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Antiferromagnetic Interaction between Two Easy-Plane Ferromagnetic Heisenberg Chains

By

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Nonlinear magnetic excitations in the Heisenberg magnetic system $CsNiF_3$, when an antiferromagnetic interchain interaction is present between two neighboring easy-plane ferromagnetic chains, are studied. Using a two-lattice model and defining coherent states on each site for the two chains the discrete coupled equation for the averages of the spin components are given. In the easy-plane limit it is found that three kinds of static magnetic excitations can exist, depending on the value of the antiferromagnetic interchain exchange interaction J_2 . The inclusion of this antiferromagnetic interchain interaction makes the problem of the nonlinear magnetic excitations appear in a new light.

1. Introduction

The magnetic salt CsNiF₃ is a system widely investigated due to the striking nonlinear magnetic excitations in the easy-plane ferromagnetic chains of spins defined ignoring the antiferromagnetic interaction present in the three dimensional system. However, systematic deviations between theory and experiments attributed to the antiferromagnetic interaction between chains have been found up to several K above the 3D ordering temperature [1].

Our scope is to investigate qualitatively the nature of the nonlinear magnetic excitations when we include this antiferromagnetic interchain interaction for the very simplified case of two neighboring ferromagnetic easy-plane chains. In fact in the three-dimensional case each chain is surrounded by six chains [2].

Starting from a spin-Hamiltonian for the two chains the averages of the spin components are expressed in terms of well defined angles and amplitudes, on each site and on each chain, using the coherent state formalism which proves to be very adapted when we consider the semiclassical limit $(S \to \infty)$ and transform the spin operators into operators of two independent harmonic oscillators (Schwinger operators). However, as the spin for CsNiF₃ equals one, this model demands the inclusion of quantum effects. The reason for our classical approach is again simplicity. We are interested in finding the nonlinear excitations usually described by the sine-Gordon model for the case of noninteracting chains, when an antiferromagnetic interchain interaction J_2 is present.

2. The Model

We take the chains, denoted by A and B, parallel to the z-axis, and the y-axis intersects perpendicularly the chains. The x-axis perpendicular to the y-z plane completes the reference

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system. Taking the applied magnetic field along the x-axis the Hamiltonian is

$$\mathcal{H} = \mathcal{H}_{A} + \mathcal{H}_{B} + \mathcal{H}_{int}, \tag{1}$$

where

$$\mathcal{H}_{A} = -J_{1} \sum_{n, \delta} S_{A, n} \cdot S_{A, n+\delta} + D \sum_{n} (S_{A, n}^{z})^{2} + g \mu_{B} H \sum_{n} S_{A, n}^{x}, \qquad (2)$$

$$\mathcal{H}_{B} = -J_{1} \sum_{n, \delta} S_{B, n} \cdot S_{B, n+\delta} + D \sum_{n} (S_{B, n}^{z})^{2} + g \mu_{B} H \sum_{n} S_{B, n}^{x},$$
(3)

$$\mathcal{H}_{\text{int}} = J_2 \sum_{n} S_{A,n} \cdot S_{B,n} . \tag{4}$$

Here $J_1>0$ is the nearest-neighbor intrachain exchange interaction in the chains, $J_2>0$ the interchain exchange interaction between the chains, D>0 the anisotropy parameter, g the g-factor, H the intensity of the external magnetic field, and $\mu_{\rm B}$ the Bohr magneton. Label n represents the lattice sites and $\delta=\pm1$.

We now make use of the Schwinger boson operators linking the spin operators with two independent bosonic fields.

For lattice A.

$$S^{\dagger} = a^{\dagger}b$$
, $S^{-} = b^{\dagger}a$, $S^{z} = \frac{1}{2}(a^{\dagger}a - b^{\dagger}b)$ (5)

and for lattice B it is convenient to use the conjugated transformation

$$S^{\dagger} = b^{\dagger} a$$
, $S^{-} = a^{\dagger} b$, $S^{z} = \frac{1}{2} (a^{\dagger} a - b^{\dagger} b)$, (6)

since the chains interact antiferromagnetically. In both cases there is a contraint on the total Bose occupation $a^{\dagger}a + b^{\dagger}b = 2S$.

