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Quantum features of two types of Dzyaloshinskii-Moriya coupling in antiferromagnetic spin chain

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A $1D$ spin quantum system ($S = 1/2$) with the Dzyaloshinskii-Moriya interaction is studied. It is shown that this type of coupling in the antiferromagnetic chain with an odd structure with respect to the main axis accounts for a staggered magnetic ordering in the ground state. For an even structure the Dzyaloshinskii-Moriya interaction causes a helicoidal spin structure only. Correlation functions are calculated under different conditions.

1. Last years, low-dimensional quantum systems attracted considerable attention of physicists. This interest was intensified by the low-dimensional nature of metal-oxides which manifest high temperature superconductivity under special conditions [1]. Anderson claimed [2] that the nature of $2D$ quantum systems is analogous in some sense one to $1D$. It is of interest to examine properties of the $1D$ spin quantum chain with the Dzyaloshinskii-Moriya (DM) interaction [3].

The reason of a theoretical study of a DM system is the existence of quasi-$1D$ compounds of site spin $1/2$ with such coupling (see, e.g., Ref. 4). Essential progress has been achieved in obtaining spin compounds with organics in which the ratio of interchain to intrachain interactions reaches values of 10^{-4}. Those compounds have Curie temperatures T_C of a few Kelvins and in the temperature interval $T_C < T < I$, I is the exchange constant along the chain, the system reveals $1D$ features. Such systems have no long-range magnetic order, but intrachain interactions, e.g., of a DM type, essentially define magnetic properties. The ground state properties of $1D$ spin models manifest peculiarities of the low-temperature phase behavior of real quasi-one-dimensional magnets.

Last year there appeared a number of theoretical papers dealing with the DM $1D$ spin systems (see, e.g., [5–9]). The most of these authors studied spin systems with DM coupling of one kind — antiferromagnetic systems with an even antiferromagnetic structure (with respect to the principal axis of the magnet). The quasiclassical treatment of an odd (with respect to principal axis) antiferromagnetic structure with DM interaction was given [10]. But, as we can see, the $1D$ quantum DM spin chains manifest some interesting properties, e.g., the absence of weak ferromagnetism [6,8]. The main purpose of this paper is to study the $1D$ quantum DM spin $1/2$ chain with two different kinds of DM coupling and to understand the features of each of them. We are studying magnetic characteristics of a spin $S = 1/2$ system with the exchange and exchange-relativistic magnetic anisotropy and the DM spin-spin short-range interactions. The DM type coupling of the first form (for an even antiferromagnetic structure) does not cause nonzero magnetization in the ground state (the weak ferromagnetism), while the other DM type interaction (of an odd structure with respect to the main axis) produces nonzero staggered magnetic momentum value for the zero temperature. Nonzero temperature, as usual, destroys order in the $1D$ system. If the magnetic order parameter is zero, there is a helicoidal spin transverse structure determined by pair spin correlation functions (that is something like the off-diagonal order parameter, see Refs. 11,12). The helicoid shift is determined by DM coupling constants. An external magnetic field does not cause the change of the shift value, but the order parameter depends on the magnetic field. A magnetic field value determines either a magnetic ordering or a helicoidal spin structure.

2. The Hamiltonian of the spin $S = 1/2$ chain has the form

$$\hat{H} = -\sum_n (J_{\alpha\beta} S_n^\alpha S_{n+1}^\beta + HS_n^z) , \qquad (1)$$

where $J_{\alpha\beta}$ are the exchange constants; $\alpha, \beta = x, y, z$; $J_{z\beta} = J_{\alpha z} = 0$; H is the magnetic field value. One can see that $(J_{xx} + J_{yy})$ is the exchange interaction constant; J_{zz} is the uniaxial magnetic anisotropy parameter; $(J_{xx} - J_{yy})$ is the biaxial magnetic anisotropy parameter; $(J_{xy} - J_{yx}) = 2D_1$ and $(J_{xy} + J_{yx}) = 2D_2$ are DM exchange-relativistic coupling constants of the first and second kinds, respectively [10].

