the size of the 1D Brillouin zone related to the motion along the stripe which is a 1D object is effectively reduced by a factor of 2. The dashed line in figure 2 represents the lower part of this band. It can be filled twice by quasiparticles which are compositions of the spin polaron and of the bonding spin-up or spin-down fermion on a rung. A stripe obtained by filling the ladder-like DW with holes is different in this respect from the

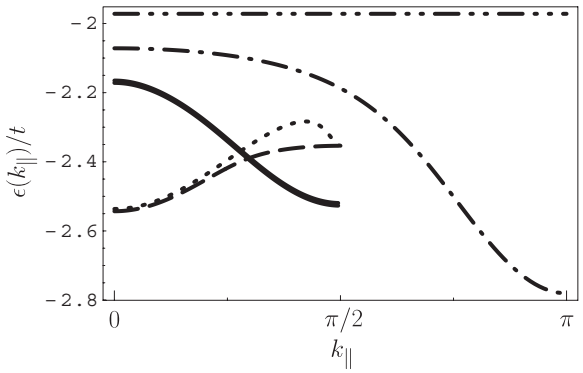

Figure 2. Energy of a single hole confined in the homogeneous Ising AF (dash–double-dotted line), energy of a quasiparticle propagating in the ladder-type stripe with singlets on rungs (dotted line and dashed line), energy of a quasiparticle propagating in the ladder-type stripe with singlets on legs (solid line) and energy of a quasiparticle in the narrow stripe (dash–dotted line). Energy is measured relative to energy of the homogeneous Ising AF or an empty DW. $k_\parallel$ is the momentum along the stripe. Only the symmetric halves of bands for positive $k_\parallel$ have been presented. For the stripe with the bond order on rungs the dotted (dashed) line refers, here and below, to a calculation with non-optimized (optimized) amplitudes $\beta_{e,\uparrow}(k_\parallel)$ and $\beta_{o,\uparrow}(k_\parallel)$ of states representing transversal spin polarons attached to even and odd numbered rungs. $J/t = 0.4$ as everywhere.

stripe obtained by filling with holes the narrow DW [17]. The quasiparticle band which forms for the latter type of stripe is represented by the dash–dotted line in figure 2. It can be filled only once because a spin-less holon is now the component of the quasiparticle propagating along the stripe [17]. The dispersion of the holon band has been also found by means of the recurrence method. The energy is measured in both cases relative to the energy of the empty DW. Irrespective of the fact that the bottom of the energy band for the stripe which is formed when the ladder-type DW is filled lies higher than the bottom of the energy band for the stripe which is formed when the narrow DW is filled, filling the ladder-type DW with holes is a more effective way of lowering the energy for higher levels of doping because the quasiparticle band is flatter in this case and it can be filled twice. The dash–double-dotted straight line represents the energy of a hole confined in the anisotropic AF described by the tJ_zM. In order to check the sensitivity of our approach to approximations which have been applied we have plotted as a dotted line in figure 2 the quasiparticle energy $\epsilon_1(k_\parallel)$ obtained when the parameters $\beta_{e,\uparrow}(k_\parallel)$ and $\beta_{o,\uparrow}(k_\parallel)$ are determined by minimizing the matrix element (11) which refers to the motion of a hole inside the DW. In this case the quasiparticle energy $\epsilon_1(k_\parallel)$ is again given by the lowest pole of $g_{11}(\omega)$ but the optimization of this pole with respect to the parameters β is not applied.

3. Hole motion along the ladder-like stripe with bond order on legs

In this part of the paper we consider a different bond-centred stripe with a slightly modified underlying magnetic structure. It is not clear what kind of bond order is energetically favourable when a ladder-like DW is filled with holes. An obvious magnetic structure alternative to the bond-ordered rungs is the bond order on legs. Figure 3(a) depicts this structure. We sketch now the calculation of the energy dispersion for a quasiparticle moving in such a spin background. The hopping of a hole along a rung gives rise to an exchange of positions between a single fermion and a singlet on parallel legs. The matrix element of the hopping term in the Hamiltonian which couples the states depicted by figures 3(b) and (c) is $t/2$. The same value

