Pseudo-particles picture in single-hole-doped two-dimensional Néel ordered antiferromagnet

2007 J. Phys.: Condens. Matter 19 156203

(http://iopscience.iop.org/0953-8984/19/15/156203)

IOP PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **19** (2007) 156203 (14pp) doi:10.1088/0953-8984/19/15/156203

Pseudo-particles picture in single-hole-doped two-dimensional Néel ordered antiferromagnet

A R Pereira[1,2], **E Ercolessi**[2,3] **and A S T Pires**[4]

[1] Departamento de Física, Universidade Federal de Viçosa, 36570-000, Viçosa, Minas Gerais, Brazil
[2] Physics Department, University of Bologna, Via Irnerio 46, I-40126, Bologna, Italy
[3] INFN, Bologna, Italy
[4] Departamento de Física, ICEX, Universidade Federal de Minas Gerais, Caixa Postal 702, 30123-970, Belo Horizonte, Minas Gerais, Brazil

E-mail: apereira@ufv.br, Elisa.Ercolessi@bo.infn.it and antpires@fisica.ufmg.br

Received 7 November 2006, in final form 22 February 2007
Published 16 March 2007
Online at stacks.iop.org/JPhysCM/19/156203

Abstract
Using the nonlinear σ model on a non-simply connected manifold, we consider the interaction effects between the elementary excitations (magnons and skyrmions) and static spin vacancy (hole) in two-dimensional quantum antiferromagnetic systems. Holes scatter magnons and trap skyrmions. The phase-shifts of the scattered magnons are obtained and used to calculate the zero point energy of spin waves measured with respect to the vacuum. It is suggested that this zero point energy lowers the energy cost of removing spins from the lattice. We also study the problems of the skyrmion–hole interactions and the skyrmion–hole (half-skyrmion–hole) bound states in the presence of magnons. We argue that two adjacent non-magnetic impurities are attracted when they are placed at the centre of half-skyrmions.

1. Introduction

The effects of impurities in quantum antiferromagnets has been an important topic in condensed matter physics since the discovery of high-temperature superconductivity. Interactions between mobile holes have attracted much interest, mainly to get some insight about the pairing mechanism in high-T_c compounds. In this respect, the static-vacancy problem is an important limiting model for understanding the interaction of mobile holes through the antiferromagnetic background. It is known that static impurities induce spin-1/2 degrees of freedom in ladders, which interact to form gapless excitations in otherwise gapped systems [1, 2]. Besides, it has been shown that static non-magnetic impurities in the magnetic background can interact via an effective potential induced by quantum fluctuations [3–5]. In this paper we would like to consider the interactions between impurities and magnons in two-dimensional (2D) Heisenberg antiferromagnets. In contrast to chains and ladders, the 2D Heisenberg antiferromagnet is not dominated by strong quantum correlations. Instead it is believed to be well described by the physics of spin waves on top of a Néel ordered state. Therefore, it would be important to study how magnons and vacancies interact in this model. Besides spin waves, nonlinear excitations may also be present in the system. Then we also consider the effects of a hole on skyrmions. Here we examine the simplest case of only one vacancy or some adjacent vacancies, i.e. the situation with a single hole with arbitrary size, which will depend on the number of neighbour impurities.

Haldane and, more properly, Chakravarty *et al* [6–8] have shown that the $d+1$-dimensional short-range isotropic Heisenberg antiferromagnetic Hamiltonian in a bipartite lattice $H = J\Sigma_{\langle ij\rangle}\vec{S}_i\cdot\vec{S}_j$ (where $J > 0$ is the exchange constant, $\vec{S}_i$ denotes the spin operator at site i, and the sum $\langle i, j\rangle$ is over nearest-neighbour pairs) is well described, at low energy and long length scales, by a quantum nonlinear σ model,

$$Z = \int D\vec{n}\delta(\vec{n}^2 - 1)\exp(\mathrm{i}2\pi S\Theta[\vec{n}])\exp[(\mathrm{i}/2ga)\int(\partial_\nu\vec{n}\partial^\nu\vec{n})\,\mathrm{d}^{d+1}x], \tag{1}$$

defined in the $d+1$-dimensional space $x^\nu \equiv (ct, x_1, \ldots, x_d)$. Here the unit vector $\vec{n} = (n_1, n_2, n_3)$ denotes the Néel sublattice magnetization, $g = 2\sqrt{d}/S$ is a dimensionless coupling constant, $\nu = 0, 1, \ldots, d$, $\partial_\nu = [\partial_0 = (1/c)\partial/\partial t, \partial/\partial x_1, \ldots, \partial/\partial x_d]$ and $c = 2\sqrt{d}JSa/\hbar$ is the velocity of the long-wavelength antiferromagnetic spin waves, with a being the lattice spacing. The exponent $\Theta[\vec{n}]$ is a topological factor associated with the Berry phase. Our interest is in $2+1$-dimensional antiferromagnets. In two spatial dimensions, the Berry phase terms vanish [8–11] if the Néel order parameter is continuous as the contributions from each sublattice cancel.

This paper is organized as follows. In section 2, the motion equations and the elementary excitations (magnons and skyrmions) are discussed in the approach of the nonlinear σ model. The impurity model (containing a single hole) is introduced. In section 3, the magnon–hole interactions are studied and the phase-shifts of the scattered magnons are obtained. In section 4 we consider the skyrmion–hole system, and in section 5 the nature of the interactions between two adjacent holes (which form a larger single hole) in the pseudo-particle's background is studied. Section 6 is dedicated to the hole–skyrmion system interacting with magnons and, finally, section 7 presents the conclusions and discussions.

2. Equations of motion and pseudoparticles

A useful way of describing the nonlinear σ model is through the stereographic projection [12] $w = (n_1 + \mathrm{i}n_2)/(1 + n_3)$. Then we can write $w = w_1 + \mathrm{i}w_2$, where w_1 and w_2 describe the complex number plane with the point at infinity added to it. In terms of these variables, the Lagrangian associated with the action in equation (1) becomes

$$L = 2\hbar\varrho_s\int\left[\frac{|\partial_0 w|^2}{(1+|w|^2)^2} - 4\frac{|\partial_{\bar{z}}w|^2}{(1+|w|^2)^2} - 2\frac{(\partial_z w)(\partial_{\bar{z}}\bar{w}) - (\partial_{\bar{z}}w)(\partial_z\bar{w})}{(1+|w|^2)^2}\right]\mathrm{d}^2x, \tag{2}$$

where $\varrho_s \equiv JS^2/\hbar$ is the spin stiffness, $\partial_z = (\partial_{x_1} - \mathrm{i}\partial_{x_2})/2$, $\partial_{\bar{z}} = (\partial_{x_1} + \mathrm{i}\partial_{x_2})/2$, $z = x_1 + \mathrm{i}x_2$ and $\bar{z} = x_1 - \mathrm{i}x_2$.

