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EFFECT OF DZYALOSHINSKII–MORIYA INTERACTION ON HEISENBERG ANTIFERROMAGNETIC SPIN CHAIN IN A LONGITUDINAL MAGNETIC FIELD

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Abstract. Using the functional integral method for the Heisenberg antiferromagnetic spin chain with the added Dzyaloshinskii–Moriya interaction in the longitudinal magnetic field, we find an expression for the free energy of the spin chain via spin fluctuations. From this expression, we derive quantities that characterize the antiferromagnetic order and the phase transition, such as staggered magnetization and total magnetization Next, we deduce the significant effect of the Dzyaloshinskii–Moriya interaction on reducing the antiferromagnetic order. The total magnetization can be deviated from the initial one due to the Dzyaloshinskii–Moriya interaction and the magnetic field causing a canting of the spins. Besides, the remarkable role of the transverse spin fluctuations of the spin chain is also indicated.

Keywords: antiferromagnetic spin chain, Dzyaloshinskii–Moriya interaction, transverse spin fluctuations, functional integral method

1 Introduction

One dimensional (1D) spin systems have studied extensively over the last years because of their unusual new magnetic phenomena which have been found out. With the mathematical simplicity of models applied for the 1D systems, they have been considered as ideal objects for investigating effect of thermal and quantum fluctuations on thermodynamic properties and the phase transitions [1, 2]. Recently some real materials in the 1D or quasi-1D magnetic systems have been found out, such as $Sr_2V_3O_9$ [3], $BaCu_2Ge_2O_7$ [4], $Cu(C_8H_6N_2)Cl_2$ [5], $(C_7H_{10}N)_2CuBr_4$ [6], $K_2CuSO_4Cl_2$ and $K_2CuSO_4Br_2$ [7], which cannot be described by a pure Heisenberg model. In other words, there are definitely the presence of anisotropies in these real materials, such as anisotropic exchange interactions, magneto-crystalline anisotropy or ones from spin-orbit couplings which may cause antisymmetric superexchange interaction.

The antisymmetric interaction was at first recommended by Dzyaloshinskii IE [8] after the observation of a weak ferromagnetism in the antiferromagnetic α-Fe_2O_3 crystals, and later, Moriya T [9] pointed out that spin-orbit couplings were the microscopic mechanism of this interaction. So the antisymmetric interaction is also known as the Dzyaloshinskii–Moriya interaction (DMI). Although the DM term is about a few per cent of the Heisenberg exchange one [10, 11], which only makes a small canting, the effect of the DMI is significant. In antiferromagnetic (AFM) systems, a small DMI favours a canting of the antiparallel arrangement of the magnetic moments producing a weak ferromagnetic (FM) behaviour which couples strongly to an external magnetic field [10]. Besides, the DMI has caused a variety of interesting effects in low dimensional magnetic systems depending on the values of this interaction, such as unusual phase diagrams [7, 12]; stabilization of chiral magnetic orderings [13]; quantum chaos in the Heisenberg spin chain [14]; or skyrmion formation in two dimensional (2D) systems [15, 16].

Recently, the Heisenberg model with AFM exchange interactions in the presence of a longitudinal external magnetic field and a DM interaction has been studied by using the mean-field approximation (MFA) and showed that the increase of either the external field or the DMI has decreased the corresponding phase transition temperature [17]. However, the significant role of the spin fluctuations which have not considered yet in [17], which is one of the restrictions of the MFA. It is noted that the fluctuations have the important influences on the thermodynamic behaviours of the low dimensional systems [1, 18, 19, 20]. Therefore, in the current article we use the functional integral method to study the effect of the DMI on the AFM spin chain via the spin fluctuations with the Heisenberg model in the presence of the longitudinal magnetic field and from that highlighting the role of the transverse spin fluctuations due to the DMI and the magnetic field.

2 Theory

Consider a the AFM 1D Heisenberg model with two sublattices labelled A $(\text{spin} \uparrow)$ and B $(\text{spin} \downarrow)$ which regularly align along the x′Ox axis in the presence of the longitudinal magnetic field $\vec{h}(0,0,h)$, Hamiltonian for this system with the added Dzyaloshinskii-Moriya interaction has form [13]:

$$
\begin{aligned}
H &= J\sum_{j,j'}\left(S_{Aj}^{x}S_{Bj'}^{x} + S_{Aj}^{y}S_{Bj'}^{y} + S_{Aj}^{z}S_{Bj'}^{z}\right) \\
&+\vec{D}\sum_{j,j'}\left(\vec{S}_{Aj}\times\vec{S}_{Bj'}\right) - g\mu_B h\sum_{j}\left(S_{Aj}^{z} + S_{Bj}^{z}\right) \\
&\frac{1}{2}I\sum_{j}\left(\left(S_{Aj}^{z}\right)^2 + \left(S_{Bj}^{z}\right)^2\right),
\end{aligned}
\qquad (1)
$$