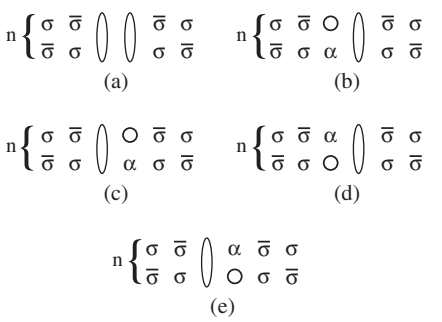

Figure 3. Graphical representation of some string states created by the hopping inside AF domains of a hole created at the ladder-like DW with bond order on legs.

has the matrix element which couples the states depicted by figures 3(d) and (e). Since that matrix element is positive, the lowest-energy state with a given momentum along the stripe may be constructed by summing odd combinations of some state pairs. The states in each pair are images of each other obtained by the reflection in the axis of the stripe. Two examples of reflected states are shown in figures 3(b), (c), and in figures 3(d), (e). In a similar way as before we define $|\Psi^{(1)}_{n,u,\alpha}\rangle$ as the normalized odd combination of states depicted by figure 3(b) and by figure 3(c). $|\Psi^{(1)}_{n,l,\alpha}\rangle$ denotes the odd combination of states depicted by figure 3(d) and by figure 3(e). A wavefunction which we use as the starting point in the recurrence procedure applied to the problem of the stripe with bond order on legs may be defined as

$$|\Psi^{(1)}_{\sigma}(k_{\parallel})\rangle = \frac{1}{\sqrt{L/2}} \sum_{n} \mathrm{e}^{\mathrm{i}2nk_{\parallel}} (\beta_{1,\sigma}(k_{\parallel})|\Psi^{(1)}_{n,l,\sigma} + \beta_{u,\sigma}(k_{\parallel})|\Psi^{(1)}_{n,u,\sigma}\rangle). \tag{16}$$

We easily deduce that the diagonal matrix element for the initial state is

$$\langle\Psi^{(1)}_{\sigma}(k_{\parallel})|H_{tJ_z}|\Psi^{(1)}_{\sigma}(k_{\parallel})\rangle = -\frac{t}{2} - t[\beta^{*}_{u,\sigma}(k_{\parallel})\beta_{1,\sigma}(k_{\parallel}) + \beta^{*}_{1,\sigma}(k_{\parallel})\beta_{u,\sigma}(k_{\parallel})]$$
$$+\frac{t}{2}[\mathrm{e}^{\mathrm{i}2k_{\parallel}}\beta^{*}_{u,\sigma}(k_{\parallel})\beta_{1,\sigma}(k_{\parallel}) + \mathrm{e}^{-\mathrm{i}2k_{\parallel}}\beta^{*}_{1,\sigma}(k_{\parallel})\beta_{u,\sigma}(k_{\parallel})] + \frac{J}{2}|\beta_{u,\sigma}(k_{\parallel})|^2. \tag{17}$$

The relations presented below may be obtained by carrying out the recurrence analysis in a way similar to that which was applied to the problem of the ladder-like stripe with the bond order on rungs

$$\langle\Psi^{(1)}_{\sigma}(k_{\parallel})|\Psi^{(1)}_{\sigma}(k_{\parallel})\rangle = 1, \tag{18}$$
$$\langle\Psi^{(n)}_{\sigma}(k_{\parallel})|\Psi^{(n)}_{\sigma}(k_{\parallel})\rangle = (z-1)^{n-2}t^{2(n-1)}, \tag{19}$$

and

$$\langle\Psi^{(n)}_{\sigma}(k_{\parallel})|H_{tJ_z}|\Psi^{(n)}_{\sigma}(k_{\parallel})\rangle = (z-1)^{n-2}t^{2(n-1)}(n-1)J, \tag{20}$$

where $n \geqslant 2$. By looking for the lowest pole of $g_{11}(\omega)$, equation (10), and optimizing that parameter with respect to $\beta_{1,\sigma}(k_{\parallel})$ and $\beta_{u,\sigma}(k_{\parallel})$, we may find the energy dispersion $\epsilon_1(k_{\parallel})$ of a hole-like quasiparticle propagating along the ladder-like stripe with bond order on legs. The solid line in figure 2 represents that dispersion. As before, $\epsilon_1(k_{\parallel})$ is measured relative to the energy of the undoped DW forming the stripe upon hole filling.