The quantum mechanics of this model can be obtained either via canonical quantization or path integrals. The former is carried out by first defining the momenta conjugate to w and $\bar{w}$, $\Pi \equiv \delta L/\delta(\partial_0\bar{w})$, $\bar{\Pi} \equiv \delta L/\delta(\partial_0 w)$ respectively, and then imposing canonical commutation relations among the momenta and coordinates. The Heisenberg equation of motion that follows from the Hamiltonian thus obtained, $H = \int[\bar{\Pi}\partial_0 w + \Pi\partial_0\bar{w} - L]\,\mathrm{d}^2x$, is identical to the classical equation (when properly ordered) and is given by

$$\partial_\mu\partial^\mu w = \frac{2\bar{w}}{1+|w|^2}\partial_\mu w\partial^\mu w \tag{3}$$

or

$$\partial_0^2 w - 4\partial_z \partial_{\bar{z}} w = \frac{2\bar{w}}{1+|w|^2}[(\partial_0 w)^2 - 4\partial_z w \partial_{\bar{z}} w]. \tag{4}$$

Linearization of this equation leads to the low-energy excitations of the nonlinear σ model, which are magnons in the Néel phase (when quantized). Therefore, we now turn our attention to the Néel ordered phase. In this case, $\vec{n}$, or equivalently w, acquires an expectation value $\langle n_3 \rangle = 1$, $\langle w \rangle = 0$, where we have chosen the order parameter pointing along the 3-direction, as it will always point in an arbitrary but fixed direction. Small oscillations about the order parameter, $w = \varepsilon$, are the Goldstone excitations (magnons) of the Néel phase, described by the linearized equation of motion,

$$\partial_\mu \partial^\mu \varepsilon = 0. \tag{5}$$

Thus there exist two pure magnon solutions to equation (5), with relativistic dispersions $\omega_q = cq$ (where q is the wavenumber) that vanish at long wavelengths, as dictated by Goldstone's theorem [13]. Magnons are, of course, spin-1 particles having only two polarizations, as they are transverse to the Néel ordered field.

Static nonlinear solutions for the complete motion equation (4) are also obtained by solving $\partial_z w = 0$ (or $\partial_{\bar{z}} w = 0$). These are the Belavin–Polyakov [12] skyrmion solutions $w = w_0 = P_0(z)/P_1(z)$ (where P_j are polynomials), which have energy $E_{\mathrm{BP}} = 4\pi\hbar\varrho_s|Q|$, where $Q = (1/\pi)\int[(\partial_z w)(\partial_{\bar{z}}\bar{w}) - (\partial_{\bar{z}} w)(\partial_z \bar{w})]/(1+|w|^2)^2\,\mathrm{d}^2x = \pm 1, \pm 2, \ldots$ is the topological charge. Topologically, the skyrmions correspond to nontrivial mappings of the spin space sphere ($\vec{n}^2 = 1$) onto the lattice plane (compactified at infinity) and $|Q|$ gives the number of times that $\vec{n}$ wraps around the plane. Here we will be interested only in the fundamental skyrmion configuration with unit topological charge $Q = 1$, given by $w_0 = \kappa/(\bar{z} - z_s)$, where κ and z_s are complex parameters associated with the skyrmion size and position, respectively. We use $|\kappa| = R$ and $|z_s| = r_s$ for its size and position in the physical space. Note that, in the pure system, the skyrmion energy does not depend on R and r_s reflecting scale and translational invariance of the model. All results obtained apply equally to anti-skyrmions $Q = -1$.

Now we would like to know how these elementary excitations (magnons and skyrmions) interact with a single hole, i.e. a vacancy obtained by removing a number of neighbouring spins. We first consider the effect of removing a single spin at the site that we label 0 (origin), which can be taken into account using the impurity potential [3] $V_1 = -J\sum_{\alpha=1}^{4} \vec{S}_\alpha^B \cdot \vec{S}_0^A$, added to the Heisenberg Hamiltonian. Here $A(down, up)$ and $B(up, down)$ refer to the sublattices and α labels to the sites neighbouring the vacancy. This can be generalized for two or more adjacent vacancies. For instance, the potential that represents two nearest-neighbour removed spins at sites 0 (origin $(0, 0)$) and 1 ($(1, 0)$) is $V_2 = -J\sum_{\alpha=1}^{4} \vec{S}_\alpha^B \cdot \vec{S}_0^A - J\sum_{\beta=5}^{7} \vec{S}_\beta^A \cdot \vec{S}_1^B$, where the sites 5, 6 and 7 are the neighbours to the second spin removed. Such impurity potentials destroy part of the Néel field. Therefore, to study the interactions between the elementary excitations and vacancies using the approach of the nonlinear σ model, we modify Lagrangian (2) by introducing an adequate impurity potential for the continuum limit. Considering the lattice defect placed at $\vec{r}_0$, the simplest picture of a vacancy is the one in which we remove a disk of radius ρ (centred at $\vec{r}_0$) from the magnetic continuous plane. The removed disk creates a circular hole in the plane [14–16], inside of which the magnetic degrees of freedom vanish (impurity potential). Then, Lagrangian (2) can be rewritten as

$$L = 2\hbar\varrho_s \int \left[\frac{|\partial_0 w|^2}{(1+|w|^2)^2} - 4\frac{|\partial_{\bar{z}} w|^2}{(1+|w|^2)^2} - 2\frac{(\partial_z w)(\partial_{\bar{z}}\bar{w}) - (\partial_{\bar{z}} w)(\partial_z \bar{w})}{(1+|w|^2)^2}\right] V_\rho(\vec{r} - \vec{r}_0)\,\mathrm{d}^2x, \tag{6}$$

where the impurity potential is essentially the step function, i.e. $V_\rho(\vec{r} - \vec{r}_0) = 0$ for $|\vec{r} - \vec{r}_0| < \rho$ and $V_\rho(\vec{r} - \vec{r}_0) = 1$ for $|\vec{r} - \vec{r}_0| \geqslant \rho$. We notice that cutting a small disk out from the plane is equivalent to substituting S by $SV_\rho(\vec{r}-\vec{r}_0)$ in equation (2), which in turn means that the field w (or $\vec{n}$) has been removed from a small region around the site $\vec{r}_0$. Such a local absence of the field degrees of freedom in the continuum system is what reproduces the vacancy of some spin degrees of freedom in the discrete lattice. Suitable boundary conditions will be discussed in the next section. Therefore, the problem of a non-simply connected magnetically coated plane is equivalent to the problem of a magnetic plane which is simply connected but contains spin vacancies (or Néel vectors vacancies) in the pure Lagrangian (2). Of course, since the response to a vacancy is local, its exact position $\vec{r}_0$ is immaterial. In addition, we can consider the size of the hole to be as small as that for a single vacancy (ρ of the order of the lattice spacing a), or any size larger than this (for the situation of two or more nearest-neighbour non-magnetic impurities). In the last case, the hole size ρ (i.e. the range of the impurity potential) would be related to the number of nearest-neighbour vacancies. For the case of only one vacancy, we will set $\rho \sim a$ for the effective hole size and $\rho \sim 2a$ for the case of two adjacent vacancies. This simple analytical model is defined on a continuum antiferromagnetic plane with a single hole, which is a non-simply connected manifold.

