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LETTER TO THE EDITOR

Long-range distortions induced by a hole in an antiferromagnet

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Abstract. We examine the long-range distortion induced by a hole in an antiferromagnet, first found by Shraiman and Siggia. We introduce a novel set of variables to treat the long-wavelength properties of an antiferromagnet. It is shown that if a static hole causes a short range ferromagnetic distortion, then the dynamical distortion follows immediately from the equations of motion of the spin system. Moreover we show explicitly that a weakly coupled particle induces such an effect perturbatively.

Interest in the motion of holes in antiferromagnets, inspired by the discovery of high-T_c cuprate superconductors, has focused on two aspects of the effect on the spin arrangement due to a single hole. First there is the effect of a hole on a set of *uncoupled* spins, considered by Nagaoka (1966). The result of such a calculation is believed to depend on the type of lattice involved: for the square lattice one finds ferromagnetism; but for a frustrated (e.g., triangular) lattice the answer is not clear. Secondly, there is the effect of the (super-) exchange coupling of the spins. The addition of the exchange coupling makes the problem intractable, so that one is forced to approximate.

As soon as the exchange coupling is added, the hole cannot determine the entire spin arrangement, but merely determines it in some more or less localised region. Physically this results in the formation of some kind of 'polaron', with the interior of the polaron being the region of disruption of the Néel state. This area has been discussed before in the context of ordinary Mott insulators and rare earth materials (for a review see Nagaev 1974). A new feature that has emerged in recent work by Shraiman and Siggia (1988) is the existence of a long-range *dynamically*-induced distortion. Thus the polaron develops two types of distortion: a short-range part which is determined by a local coupling of the hole to the spin system, perhaps of a Nagaoka form, and which remains in the stationary limit; and secondly the dynamical long-range part.

In this Letter we show, without recourse to explicit discussion of the hole motion, that if the hole develops a ferromagnetically magnetised (not necessarily saturated) region statically, then an immediate consequence of the hole's motion is the long range distortion found by Shraiman and Siggia (1988). All that is needed are the classical equations of motion of the spin system. Moreover we show that the same phenomenon occurs in a model with a weak local coupling of the hole to the spins (the Hubbard model implicit in the work of Shraiman and Siggia is strong coupling). We also introduce some novel variables to facilitate the 'long-wavelength' discussion of an antiferromagnet which have some advantages over previous methods.

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There is no exact treatment of the form of the spin distortion around a stationary ferromagnetic spin polaron (for a review see Nagaev 1974). Here we will make some qualitative comments on the orientation of the magnetisation associated with the short range part of the distortion and the absence of a long range part for the *stationary* case.

Initially, let us assume that the hole causes a net magnetisation in a finite region of the lattice. The orientation of this magnetisation, if it is not saturated, may be deduced from the susceptibility of an antiferromagnet in the limit of zero temperature. Classically, in that limit, the longitudinal susceptibility (i.e. in the direction of the sublattice magnetisation) is zero while the transverse susceptibility is non-zero. Thus regarding the effect of the hole as resembling an external field (which induces the magnetisation), we deduce that the induced magnetisation will be perpendicular to the sublattice magnetisation. If the magnetisation *is* saturated then the issue is more subtle and will involve the effects of the boundaries of the region; henceforth we shall assume that we are dealing with the former case.