4. Bond-ordered anti-phase domain wall in the 2D AF

Now, we temporarily concentrate on the undoped system and analyse the energy of a DW with a given internal magnetic structure. We use a simple approach, which is the second-order

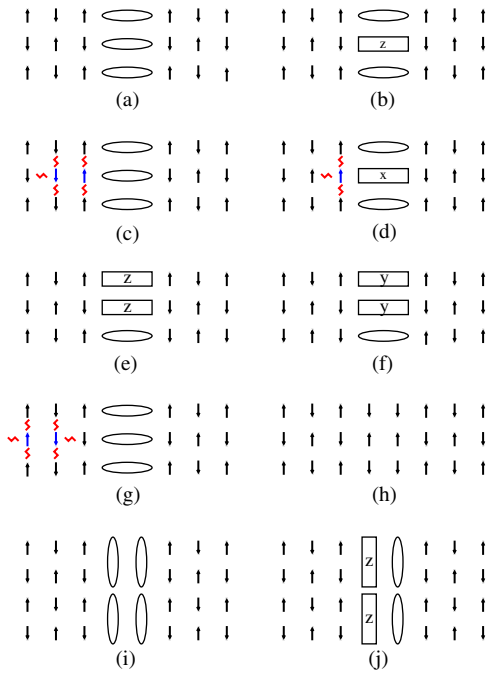

Figure 4. Graphical representation of the DW which takes the form of a two-leg ladder with bond order on rungs, (a); and some excitations in this DW, (b)–(g). Graphical representation of the narrow DW representing two directly merged anti-phase domains which are not separated by an intermediate region with additional order, (h). Magnetic structure of a stripe formed by hole-filling the DW with bond-order on legs, (i), and an excitation created in that structure by the transversal part of the Heisenberg model, (j).

(This figure is in colour only in the electronic version)

perturbation theory applied to the Heisenberg model. As has been shown in the case of the homogeneous 2D AF, such a simple approach gives rise to a correct lowest-order description of the system [24, 25]. First we discuss a DW with dominating bond order on rungs. Our starting point is an unperturbed Hamiltonian H_0 with a ground state $|\Phi_0\rangle$, shown in figure 4(a), which depicts two AF domains separated by a column formed by singlets,

$$H_0 = \sum_{\langle i,j\rangle} S_i^z S_j^z + \sum_{\langle m,n\rangle} \mathbf{S}_m \mathbf{S}_n, \tag{21}$$

where $\langle i, j\rangle$ refers to all pairs of NN sites belonging to domains and $\langle m, n\rangle$ refers to all pairs of NN sites belonging to rungs in the ladder-like DW. As before, ovals in figure 4(a) denote singlets on rungs. The full exchange interaction of sites which belong to domains with sites belonging to ladder-like DWs is treated here as a perturbation. The energy of an eigenstate $|\Phi\rangle$ of H may be found by means of the standard second-order perturbation theory. This goal can be achieved by analysing matrix elements $\langle\Psi_i^{(0)}|H_1|\Phi^{(0)}\rangle$, where $H_1 = H - H_0$ and H is the Hamiltonian of the Heisenberg model. $|\Psi_i^{(0)}\rangle$ are excited states of H_0 with eigenenergy E_i, while $|\Phi^{(0)}\rangle$ is its ground state with eigenenergy E_0. Figures 4(b)–(g) depict typical examples of excited states $|\Psi_i^{(0)}\rangle$ which contribute to non-vanishing matrix elements $\langle\Psi_i^{(0)}|H_1|\Phi^{(0)}\rangle$. A zig-zag line represents a 'broken' bond with a higher contribution to the energy of the Ising model relative to the energy of the Néel state. A letter $o = x, y, z$ inside a rectangle denotes a

triplet state created by the operator

$$t_{ij,o} = \frac{\mathrm{i}}{\sqrt{2}}[\sigma^o\sigma^y]_{\alpha,\beta}c^\dagger_{i,\alpha}c^\dagger_{j,\beta}, \tag{22}$$

