Linear spin waves in a frustrated Heisenberg model

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A Heisenberg model, which has the property that its classical ground state shows a continuous transition from the Néel to an incommensurate spiral state, is investigated. It is shown that even for arbitrarily large spin these states are not stable with respect to quantum spin fluctuations in a finite region of the parameter space. Outside this region the order of the classical ground state is not destroyed. Thus, the results of linear spin-wave theory suggest the existence of a quantum-spin-liquid state between the Néel and an ordered incommensurate spiral phase.

There is experimental and theoretical evidence that for small doping the ground state of a two-dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnet with only nearest-neighbor coupling has incommensurate antiferromagnetic order.[1,2] In an undoped Heisenberg model with next- and additional third-nearest-neighbor antiferromagnetic couplings along the two coordinate axis the classical ground state shows a continuous transition from Néel to incommensurate spiral order as the ratio of the two coupling constants J_1, J_3 is changed. The following questions arise: Are the incommensurate spiral and the Néel state stable with respect to quantum spin fluctuations at zero temperature or is there a new disordered quantum phase arising, and if yes, what are the properties of this new state and of the phase transition?

In the following I am interested in the ground-state properties of the Hamiltonian

$$H=\frac{1}{2}\sum_{l,\delta}(J_1\mathbf{S}_l\cdot\mathbf{S}_{l+\delta}+J_3\mathbf{S}_l\cdot\mathbf{S}_{l+2\delta}) \qquad (1)$$

(where $J_1,J_3\geq 0$, δ is a vector between nearest neighbors), as a function of the frustration parameter $\alpha=J_3/J_1$.

The model is investigated by conventional linear spin-wave theory.[3] Classically, or equivalently in the limit $S\rightarrow\infty$ (S is the spin quantum number), the ground state has (for arbitrary couplings J_{lm} between site l and m) a spiral spin structure which can be characterized by a wave vector $\mathbf{Q}$:

$$S_l^y=S\sin(\mathbf{Q}\cdot\mathbf{r}_l)\ ,$$

$$S_l^z=S\cos(\mathbf{Q}\cdot\mathbf{r}_l)\ .$$

$\mathbf{Q}$ satisfies the minimal energy condition

$$J_{\mathbf{Q}}\leq J_{\mathbf{k}},\forall\mathbf{k}\ , \qquad (2)$$

where $J_{\mathbf{k}}$ is the Fourier transform of the coupling constants J_{lm},

$$J_{\mathbf{k}}=\sum_m J_{lm}e^{i\mathbf{k}\cdot(\mathbf{r}_l-\mathbf{r}_m)}\ . \qquad (3)$$

In my case, Eq. (2) leads to $\mathbf{Q}=Q(1,1)$, where Q satisfies

$$J_1\sin Q+2J_3\sin(2Q)=0\ , \qquad (4)$$

with the solution corresponding to minimal classical energy

$$Q=\pi,\ \text{for}\ \alpha\leq\frac{1}{4}\ ,$$

$$\pi/2<Q<\pi,\ \text{for}\ \alpha>\frac{1}{4}\ .$$

For $\alpha=\frac{1}{4}+\epsilon$ the wave vector $\mathbf{Q}$ departs $\propto\sqrt{\epsilon}$ from (π,π) for small $\epsilon>0$. Therefore, the classical ground state has Néel order for $\alpha\leq\frac{1}{4}$, which goes over to an incommensurate phase for $\alpha>\frac{1}{4}$, finally reaching the state of two decoupled Néel sublattices for very large α. The classical spin structure for $Q=2\pi/3$ (corresponding to $\alpha=0.5$) is shown in Fig. 1.

A similar model has been studied by Chandra and Doucot[4] and by Chakravarty, Halperin, and Nelson,[5] but with frustration originating from next-nearest-neighbor coupling J_2 instead of J_3. In contrast to the present model the classical spin structure changes discontinuously at $\alpha'=J_2/J_1=\frac{1}{2}$ between the Néel state ($Q=\pi$) and two decoupled Néel sublattices ($Q=\pi/2$). At this critical value of frustration, every state with total spin equal to zero for an elementary square is a ground state. Hence, classically there is a large degeneracy, including many states with no long-range order. It is not surprising then that the ground state is found to be a disordered spin-liquid state in a finite region of the (α,S) parameter space upon including quantum spin fluctuations. It is shown in this paper that the J_1,J_3 model also contains a quantum-

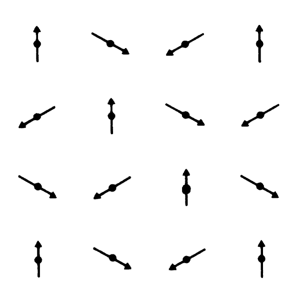

FIG. 1. Classical ground-state spin configuration for $J_3/J_1=0.5$ corresponding to $Q=2\pi/3$.

spin-liquid phase. The results of Chandra and Doucot,[4] who also used linear spin-wave theory, have been supported by exact numerical calculations on small clusters,[6] where it has been found that the lowest excited states are singlets rather than triplets in a critical region of the parameter space, indicating the existence of a new phase in the thermodynamic limit.