3. Magnon–hole interactions

The problem of magnons scattering through a single vacancy in the discrete lattice was studied and solved exactly by use of the T-matrix formalism [17, 18]. However, it is not a direct task to obtain the phase-shifts of the scattered magnons from these previous results and so, here, we study the magnon–vacancy interactions in the continuum approach. The magnetic degrees of freedom are defined only outside the hole, which can be considered to be centred at the origin, $\vec{r}_0 = (0, 0)$. Then, due to the presence of the hole (vacancy), the magnon wavefunctions need only to be defined in the outer region, $r \geqslant \rho$. Obviously, this problem is completely specified only if the boundary conditions at $r = \rho$ are given. From the physical point of view, the correct boundary condition is determined by the requirement of no net flux of spin wave energy into the hole, which is a region absent of spin degrees of freedom. Of course, the magnon flux is proportional to $\vec{F} = \varepsilon\vec{\nabla}\bar{\varepsilon}$, and then we have either $\varepsilon = 0$ or $\vec{\nabla}\varepsilon = 0$ at the hole boundary. For instance, consider the square lattice nearest-neighbour Heisenberg antiferromagnet in the homogeneous Néel state ($q = 0$) at zero temperature. If one removes a spin from the lattice, the nearest neighbours of that spin will have a coordination number of three, instead of the bulk-spin coordination number of four. Therefore, such boundary spins are free to vibrate as the rest of the neighbouring spins exert forces on them. This corresponds to free boundary conditions at $r = \rho$ applied to magnon fields. This means that these fields can be set to a non-zero constant at $r = \rho$ and then the Dirichlet boundary condition leading to $\vec{F} = 0$, i.e. $\varepsilon = 0$, is not useful. Hence we apply the Neumann boundary condition, $\vec{\nabla}\varepsilon = 0$ ($\mathrm{d}\varepsilon/\mathrm{d}r = 0$), at the hole boundary $r = \rho$.

Outside the hole, general solutions to equation (5) are given by (in polar coordinates $\vec{r} = (r, \varphi)$)

$$\varepsilon_m(r,\varphi,t) = [b_m J_{|m|}(qr) + d_m N_{|m|}(qr)]\exp(-\mathrm{i}m\varphi)\exp(-\mathrm{i}qct), \tag{7}$$

where m is the angular momentum channel and $J_m(qr)$, $N_m(qr)$ are the Bessel functions. The values of the constants b_m and d_m are determined using the Neumann boundary condition. We get

$$\varepsilon_m(r,\varphi,t) = \left[J_{|m|}(qr) - \tan(\Delta_m(q))N_{|m|}(qr)\right]\exp(-\mathrm{i}m\varphi)\exp(-\mathrm{i}qct), \tag{8}$$

with

$$\Delta_m(q,\rho) = \arctan\left[\frac{|m|J_{|m|}(q\rho) - q\rho J_{|m|+1}(q\rho)}{|m|N_{|m|}(q\rho) - q\rho N_{|m|+1}(q\rho)}\right]. \tag{9}$$

Therefore, solutions (8) are given by phase-shifted cylindrical spin waves

$$\varepsilon_m(r,\varphi,t) \propto \left[H^{(1)}_{|m|}(qr) + \exp(-2\mathrm{i}\Delta_m(q,\rho))H^{(2)}_{|m|}(qr)\right]\exp(-\mathrm{i}m\varphi)\exp(-\mathrm{i}qct), \quad (10)$$

where $\Delta_m(q,\rho) = \Delta_{-m}(q,\rho)$ are the phase-shifts. Here, the phase-shift matrix $\Delta_{mn}(q,\rho)$ is diagonal, since we have assumed a circular shape for the hole. The asymptotic phase-shifted spin waves are an indication that the system is affected by the impurity over relatively large distances. Note that the phase-shifts are extremely sensitive to the hole size ρ.

We remark here that it is not completely clear whether our simple semiclassical approach (complemented by the use of the Neumann boundary condition at the border of the hole) is equivalent to excluding spins in the original Heisenberg lattice Hamiltonian, as done, for example, in [17, 18]. Indeed, a direct comparison of our calculations with the results of the latter papers is difficult: in these references, no explicit expression for the phase-shift is given and the magnon density of states is known only as a function of the impurity concentration, which is a continuum variable. A complete comparison could be carried out only after having used our results to calculate the dynamic and thermodynamic properties (dynamical structure factor, specific heat etc) of the system at a low concentration of impurities. Although this is an interesting problem, it is out of the scope of the paper. At this stage, only some qualitative remarks can be made. In particular, we notice that equation (9) shows that the spin waves in the $m = 0, 1, 2$ angular momentum channels are the most affected by the vacancy and give the main contributions to the properties of the system, in agreement with the results of [17]. It is also worth mentioning that the method that we use here works relatively well in other realistic systems, when compared, for example, to numerical calculations, as is done in [16] for an easy-plane Heisenberg model on a discrete lattice containing a static hole (removed spin). Therefore, we believe that, in general, our results lead to good approximations for the magnon–vacancy interactions in the model considered.

As we have seen, the main effect of the lattice defect (the spin vacancy) is, in the lowest-order, to produce an elastic scattering centre for the spin waves modifying their wavefunctions. Therefore, at zero temperature there is a clear distinction in the magnon spectrum when a vacancy in the spin field is present or absent. This causes a change in the magnon density of states, which changes the magnon free energy. These results are very important for the thermodynamics of systems doped with a small concentration of non-magnetic impurities. Indeed, for a low density of vacancies, the behaviour of small oscillations in regions between the vacancies will be very similar to the behaviour of such oscillations in the pure system as a whole. Therefore one can assert that the total change in the magnon density of state is given approximately by the sum of changes caused by each hole independently. Our calculations represent a first step in this direction. In addition, these calculations are also important for other purposes. For example, in section 5 we use the above results to argue that magnon–hole interactions affect the energy cost of removing spins from the lattice, i.e. the energy cost of removing a disk from the plane. They will be also useful for studying the interactions between magnons with a pinned skyrmion (see section 6).