acting on a an empty pair $\langle i, j\rangle$ of NN sites. We would like to emphasize that the operator $t_{ij,o}$ creates in the vacuum a triplet on sites i and j. By counting the contributions from excited states, we get, for the difference between the energy of the ladder-like DW of length L and the energy of the homogeneous ground state of the quantum AF in two dimensions (Heisenberg model),

$$\delta E_1 = \tfrac{13}{40}JL. \tag{23}$$

The ground-state energy of the homogeneous AF used to derive the value of δE_1 in (23) has also been obtained by means of the second-order perturbation theory. The Ising model and the Néel state have been applied in the derivation as the unperturbed Hamiltonian and its ground state, respectively.

We proceed now to discuss the energy of the narrow DW between two AF domains with the opposite staggered magnetization. The domains are in this case in more direct contact with each other, as shown in figure 4(h). An increase of the energy due to the formation of the narrow DW is lower than for the wider DW depicted by figure 4(a),

$$\delta E_n = \tfrac{1}{6}JL. \tag{24}$$

The quantity δE_n has also been obtained by means of the second-order perturbation theory applied to the Heisenberg model.

Quantum fluctuations in the isotropic AF reduce the increase of the energy caused by the DW. We may draw this conclusion by noticing that in the extremely anisotropic case of the Ising model the energy of the ladder-like DW, figure 4(a), is JL while the energy of the narrow DW, figure 4(h), is $\frac{1}{2}JL$.

We also need to know the energy of the wide DW with dominating bond order on legs. The unperturbed Hamiltonian H_0 may be written in this case also in the form given by (21), but with pairs $\langle m, n\rangle$ referring to legs on which singlets are formed, as has been presented in figure 4(i). Again, by analysing excitations created in the ground state of H_0 by the remaining part of the Hamiltonian we may get an approximation to the energy of the DW with bond order on legs. It turns out that this energy is $\frac{27}{160}JL$, which is lower than for the DW with bond-ordered rungs. This lowering may be attributed to the existence of a bigger number of accessible excitations than in the previous case. An example of a new kind of excitation has been presented in figure 4(j). The energy of the DW with bond-ordered legs is JL in the Ising limit. This value is the same as for the DW with bond-ordered rungs. Again we notice that quantum fluctuations diminish the energy difference between the wide and the narrow DWs. We will show that this reduction is crucial for the stability of the ladder-like stripe.

5. Stability analysis

The energy per doped hole of the stripe obtained by hole filling the ladder-like DW with bond order on rungs, e_1, is given by an obvious formula,

$$e_1 = \frac{\frac{1}{\pi}\int_{-k_\mathrm{F}}^{k_\mathrm{F}} \epsilon_1(k_\parallel)\,\mathrm{d}k_\parallel + \delta E_1}{\frac{1}{\pi}\int_{-k_\mathrm{F}}^{k_\mathrm{F}} \mathrm{d}k_\parallel}, \tag{25}$$

where δE_1 is the energy of the DW per lattice spacing along the stripe. e_1 and δE_1 are measured relative to the energy of the undoped AF. The linear filling level of the stripe is

$$\delta_1^\parallel = \frac{1}{\pi}\int_{-k_\mathrm{F}}^{k_\mathrm{F}} \mathrm{d}k_\parallel = \frac{2k_\mathrm{F}}{\pi}. \tag{26}$$

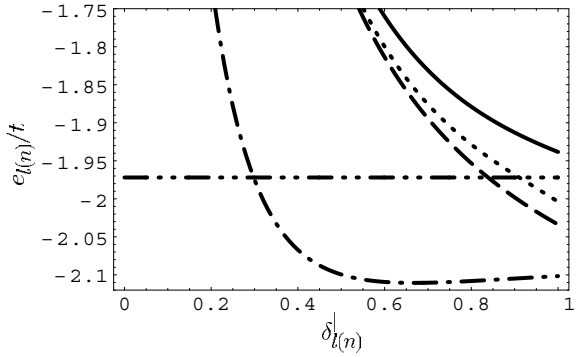

Figure 5. $e_{\rm l}$, the energy per doped hole relative to the energy of the homogeneous Ising AF for the ladder-like stripe with bond order on rungs, dotted line and dashed line, and for the ladder-like stripe with bond order on legs, solid line. e_n, the energy per doped hole for the site-centred stripe, dash–dotted line, as a function of linear doping $\delta^{\|}_{{\rm l}(n)}$. The dash–double-dotted line represents the energy of a hole confined in the homogeneous system.