Using the Jordan-Wigner transformation [13]

$$S_n^+ = S_n^x + iS_n^y = \prod_{m<n} \sigma_m a_n ;$$

$$S_n^- = S_n^x - iS_n^y = a_n^+ \prod_{m<n} \sigma_m ; \qquad (2)$$

$$2S_n^z = \sigma_n = 1 - 2a_n^+ a_n ,$$

one obtains

$$\hat{H} = -I \left\{ \frac{1}{2} Nh + \Sigma_n \left[-ha_n^+ a_n + \frac{1}{2}(a_n^+ a_{n+1} e^{-i\varphi} + \text{h.c.}) + \right.\right.$$
$$\left.\left. + \frac{\gamma}{2}(a_{n+1} a_n e^{-i\psi} + \text{h.c.}) + \frac{\Delta}{4}(1 - 2a_n^+ a_n)(1 - 2a_{n+1}^+ a_{n+1}) \right] \right\} , \qquad (3)$$

where

$$I = \frac{1}{2}[(J_{xx} + J_{yy})^2 + (J_{xy} - J_{yx})^2]^{1/2} ,$$

$$h = H/I ,$$

$$\gamma = \frac{1}{2I}[(J_{xx} - J_{yy})^2 + (J_{xy} + J_{yx})^2]^{1/2} ,$$

$$\Delta = J_{zz}/I ,$$

$$\text{tg}\,\varphi = \frac{J_{xy} - J_{yx}}{J_{xx} + J_{yy}} ,$$

$$\text{tg}\,\psi = \frac{J_{xy} + J_{yx}}{J_{xx} - J_{yy}} . \qquad (4)$$

Using the Fourier transformation

$$a_n = N^{-1/2} \sum_k a_k e^{ikn} ,$$

we have

$$\hat{H} = -I \left\{ \frac{1}{2} Nh + \frac{\Delta}{4} N - \Sigma_k \left[(h - \cos(k + \varphi)) a_k^+ a_k - \right.\right.$$
$$\left.\left. - \frac{\gamma}{2}(a_k a_{-k} e^{-i(\psi + k)} + \text{h.c.}) - \frac{\Delta}{N} \cos k \rho_{-k} \rho_k \right] \right\}, \qquad (5)$$

where

$$\rho_k = \sum_p a_{p+k}^+ a_p . \qquad (6)$$

3. Let us start with the simple case of a noninteracting Fermi gas (*XY* model): $J_{zz} = 0$. For the diagonalization of the quadratic form, see Eq. (5), $\Delta = 0$, we use the Bogolyubov-Valatin transformation:

$$a_k = u_k b_k + v_{-k}^* b_{-k}^+ ,$$

$$a_k^+ = u_k^* b_k^+ + v_{-k} b_{-k} ,$$

$$|u_k|^2 + |v_{-k}|^2 = 1 ,$$

$$|u_{-k}|^2 + |v_k|^2 = 1 ,$$

$$u_k v_k^* + u_{-k} v_{-k}^* = 0 ,$$

$$u_k^* v_k + u_{-k}^* v_{-k} = 0 ,$$

$$v_k = u_k \frac{A_k - \varepsilon_k}{B_k^* - B_{-k}^*} ,$$

$$|u_k|^2 = \frac{|B_k - B_{-k}|^2}{|B_k - B_{-k}|^2 + (\varepsilon_k - A_k)^2} , \qquad (7)$$

where

$$A_k = I[h - \cos(k + \varphi)] ,$$

$$B_k = \frac{\gamma}{2} I e^{-i(k - \psi)} , \qquad (8)$$

$$\varepsilon_k = \frac{1}{2}\left[(A_k - A_{-k}) \pm [(A_k + A_{-k})^2 + \right.$$
$$\left. + 4|B_k - B_{-k}|^2]^{1/2} \right] . \qquad (9)$$

One can use any sign in Eq. (9), because that sign determines the difference between the time evolution of the modes b_k and b_{-k}^+ only. We take the sign «+» from here.

We can study the influence of DM couplings for two different symmetry classes of the lattice separately.

(i). The case $D_2 = 0$, $J_{xx} = J_{yy}$ was studied earlier (see, e.g., Ref. 11). From that paper we know that the DM coupling D_1 for the $1D$ case causes a transverse helical spin structure for nonzero temperature case with any magnetic field (along the Z axis) value. Please note that, even for the interacting case $\Delta \neq 0$, there is a transverse spin structure for the case $\Delta < 1$, if a magnetic field is less than the critical one (a spin-flip transition value), and there is no transverse structure for the easy-axis ferromagnetic case $\Delta > 1$ and for the spin-flip phase of the $\Delta < 1$ case [8]) for the ground state. The shift ξ of the helicoid is equal to

$$\operatorname{tg} \xi = \frac{2D_1}{J_{xx} + J_{yy}} = \operatorname{tg} \varphi \ ,$$

and there is no spontaneous magnetization, caused by the DM interaction, even for the ground state [6,8]. The transverse spin structure is determined by the pair correlation functions $\langle S_n^{x,y} S_{n+r}^{x,y} \rangle$ [11].