4. Skyrmion–hole interactions

Now we consider the skyrmion–single-hole interactions. Here, a hole placed at the origin is in the presence of a unit skyrmion of size R centred at a distance $|\vec{r}_s| = r_s$ away. It is assumed that the hole just excludes the part of the skyrmion configuration that would exist if the hole were absent, without modifying the remaining spin structure. Such an assumption is based on numerical results on the discrete lattice by Subbaraman *et al* [20]. These authors have shown that a skyrmion centralized at a vacancy has practically the same configuration

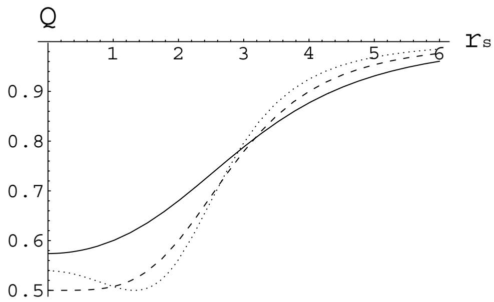

Figure 1. Fractional topological charge of skyrmions with $R < \rho$ (dotted line), $R = \rho$ (dashed line) and $R > \rho$ (solid line) as a function of the skyrmion–hole separation r_s (in units of a). The different types of half-skyrmions discussed in this paper are obtained from the excitations of lowest energy for the first two cases. Here we have used $\rho = 2a$ and $R = 1.5a$, $2a$ and $3a$, respectively.

of the Belavin–Polyakov skyrmion. There is only a small deformation in the out-of-plane structure (polar spin angles) in a small region of radius $\sim 4a$ around the hole, while beyond this distance the deformation vanishes. Other results obtained by numerical simulations on a discrete lattice for easy-plane magnets also confirm this picture. Such results have shown that the in-plane structure (azimuthal spin angles) of a vortex is practically unaffected by one or more vacancies [14, 21], even when the vortex is not centralized at the lattice defect [14]. Indeed, a hole modifies the configuration of these structures only locally, around itself. To reinforce this argument, we remember that topological excitations are objects that cannot be made to disappear by any continuous deformation of the order parameter and therefore they are said to be topologically stable. Then, it is not so easy to deform the configurations of these structures considerably without giving a large amount of energy. A large deformation is very costly energetically. Therefore, in the lowest approximation we can neglect possible small deformations and then, basically, the lowest-order effect of the hole is to decrease the topological charge (and consequently the energy) of the skyrmion in such a way that $0 < |Q| < 1$. This is a consequence of the fact that part of the spin space sphere is not included in the mapping due to the absence of spins inside the hole. The value of $|Q|$ depends on the position $|\vec{r}_s|$ and size R of the skyrmion as well as the hole radius ρ. As we have already said, the last is associated with the number of adjacent spins removed from the lattice. Removing a disk of radius ρ placed at the origin from the plane leads to the following topological charge of the skyrmion placed at $\vec{r}_s$:

$$|Q| \approx 1 - \frac{2\rho^2 R^2}{(r_s^2 + 2r_s\rho + \rho^2 + R^2)(r_s^2 - 2r_s\rho + \rho^2 + R^2)}, \tag{11}$$

and, therefore, the effective interaction potential between the hole and the skyrmion is attractive and given by

$$U_{\text{eff}}(r_s) \approx \frac{-8\pi\hbar\varrho_s\rho^2 R^2}{(r_s^2 + 2r_s\rho + \rho^2 + R^2)(r_s^2 - 2r_s\rho + \rho^2 + R^2)}. \tag{12}$$

The above results show that the charge is always $|Q| \geqslant 1/2$ (see figure 1). In fact, for large enough skyrmions ($R > \rho$), we have $|Q| > 1/2$ and the minimum energy is achieved for $r_s = 0$, i.e. when the excitation centre coincides with the hole centre. The pinned-skyrmion energy decreases as R/ρ decreases, which means that, in the continuum limit, such large skyrmions must be unstable. The question of the stability of this solution will be discussed later, after considering the other possible topological structures. On the other hand, for small

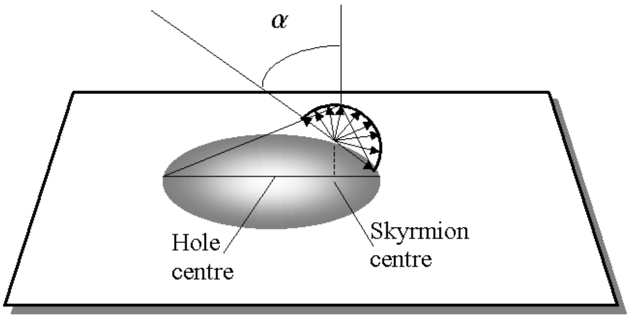

Figure 2. Magnetic plane with a hole. The base of the spin half-sphere makes an angle α with the vertical line that passes through the north pole (the eye of the stereographic projection). There are two types of half-skyrmions: when $\alpha = \pi/2$, the half-skyrmion is cylindrically symmetric and its size is equal to the hole size ρ; for $0 < \alpha < \pi/2$, the half-skyrmions are not cylindrically symmetric, their sizes are smaller than ρ, and their centres are shifted by a distance $\sqrt{\rho^2 - R^2}$ from the hole centre.

skyrmions ($R \leqslant \rho$), the minimum energy always arises for $|Q| = 1/2$, leading to two different types of half-skyrmion solutions: (1) for $R = \rho$, the stable half-skyrmion configuration is cylindrically symmetric, with the excitation centre coinciding with the hole centre ($r_s = 0$)—the binding energy of this state is $-2\pi\hbar\varrho_s$, and then for half-spin systems it is equal to -1.57 J; (2) for $R < \rho$, the equilibrium position of the excitation centre does not coincide with the hole centre, but it is given by $r_s = r_{s(\mathrm{eq})} = \sqrt{\rho^2 - R^2}$. This last small skyrmion does not have a symmetric configuration. Indeed, for R smaller than ρ, the Néel vector $\vec{n}$ has out-of-plane components pointing up along part of the boundary of the circular hole, while around the complementary part of the circumference there are out-of-plane components pointing down. It is important to remark that the relevance of these small structures with $R < \rho$ is not clear. In general, for half-skyrmions, the spin sphere mapping on the plane consists of a half-sphere, as shown in figure 2. One can see that, if the angle $\alpha = \pi/2$, then the solution is the cylindrically symmetric skyrmion with $R = \rho$. However, as α decreases from $\pi/2$, the solutions are half-skyrmions with $R < \rho$. In this case, the skyrmion centre does not coincide with the hole centre and the distance between them increases from zero (when $\alpha = \pi/2$) to ρ (when $\alpha = 0$). At the same time, the skyrmion size decreases as α decreases. For $\alpha \to 0$, the skyrmion size tends to zero. This is a limiting situation which may not be much relevant for the system. Half-skyrmion solutions must be relevant only for relatively large holes, $\rho > a$. Indeed, for $R \leqslant \rho \sim a$, the discreteness and quantum effects should be very important. For instance, the topological charge (11) has no sense for the case $R < a$, since discreteness effects break the scale and conformal invariance of the model, and quantum effects (e.g. the Casimir correction to the skyrmion energy) can cause the skyrmion to collapse. We notice also that it is expected that the centre of the structures with plausible $a < R < \rho$, or equivalently $0 < \alpha < \pi/2$, may develop an orbital circular motion with radius $\langle r_{s(\mathrm{eq})}\rangle$ around the hole centre. In conclusion, the effective potential (12) may produce two possible types of bound states between a hole and a half-skyrmion. Although the two half-skyrmions have the same energy, they have different sizes and configurations.

