Nematic state in an exchange Heisenberg Hamiltonian

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A qualitative case is made for the possibility of a spin-nematic state in a system of quantum-mechanical spins with a binary exchange interaction causing a frustration. The arguments are based on a possible instability of the spin-wave spectrum in the Néel state with respect to the formation of pairs of quasiparticles.

An antiferromagnetic state has been observed experimentally in high-T_c superconductors such as $La_2CuO_{4+\delta}$ and $YBa_2Cu_3O_{6+\delta}$. This state is usually attributed to a Cu^{2+} (d^9) configuration. Although the copper d shell does undoubtedly hybridize with oxygen p orbitals in the sublattice of CuO_2 planes, the existence of a localized moment is an experimental fact. One is naturally led to ask whether doping would suppress the localized moments. We have repeatedly stressed (Ref. 1, for example) that the antiferromagnetic phase should be separated from a metallic state on the side of a low dopant density by a first-order phase transition. A question which remains is just what happens to the localized magnetic moment in the metallic region. One might of course suggest that a first-order insulator-to-metal Mott transition occurs, and that in the course of this transition all the highly correlated electrons would become delocalized. In this case there would be no problem of magnetic moments. However, the entire body of experimental evidence shows convincingly that this is not the case: The first-order transition is apparently weak, and the presence of local moments is demonstrated in spin fluctuations.

We would accordingly like to discuss the possible existence of—in addition to antiferromagnetic and paramagnetic states—other order parameters, e.g., a nematic (quadrople) state. The possibility of a quadrople ordering has been discussed in several places.[2-4] It has been assumed, however, that a quadrople ordering is promoted by an exchange of high order (fourth or higher). Our purpose in the present letter is to show that frustration in an exchange Heisenberg Hamiltonian (for example) is a possible source of a nematic state.[5] The problem obviously has no small parameters and cannot be solved exactly, so we will content ourselves with some simple qualitative arguments.

We consider a Heisenberg model with the Hamiltonian

$$\hat{H} = \frac{1}{2} \sum_{nm} I(\vec{R}_n - \vec{R}_m)\, \hat{\vec{\sigma}}_n \hat{\vec{\sigma}}_m \tag{1}$$

($\vec{\sigma}$ are the Pauli matrices). We assume $T=0$, so that there are no thermodynamic fluctuations. The results will thus be valid in both two and three dimensions. Our qualitative arguments in favor of the existence of a nematic ground state can be summarized as follows: In a certain interval of values of the parameters of the problem, the spin-wave spectrum in the Néel state may become unstable with respect to the formation of pairs of quasiparticles.

Let us assume for definiteness that we are dealing with a two-dimensional square lattice and that there is no exchange except for nearest neighbors ($I_1>0$) and for nearest neighbors along a diagonal ($I_2>0$). The quantity I_2 thus plays a frustrating role. At parameter values corresponding to $I_2<I_1/2$, the Fourier transform of the exchange,

$$I_q = \sum_R I(\vec{R}) \exp[i\vec{q}\vec{R}] \ , \tag{2}$$

has a minimum at a vertex of the Brillouin zone, $\vec{Q}=(\pi/a,\ \pi/a)$ (a is the lattice constant). In this case the classical Néel state contains two collinear sublattices, so the projection of $\hat{\sigma}_n^z$ onto its wave function $|\Phi_0\rangle$ gives us $\sigma^z = \pm 1$:

$$\hat{\sigma}_n^z|\Phi_0\rangle = \exp(i\vec{Q}\vec{R}_n)|\Phi_0\rangle. \tag{3}$$

Against the background of the Néel state $|\Phi_0\rangle$ we can introduce the operators $b_{q\alpha}$ and $b^\dagger_{q\alpha}$, which respectively annihilate and create transverse magnons; here $\vec{q}$ is the wave vector which takes on values in the Brillouin zone for the doubled lattice $B_{1/2}$ (Fig. 1), and $\alpha=\uparrow,\downarrow$ is the polarization. It is not difficult to verify that for the operators

$$b_{q\uparrow} = \frac{1}{2}\left\{u_q\hat{\sigma}_q^- - u_{q+Q}\hat{\sigma}_{q+Q}^-\right\}, \quad b_{q\downarrow} = \frac{1}{2}\left\{u_q\hat{\sigma}_q^+ + u_{q+Q}\hat{\sigma}_{q+Q}^+\right\}, \tag{4}$$