The Hamiltonian now read

$$\mathcal{H} = \sum_{m} \left\{ -\frac{J_{1}}{2} \left[a_{A, m}^{\dagger} b_{A, m} b_{A, m}^{\dagger} b_{A, m+1}^{\dagger} a_{A, m+1} + b_{A, m}^{\dagger} a_{A, m} a_{A, m}^{\dagger} a_{A, m+1}^{\dagger} b_{A, m+1} \right. \right. \\ + \frac{1}{2} \left(n_{A, m}^{a} - n_{A, m}^{b} \right) \left(n_{A, m+1}^{a} - n_{A, m+1}^{b} \right) \right] \\ - \frac{J_{1}}{2} \left[a_{B, m}^{\dagger} b_{B, m} b_{B, m}^{\dagger} b_{B, m+1}^{\dagger} a_{B, m+1} + b_{B, m}^{\dagger} a_{B, m} a_{B, m}^{\dagger} a_{B, m+1}^{\dagger} b_{B, m+1} \right. \\ + \frac{1}{2} \left(n_{A, m}^{a} - n_{B, m}^{b} \right) \left(n_{B, m+1}^{a} - n_{B, m+1}^{b} \right) \right] \\ + \frac{D}{4} \left[\left(n_{A, m}^{a} - n_{A, m}^{b} \right)^{2} + \left(n_{B, m}^{a} - n_{B, m}^{b} \right)^{2} \right] \\ - \frac{g\mu_{B}H}{2} \left[\left(a_{A, m}^{\dagger} b_{A, m} + b_{A, m}^{\dagger} a_{A, m} \right) + \left(a_{B, m}^{\dagger} b_{B, m} + b_{B, m}^{\dagger} a_{B, m} \right) \right] \\ + J_{2} \left[\frac{1}{2} \left(a_{A, m}^{\dagger} b_{A, m} a_{B, m}^{\dagger} b_{B, m} + b_{A, m}^{\dagger} a_{A, m} b_{B, m}^{\dagger} a_{B, m} \right) \\ - \frac{1}{4} \left(n_{A, m}^{a} - n_{A, m}^{b} \right) \left(n_{B, m}^{a} - n_{B, m}^{b} \right) \right] \right\}.$$
 (7)

Here $n^a = a^{\dagger}a$ and $n^b = b^{\dagger}b$.

We take the extremal state $|0\rangle$ of this magnetic system as that with all the spins pointing parallel to the magnetic field (x-axis) in chain A, and the opposite for chain B. In the Schwinger representation any quantum state is defined giving the excitation state of the independent harmonic oscillators associated to each site; then $|0\rangle$ corresponds to vacuum states of all the harmonic oscillators. Following Glauber [3] we define the displacement operators

$$D(\alpha_{vi}) = \exp \left(\alpha_{vi} a_{vi}^{\dagger} - \alpha_{vi}^{*} a_{vi}\right),$$

$$D(\beta_{vi}) = \exp \left(\beta_{vi} b_{vi}^{\dagger} - \beta_{vi}^{*} b_{vi}\right),$$
(8)

to introduce the field coherent states

$$|\alpha_{vi}\beta_{vi}\rangle = |\alpha_{vi}\rangle |\beta_{vi}\rangle = D(\alpha_{vi}) D(\beta_{vi}) |0\rangle,$$
 (9)

where v refers to the two chains, and i to the chain sites.