While small skyrmions ($|Q| = 1/2$) can be stabilized by removing a disk from an infinite plane and, in view of the fact that fractional skyrmions with topological charge varying between zero and half ($0 < |Q| < 1/2$) can also exist if the underlying manifold represents an annulus with an inner radius ρ and outer radius R [22], we have to mention something about the conditions of stability of large skyrmions ($1/2 < |Q| < 1$). As we have already seen, such excitations seem to be unstable in the continuum approach. In fact, the size of these large skyrmions pinned to a vacancy can be determined by minimizing $U_{\text{eff}}(0)$ for a given hole size ρ. This leads to a preferential size for skyrmions given by $R = \rho$, and so they should decay into cylindrically symmetric half-skyrmions (at zero temperature). However, the large skyrmions described above may appear in a discrete lattice for $T \neq 0$, being therefore relevant for the static and dynamic properties of the system. In fact, structures with $|Q| > 1/2$ (or equivalently $R > \rho$) pinned to non-magnetic impurities were studied numerically in a discrete lattice [20] and observed experimentally [20, 23] in the nearly classical layered spin-5/2 antiferromagnetic compounds $(C_3H_7NH_3)_2M_xMn_{1-x}Cl_4$ under non-magnetic doping ions (such as Mg or Cd) through electron paramagnetic resonance (EPR) measurements.

5. Interactions between adjacent holes in the pseudoparticles' background

Considering the $S = 1/2$ Heisenberg antiferromagnet and using the linear spin-wave approximation, Bulut *et al* [3] found that the energy cost of removing one spin from an infinite lattice is $E_1 = 1.1552$ J. They also found that the energy cost of two adjacent vacancies is $E_2 = 2.0436$ J, which is less than twice the cost of a single vacancy and, therefore, the binding energy is $\upsilon = E_2 - 2E_1 = -0.2666$ J. These results compare well with the recent calculations of Anfuso and Eggert [5] based on a small quantum valence bond character on top of the Néel order. However, these calculations did not take into consideration the magnon–hole interactions or the presence of topological excitations. This is the object of this section.

As we have seen in section 3, the main effect of the lattice defect (the spin vacancy) is, in the lowest order, to produce an elastic scattering centre for the spin waves, modifying their wavefunctions. Then, at zero temperature there is a clear distinction in the magnon spectrum when a vacancy in the spin field is present or absent. This distinction, which implies a difference in the magnon zero-point energy in the presence ($\frac{1}{2}\hbar\omega_q$) and absence ($\frac{1}{2}\hbar\omega_k$) of the hole can be written as $E_{\text{zp}} \sim (1/2)\hbar[\sum_q \omega_q - \sum_k \omega_k] + O(\hbar^2)$, where ω_q and ω_k are the possible frequencies (for a determined system size L) of the magnons in the presence and absence of the vacancy defect, respectively. Considering an infinite plane ($L \to \infty$), the discrete sum becomes an integral, and this zero-point energy becomes

$$E_{\text{zp}}(\rho) \approx -\frac{\hbar}{\pi} \sum_{m=-\infty}^{\infty} \int_0^{1/a} \frac{\partial \omega_q}{\partial q} \Delta_m(q, \rho)\, \mathrm{d}q, \tag{13}$$

where we have introduced a cut-off for the integration, assuming a Debye model for the spin waves. The value $1/a$ is due to the fact that solid-state systems have a natural cut-off that makes the theory finite. We suggest that this change in the zero-point energy due to the presence of the hole is associated with the hole creation energy. Therefore, due to the magnon–hole interactions, the energy cost to remove a spin from the lattice should be modified to $E_1 + E_{\text{zp}}(a)$. For removing two adjacent spins, we have $E_2 + E_{\text{zp}}(2a)$. In figure 3 we plot E_{zp} as a function of the hole size ρ for $S = 1/2$ antiferromagnets. Then, some estimates can be made. Using $\rho \approx a$ for one vacancy, we get $E_{\text{zp}}(a) \approx -0.09$ J and hence the energy cost for creating a vacancy should be lowered, being approximated by $E_{1C} \approx 1.065$ J. For two adjacent vacancies, the hole size is $\rho \approx 2a$, leading to $E_{\text{zp}}(2a) \approx -0.06$ J, and the energy cost to remove two spins from the $2D$ antiferromagnet is lowered to $E_{2\text{C}} \approx 2$ J. The bound energy is $\upsilon = E_{2\text{C}} - 2E_{1\text{C}} \approx -0.15$ J. Thus, the interaction energy of two adjacent vacancies may be substantially lower than expected due to changes in the vacuum fluctuations associated with magnon–hole interaction effects. We are aware of the fact that this approach does not necessarily give the precise results, since the strong dependence of the phase-shifts on the hole size makes our estimates not so trustworthy.

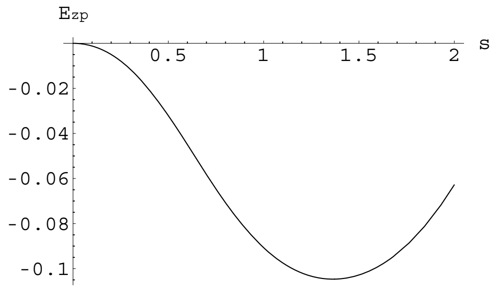

Figure 3. Zero-point energy E_{zp} (in units of J) for $S = 1/2$ as a function of the hole size $s = \rho/a$. The phase-shift sum converges rapidly. In our computation we use 61 angular momentum channels m.

