Characteristics of two-sublattice spin chain with Dzyaloshinskiĭ interaction

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The stationary states of a two-sublattice quantum spin chain with a Dzyaloshinskiĭ interaction are analyzed exactly. The corresponding thermodynamics is constructed. Certain distinctive features are found in the magnetic characteristics of this spin system, in particular, helical structure.

There is no waning of interest in research on low-dimensional spin systems. Experimentally, these systems exhibit some special properties (Ref. 1, for example). From the theoretical standpoint, low-dimensional systems are interesting primarily because in these cases exact solutions can be found for problems of both classical dynamics[2-4] and quantum mechanics.[5-7] Multiple-sublattice low-dimensional systems have been attracting particular research interest in recent years.[8] These systems are interesting because of the diverse properties of these magnetic materials and also because of aspects of their behavior which stem from the low dimensionality.

Some very interesting entities for study are weak ferromagnets, in which there is a nonzero magnetic moment in the absence of a magnetic field because of the Dzyaloshinskiĭ exchange-relativistic interaction.[9] In addition, the Dzyaloshinskiĭ interaction may lead to particular features in the spin structure, noncollinear helical structures.[10] A theory describing the behavior of three-dimensional multiple-sublattice weak ferromagnets has been derived for various types of magnetic structures.[11] The customary approach is to seek the equilibrium configuration of magnetic moments for the ground state; the excited states are slight deviations of the magnetic sublattices from this equilibrium position. This approximation usually works quite well in describing the low-temperature behavior of magnetic systems, provided that the spin at a site is far greater than unity. Quantum-mechanical corrections, however, may prove important if this "site spin" is on the order of unity.

In this paper we are reporting a study of the quantum-mechanical aspects of the behavior of a two-sublattice spin chain ($s = 1/2$) with the Dzyaloshinskiĭ exchange-relativistic interaction. In this system, the Dzyaloshinskiĭ interaction takes a special form. For simplicity we will discuss the situation in which the easy-plane magnetic anisotropy is extremely pronounced, i.e., the case of an XY chain (the consequences of incorporating a Z–Z interaction between spins in chains with a Dzyaloshinskiĭ interaction were demonstrated in Ref. 12 by the present author).

The Hamiltonian of this system is

$$H=\sum_n \{J_1(s^x_{n,1}s^x_{n,2}+s_{n,1}s_{n,2})+J_2(s_{n,2}s_{n+1,1}+s_{n,2}s_{n+1,1})$$
$$+D_1(s^x_{n,1}s^y_{n,2}-s^y_{n,1}s^x_{n,2})+D_2(s^x_{n,2}s^y_{n+1,1}-s^y_{n,2}s^x_{n+1,1})$$
$$+h(\mu_1 s_1{}^z+\mu_2 s_2{}^z)\}, \qquad (1)$$

where $J_{1,2}$ are exchange constants, $D_{1,2}$ are Dzyaloshinskiĭ interaction constants, $h > 0$ is a constant magnetic field, $\mu_1 \geqslant \mu_2 > 0$ are the sublattice magnetons, $s^{x,y,z}_{n,1,2}$ are the spin projection operators ($s = 1/2$) in cell n, and 1 and 2 are the indices of the sublattices. Using the transformations of Ref. 13, we obtain the Fermi operators

$$s^+_{n,1}=\prod_{m<n}\sigma_{m,1}\sigma_{m,2}a_{n,1}, \qquad s^+_{n,2}=\prod_{m<n}\sigma_{m,1}\sigma_{m,2}\sigma_{n,1}a_{n,2},$$
$$s^-_{n,1}=(s^+_{n,1})^+, \quad s^-_{n,2}=(s^+_{n,2})^+ \quad 2s^z_{n,1,2}=\sigma_{n,1,2}=1-2a^+_{n,1,2}a_{n,1,2}, \qquad (2)$$

where $s^{\pm}_{n,1,2} = s^x_{n,1,2} \pm is^y_{n,1,2}$ and $a^+_{n,1,2}, a_{n,1,2}$ obey Fermi commutation relations. Here and below, we are uninterested in edge effects, being concerned only with the thermodynamic limit $N\to\infty$. Taking Fourier components, we have

$$H=-(N/2)h(\mu_1+\mu_2)$$
$$+\sum_k\{h(\mu_1 a^+_{k,1}a_{k,1}+\mu_2 a^+_{k,2}a_{k,2})-{}^1/_2[a^+_{k,1}a_{k,2}((J_1-iD_1)$$
$$+e^{-ik}(J_2+iD_2))+\text{H.a.}]\}, \qquad (3)$$

where N is the number of cells. The Hamiltonian (3) can be diagonalized easily by means of the unitary transformation

$$a_{k,1}=u_{k,11}b_{k,1}+u_{k,12}b_{k,2}, \qquad a_{k,2}=u_{k,21}b_{k,1}+u_{k,22}b_{k,2}. \qquad (4)$$