In the classical ground state the full lattice translation and rotation symmetry of the Hamiltonian (1) is broken to a subgroup of combined translation rotations $TR_{\mathbf{r}}$ ($\mathbf{r}$ is a lattice vector),

$$(TR_{\mathbf{r}}\mathbf{S})(\mathbf{r}_i) = (R_{\mathbf{r}}\mathbf{S})(\mathbf{r}_i + \mathbf{r}) .$$

In this equation, R_r is a rotation by an angle $\mathbf{Q}\cdot\mathbf{r}$. When the spin operators are written in a (locally defined) primed reference system

$$\mathbf{S}'(\mathbf{r}_i) = (R_{\mathbf{r}_i}\mathbf{S})(\mathbf{r}_i) ,$$

$TR_{\mathbf{r}}$ formally acts as the full lattice translation group on the primed spin operators,

$$(TR_{\mathbf{r}}\mathbf{S}')(\mathbf{r}_i) = \mathbf{S}'(\mathbf{r}_i + \mathbf{r}) .$$

Starting from the classical ground state, the application of a Holstein-Primakoff transformation[7] yields a Hamiltonian which has the full lattice translation symmetry. Neglecting higher-order terms it can be diagonalized by Fourier and subsequent Bogoliubov transformation. The noninteracting spin waves can be classified by a wave vector $\mathbf{k}$ with values in the first Brillouin zone of the given lattice and no description within a reduced Brillouin zone is needed. I obtain the following spin-wave dispersion relation:

$$E(\mathbf{k}) = S\{(J_{\mathbf{k}} - J_{\mathbf{Q}})[\tfrac{1}{2}(J_{\mathbf{k}+\mathbf{Q}} + J_{\mathbf{k}-\mathbf{Q}}) - J_{\mathbf{Q}}]\}^{1/2} , \quad (5)$$

where $J_{\mathbf{k}}$ is given by Eq. (3). There are two types of zeros in the dispersion,

$$J_{\mathbf{k}} - J_{\mathbf{Q}} = 0 \quad \text{for } \mathbf{k} = Q(\pm 1, \pm 1) ,$$

and

$$\tfrac{1}{2}(J_{\mathbf{k}+\mathbf{Q}} + J_{\mathbf{k}-\mathbf{Q}}) - J_{\mathbf{Q}} = 0 \quad \text{for } \mathbf{k} = 0 .$$

Considering the Taylor expansions around these zeros, it is easy to see that the dispersion is linear, unless

$$J_1 \cos Q + 4J_3 \cos(2Q) = 0 .$$

In this case the linear term vanishes. The above relation and Eq. (4) are simultaneously satisfied only for $\alpha = \frac{1}{4}$ with the solution $Q = \pi$, corresponding to a softened spin-wave mode with quadratic dispersion. This coincides with the value of α, where $\mathbf{Q}$ starts to move away from (π,π) towards incommensurate values $\pi/2 < Q < \pi$. The dispersion relation (5) is shown for $\alpha = 0$, 0.15, and 0.25 in Fig. 2 and for $\alpha = 0.309$, 0.5, and 0.653 in Fig. 3.

The ground-state energy per spin E_0 and the staggered magnetization M are given by the following expressions:

$$E_0 = \langle H \rangle_0 = \tfrac{1}{2} S^2 J_{\mathbf{Q}} - \frac{1}{N} \sum_{\mathbf{k}} E(\mathbf{k}) v_{\mathbf{k}}^2 ,$$

$$M = S - \frac{1}{N} \sum_{\mathbf{k}} v_{\mathbf{k}}^2 ,$$

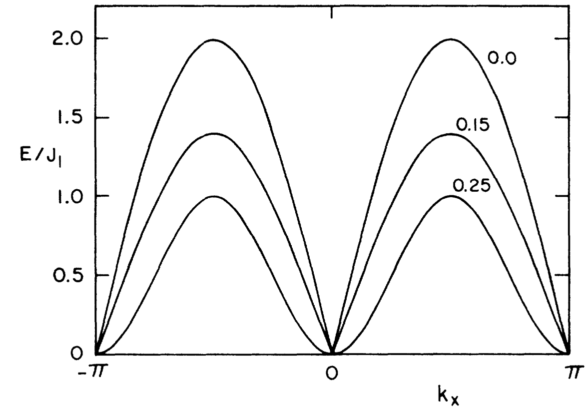

FIG. 2. Spin-wave dispersion relation $E(\mathbf{k})$ along the (1,1) direction for given values $\alpha = 0$, 0.15, 0.25, corresponding to a Néel ground state ($Q = \pi$).