In fact, we do not have the exact dimensions of a hole for one, two or more adjacent vacancies in this simple analytical model. Therefore, our semiclassical calculations of the energies is not so rigorous. Nevertheless, our discussion may give some insight about how one can include corrections due to magnon-impurity interactions (and the Casimir energy).

Now we investigate the nature of the interaction between two adjacent vacancies through the skyrmion background. The energy of an impurity-pinned skyrmion of generic size R, centralized at a hole of size ρ is given by (see expression (11))

$$E_{\mathrm{I(sk)}} \approx 4\pi\hbar\varrho_s\left[1 - \frac{2\rho^2R^2}{(\rho^2+R^2)^2}\right]. \tag{14}$$

Substituting $\rho \approx a$ in $E_{\mathrm{BP}} - E_{\mathrm{I(sk)}} = 4\pi\hbar\varrho_s[2\rho^2R^2/(\rho^2+R^2)^2]$, we get the energy cost of removing one spin located at the origin of an infinite plane containing a skyrmion (also centred at the origin): $\varepsilon_1 \approx 8\pi R^2a^2\hbar\varrho_s/(R^2+a^2)^2$. At the same time, the energy cost of removing two adjacent spins placed about the skyrmion centre from the plane is obtained by substituting $\rho \approx 2a$ in $4\pi\hbar\varrho_s[2\rho^2R^2/(\rho^2+R^2)^2]$: $\varepsilon_2 \approx 32\pi R^2a^2\hbar\varrho_s/(R^2+4a^2)^2$. Therefore, there is an effective interaction potential between two static adjacent spins through the skyrmion background, which depends on the skyrmion size, given by

$$u = \varepsilon_2 - 2\varepsilon_1 = \frac{16\pi R^2a^2(R^4 - 4R^2a^2 - 14a^4)\hbar\varrho_s}{(4a^2+R^2)^2(a^2+R^2)^2}. \tag{15}$$

In figure 4 we plot this effective potential of adjacent vacancies as a function of the skyrmion size R. For skyrmions with $R < 2.5a$, this interaction is attractive. However, for large enough skyrmions ($R > 2.5a$), it becomes repulsive. Skyrmions with size $R \approx 2.5a$ do not generate any potential for the impurities at their centres. Note that the hole size is $\rho_2 \approx 2a$ (the effective size of two adjacent vacancies) and, consequently, skyrmions with sizes equal to or smaller than this value (e.g. half-skyrmions) tend to create an attractive interaction between two adjacent impurities put at their centres. In addition, half-skyrmions with $R < \rho_2$ (not symmetric) induce a stronger effective attractive interaction between the vacancies than the symmetric ones ($R = \rho_2$). In contrast, large skyrmions give rise to a repulsive interaction. For the attractive cases, the binding energy is a minimum when $R \approx 0.83a$, which leads to a very strong potential $u \approx -9\hbar\varrho_s$ (for spin-1/2 systems, it is equal to -2.24 J). However, this is not a plausible situation, since $R < a$. For the more realistic case of a symmetric half-skyrmion with $R \sim \rho_2$, we have $u \approx -0.44$ J, which is almost twice the binding energy calculated in [3, 5] of two adjacent vacancies in the absence of topological excitations. Hence, skyrmions generate a stronger potential ($u > v$). The fact that half-skyrmions can also bind two holes, as suggested by our calculations, is of interest for superconductivity, since it may result in a Cooper pairing

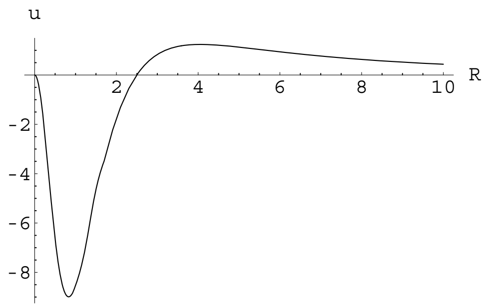

Figure 4. Effective interaction energy (in units of $\hbar\varrho_s$) of two adjacent vacancies placed at the skyrmion centre as a function of the skyrmion size R. We remark that discreteness and quantum effects should be very important for skyrmions with $R < a$ and so they may collapse. In addition, large skyrmions ($R > \rho$) are also unstable in the continuum limit and they may decay in symmetric half-skyrmions. Then, for this situation, the relevant range of sizes for skyrmions ($a < R \leqslant \rho_2$) implies in an attractive effective potential for two holes.

mechanism. We see, therefore, that half-skyrmions may be of some relevance in quantum spin systems: first, they are stabilized by the hole (even in the continuum approach); second, these are excitations which are gapped in the ordered phase, contributing to the physics of the system only at energy scales larger than their energy. For half-skyrmions, the latter is $2\pi\hbar\varrho_s$, which is much smaller than the large skyrmions' gap. Besides, small skyrmions give rise to an effective attractive potential between adjacent vacancies and, assuming that the resulting hole–skyrmion mixtures have metallic mobilities, then such interaction may have some relevance for high-temperature superconductivity in doped layered antiferromagnets [24, 25].

6. Hole–skyrmion system interacting with magnons

Until now we have considered only the interactions of an isolated hole with either magnons or skyrmions. A more realistic situation for the two elementary excitations is, however, a consideration in which they are both present simultaneously around the hole. Therefore, finally we study the effects of a hole–skyrmion system through the magnon background. As we have already seen, the skyrmion solution is given approximately by w_0 for $r > \rho$. Hence, the presence of small deviations $\xi(\vec{r}, t)$ (spin waves) modifies the skyrmion structure as $w = w_0 + \xi(\vec{r}, t)$. Considering only one scattering centre, i.e. pinned skyrmions centralized at the hole centre (which implies $R \geqslant \rho$), and substituting w into the motion equation (4), one obtains, in the linear approximation, the following Schrödinger equation $-\nabla^2\xi_0 + U\xi_0 = (\omega_q^2/c^2)\xi_0$, where the potential is given by [25] $U = 8[\partial_{\bar{z}} \ln(1+|w_0|^2)]\partial_z$ and we have used the temporal dependence $\xi(\vec{r}, t) = \xi_0(\vec{r}) \exp(-i\omega_q t)$. Then, the presence of the potential U in the region $r > \rho$ changes the solutions ε_m (see equation (7)) obtained in section 3 and also causes an elastic centre for spin waves. The phase-shifts cannot be calculated exactly for this case and hence we apply a usual method: the Born approximation. In the absence of the skyrmion, the magnon solutions are given by equation (7) and, therefore, the first-order Born term can be written as $\delta_m^{(1)} = (-\pi/2) \int_\rho^\infty r\,\mathrm{d}r < \varepsilon_m \exp(\mathrm{i}m\varphi) U \exp(-\mathrm{i}m\varphi)\varepsilon_m >_\varphi$, which leads to

$$\delta_m^{(1)} = -\frac{\pi}{2}\int_\rho^\infty r\,\mathrm{d}r[J_{|m|}(qr) - \tan\Delta_m N_{|m|}(qr)] \times \left(\frac{2r}{r^2+R^2}\frac{\mathrm{d}}{\mathrm{d}r}\right)[J_{|m|}(qr) - \tan\Delta_m N_{|m|}(qr)], \quad (16)$$