The coefficients of transformation (4) are

$$\begin{pmatrix}u_{k,11}\\ u_{k,21}\end{pmatrix}=\left[\frac{\mu_2 h-\varepsilon_{k,1}}{\varepsilon_{k,2}-\varepsilon_{k,1}}\right]^{1/2}\begin{pmatrix}e^{i\varphi}\\ e^{i\varphi}\dfrac{(J_1+iD_1)+(J_2-iD_2)e^{ik}}{2(\mu_2 h-\varepsilon_{k,1})}\end{pmatrix},$$
$$\begin{pmatrix}u_{k,12}\\ u_{k,22}\end{pmatrix}=\left[\frac{\mu_2 h-\varepsilon_{k,1}}{\varepsilon_{k,2}-\varepsilon_{k,1}}\right]^{1/2}\begin{pmatrix}e^{i\psi}\dfrac{(J_1-iD_1)+(J_2+iD_2)e^{ik}}{2(\mu_1 h-\varepsilon_{k,2})}\\ e^{i\psi}\end{pmatrix}, \qquad (5)$$

where φ and ψ are arbitrary phases, and the Hamiltonian becomes

$$H=\sum_{k,j}\varepsilon_{k,1,j}(b^+_{k,j}b_{k,j}-{}^1/_2), \quad j=1,2, \qquad (6)$$

where

$$2\varepsilon_{k,1,2}=(\mu_1+\mu_2)h\pm\{(\mu_1-\mu_2)^2h^2+J_1{}^2+J_2{}^2+D_1{}^2+D_2{}^2$$
$$+2[(J_1{}^2+D_1{}^2)(J_2{}^2+D_2{}^2)]^{1/2}\cos(k-\xi)\}^{1/2},$$
$$\xi=\arcsin\{(J_1D_2+J_2D_1)/[(J_1{}^2+D_1{}^2)(J_2{}^2+D_2{}^2)]^{1/2}\}. \qquad (7)$$

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We introduce

$$h_{1,2}=\{(J_1^2+J_2^2+D_1^2+D_2^2\mp 2[(J_1^2+D_1^2)(J_2^2+D_2^2)]^{1/2})/4\mu_1\mu_2\}^{1/2}, \quad (8)$$

$$k^c_{1,2}=\xi\mp\arccos\{[4\mu_1\mu_2h^2-(J_1^2+J_2^2+D_1^2+D_2^2)]/2[(J_1^2+D_1^2)(J_2^2+D_2^2)]^{1/2}\}=\xi\mp\arccos\alpha. \quad (9)$$

It can be seen from (7) that we have $\varepsilon_{k,1}\geqslant 0$ for all h and k. For $\varepsilon_{k,2}$, on the other hand, in the interval $0\leqslant h\leqslant h_1$ we have $\varepsilon_{k,2}\leqslant 0$ for all k. For $h\geqslant h_2$, we have $\varepsilon_{k,2}\geqslant 0$ for all k. If, on the other hand, we have $h_1\leqslant h\leqslant h_2$, than we have $\varepsilon_{k,2}\leqslant 0$ for $k^c_1\leqslant k\leqslant k^c_2$ and $\varepsilon_{k,2}\geqslant 0$ for all k outside this interval. The energy of the ground state of the spin chain is

$$E_0=-(N/2)(\mu_1+\mu_2)h+\sum_k \varepsilon_{k,2}. \quad (10)$$

For $0\leqslant h\leqslant h_1$, the summation in (10) runs over all values of k; for $h_1\leqslant h\leqslant h_2$, the summation is over k values in the interval $k^c_1\leqslant k\leqslant k^c_2$. For $h\geqslant h_2$, the corresponding interval is empty. Corresponding to the creation of a genuine excitation is the creation of fermions with positive energies or the creation of "holes" in the "Dirac ocean," which forms the ground state of this system and which has been discussed previously.