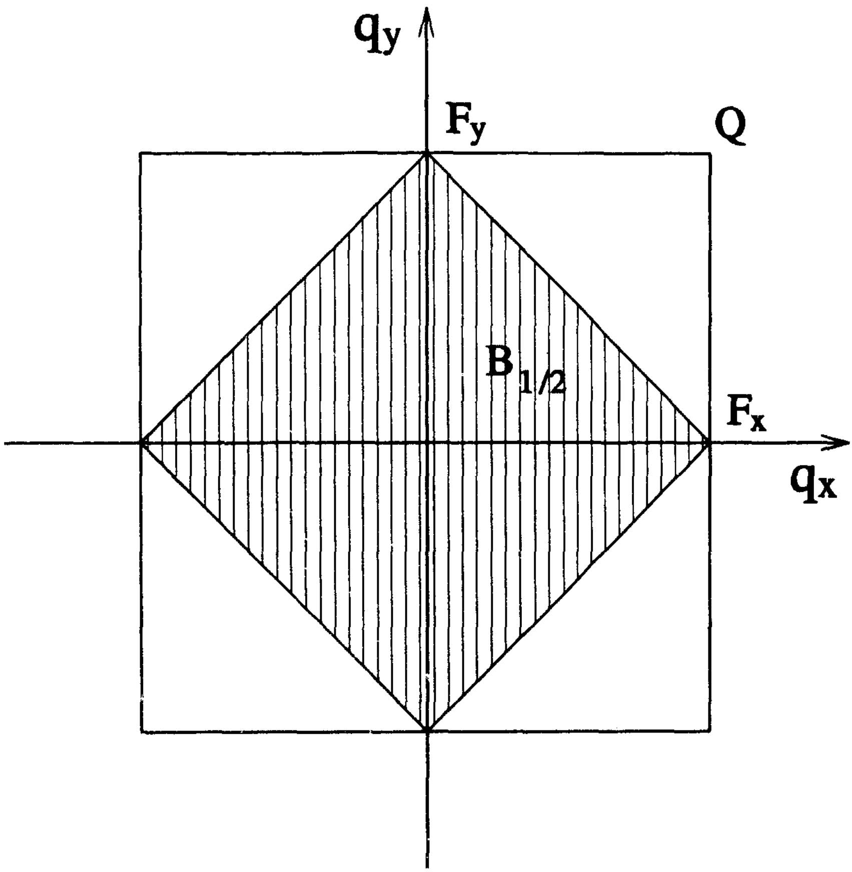

FIG. 1. Position of the points $\vec{Q}=(\pi/a,\pi/a)$, $\vec{F}_x=(\pi/a,0)$ and $\vec{F}_y=(0,\pi/a)$ in reciprocal space.

where

$$\hat{\sigma}_q^{\pm}=\sum_a \hat{\sigma}_a^{\pm}\exp(-i\vec{q}\vec{R}_a), \quad u_q=\left[\frac{\beta_q}{\beta_{q+Q}}\right]^{1/4}, \quad \beta_q=2(I_q-I_Q)>0, \tag{5}$$

the following "commutation relations" hold:

$$[b_{q\alpha},b^{\dagger}_{q'\alpha'}]_-|\Phi_0\rangle=\delta_{\alpha\alpha'}\delta(\vec{q}-\vec{q}')|\Phi_0\rangle, \quad [b_{q\alpha},b_{q'\alpha'}]_-|\Phi_0\rangle=0,$$
$$[b^{\dagger}_{q\alpha},b^{\dagger}_{q'\alpha'}]_-|\Phi_0\rangle=0. \tag{6}$$

The operators in (4) are thus "boson" operators when projected onto the Néel state. The commutator of the operator $b^{\dagger}_{q\alpha}$ with Hamiltonian (1) is

$$[\hat{H},b^{\dagger}_{q\alpha}]_-|\Phi_0\rangle=\epsilon_q b^{\dagger}_{q\alpha}|\Phi_0\rangle, \tag{7}$$

where ϵ_q, which serves as the magnon energy, is given by

$$\epsilon_q = \sqrt{\beta_q \beta_{q+Q}}. \tag{8}$$

The one-particle Hamiltonian of the magnons (without the interaction) is thus

$$\hat{H}_1 = \frac{1}{(2\pi)^2} \sum_\alpha \int_{B_{1/2}} d\vec{q}\, \epsilon_q b^\dagger_{q\alpha} b_{q\alpha}. \tag{9}$$