To deduce the form of any static long range distortion induced outside the magnetised region, we regard the magnetisation as a weak transverse field applied to the rest of the antiferromagnet. Consider first the effect of a small transverse field applied to only one site. It is easy to see that the Euler–Lagrange equation for the large distance part of the distortion is Poisson's equation, with the transverse field acting as a source, the sign of which depends on which sublattice the field is applied to. The azimuthally symmetric solutions in two dimensions are proportional to $\ln r$ or a constant. Happily, these radial dependencies are not present in the case of interest, since the transverse field is applied to a finite region. The effect of the transverse field on the two sublattices is opposite in sign, so we may guess that one sees a multipolar superposition of many of the above solutions. This is consistent with the solution of a problem in which a transverse field is applied to the spins at the edge of a semi-infinite plane of antiferromagnetically-coupled Heisenberg spins: apart from the single Fourier component of the field that causes rotation of the spins across the entire plane, one finds that the induced distortion dies away exponentially with distance from the surface. Hence we expect the distortion around a region of radius ρ (in units of the lattice parameter) to decay as $r^{-\rho}$, if we can regard the surface of the region as a multipole of order ρ. We will assume that we are dealing with spin polarons with an extent much larger than the lattice parameter so that we may discard the above distortion.

Finally we come to the possibility of a *dynamic* distortion, in particular its long range part. (One expects any dynamical modification of the short range part to be model-dependent.) Since we are interested in long wavelength effects it is more convenient to use a continuum approximation for the antiferromagnet. The natural variable to focus upon is the direction of the local sublattice magnetisation as it is that which varies slowly, rather than the spin directions themselves. Moreover, if a formulation is desired which is well-defined even for disordered ground states, then one cannot define the sublattice magnetisation in a way that distinguishes between the 'A' and 'B' sublattices.

One definition which *does* make such a distinction is the 'brick' definition used by Affleck (1985) for the one-dimensional spin chain. Here the sublattice magnetisation, $\Omega^{\mathrm{br}}_{n+1/2}$, is defined on alternate links as the difference of the spin vectors on the neighbouring sites n and $n+1$:

$$\boldsymbol{\Omega}^{\mathrm{br}}_{n+1/2} = (\boldsymbol{S}_{n+1} - \boldsymbol{S}_n)/2 \tag{1}$$

The difficulty with such a definition is that it requires an arbitrary choice of magnetic unit cell. In one dimension this amounts to a decision to pair a given site with the neighbour on its left rather than than on its right. In higher dimensions it leads to less palatable choices that break rotational symmetries.

We would like to deal in a fully symmetrical way with quantum mechanical analogues of staggered magnetisation $\boldsymbol{\Omega}^{\mathrm{br}}$ and net magnetisation, $\boldsymbol{M}^{\mathrm{br}}$, defined by changing the sign in (1). The difficulties arise from combining dynamical varibles from different sites, and can be circumvented by introducing *two* vectors, $\boldsymbol{\omega}$ and $\boldsymbol{\mu}$, on each site. We will later interpret the redundant variables of this description in terms of the sublattice magnetisation, $\boldsymbol{\Omega}^{\mathrm{br}}$, and the net magnetisation, $\boldsymbol{M}^{\mathrm{br}}$. The redundancy of having an extra vector on each site allows us considerable freedom in determining the commutation relations and equations of motion of $\boldsymbol{\omega}$ and $\boldsymbol{\mu}$. In making our choices of these quantities we will be guided by the bricking procedure and simplicity.

We make the initial stipulation that the physical spins, $\boldsymbol{S}$, are related to $\boldsymbol{\omega}$ and $\boldsymbol{\mu}$ by

$$\boldsymbol{S} = \boldsymbol{\mu} \pm \boldsymbol{\omega} \tag{2}$$

where the upper (lower) sign refers, arbitrarily, to the A (B) sublattice. This is the same as the relation between $\boldsymbol{S}_n$ and $\boldsymbol{\Omega}^{\mathrm{br}}$ and $\boldsymbol{M}^{\mathrm{br}}$. To aid the interpretation of $\boldsymbol{\mu}$ and $\boldsymbol{\omega}$ as the magnetisation and sublattice magnetisation, we further require them to satisfy the same relation $\boldsymbol{\mu} \cdot \boldsymbol{\omega} = 0$ as the brick variables, and to have also the same commutation relations

$$[\mu_i, \mu_j] = \tfrac{1}{2}\mathrm{i}\varepsilon_{ijk}\mu_k \qquad [\omega_i, \omega_j] = \tfrac{1}{2}\mathrm{i}\varepsilon_{ijk}\mu_k \qquad [\mu_i, \omega_j] = \tfrac{1}{2}\mathrm{i}\varepsilon_{ijk}\omega_k. \tag{3}$$