In the ground state, the expectation values of the z projections of the sublattice spins are

$$\langle s^z_{1,2}\rangle=\tfrac{1}{2}\Big\{1-(1/N)\sum_k[1\pm(\mu_1-\mu_2)h/\{(\mu_1-\mu_2)^2h^2+J_1^2+J_2^2+D_1^2+D_2^2+2[(J_1^2+D_1^2)(J_2^2+D_2^2)]^{1/2}\cos(k-\xi)\}^{1/2}]\Big\}. \quad (11)$$

The summation is over the same intervals of k as in expression (10). It can be seen from (11) that in the interval $0\leqslant h\leqslant h_1$ we have $\langle s^z_1\rangle=-\langle s^z_2\rangle$, while for $h\geqslant h_2$ the z projections of the site spins are equal to the nominal value. In this spin chain, there are accordingly three phases at absolute zero: an "antiferromagnetic phase" for $0\leqslant h\leqslant h_1$, a "spin-flip phase" for $h\geqslant h_2$, and an intermediate phase at values of h which are not in either of these regions. At the points $h=h_{1,2}$, the magnetic susceptibility of the spin chain has square-root singularities; i.e., second-order phase transitions in the magnetic field occur at these points at absolute zero.

The free energy of the spin system is

$$F=-T\sum_{k,j}\ln[2\,\mathrm{ch}(\varepsilon_{k,j}/2T)], \quad (12)$$

where T is the temperature in energy units. Clearly, a nonzero temperature will disrupt the phase transitions; this is the customary situation for one-dimensional systems.

Let us take a look at the transverse structure of the spin system. Since the expectation values are zero, $\langle s^{x,y}_{n,1,2}\rangle=0$, a planar spin structure is determined substantially by binary spin correlation functions of the type $\langle s^\alpha_{n,j}s^\beta_{n+m,i}\rangle$, where $\alpha,\beta=x,y$, and $i,j=1,2$. It was shown in Ref. 14 that the angles φ_n and φ_{n+m} which satisfy the relation

$$\mathrm{tg}(\varphi_n-\varphi_{n+m})=\langle s_n^x s^y_{n+m}\rangle/\langle s_n^x s^x_{n+m}\rangle \quad (13)$$

maximize the probability that in cell n the spin projection onto the axis making an angle φ_n with the x axis is one-half, and in cell $n+m$ the spin projection onto the axis making an angle φ_{n+m} with the x axis is also one-half. An analogous relation can easily be derived for the case of a two-sublattice spin chain. The corresponding angles thus characterize the planar structure of the spin chain.

We know that there is no long-range order in one-dimensional systems at nonzero T. We will accordingly examine the correlation functions of the spins of nearest neighbors, in order to bring out the features of the short-range order in a spin chain with the Dzyaloshinskiĭ interaction. At $T=0$, for $0\leqslant h\leqslant h_1$, and in the limit $N\to\infty$, we have

$$2\pi\langle s^x_{n,1}s^x_{n,2}+s^y_{n,1}s^y_{n,2}\rangle=-J_1\int_0^\pi dk\{[1+[(J_2^2+D_2^2)/(J_1^2+D_1^2)]^{1/2}\cos k]/R\},$$

$$2\pi\langle s^x_{n,2}s^x_{n+1,1}+s^y_{n,2}s^y_{n+1,2}\rangle=-J_2\int_0^\pi dk\{[1+[(J_1^2+D_1^2)/(J_2^2+D_2^2)]^{1/2}\cos k]/R\},$$

$$2\pi\langle s^x_{n,2}s^y_{n+1,1}-s^y_{n,2}s^x_{n+1,1}\rangle=-D_1\int_0^\pi dk\{[1+[(J_2^2+D_2^2)/(J_1^2+D_1^2)]^{1/2}\cos k]/R\},$$

$$2\pi\langle s^x_{n,2}s^y_{n+1,1}-s^y_{n,2}s^x_{n+1,1}\rangle=-D_2\int_0^\pi dk\{[1+[(J_1^2+D_1^2)/(J_2^2+D_2^2)]^{1/2}\cos k]/R\},$$

$$R=\{(\mu_1-\mu_2)^2h^2+J_1^2+J_2^2+D_1^2+D_2^2+2[(J_1^2+D_1^2)(J_2^2+D_2^2)]^{1/2}\cos k\}^{1/2}. \quad (14)$$

It can thus be seen from (14) that we have $\tan(\varphi_{n,1}-\varphi_{n,2})=D_1/J_1$ and $\tan(\varphi_{n,2}-\varphi_{n+1,1})=D_2/J_2$. For $h_1\leqslant h\leqslant h_2$, we find the same spin structure, while the correlation functions take a form similar to (14); for example,

$$2\pi\langle s^x_{n,1}s^x_{n,2}+s^y_{n,1}s^y_{n,2}\rangle=-J_1\int_0^{\arccos\alpha} dk\{[1+[(J_2^2+D_2^2)/(J_1^2+D_1^2)]^{1/2}\cos k]/R\}+\frac{2J_1(\mu_1+\mu_2)h[4\mu_1\mu_2h^2+J_1^2+D_1^2-J_2^2-D_2^2]}{2(J_1^2+D_1^2)^{3/2}(J_2^2+D_2^2)^{1/2}(1-\alpha^2)^{1/2}},$$