Taking the classical limit of the spin variable, i.e. $S \to \infty$, these field coherent states can be expanded in terms of the eigenstates of the harmonic oscillator number operators

$$|\alpha_{vi}\rangle = \exp\left(-\frac{1}{2}\alpha_{vi}^*\alpha_{vi}\right)\sum_{n=0}^{\infty}(\alpha_{vi})^n(n!)^{-1/2}|n\rangle,$$
 (10)

$$|\beta_{vi}\rangle = \exp\left(-\frac{1}{2}\beta_{vi}^*\beta_{vi}\right) \sum_{n=0}^{\infty} (\beta_{vi})^n (n!)^{-1/2} |n\rangle.$$
 (11)

In this way the states $|\alpha_{vi}\rangle$ and $|\beta_{vi}\rangle$ are, respectively, the eigenstates of the annihilation operators a_{vi} and b_{vi} of the independent harmonic oscillators.

We now write the general coherent state of the system as

$$|\alpha\beta\rangle = \prod_{vi} |\alpha_{vi}\beta_{vi}\rangle \,, \tag{12}$$

from which, using the above properties, the average energy $\langle \alpha\beta | \mathcal{H} | \alpha\beta \rangle$ can readily be obtained.

The correspondence between the coherent states and points in the complex plane permits a physical interpretation of each pair of points in the complex plane. In fact, writing

$$\alpha_{vi} = \varrho(\alpha_{vi}) \exp(i\varphi(\alpha_{vi})),$$

$$\beta_{vi} = \varrho(\beta_{vi}) \exp(i\varphi(\beta_{vi})),$$
(13)

the averages of the spin components at site i of chain v are

$$\langle S_{vi}^{x} \rangle = \varrho(\alpha_{vi}) \varrho(\beta_{vi}) \cos(\Phi_{vi}),$$

$$\langle S_{vi}^{y} \rangle = \varrho(\alpha_{vi}) \varrho(\beta_{vi}) \sin(\Phi_{vi}),$$

$$\langle S_{vi}^{z} \rangle = \frac{1}{2} (\varrho^{2}(\alpha_{vi}) - \varrho^{2}(\beta_{vi}))$$
(14)

with $\Phi_{vi} \equiv \varphi(\alpha_{vi}) - \varphi(\beta_{vi})$. We have then that to some selected pair of points inside the circle of radius $\sqrt{2S}$ in the complex plane there corresponds one point in the spin space, since the constraint now reads $\varrho^2(\alpha_{vi}) - \varrho^2(\beta_{vi}) = 2S$. This permits to clasify some configurations of the spins in terms of the relative position of the complex numbers of the pair in the complex plane. For example any easy-plane configuration corresponds to α and β in the circumference of radius \sqrt{S} , any y-z configuration corresponds to α and β forming right angles, etc.

Our interest is the easy-plane case, for which the average energy of our system is

$$\langle \alpha \beta | \mathcal{H} | \alpha \beta \rangle = -J_1 \sum_{v} \left[\cos \left(\Phi_{v+1}^{A} - \Phi_{v}^{A} \right) + \cos \left(\Phi_{v+1}^{B} - \Phi_{v}^{B} \right) \right]$$

$$- g \mu_{B} H \sum_{v} \left[\cos \Phi_{v}^{A} + \cos \Phi_{v}^{B} \right] + J_2 \sum_{v} \left[\cos \left(\Phi_{v}^{A} + \Phi_{v}^{B} \right) \right].$$
 (15)

The stationary configurations are obtained minimizing $\langle \mathcal{H} \rangle$ with respect to Φ_v^A and Φ_v^B , we obtain in this way the following two coupled nonlinear recurrence equations:

$$\begin{split} J_1 \sin{(\Phi_n^{\rm A} - \Phi_{n-1}^{\rm A})} &- J_1 \sin{(\Phi_{n+1}^{\rm A} - \Phi_n^{\rm A})} \\ &+ g \mu_{\rm B} H \sin{\Phi_n^{\rm A}} - J_2 \sin{(\Phi_n^{\rm A} + \Phi_n^{\rm B})} = 0 \;, \\ J_1 \sin{(\Phi_n^{\rm B} - \Phi_{n-1}^{\rm B})} &- J_1 \sin{(\Phi_{n+1}^{\rm B} - \Phi_n^{\rm B})} \\ &+ g \mu_{\rm B} H \sin{\Phi_n^{\rm B}} - J_2 \sin{(\Phi_n^{\rm B} + \Phi_n^{\rm A})} = 0 \;. \end{split}$$