Formulae which may be applied to derive the energy per doped hole and the linear filling parameter for the stripe with bond order on legs are similar. The main difference is that the energy band now has its minimum at the point $\pi/2$,

$$e_{\rm l} = \frac{\frac{1}{\pi}\int_{-\pi/2}^{-\pi/2+k_{\rm F}} \epsilon_{\rm l}(k_{\|})\,{\rm d}k_{\|} + \frac{1}{\pi}\int_{\pi/2-k_{\rm F}}^{\pi/2} \epsilon_{\rm l}(k_{\|})\,{\rm d}k_{\|} + \delta E_{\rm l}}{\frac{1}{\pi}\int_{-\pi/2}^{-\pi/2+k_{\rm F}} {\rm d}k_{\|} + \frac{1}{\pi}\int_{\pi/2-k_{\rm F}}^{\pi/2} {\rm d}k_{\|}}, \tag{27}$$

$$\delta^{\|}_{\rm l} = \frac{1}{\pi}\left(\int_{-\pi/2}^{-\pi/2+k_{\rm F}} {\rm d}k_{\|} + \int_{\pi/2-k_{\rm F}}^{\pi/2} {\rm d}k_{\|}\right) = \frac{2k_{\rm F}}{\pi}. \tag{28}$$

The site-centred stripe is formed by filling with holes only one of two vertical chains in the middle of figure 4(h). The energy band of holon-like quasiparticles which propagate along the narrow stripe can be filled only once because holons are spin-less objects [17]. Thus, the energy per doped hole, e_n, is given by

$$e_n = \frac{\frac{1}{2\pi}\int_{\pi-k_{\rm F}}^{\pi+k_{\rm F}} \epsilon_n(k_{\|})\,{\rm d}k_{\|} + \delta E_n}{\frac{1}{2\pi}\int_{\pi-k_{\rm F}}^{\pi+k_{\rm F}} {\rm d}k_{\|}}, \tag{29}$$

where δE_n is the energy of the narrow DW per lattice spacing along the stripe. The linear filling parameter $\delta^{\|}_n$ is

$$\delta^{\|}_n = \frac{1}{2\pi}\int_{\pi-k_{\rm F}}^{\pi+k_{\rm F}} {\rm d}k_{\|} = \frac{k_{\rm F}}{\pi}. \tag{30}$$

We start the stability analysis with the discussion of a single stripe in the extremely anisotropic limit of the $t\,J_z$M. Figure 5 depicts the total energy per doped hole in the ladder-like DW (dashed line and solid line) and the total energy per one hole in the narrow DW (dash–dotted line) as a function of linear filling $\delta^{\|}_{{\rm l}(n)}$. The dash–double-dotted horizontal line represents the energy of the single spin polaron confined in the homogeneous Néel state. It has been calculated by means of the recursion method. Earlier, that quantity was analysed by Starykh and Reiter [23]. It was also compared by Chernyshev *et al* [16] to the energy of a hole in a stripe formed in the narrow DW. That comparison has demonstrated that for $t\,J_z$M, at the linear hole filling level above ∼0.25, a stripe without intermediate bond order in the DW between two AF domains is more stable than a system of holes homogeneously distributed in the Néel