$$2\pi\langle s^x_{n,1}s^y_{n,2}-s^y_{n,1}s^x_{n,2}\rangle=-D_1\int_0^{\arccos\alpha} dk\{[1+[(J_2^2+D_2^2)/(J_1^2+D_1^2)]^{1/2}\cos k]/R\}+\frac{2D_1(\mu_1+\mu_2)h[4\mu_1\mu_2h^2+J_1^2+D_1^2-J_2^2-D_2^2]}{2(J_1^2+D_1^2)^{3/2}(J_2^2+D_2^2)^{1/2}(1-\alpha^2)^{1/2}},$$

$$2\pi\langle s^x_{n,2}s^x_{n+1,1}+s^y_{n,2}s^y_{n+1,1}\rangle$$

$$=-J_2\int_0^{\arccos\alpha} dk\{[1+[(J_1^2+D_1^2)/(J_2^2+D_2^2)]^{1/2}\cos k]/R\}$$

$$+\frac{2J_2(\mu_1+\mu_2)h[4\mu_1\mu_2h^2+J_2^2+D_2^2-J_1^2-D_1^2]}{2(J_2^2+D_2^2)^{3/2}(J_1^2+D_1^2)^{1/2}(1-\alpha^2)^{1/2}},$$

$$2\pi\langle s_{n,2}s^y_{n+1,1}-s^y_{n,2}s^x_{n+1,1}\rangle$$

$$=-D_2\int_0^{\arccos\alpha} dk\{[1+[(J_1^2+D_1^2)/(J_2^2+D_2^2)]^{1/2}\cos k]/R\}$$

$$+\frac{2D_2(\mu_1+\mu_2)h[4\mu_1\mu_2h^2+J_2^2+D_2^2-J_1^2-D_1^2]}{2(J_2^2+D_2^2)^{3/2}(J_1^2+D_1^2)^{1/2}(1-\alpha^2)^{1/2}}. \qquad (15)$$

For magnetic fields $h \geqslant h_2$, the correlation functions are of course zero, and there is no helical planar spin structure. The introduction of a nonzero temperature does not alter the planar structure of this spin system. We wish to stress that it prevails at all values of the field h for $T \neq 0$.

When we compare the results of an exact quantum-mechanical calculation with the result found by replacing the spin operators by Bose operators (the Holstein–Primakoff representation disregarding Boson interactions), we see that there is no "antiferromagnetic" phase in that semiclassical description. Although the planar correlation functions of nearest neighbors in the ground state do not behave as described by (14) and (15), the complex helical structure is the same as that predicted by the exact quantum-mechanical theory.

Let us examine the case with a field $h = 0$. One can show fairly easily, by analogy with Ref. 15, that there is cooperative Jahn–Teller phase transition in this chain. Assume

$$J_{1,2}=J(1\pm b\delta), \quad D_{1,2}=D(1\pm b\delta),$$

where δ is the displacement of an atom of the chain, and b is the magnetoelastic constant. The ground-state energy of the chain of spins is, at small values of δ,

$$U=-(2/\pi)N(J^2+D^2)^{1/2}E(1-b^2\delta^2)+NC\delta^2, \qquad (16)$$

where C is an elastic constant, and $E(x)$ is the elliptic integral of the first kind. Minimizing expression (16) with respect to δ, we find that in the case $\delta \ll 1$, in the ground state, an equilibrium corresponds to

$$b\delta \approx \exp[-\pi C/b^2(J^2+D^2)^{1/2}]. \qquad (17)$$

In other words, Peierls period doubling occurs in the chain. In a chain with such period doubling, simple helical planar structure occurs, as can be seen from (14): $\tan(\varphi_{n+1,1}-\varphi_{n,2}) = \tan(\varphi_{n,2}-\varphi_{n,1}) = D/J$. At high temperatures, there is a phase without period doubling.

We have studied the quantum-mechanical aspects of the behavior of a low-dimensional two-sublattice spin chain with the Dzyaloshinskiĭ interaction. Although this interaction generally does not give rise to weak ferromagnetism (the imposition of a magnetic field in the basal plane in XY systems poses serious difficulties to a theoretical description), in agreement with Mermin and Wagner's assertion[16] that there is no long-range order in one-dimensional uniaxial spin systems in a magnetic field directed perpendicular to the special axis, this interaction does renormalize the fields of the phase transitions. In addition, the Dzyaloshinskiĭ interaction in this spin chain leads to some special helical planar spin structures. These helical structures occur in the antiferromagnetic and intermediate phases if the magnetic field is below the level corresponding to the spin–flip transition, h_2.

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