To within factors of 2, these are the commutation relations of the generators of the rotation group in four dimensions, which are met also in Pauli's treatment of the hydrogen atom (Landau and Lifshitz 1977) where $\boldsymbol{l}$, the orbital angular momentum, and $\boldsymbol{u}$, related to the Runge–Lenz vector, correspond respectively to our $\boldsymbol{\mu}$ and $\boldsymbol{\omega}$.

We have given $\boldsymbol{\omega}$ and $\boldsymbol{\mu}$ the commutation relations of a sum and difference of angular momenta, and only the combination $\boldsymbol{\mu} + \boldsymbol{\omega}$ has so far been accounted for. It follows that the other combination

$$\boldsymbol{L} = \boldsymbol{\mu} \mp \boldsymbol{\omega} \tag{4}$$

corresponds to a 'phantom' spin, $\boldsymbol{L}$, obeying standard angular momentum commutation relations. This is the redundancy introduced when the spin system is described by the variables $\boldsymbol{\mu}$ and $\boldsymbol{\omega}$.

To see the relation of $\boldsymbol{\mu}$ and $\boldsymbol{\omega}$ to the variables $\boldsymbol{M}^{\mathrm{br}}$ and $\boldsymbol{\Omega}^{\mathrm{br}}$, choose $\boldsymbol{S}_1$ and $\boldsymbol{S}_0$ to be neighbours on the A and B sublattice, respectively. Since the brick variables are defined on links, we make the comparison at the midpoint of the link, imagining for this purpose that $\boldsymbol{\mu}$ and $\boldsymbol{\omega}$ are smooth, classical functions of position. Then we have

$$\boldsymbol{\Omega}^{\mathrm{br}}_{\frac{1}{2}} = \tfrac{1}{2}(\boldsymbol{S}_1 - \boldsymbol{S}_0) \simeq \boldsymbol{\omega}_{\frac{1}{2}}; \boldsymbol{M}^{\mathrm{br}}_{\frac{1}{2}} = \tfrac{1}{2}(\boldsymbol{S}_1 + \boldsymbol{S}_0) \simeq \boldsymbol{\mu}_{\frac{1}{2}} \pm \tfrac{1}{2}a\, \partial\boldsymbol{\omega}/\partial x. \tag{5}$$

The upper and lower signs refer here to the two possible choices of brick in one dimension: the correspondence between $\boldsymbol{M}^{\mathrm{br}}$ and $\boldsymbol{\mu}$ is therefore defined only to within the lattice derivative of $\boldsymbol{\omega}$. In (5) we have neglected $\partial\boldsymbol{\mu}/\partial x$ and $\partial^2\boldsymbol{\omega}/\partial x^2$ compared with $\boldsymbol{\mu}$ and $\partial\boldsymbol{\omega}/\partial x$, This can be shown explicitly to be valid for a long-wavelength spin wave, or for a superposition of spin waves, and this will be sufficiently general for our purposes.

So we see that our new variables may be chosen to correspond to the sublattice magnetisation and the slowly varying net magnetisation for a state which deviates only slightly from the classical Néel state. Unlike these latter quantities, however, $\boldsymbol{\omega}$ and $\boldsymbol{\mu}$ are defined even in a disordered spin state, so that there is no artificial discontinuity in the description in passing from an ordered to a disordered state.