state. For the interesting case of the global doping level 1/8, this result has been confirmed by a numerical calculation based on the string scenario [26]. The dashed line in figure 5 represents the energy e_1 for the ladder-like stripe with the bond order on rungs derived from the formula (25) in which we have applied the quasiparticle energy $\epsilon_1(k_\parallel)$ obtained by minimizing the value of the lowest pole in (10) as a function of the parameters $\beta_{e,\uparrow}(k_\parallel)$ and $\beta_{o,\uparrow}(k_\parallel)$. For comparison, the dotted line has been obtained for the same type of stripe by using an ansatz for these parameters. This ansatz minimizes the value of the matrix element (11). The solid line refers to the wide stripe with bond order on legs. The energy is measured in all cases relative to the energy of the Néel state. We have set $J/t = 0.4$. This estimate is based on experimental data. The stripe obtained by filling the narrow DW becomes stable slightly above quarter-filling [17] in the limit of extremely anisotropic exchange interaction of the tJ_zM. The energy per doped hole of the stripe obtained by hole filling the ladder-like stripe with bond order on rungs is lower than the energy of the hole confined in the Néel AF at a linear filling above $\delta_1^{\parallel} \simeq 0.8$. The energy per doped hole for a ladder-like stripe with bond order on legs is higher than the energy of the hole confined in the anisotropic AF for the whole range of the linear filling parameter. Since the energy of the ladder-like DW is much higher than the energy of the narrow DW, the ladder-like stripe has higher energy than the narrow stripe up to the linear filling parameter $\delta_1^{\parallel} = 1.0$. Nevertheless, as may be seen in figure 2, for higher values of $\delta_{1(n)}^{\parallel}$, hole-filling the ladder-like DW is a more effective way of lowering the energy relative to the energy of the empty DW than filling the narrow DW. In addition, by looking at formulae (25)–(30) we notice that the reduction of the difference between energies of the narrow DW, δE_n (29) and the ladder-like DW, δE_1 in (25) and (28) may give rise to the stability of the ladder-like stripe at finite doping. As we have already shown, that difference is reduced in the isotropic AF and one may expect that the ladder-like stripe may be more favourable in the system described by the tJM. An additional factor which may influence the stripe energy is the distance between stripe axes and the width of domains. Thus, from now on we discuss the stripe system formed in the anisotropic AF. In such a system the length of strings created by holes which hop in domains is to some extent limited by the width of these domains. This limitation influences the band-energy renormalization which is brought about by intrusions into domains of the hole moving along the DW. Neutron scattering experiments suggest that the width of AF domains is 2–3 lattice spacings for the doping level 1/8. The domain-width limitation induced by the finite spacing between stripes may influence the stripe energy. In order to analyse that influence we have limited the length of strings to two lattice spacings. By the string length is meant here the number of hops needed to create a given string state from a state representing the single hole created on a bond. By analysing the construction of the sequence $|1\rangle, |2\rangle \cdots$ by means of the recursion method applied to the stripe problem we easily infer that the state $|n\rangle$ represents strings of length $n - 1$. Thus, by stopping the recurrence procedure at the $(n + 1)$th step we may impose the restriction of the string length to n lattice spacings.

It turns out that for a linear filling $\delta_{1(n)}^{\parallel} \sim 0.5$ and above, which for the distance of four lattice spacings between stripe axes corresponds to the doping level 12.5% and above, the ladder-like stripe with bond order on legs becomes stable in a system with fully isotropic exchange energy; see figure 6. At some higher values of the doping parameter, the DW with bond order on rungs is stable. In the calculation performed to derive numbers which have been used to plot figure 6, we have applied in formulae (25), (28) and (29) DW energies per site, δE_1, and δE_n, obtained for the isotropic AF. The string length was by definition limited by the distance of two lattice spacings.

We do not assume that nearest DWs are impenetrable for a hole which has been created at a given DW. The hole may penetrate a nearest DW without raising the exchange energy only if

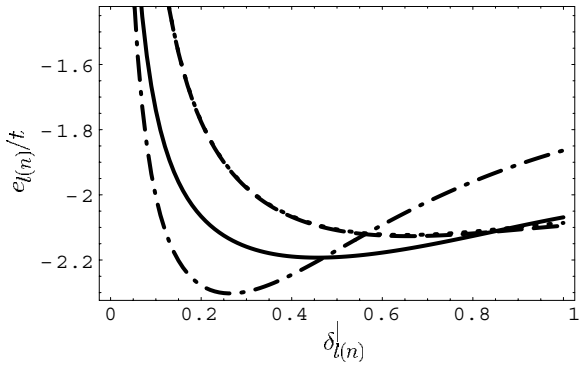

Figure 6. $e_{l(n)}$, the energy per doped hole relative the energy of the empty homogeneous isotropic AF. The dashed line and the dotted line merging with it represent that parameter calculated for the DW with bond order on rungs and the optimized and non-optimized parameters $\beta_{e,\uparrow}(k_\parallel)$, $\beta_{o,\uparrow}(k_\parallel)$, respectively, while the solid line refers to the DW with bond order on legs and the dash–dotted line refers to the site-centred stripe.