How does ϵ_q depend on the parameters of the problem? In the $B_{1/2}$ Brillouin zone for a tetragonal doubled lattice (Fig. 1), the magnon energy vanishes at $\vec{q} = 0$ and has local minima at $\vec{q} = \pm \vec{F}_x, \pm \vec{F}_y$, where $\vec{F}_x = (\pi/a, 0)$, $\vec{F}_y = (0, \pi/a)$ (all four points are equivalent in $B_{1/2}$: $\vec{F}_x \equiv \vec{F}_y \equiv \vec{F}$). Near a local minimum we have

$$\epsilon_q \approx \Delta + \frac{(\vec{q} - \vec{F})^2}{2m^*}, \quad \Delta = 8(I_1 - 2I_2), \quad m^* = \frac{1}{8a^2 I_2}. \tag{10}$$

The gap Δ at the point $\vec{F}$ vanishes in the case $I_2 = I_1/2$, in which the structure in (3) becomes less favorable than two "nested" Néel structures (the total number of sublattices is four). In structural transitions, the vanishing of Δ is interpreted as a phase transition by the "soft-mode" scheme. The anharmonicity is not slight for the spin problem, so new possibilities open up for a restructuring of the ground state.

We first note that we have $b_{q\alpha} |\Phi_0\rangle \to 0$ at $\vec{q} \approx \vec{F}$, so the Néel state is the "vacuum" for spin waves in this region of wave vectors. We are thus justified in speaking of one-magnon, two-magnon, etc., states near $\vec{F}$. We can construct a magnon Hamiltonian $\hat{H}_2$ which correctly describes the equations of motion for the two-magnon state $|\Phi_2\rangle = b^\dagger_{q\alpha} b^\dagger_{q'\alpha'} |\Phi_0\rangle$:

$$[H_2, b^\dagger_{q\alpha} b^\dagger_{q'\alpha'}]|\Phi_0\rangle = [H, b^\dagger_{q\alpha} b^\dagger_{q'\alpha'}]|\Phi_0\rangle. \tag{11}$$

For a general position $\vec{q}, \vec{q}\,'$ in the Brillouin zone, the Hamiltonian H_2 has terms of the type $bbbb$ + H.a., $b^\dagger bbb$ + H.a., and $b^\dagger b^\dagger bb$. The interaction of magnons has been studied in many places (e.g., Ref. 6). An important point for the discussion below is that if all the wave vectors lie near $\vec{F}$, then the terms which do not conserve the number of particles are small $[\sim a^2(\vec{q} - \vec{F})^2]$. The interaction near $\vec{F}$ reduces to a scattering of magnons with an amplitude

$$U^{\alpha\alpha'}_{q,q' \to q+p, q'-p} = \begin{cases} 64 I_2 > 0, & \alpha = \alpha' \\ -32 I_1 < 0, & \alpha \neq \alpha' \end{cases}. \tag{12}$$

In other words, there is a region near point $\vec{F}$ in the Brillouin zone in which magnons differing in polarization attract each other. Since the amplitude in (12) is not small, this attraction means that a bound state of magnons may form with a center-of-mass wave vector that lies near $\vec{F}$. Since we have $U^{\alpha\alpha'} \neq 0$ for $I_2 = I_1/2$, with $\Delta = 0$, an increase in the frustration will eventually cause the total energy of the bound state, $2\Delta + E_c$, to vanish (the binding energy is negative: $E_c < 0$).

The spin-wave spectrum in the Néel state can thus become unstable. A collapse involving the formation of pairs of magnons occurs in the system. One example of this collapse might be a nematic ordering, $\langle \sigma^\mu_n \sigma^\nu_m \rangle \neq \delta_{\mu\nu} \delta_{nm}$, $\langle \sigma^\mu_n \rangle = 0$. A $\langle b^\dagger_1 b^\dagger_1 \rangle$ spin symmetry, for example, does not contradict this suggestion. The case $\Delta = 0$ was studied in Ref. 5, where it was shown that fluctuations lead to a quadrupole interaction for Hamiltonian (1). However, only a scalar order parameter was found in Ref. 5.

For a large spin S, the interaction of magnons is on the order of $1/S$. The problem reduces to one of calculating the energy level of a particle with a mass $m^*/2$ in a weak attractive potential. We can thus restrict the discussion to $\vec{q} \approx \vec{F}$. In the 2D case, there definitely exists at least one discrete level.

We note in conclusion that the example discussed above, of a frustration due to the interaction of nearest neighbors along a diagonal, is not the only possibility. Any long-range antiferromagnetic interaction (Ref. 7, for example) could lead to an attraction of magnons near the point $\vec{F}$ (there is no minimum of ϵ_q here, but the relation $b_{q\alpha}|\Phi_0\rangle \approx 0$ holds). For a momentum transfer $p \sim R_0^{-1}$ the interaction amplitude would exceed the magnon energy by a factor of $(R_0/a)^2$, where $R_0 \gg a$ is the interaction radius. We will analyze that case in a subsequent paper.

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