(ii). One can see that the case $D_1 = 0$ differs drastically from the former one. The dispersion law (9) has a gap, caused by the DM coupling D_2 (even for the uniaxial case, $J_{xx} = J_{yy}$, the gap has nonzero value). That is why the behavior of the spin structure has features of the effectively biaxial case. That result is in contrast with the statement of Ref. 9, that the DM coupling does not change the class of the system's behavior, determined by the anisotropy constants. That statement is valid for the case (i) (studied only in Ref. 9), but not for the case of nonzero D_2 coupling constant.

Using the results of Ref. 14 one can calculate long-distance pair correlators. The physical result is the following: for $h < 1$ the DM coupling D_2 causes spontaneous staggered magnetization (the weak antiferromagnetism) for the ground state (let $0 < \gamma < 1$):

$$\langle S_n^x S_{n+r}^x \rangle = (-1)^r \frac{\gamma^{1/2}(1 - h^2)^{1/4}}{2 + 2\gamma} \left(1 + \frac{A_x}{\pi r^2}\right) + \dots \ , \tag{10}$$

$$A_x^{-1} = [2\lambda_2^{2r}(\lambda_2 - \lambda_1)^2] \ , \quad 1 - \gamma^2 < h^2 < 1 \ ,$$

$$A_x = \alpha^{-2r} \operatorname{Re} \frac{\exp(i\Psi r)}{[\alpha^{-1} \exp(-i\Psi) - \alpha \exp(i\Psi)]^2} \ ,$$
$$h^2 < 1 - \gamma \ ,$$

$$\langle S_n^y S_{n+r}^y \rangle = (-1)^r A_y \frac{(1 - h^2)^{1/4}}{\gamma^{1/2}[2\pi(1 - \lambda_2^{-2})(1 - \lambda_1 \lambda_2)]} + \dots , \tag{11}$$

$$A_y = -(4\lambda_2^{2r} r^3)^{-1} \ , \quad 1 - \gamma^2 < h^2 < 1 \ ,$$

$$A_y = 2\,\alpha^{2r} r^{-1} \sin^2 \Psi \ , \quad h^2 < 1 - \gamma \ ,$$

$$\langle S_n^x S_{n+r}^x \rangle = (-1)^r \left[\frac{\lambda_2^{2r}\gamma}{8\pi r(1 + \gamma)}\right]^{1/2} \left[\frac{1 - \lambda_1^2}{1 - \lambda_2^2}\right]^{1/4} + \dots ,$$
$$h^2 > 1 \ , \tag{12}$$

$$\langle S_n^y S_{n+r}^y \rangle =$$
$$= -(-1)^r \frac{\lambda_2^r}{8} \frac{[\pi(1+\gamma)]^{1/2}(1 - \lambda_2^2)^{3/4}(1 - \lambda_1^2)^{1/4}}{(2\gamma r^3)^{1/2}(1 - \lambda_1 \lambda_2)} + \dots ,$$
$$h^2 > 1 \ , \tag{13}$$

where

$$\alpha = \left(\frac{1 - \gamma}{1 + \gamma}\right)^{1/2} ,$$

$$\cos \Psi = \frac{h}{(1 - \gamma^2)^{1/2}} \ ,$$

$$\lambda_{1,2} = \frac{h - (h^2 - 1 + \gamma^2)^{1/2}}{1 \pm \gamma} \ . \tag{14}$$

For $h > 1$, the spontaneous staggered magnetization is equal to zero, but the helical spin transverse structure takes place:

$$\operatorname{tg}(\varphi_n + \varphi_{n+1}) = \frac{\langle S_n^x S_{n+1}^y + S_n^y S_{n+1}^x \rangle}{\langle S_n^x S_{n+1}^x - S_n^y S_{n+1}^y \rangle} \ , \tag{15}$$

where φ_n (φ_{n+1}) is the most probable site n $(n+1)$ spin angle value with the axis X. One can see from Eqs. (5), (9) that the phase shift ζ of the helicoid is equal to

$$\operatorname{tg} \zeta = \frac{2D_2}{J_{xx} - J_{yy}} = \operatorname{tg} \psi \tag{16}$$

for any temperature and external field value h. It is easy to see from Eq. (16) that for the uniaxial case $J_{xx} = J_{yy}$, the phase shift ζ is equal to $\pm \pi/2$.

4. Let us study the interacting case $\Delta \neq 0$. One can see that the Hamiltonian (5) is the general lattice form of the Thirring model Hamiltonian [16]. We can write the Bethe ansatz equation for our system [17]:

$$-N|\gamma| \operatorname{sh} \beta_j = 2\pi I_j + \varphi +$$
$$+ 2 \sum_{k=1}^{M} \operatorname{arctg} [\operatorname{ctg} \mu \operatorname{th}((\beta_j - \beta_k)/2)] \ , \tag{17}$$

where $j = 1, \dots, M$, M is the number of down spins; $\operatorname{ctg}\mu = -\Delta$; I_j are integer or half-integer numbers, depending on M value. The energy of the state is

$$E = I\sum_{k=1}^{M}[|\gamma|\operatorname{ch}\beta_k + h] \ . \tag{18}$$

Solving Eqs. (17) we can obtain the energy dependence on the DM constants. One can get the solution by using the results of Refs. 16,17.