To determine the Hamiltonian, we note that the phantom spins cannot be coupled to the real spins, as the dynamics of the latter must not be altered. Thus we may only couple the phantom spins among themselves. The choice that yields the simplest Hamiltonian (in terms of $\boldsymbol{\omega}$ and $\boldsymbol{\mu}$) is that the coupling of the $\boldsymbol{L}_n$ parallels that of $\boldsymbol{S}_n$

$$H = J \sum_{\langle n,n' \rangle} (\boldsymbol{S}_n \cdot \boldsymbol{S}_{n'} + \boldsymbol{L}_n \cdot \boldsymbol{L}_{n'}) = 2J \sum_{\langle n,n' \rangle} (\boldsymbol{\mu}_n \cdot \boldsymbol{\mu}_{n'} - \boldsymbol{\omega}_n \cdot \boldsymbol{\omega}_{n'}) \tag{6}$$

If, for instance, we had not coupled the $\boldsymbol{L}$s at all (an apparently simpler choice), then we would have obtained terms in $\boldsymbol{\omega} \cdot \boldsymbol{\mu}$.

The commutation relations (3) and the Hamiltonian (6) expresed in terms of $\boldsymbol{\mu}$ and $\boldsymbol{\omega}$ give the following equations of motion

$$\begin{aligned} \dot{\boldsymbol{\omega}}_n &= J \sum_{n'} (\boldsymbol{\mu}_n \times \boldsymbol{\omega}_{n'} - \boldsymbol{\omega}_n \times \boldsymbol{\mu}_{n'}) \\ \dot{\boldsymbol{\mu}}_n &= J \sum_{n'} (\boldsymbol{\omega}_n \times \boldsymbol{\omega}_{n'} - \boldsymbol{\mu}_n \times \boldsymbol{\mu}_{n'}) \end{aligned} \tag{7}$$

and these equations of motion, being respectively odd and even in $\boldsymbol{\omega}_n$, take the same form on the two different sublattices, a virtue of this formulation.

Equations (6) and (7) facilitate the derivation of the non-linear sigma Lagrangian for the long-wavelength properties of the Heisenberg antiferromagnet. The fields $\boldsymbol{\omega}$ and $\boldsymbol{\mu}$ are written in a gradient expansion and inserted into expression (6) for the Hamiltonian. We have

$$\sum_{\langle n,n' \rangle} (\boldsymbol{\mu}_n \cdot \boldsymbol{\mu}_{n'} - \boldsymbol{\omega}_n \cdot \boldsymbol{\omega}_{n'}) = \text{const.} + \int \frac{\mathrm{d}^2 x}{2a^2} [8\mu^2 + a^2 (\nabla \boldsymbol{\omega})^2] \tag{8}$$

From the equation for $\dot{\boldsymbol{\omega}}$ and the condition $\boldsymbol{\mu} \cdot \boldsymbol{\omega} = 0$ we find

$$\boldsymbol{\mu} \simeq \boldsymbol{\omega} \times \dot{\boldsymbol{\omega}} / 8JS^2 \tag{9}$$

so that the μ^2 term in the long-wavelength expansion of the Hamiltonian is a kinetic energy. In that limit the equations of motion are obtainable from a Lagrangian

$$\mathscr{L} = \tfrac{1}{2} \int \mathrm{d}^2 x \, (\dot{\boldsymbol{\omega}}^2 - (\nabla \boldsymbol{\omega})^2) \tag{10}$$

together with a constraint $\boldsymbol{\omega}^2 = 1$. (This constraint is conserved only in the continuum limit of the equations of motion.) To simplify (10) and the subsequent formulae we have set $2\sqrt{2}JS = a = 1$ and redefined our variables by $\boldsymbol{\mu} \to 2\sqrt{2}\boldsymbol{\mu}/S$ and $\boldsymbol{\omega} \to \boldsymbol{\omega}/S$, making $\boldsymbol{\omega}$ a unit vector.