Defining now

$$u_n^{A} = \sin \left(\Phi_n^{A} - \Phi_{n-1}^{A} \right), \tag{16}$$

$$u_n^{\rm B} = \sin \left(\Phi_n^{\rm B} - \Phi_{n-1}^{\rm B} \right), \tag{17}$$

we get the four-dimensional mapping

$$u_{n+1}^{A} = u_{n}^{A} + h \sin \Phi_{n}^{A} - J \sin (\Phi_{n}^{A} + \Phi_{n}^{B}),$$

$$u_{n+1}^{B} = u_{n}^{B} + h \sin \Phi_{n}^{B} - J \sin (\Phi_{n}^{B} + \Phi_{n}^{A}),$$

$$\Phi_{n+1}^{A} = \Phi_{n}^{A} + \arcsin \left[u_{n}^{A} + h \sin \Phi_{n}^{A} - J \sin (\Phi_{n}^{A} + \Phi_{n}^{B})\right],$$

$$\Phi_{n+1}^{B} = \Phi_{n}^{B} + \arcsin \left[u_{n}^{B} + h \sin \Phi_{n}^{B} - J \sin (\Phi_{n}^{B} + \Phi_{n}^{A})\right],$$
(18)

where $J \equiv J_2/J_1$ and $h \equiv g\mu_B H/J_1$.

3. Results and Discussion

The structure of this map can be understood in terms of the fixed points and their stability. We restrict the angles to the interval between 0 and 2π . The fixed points are

$$P_{f1}(n) = \begin{pmatrix} u_{f1(n)}^{A} \\ u_{f1(n)}^{B} \\ \Phi_{f1(n)}^{A} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ n\pi \\ n\pi \end{pmatrix}; \qquad n = 0, 1, 2,$$

$$(19)$$

$$P_{f2} = \begin{pmatrix} u_{f2}^{A} \\ u_{f2}^{B} \\ \Phi_{f2}^{A} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \arccos \frac{h}{2J} \\ \arccos \frac{h}{2J} \end{pmatrix}. \tag{20}$$

In Fig. 1 we show the bifurcation diagram for these equilibrium angles with respect to J where we put h=0.1 and define $\Phi^A=\Phi^B\equiv\Phi$. The fixed points $P_{f1}(n)$ are independent of the parameters, in contrast with P_{f2} (spin-flop point) which is defined up to h/2J=1.

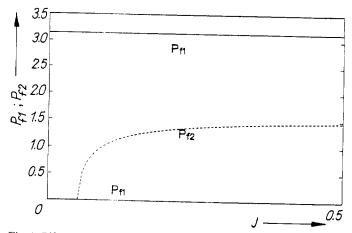


Fig. 1. Bifurcation diagram for the equilibrium angles as a function of J. Here h=0.1 and $\Phi^A=\Phi^B=\Phi$

Regarding the stability we found that for the case of the fixed points $P_{\rm f1}(n)$ with even n, two eigenvalues depend on h and J, whereas the other two depend only on h. For the case h/2J>1 all these points are real, two of them being greater than one and the others less than one so the $P_{\rm f1}(n)$ branch is unstable. As h/2J approaches one, two eigenvalues are close to one and the other two remain unaltered, one being greater than one and the other less than one. If h/2J=1 there are two eigenvalues equal to one (parabolic), and if h/2J<1 they are on the unit circle (elliptic). For odd n all four eigenvalues are always complex and on the unit circle. On the other hand, all the $P_{\rm f2}$ branch corresponds to a saddle-point-like unstable equilibrium point for each allowed value of h and J.

The static configurations of the N spins of chain A projected on the plane (u^A, Φ^A) from the trajectory on the $(u^A, u^B, \Phi^A, \Phi^B)$ phase space, are presented in Fig. 2 (the same we have for chain B).