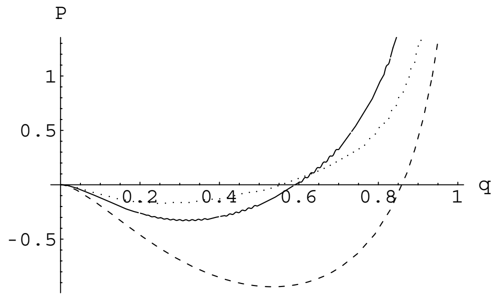

Figure 5. Magnon phase-shifts $P = \delta_0^{(1)}(q)$ due to the presence of a topological excitation centralized at the hole centre. Here we consider the hole size $\rho = 2a$ and the skyrmions sizes $R = 2a$ (solid line) and $R = 4a$ (dotted line). The dashed line is the function Λ_0. The wavevector q is in units of $1/a$.

and are dependent of the hole size ρ as well as of the skyrmion size R. For impurity systems, the new magnon wavefunction on the top of a hole–skyrmion can be approximated, in the limit $\vec{r} \to \infty$, as follows:

$$\xi_m(\vec{r} \to \infty, t) \sim \tfrac{1}{2}[H_{|m|}^{(1)}(qr) + \exp(-2\mathrm{i}\delta_m^{(1)}(q, \rho, R))H_{|m|}^{(2)}(qr)]\exp(-\mathrm{i}m\varphi)\exp(-\mathrm{i}qct). \tag{17}$$

It is important to say that the resulting phase-shifts are not a simple addition of the contributions of the hole and of the skyrmion independently. In fact, the interaction skyrmion–hole transforms the two defects (one in the lattice and the other in the spin field) in only one object coupling their individual contributions, producing a different scattering. Of course, one of the differences comes from the absence of spin degrees of freedom inside the hole, which is the region where the potential U would be stronger with more appreciable variation. Consequently, it is expected that the hole–skyrmion system produces smaller phase-shifts than an usual skyrmion. Another difference is associated with the fact that the hole naturally changes the magnon waveform, which must be taken into consideration around the skyrmion. For the effect of comparison, it should be interesting to analyse the linear combination of the individual contributions with the actual phase-shift generated by the hole–skyrmion system. The individual contribution of the skyrmion in pure systems, $\gamma_m^{(1)}(q)$, can be obtained by substituting $\rho = 0$ and $\Delta_m = 0$ in equation (16). It can easily be calculated analytically and one gets [25] $\gamma_m^{(1)}(q, R) = 2\pi RqK_{m-1}(qR)I_m(qR)$ for $m \geqslant 1$ and $\gamma_m^{(1)}(q, R) = -\gamma_{1-m}^{(1)}(q)$ for $m < 1$. On the other hand, the individual contribution of the hole is given by equation (9) and therefore we define the relation $\Lambda_m = \gamma_m^{(1)}(q, R) \pm \Delta_m(q, \rho)$, which considers both contributions (skyrmion and hole). Below, the combined individual contributions Λ_m will be compared with equation (16) for some particular cases.

We have numerically evaluated the phase-shifts using equation (16) for several finite lattices up to size $L = 200a$. Figure 5 plots $\delta_0^{(1)}(q)$ for a hole of size $\rho = 2a$ and skyrmion sizes $R = 2a, 4a$. Besides, we have also plotted the function $\Lambda_0 = \gamma_0^{(1)}(q) - \Delta_0(q, 2a)$. Note that the magnon wavefunction has a similar behaviour for different skyrmion sizes, but it is more shifted for the case $R = 2a$ (half-skyrmion). As R increases, the strength of $\delta_0^{(1)}(q)$ decreases. Note also that, in the case $m = 0$, the subtraction (and not the sum) of the individual contributions produces a function similar to $\delta_0^{(1)}(q)$. It suggests that, for s-waves, the hole and the skyrmion contribute to the scattering in an opposite way. However, it is not a definitive conclusion. For other hole sizes, the similarity between Λ_0 and $\delta_0^{(1)}(q)$ is not so evident. In general, the magnon scattering by the hole–skyrmion system, described by the phase-shifts

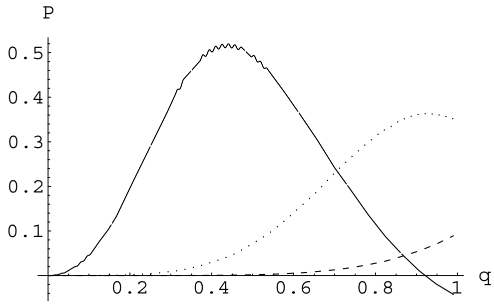

Figure 6. Magnon phase-shifts $P = \delta_1^{(1)}(q)$, $\delta_2^{(1)}(q)$ and $\delta_3^{(1)}(q)$ due to the presence of a half-skyrmion centralized at the hole with size $\rho = 2a$. The angular momentum channels are $m = 1$ (solid line), $m = 2$ (dotted line) and $m = 3$ (dashed line).

$\delta_0^{(1)}(q)$, have a characteristic that is independent of the individual contributions, at least in part of the range of q. The main differences arise for large wavevectors. The behaviour of the phase-shifts for different angular momentum channels m is plotted in figure 6 (also for $\rho = 2a$). As expected, $\delta_m^{(1)}$ decreases considerably as m increases due to the fact that, for large enough m, the centrifugal barrier m^2/r^2 expels the magnons from the central region of scattering where U is more appreciable. Here, for the function Λ_m (not shown), it is the sum of the individual contributions (not the subtraction) that has some similarity with $\delta_m^{(1)}(q)$, in contrast to the case $m = 0$. Again, Λ_m is much larger than $\delta_m^{(1)}(q)$. An interesting fact to be observed (for q not large enough) is that the intensity of the phase-shifts are larger for $m = 1$ and even $m = 2$ than for the case $m = 0$ which, in principle, should generate larger scattering, since the centrifugal barrier is zero. A possible justificative is that the hole and the skyrmion contribute to the scattering in opposite ways for $m = 0$, while they are inverse for $m \neq 0$.