A form for the coupling between the polaron and the spin system can be deduced from our earlier, qualitative considerations in which we argued that the spins near the hole show a tendency toward ferromagnetic alignment. We do not enquire closely into the internal structure of this region, but note simply that the canted spins at its boundary are coupled directly to the remainder of the antiferromagnet. The spins of the 'external' region therefore move in response to a certain distribution of magnetic moment, $\boldsymbol{\mu}^{\text{srce}}$, which will appear as a source on the right-hand side of (7) for $\dot{\boldsymbol{\omega}}$. Therefore we write the long-wavelength expansions of (7) in the form

$$\dot{\boldsymbol{\mu}} = \boldsymbol{\omega} \times \nabla^2 \boldsymbol{\omega} \qquad \dot{\boldsymbol{\omega}} = (\boldsymbol{\mu} + \boldsymbol{\mu}^{\text{srce}}) \times \boldsymbol{\omega}. \tag{11}$$

We have observed already that, because of the vanishing of the parallel component of the magnetic susceptibility of the antiferromagnet, a distribution of magnetisation,

$\boldsymbol{\mu}$, will lie perpendicular to the sublattice magnetisation $\boldsymbol{\omega}$. We therefore seek solutions of (11) in which $\boldsymbol{\mu}$ lies in some fixed direction and $\boldsymbol{\omega}$ lies in the plane perpendicular to it. With the substitutions $\boldsymbol{\mu} = m\hat{z}$ and $\omega_z + \mathrm{i}\omega_y = \exp(\mathrm{i}\varphi)$ we obtain, after eliminating m, an equation of motion for φ

$$\ddot{\varphi} - \nabla^2\varphi = \dot{m}^{\mathrm{srce}}. \tag{12}$$

For the calculation of the spin distortion at large distances from the spin polaron we may replace m^{srce} by a delta function $\lambda\delta^2(\boldsymbol{x} - \boldsymbol{v}t)$ where the strength λ may be expected in general to depend on the velocity, $\boldsymbol{v}$. The appearance of the d'Alembertian operator on the left-hand side of (12) allows us to pass to the frame of rest of the spin pattern by means of a Lorentz transformation in which the spin-wave speed (here equal to unity) plays the part of the speed of light

$$x' = \gamma(x - vt) \qquad y' = y \qquad \gamma = (1 - v^2)^{-1/2} \tag{13}$$

so that the shape of the spin distortion is given by

$$-(\nabla')^2\varphi = -\lambda\gamma v\, \partial[\delta(x'/\gamma)\delta(y')]/\partial x' \tag{14}$$

(Note that for $v > 1$ the equation we obtain in place of (14) is hyperbolic (the γ-factors become imaginary) and there is no solution tending smoothly to zero at infinity. This corresponds to the emission of spin waves by the moving polaron.) For $v < 1$ we have (noting the dipolar form of the right hand side of (14)), in the stationary frame, the following solution

$$\varphi(\boldsymbol{x}, t) = (\lambda/2\pi)\, v\gamma^3(x - vt)/[\gamma^2(x - vt)^2 + y^2]. \tag{15}$$

The last result (15) shows that the moving polaron carries with it a long-range dipolar distortion of the sublattice magnetisation. Despite the Lorentz invariance of the equations of motion of the free spin system, the form of the coupling to the hole is not Lorentz-invariant, so that the spin pattern does not simply Lorentz contract with increasing speed. In particular, the distortion vanishes with v, in keeping with its dynamical origin.

The result for the angular deviation φ has a parallel in the result of a simpler, perturbative, calculation in which the approximations made are more easily understood. We consider an $S \rightarrow \infty$ Heisenberg antiferromagnet with weak exchange coupling to an electron near the bottom of a band. The interaction Hamiltonian is

$$H^{(1)} = j\sum_n \boldsymbol{S}_n \cdot (c_n^\dagger \boldsymbol{\sigma} c_n). \tag{16}$$