at a certain stage of this process the transversal part of the Heisenberg Hamiltonian is applied to an intermediate state. The transversal term is proportional to J. Thus it seems that hole propagation transverse to stripes influences to a lesser extent the value of the energy than hole propagation along them for which the energy scale is $\sim t$, and therefore the propagation in the transverse direction may be neglected in a simple analysis.

6. Discussion and outlook

The crucial question which needs to be answered, before the puzzle of high-temperature superconductivity and non-Fermi liquid behaviour observed in cuprates is solved, is how the Mott insulating AF is transformed, upon doping, into the unconventional metal and the superconductor. Many interesting efforts, which concentrate mainly on the homogeneous phase, have been made to give at least partial answer to this question [27]. On the other hand, much experimental evidence has been obtained that inhomogeneity plays an important role in the physics of cuprates and doped AFs, at least for some doping levels. Some theoretical results give also rise to the same conclusion [28]. Recent experiments [3, 4] and theoretical papers [11–13] directly point at the possibility of the coexistence between bond and AF orders in the stripe phase. In our work we have analysed mechanisms which may give rise to this coexistence, by comparing the energy of several optional states, including the homogeneous state. The form of the tested states has been suggested either by experiments or by recent numerical results. In the past, much effort has been made to develop theories of stripe states in doped AFs [10, 17, 26, 29, 30]. On the other hand, the experimental detection of stripes is far from being trivial. Their shape has not been identified yet with full certainty. The experimental evidence of nanoscale phase separation and its theoretical interpretation is not always unique [31]. The width and the magnetic structure of stripes, defined as hole-rich regions which play the role of DWs for magnetically ordered regions, belongs to issues that are still under debate. The concept of magnetically ordered states in doped AFs has been recently confronted with the idea of bond-ordered states. The classification presented in an article [8] suggests that magnetic and bond orders are optional types of ordering, which do not coexist. A similar confrontation was already performed in an earlier paper [32] in which energy changes upon doping in the columnar spin dimerized phase and the Néel state have

been compared. In some other articles [33] the quantum critical point between the Néel state and the columnar dimerized phase has been examined. It is worth emphasizing that in all these publications it was assumed that dimers in the columnar phase were covering the whole square lattice. We have presented in our paper a different point of view, according to which the coexistence of bond order with AF order is possible due to nanoscale phase separation. The doped AF favours magnetic order with a non-vanishing value of the sublattice magnetization in hole-poor parts of the system, while the bond order develops in hole-rich regions which take the form of unidirectional stripes separating AF domains. The formation of the bond order in stripes which play the role of DWs is favourable, because holes may propagate more freely in such a spin background and the kinetic energy is substantially lowered in this way. Within the scenario of coexisting bond, AF, and charge orders we have considered a DW between two AF domains with opposite directions of the sub-lattice magnetization. This DW takes the form of the two-leg ladder with bond order either on legs or on rungs. We have also assumed that a strong tendency towards confinement manifests in the motion of a hole which has left a stripe (a DW) and has entered one of two AF domains which are separated by the stripe. After calculating the band energy of such a propagating complex quasiparticle we have deduced that the system of bond-centred, ladder-like stripes is energetically more stable than the system of site-centred stripes in the isotropic AF at the linear hole-filling 0.5, and above this value. There exists some experimental evidence that the linear filling of stripes observed in cuprates is about 0.5. The finite width of domains in a system of stripes is an important factor which gives rise to stability of bond-ordered stripes. We have taken into account in our analysis that the form of bond order in the ladder-like stripe, treated as a DW, strongly influences the value of the exchange energy. We have also argued that processes related to the coherent hole propagation in the AF background and to the hole tunnelling between stripes are of higher order and that they change the energy to a lesser extent. The outcome of our analysis shows that the system prefers the formation of singlets on bonds parallel to stripe axes. Such a direction of bond order in stripes has also been observed in results of exact diagonalizations [12, 13]. Our calculation has demonstrated that bond-centred stripes are formed for higher levels of global doping at which the distance between stripes is shorter. Since the limiting value of the linear filling parameter at which the bond-centred stripe becomes stable lies in figure 6 below the value 0.5, which refers to the global doping level about $1/8$ and to the width of AF domains about 2–3 lattice spacings, we may deduce that bond order is very likely for this and higher values of doping.