The above calculations are useful for perturbation theories involving a skyrmion (half-skyrmion) response to external perturbations or forces, statistical mechanics and quantization procedures for skyrmion states. In particular here, unfortunately the trace of equation (16) vanishes ($\sum_{m=-\infty}^{\infty} \delta_m^{(1)}(q) = 0$) and therefore, using only the first-order Born terms, we cannot calculate the quantum corrections E_{zp} to the classical energy of a pinned skyrmion (or half-skyrmion) as given by equation (13). One may try to calculate the second-order Born terms [25] but, nevertheless, such calculations are not so trustworthy, as suggested in [29]. In addition, for a given skyrmion of size R centralized at the hole, the range of the potential U is of the order of $R-\rho$ and, in particular, for half-skyrmions, the potential has a very small range, restricted to the region in which its strength is less efficient and, therefore, the second-order Born terms (which involve an expression proportional to U^2) may be neglected, not contributing substantially to the quantum corrections. Then, the Born approximation suggests that quantum fluctuations of half-skyrmions may change their energy only for a very small quantity and may produce only a small influence on the value of u, i.e. on the attraction between two vacancies put at the excitation centre.

7. Conclusions and discussions

In conclusion, in this paper we have used a simple analytical model for static holes in 2D quantum antiferromagnets to study the interactions between elementary excitations and impurities. To the authors' knowledge, this approach was used for the first time in [26] to study the vortex behaviour near a non-magnetic impurity in classical easy-plane magnets, and later [14] improved and extended to the case of many adjacent impurities. For easy-plane magnets, comparison of the results of this simple model with simulations and numerical calculations on a discrete lattice has shown good agreement [14–16, 19]. A similar model was also examined by Saxena and Dandoloff [22] in the context of quantum Hall systems and also by Morinari [27, 28] in the context of quantum magnetism. Here, the hole breaks the conformal and translational symmetries of the system, so that there is a preferred size and position for the nonlinear excitations. Also, for a bound state half-skyrmion–hole, oscillatory motion about the impurities may be possible. This conclusion is based on the vortex oscillatory motion around either only one non-magnetic impurity or many neighbouring non-magnetic impurities [14]. Differences from the vortex case may appear for half-skyrmions with $R < \rho$ (not centred at the hole centre). In this case, the half-skyrmion centre may develop an orbital circular motion around the hole centre, causing interesting spin correlations at the hole boundary. However, the study of these possibilities is outside the scope of this paper.

In summary, we have obtained the phase-shifts of linearized spin-wave fluctuations around a static single-hole of the 2D Néel state. Such phase-shifts are relevant for the study of the statistical mechanics of 2D antiferromagnets containing a small amount of non-magnetic impurities in the magnetic sites. In addition, the change in the magnon density of states due to the presence of the hole suggests that the energies for removing spins from the lattice [3, 5] may undergo small modifications. We have also considered the interactions between skyrmions and vacancies and found generic skyrmion solutions, which are dependent on the ratio R/ρ. Two bound state hole–skyrmions in the limit of small half-skyrmions were found. The nature of the interaction between two adjacent vacancies placed at the skyrmion centre was studied: it is attractive for half-skyrmions and repulsive for large skyrmions. Nevertheless, in the relevant range of skyrmion sizes, $a < R \leqslant \rho_2$ (associated with their stability in the continuum approach and zero temperature) the interaction is always attractive. As suggested by Voruganti and Doniach [24], if a skyrmion can bind two holes and no more, then the other half of the picture, namely Cooper pairs, provides an explanation for the superconductivity. Our main assumption for the calculations is that the hole size is related to the number of adjacent non-magnetic impurities.

Acknowledgments

The authors thank CAPES (the Brazilian agency) for financial support. This work was partially supported by the TMR network EUCLID and the Italian MIUR through COFIN projects.

References

[1] Mikeska H J and Neugebauer U 1997 *Phys. Rev.* B **55** 2955
[2] Sigrist M and Furusaki A 1996 *J. Phys. Soc. Japan* **65** 2385
[3] Bulut N, Hone D, Scalapino D J and Loh E Y 1989 *Phys. Rev. Lett.* **62** 2193
[4] Silva R L, Guimarães P R C and Pereira A R 2005 *Solid State Commun.* **134** 313
[5] Anfuso F and Eggert S 2006 *Europhys. Lett.* **73** 271
[6] Chakravarty S, Halperin B I and Nelson D R 1989 *Phys. Rev.* B **39** 2344
[7] Haldane F D M 1983 *Phys. Rev. Lett.* **50** 1153
[8] Haldane F D M 1988 *Phys. Rev. Lett.* **61** 1029
[9] Dombre T and Read N 1988 *Phys. Rev.* B **38** 7181
[10] Fradkin E and Stone M 1988 *Phys. Rev.* B **38** 7215
[11] Ercolessi E, Morandi G and Pietri P 1997 An introduction to the Hubbard model *Strongly Correlated Magnetic and Superconducting Systems* ed G Sierra and M A Martin-Delgado (Berlin: Springer)
[12] Belavin A A and Polyakov A M 1975 *JETP Lett.* **22** 245
Gross D J 1978 *Nucl. Phys.* B **132** 439

[13] Goldstone J 1961 *Nuovo Cimento* **19** 154
[14] Pereira A R, Leonel S A, Coura P Z and Costa B V 2005 *Phys. Rev.* B **71** 014403
[15] Paula F M, Pereira A R and Mól L A S 2004 *Phys. Lett.* A **329** 155
[16] Pereira A R and Wysin G M 2006 *Phys. Rev.* B **73** 214402
[17] Chernyshev A L, Chen Y C and Castro Neto A H 2002 *Phys. Rev.* B **65** 104477
[18] Harris A B and Kirkpatrick S 1977 *Phys. Rev.* B **16** 542
[19] Paula F M, Pereira A R and Wysin G M 2005 *Phys. Rev.* B **72** 094425
[20] Subbaraman K, Zaspel C E and Drumheller J E 1998 *Phys. Rev. Lett.* **80** 2201
[21] Wysin G M 2003 *Phys. Rev.* B **68** 184411
[22] Saxena A and Dandoloff R 2002 *Phys. Rev.* B **66** 104414
[23] Zaspel C E, Drumheller J E and Subbaraman K 2002 *Phys. Status Solidi* a **189** 1029
[24] Voruganti P and Doniach S 1990 *Phys. Rev.* B **41** 9358
[25] Rodriguez J P 1989 *Phys. Rev.* B **39** 2906
[26] Mól L A S, Pereira A R and Pires A S T 2002 *Phys. Rev.* B **66** 052415
[27] Morinari T 2006 *J. Magn. Magn. Mater.* **302** 382
[28] Morinari T 2005 *Phys. Rev.* B **72** 104502
[29] Walliser H and Holzwarth G 2000 *Phys. Rev.* B **61** 2819