The unperturbed spin state is the spin-wave ground state corresponding to Néel alignment along the z axis. The effect of the $S^z\sigma^z$ coupling is to open up a small gap for the electron states at the boundary of the magnetic Brillouin zone, and is of little interest here. On the other hand, the perpendicular coupling mixes the state $|k_1;\rangle$ with $|\boldsymbol{k} - \boldsymbol{q}\downarrow; \boldsymbol{q}\rangle$ and $|\boldsymbol{k} - \boldsymbol{q}\downarrow; \boldsymbol{q} + \pi(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}})\rangle$, which are degenerate spin-flipped states with one antiferromagnon of wavevector $\boldsymbol{q}$ or $\boldsymbol{q} + \pi(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}})$. In the perturbed state, the spin motion is correlated with that of the electron, and the expectation value $\langle\sigma_0^+ S_r^-\rangle$ measures the correlation between the azimuthal angle of the electron spin on site $\mathbf{0}$ and that of the spin on site $\boldsymbol{r}$.

To understand more fully the nature of this correlation function we write (for any spin) $S^+ = \sqrt{(2S - n)(n + 1)}\exp(\mathrm{i}\varphi_S)$ where n is the operator $(S - S^z)$ and $\exp(\mathrm{i}\varphi_S)$ is an (almost) unitary operator specified by its commutation relation with n: $[\exp(\mathrm{i}\varphi_S), n] = \exp(\mathrm{i}\varphi_S)$. The physical interpretation of φ is that it is the azimuthal angle of the spin. (This is a variation on Villain's representation of spin operators (Villain 1974).) For the states of interest, which are superpositions of 0- and 1-magnon states, the expectation value $\langle \sigma_0^+ S_r^- \rangle$ reduces to $2\sqrt{2S}\,\langle \exp \mathrm{i}(\varphi_\sigma - \varphi_S)\rangle$, which we take to define the average azimuthal angle between the spins. For the correlation function we find

$$\langle \sigma_0^+ S_r^- \rangle = 2\frac{jS}{N^2}\sum_q \frac{\mathrm{e}^{\mathrm{i}q\cdot r}(\mathrm{e}^{2u_q} \pm 1)}{\varepsilon(k) - \varepsilon(k-q) - \omega_q} = 2\frac{jSa^2}{N}\int \frac{\mathrm{d}^2 q}{(2\pi)^2}\frac{\mathrm{e}^{\mathrm{i}q\cdot r}(\mathrm{e}^{2u_q} \pm 1)}{v\cdot q - qc + \mathrm{O}(q^2)} \tag{17}$$

where the upper (lower) signs refer to the $\downarrow$ ($\uparrow$) sublattices of the classical Néel state. The overall factor of two arises from the two species of AF magnons, and the term $\exp(2u_q)$ comes from a Bogoliubov factor, and vanishes as q for small q. In the energy denominator $\partial\varepsilon(k)/\partial k$ has been replaced by v, the electron velocity, and the remaining recoil terms, of order q^2, may be neglected in the limit $r \to \infty$. The integral can now be completed analytically, giving

$$\varphi \simeq \sin\varphi = \mathrm{Im}[\langle \sigma_0^+ S_r^- \rangle / 2\sqrt{2S}\langle c_0^\dagger c_0\rangle] \propto (j/J\sqrt{S})(v/c)[\gamma^3 ax/(\gamma^2 x^2 + y^2)] + \mathrm{O}(1/r^2) \tag{18}$$

where x, y are the relative coordinates of electron and spin and γ is the factor defined in (13). In its velocity- and space-dependence this expression is identical to the one found for the spin distortion far from a spin polaron. We should bear in mind, however, that there is a limit to the comparability, since the axis of quantisation of the electron spin does not correspond to the direction of the magnetic moment in the spin polaron problem, which was fixed perpendicular to the unperturbed direction of the sublattice magnetisation.

To conclude, we have introduced a new mode of description of an antiferromagnet at long wavelengths which allows a simple derivation of the non-linear sigma model. We have applied such a formulation to show, using only the classical equations of motion, that a dynamical long-range distortion can be expected if the coupling between a hole and the antiferromagnet yields a tendency toward spin polarisation. We have shown explicitly how this occurs in a weak coupling, quantum-mechanical model.

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