Magnetic excitations in the stripe phase have been discussed in the literature. Spin wave theory of these excitations, based on a scenario of site-centred stripes separating AF domains [34], does not capture the high energy part of the spectrum measured by means of neutron scattering [3, 4]. Assuming spin dimerization and formation of bond-centred stripes, the authors of two recent preprints have been able to formulate a theory which correctly describes the measured spectrum [35]. On the other hand, they have assumed that hole-rich regions taking the form of two-leg ladders do not participate in spin dynamics, which is hard to justify because at the linear filling $1/2$, three sites out of four are occupied by spins in such structures. The two-leg ladder in the effective staggered magnetic field was already discussed, in the context of stripes, in some previous publications [36], but the authors of these papers either did not consider bond order inside the ladder or did not consider the formation of strings in domains and hole intrusions into them.

The experimental identification of bond order in stripes and its shape is a difficult task. There is no direct method to achieve that goal. Important information is provided by inelastic neutron scattering experiments [3, 4]. On the other hand, results of theoretical analyses [35] seem to indicate that the shape of measured spectra is not very sensitive to the form of the

underlying bond order. Thus, it seems that by means of neutron scattering measurements alone it is not possible to identify the exact form of the bond order which is formed in stripes. The interpretation of ARPES experiments may be additionally helpful in this task, because the formation of a bond-ordered state influences the electronic structure of any system [13]. The single-particle spectral weight in the stripe phase was discussed in several theoretical papers [30, 37]. On the other hand, the impact which the shape of hypothetical bond order in stripes, understood as hole-rich DWs between AF domains, may have on spectral properties of cuprates has not been carefully analysed until now. Results of such an analysis recently performed by us confirm conclusions which we draw in this paper. In a different work [38], which cannot be reported now in detail due to lack of space, we have computed the single-particle spectral density of stripe arrays, the stability of which we have analysed here. In the case of the stable stripe system, with bond order parallel to their axes, the intensity maps reproduce quite well the ARPES spectra from the cuprates belonging to the 214 family of compounds when they are doped with 15% of holes. It seems that this additional consistency check is necessary because, as we may see in figure 6, the margin by which the energy of bond-ordered stripes is lower than the energy of narrow stripes at the linear filling level 0.5 and the doping level 0.125 is small, and it is not clear whether the precision of the simple method applied by us is sufficient to find correctly the doping level at which the transition between narrow and wide stripes takes place.

Much evidence has been accumulated that in some cases the charge and spin inhomogeneity observed in cuprates has purely 2D character [39]. Such modulations seem to be also consistent with the scenario of fluctuations between some bond-ordered states [40]. An analysis of this category of states is beyond the scope of the discussion presented in our paper.

We do not consider the conclusions which we draw from the results of our calculation to be absolutely final. The method which we have used is not precise enough to let us determine the phase diagram of doped AFs with great precision, because the energy margin between different phases is rather small. On the other hand, the results of our calculation show that there exists a mechanism which might give rise to coexistence of bond order with AF order in doped cuprates. That mechanism is based on nanoscale phase separation between hole-rich bond-ordered regions in which kinetic energy is lowered and hole-poor AF regions in which exchange energy is lowered. Further research on that subject by means of both theoretical and experimental methods is required. This suggestion concerns first of all the relation between superconductivity and the tendency towards charge ordering or phase separation which is manifest by stripe formation. Some scenarios which attributed the cause of superconductivity to stripe formation have been put forward. It seems that there is not enough convincing evidence to support these suggestions.

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