where

$$v_{\mathbf{k}}^2 = [\beta_{\mathbf{k}} - E(\mathbf{k})]/2E(\mathbf{k}) ,$$

and

$$\beta_{\mathbf{k}} = \tfrac{1}{2} J_{\mathbf{k}} - J_{\mathbf{Q}} + \tfrac{1}{4}(J_{\mathbf{k}+\mathbf{Q}} + J_{\mathbf{k}-\mathbf{Q}}) .$$

N is the total number of spins. In the thermodynamic limit the staggered magnetization is given by the integral:[7]

$$M = S + \frac{1}{2} - \frac{1}{2\pi^2} \int_0^{\pi} \int_0^{\pi} d^2k \frac{\beta_{\mathbf{k}}}{E(\mathbf{k})} .$$

The integrand diverges for $\mathbf{k} = 0$ and $\mathbf{k} = \mathbf{Q}$, since $E(\mathbf{k})$ vanishes, but $\beta_{\mathbf{k}}$ remains finite for these values. As the dispersion is linear near the zeros for $\alpha \neq \frac{1}{4}$, the integral converges for dimensions $D \geq 2$ and the contribution to the staggered magnetization due to the spin fluctuations is finite. However, near the critical value $\alpha = \frac{1}{4}$, where the dispersion becomes quadratic, the spin fluctuations are arbitrarily large due to soft modes contributing to the amplitude of the zero-point motion, melting any ordered state

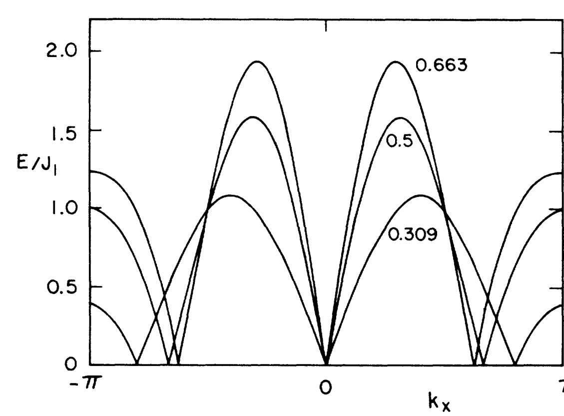

FIG. 3. Spin-wave dispersion relation $E(\mathbf{k})$ along the (1,1) direction for given values $\alpha = 0.309$, 0.5, 0.653 corresponding to $Q = 4\pi/5$, $2\pi/3$, $5\pi/8$.

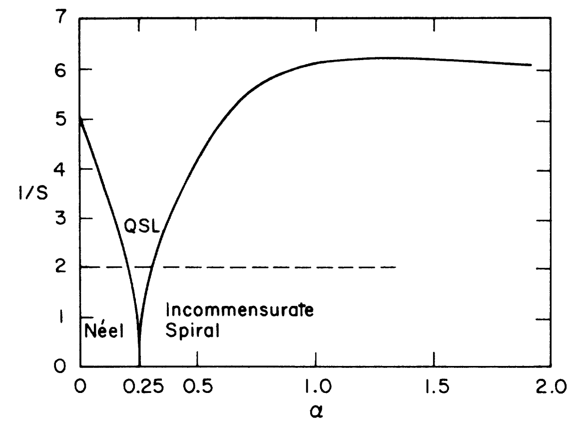

FIG. 4. Phase diagram of the considered J_1,J_3 model. The two lines, along which the staggered magnetization M is vanishing within linear spin-wave theory are shown (QSL is the quantum spin liquid). The range of physical spin values is indicated by a dashed line.

for arbitrary large spin S in dimensions $D \leq 2$. As the linear spin-wave theory becomes exact in the limit $S \rightarrow \infty$ and the fluctuations become larger for decreasing S, I conclude that the exact ground state is also disordered in some region of the parameter space (α, S) for dimensions $D \leq 2$. The two lines along which the staggered magnetization vanishes as shown in Fig. 4. Within the linear theory there is a quantum-spin-liquid phase between.

In conclusion I have presented evidence that the classical spiral states considered above are unstable, even at zero temperature and for large spin, as quantum fluctuations become arbitrarily large in a narrow region around a critical value of frustration which determines the onset of incommensurability. In this region a disordered state usually called quantum spin liquid is stabilized as a result of a softened spin-wave mode. It cannot be ruled out, however, that classes of ordered states other than the classical spiral one are stable with respect to quantum spin fluctuations for all values of frustration (and large enough spin). An investigation with other analytical (e.g., including spin-wave interactions) or numerical methods would be necessary to characterize the correlation functions of the disordered quantum spin liquid. For larger values of α an incommensurate spiral phase, and for small enough α, the Néel state are stable.

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