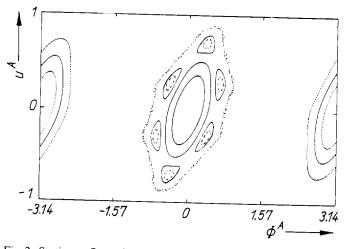
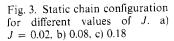
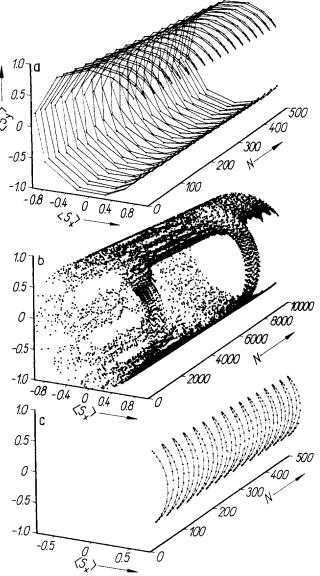


Fig. 2. Static configurations of the N spins of chain A projected on the plane (u^A, Φ^A) from the trajectory on the $(u^A, u^B, \Phi^A, \Phi^B)$ phase space (the same we have for chain B). A KAM (Kolmogorov-Arnold-Moser) behavior is observed





A KAM behavior is observed, in fact periodic, quasiperiodic, and chaotic trajectories coexist in the phase space. There are closed orbits about elliptic points at (0, 0) and $(0, \pi)$. There is a zone where orbits break to give rise to other elliptic fixed points of period six (the six small islands); finally we get into a chaotic region, far from the origin, where orbits disintegrate.

The static chain configuration for each zone is shown in Fig. 3 for given initial conditions and $J=0.02,\ 0.08,\$ and 0.18, respectively. Three well defined kinds of structure can be obtained. Defining $\Phi_1-\Phi_0$ as the opening angle and $\Delta\equiv\cos{(\Phi_1-\Phi_0)}$ we have for $J< h/2\Delta$ the spin forming a wave that oscillates pointing opposite to the magnetic field. The number of oscillations increases linearly along the chain. For $J\approx h/2\Delta$ the configuration

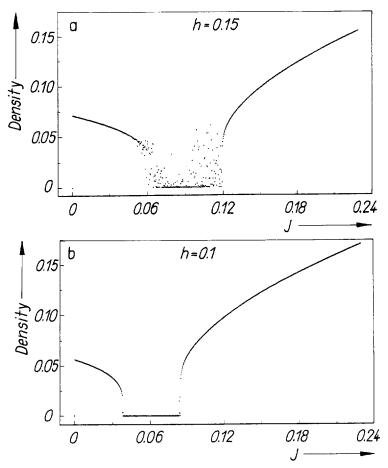


Fig. 4. Density of oscillations and solitons as a function of J for two values of the magnetic field h and identical initial conditions

can have full-turn oscillations in a very stochastic way, breaking its linear characteristic. For $J > h/2\Delta$ oscillations point parallel to the magnetic field and also there is a linear increase of the number of oscillations as we go along the chain. Fig. 4 shows the density of oscillations and solitons as a function of J for two values of the magnetic field h and identical initial conditions. We see that there is a structural phase transition around $J > h/2\Delta$. The interphase is larger as we increase J.

4. Conclusion

The main conclusion of our results is that the interchain antiferromagnetic interaction plays an important role in the theory of very low temperature excitations in magnetic chains.

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References

- [1] T. DELICA, W. J. M. DE JONGE, K. KOPINGA, H. LESCHKE, and H. J. MIKESKA, Phys. Rev. B 44, 11773 (1991).
 [2] M. STEINER, J. VILLAIN, and C. G. WINDSOR, Adv. Phys. **25**, 1 (1976).
 [3] R. J. GLAUBER, Phys. Rev. **131**, 2766 (1963).

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