For estimation of a long-range behavior of the spin chain we shall use the bosonization method [18,19]. For the thermodynamic limiting case $s \to 0$ (s is the lattice constant), $Ns = L$ (L is the chain length) one can obtain (for $-1 < \Delta < 0$, the «easy-plane» liquid-like case for simplicity, without the «cosine» mass term [20])

$$\hat{H} = 2\pi L^{-1}I\Sigma_k[(\rho_{1,k}\rho_{1,-k} + \rho_{2,-k}\rho_{2,k}) + \gamma(e^{-i\psi}a_{2,-k}\,a_{1,k} + \text{h.c.}) + \frac{2\Delta}{\pi}\rho_{1,k}\rho\,\rho_{2,-k}] + \\ + \pi L^{-1}[v_N(N - N_0)^2 + v_J(J + \varphi)^2] - \frac{I}{2}\pi L^{-1}\Sigma_k|k - k_F| \ , \tag{19}$$

instead of Eq. (5), where indices «1» and «2» describe operators with the positive and negative group velocity near the Fermi points k_F; $v_N = I(\pi + 2\Delta)$, $v_J = I(\pi - 2\Delta)$; N and J are the topological excitations [21]; N_0 is determined by the magnetic field value h; $k_F = \pi N_0/L$. The operators $\rho_{1,2,k}$ and $\rho_{1,2,-k}$ have the Bose-like commutation rules [18]. Using the method of Ref. 18 one can diagonalize the Bose part of the Hamiltonian (19) near the Fermi points for $\gamma = 0$. The dispersion law is

$$\varepsilon(k) = I|k - k_F|\sec^2\alpha \ , \tag{20}$$

$$\operatorname{th}\alpha = -2\Delta/\pi \ .$$

From Eqs. (19), (20) one can obviously derive long-range pair spin transverse correlation functions [19]:

$$-4s^2\langle S^{x,y}(x)S^{x,y}(0)\rangle \propto e^{i\varphi x/s}(s/x)^{\theta}f(mx/s) \ , \tag{21}$$

where θ is the zero-mass exponent:

$$2\theta = \left[\frac{\pi + 2\Delta}{\pi - 2\Delta}\right]^{1/2} , \tag{22}$$

$f(x)$ is an undetermined function, $f(x) = \exp(-x)$ for $m_0 \neq 0$; m is the «dressed» mass (the excitation gap),

$$m \propto m_0^{\nu} \ ,$$

$$2\nu = (1 - \theta)^{-1} \ ,$$

and m_0 is the bare mass:

$$m_0 = I\gamma \ .$$

The DM interaction D_2 changes the value of the initial mass (gap) of the excitation, and a fermion-fermion interaction for $\Delta \neq 0$ renormalizes the mass term. That is why one can use the conclusions of the $\Delta = 0$ case on the role of the DM coupling D_1 and D_2. For the uniaxial case $J_{xx} = J_{yy}$, $D_2 = 0$, one can see the transverse helical spin structure, the phase shift is determined by the $2D_1/(J_{xx} + J_{yy})$ constant. This conclusion coincides with the exact solutions [6,8] and the conformal field theory [7], where the DM interaction D_1 causes a twist of boundary conditions.

For the case $D_1 = 0$, $D_2 \neq 0$, one can see that there is an excitation gap (even for the uniaxial case $J_{xx} = J_{yy}$) and the behavior of correlations changes from the power law case into the exponential one. That difference determines a longe-range staggered magnetic ordering (the weak antiferromagnetism) in the XY spin plane.

The choice between the weak antiferromagnetic order and the helicoidal spin structure which is determined by the pair correlators depends for the ground state of an easy-plane magnet on the magnetic field value.

In conclusion, we have studied the $1D$ quantum spin 1/2 chain with the DM interaction. The DM coupling for an even (with respect to the main axis of the magnet) magnetic structure does not cause weak ferromagnetism even in the ground state. The DM interaction of odd-type accounts for a staggered magnetic order in the ground state even for the uniaxial antiferromagnetic chain for the external magnetic field interval defined by the magnetic anisotropy. Nonzero temperature destroys a weak staggered magnetic order. In another cases one deals with a helicoidal magnetic structure; its phase shifts are determined by DM and exchange constants.

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