where the first term in Hamiltonian (1) favours parallel/antiparallel exchange coupling of the spins (depending on the sign of J, $J > 0$ for the AFM system and $J < 0$ for the FM system), whereas the second term shows preference for an orthogonal alignment, which causes the canting of the spins; the third term is the interaction between the spins with the magnetic field, here $h > 0$, μ_B is the Bohr magneton and g is the gyromagnetic ratio; and the last term shows the single-ion anisotropy of the spins given in (1) to suppress the spin fluctuations and thus maintains the AFM ground state in the system, the anisotropy is chosen to be parallel to the direction of the applied magnetic field, *i.e.*, $\vec{I}//\vec{h}$. Both the exchange parameter J and the DM vector $\vec{D}$ depend on the relative positions of the spins and here only the interactions between the nearest neighbor spins are considered. In this article $\vec{D}$ is chosen in the z-direction, thus Hamiltonian (1) is rewritten as follows:

$$
\begin{aligned}
H &= J\sum_{j.j'}\left(S_{Aj}^{x}S_{Bj'}^{x} + S_{Aj}^{y}S_{Bj'}^{y} + S_{Aj}^{z}S_{Bj'}^{z}\right) \\
&+D\sum_{j,j'}\left(S_{Aj}^{x}S_{Bj'}^{y} - S_{Aj}^{y}S_{Bj'}^{x}\right) - g\mu_B h\sum_{j}\left(S_{Aj}^{z} + S_{Bj}^{z}\right) \\
&-\frac{1}{2}I\sum_{j}\left(\left(S_{Aj}^{z}\right)^2 + \left(S_{Bj}^{z}\right)^2\right).
\end{aligned}
\qquad (2)
$$

Next, the Hamiltonian (2) is diagonalized by performing a spin coordinate transformation, *i.e.*, a spin rotation about the z-axis with a specific angle $\tan\varphi = D/J$ [21]

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$$S_j^x \to S_j^x \cos\varphi + S_j^y \sin\varphi,$$
$$S_j^y \to -S_j^x \sin\varphi + S_j^y \cos\varphi \tag{3}$$

is done, thus the Hamiltonian (2) becomes:

$$H = \frac{J}{\cos\varphi}\sum_{j,j'}\left(S_{Aj}^x S_{Bj'}^x + S_{Aj}^y S_{Bj'}^y\right) + J\sum_{j=1}^{N} S_{Aj}^z S_{Bj'}^z$$
$$-g\mu_B h\sum_j\left(S_{Aj}^z + S_{Bj}^z\right) - \frac{1}{2}I\sum_j\left(\left(S_{Aj}^z\right)^2 + \left(S_{Bj}^z\right)^2\right). \tag{4}$$

From (4), it can be seen that the Heisenberg model with the added Dzyaloshinskii-Moriya interaction (1) is transformed into the XXZ anisotropic Heisenberg model with the anisotropic exchange parameter $\alpha = \cos\varphi$.

In this article, we only consider the case of the small DM term causing a modest canting of the spins in the AFM order, thus the ground state of the spin chain remains AFM, so the spin variables $S_{A(B)j}^{\alpha}$ can still be transformed by introducing the fluctuations from its mean value $\langle S_{A(B)}\rangle^z$ along the spin chain:

$$\delta S_{A(B)j}^z = S_{A(B)j}^z - \left\langle S_{A(B)}^z\right\rangle,$$
$$\delta S_{A(B)j}^x = S_{A(B)j}^x,\ \delta S_{A(B)j}^y = S_{A(B)j}^y. \tag{5}$$

Therefore, Hamiltonian (4) is divided into part:

$$H_0 = -NJ_{AB}\left\langle S_A^z\right\rangle\left\langle S_B^z\right\rangle$$
$$-\sum_j\left(g\mu_b h + 2J_{AB}\left\langle S_B^z\right\rangle + I\left\langle S_A^z\right\rangle\right)S_{Aj}^z \tag{6}$$
$$-\sum_j\left(g\mu_b h + 2J_{AB}\left\langle S_A^z\right\rangle + I\left\langle S_B^z\right\rangle\right)S_{Bj}^z,$$

and

$$H_{\text{int}} = -\sum_{k_x}\sum_{\alpha=x,y}\frac{J_{AB}}{\cos\varphi}(k_x)\delta S_A^{\alpha}(k_x)\delta S_B^{\alpha}(-k_x)$$
$$-\sum_{k_x}J_{AB}(k_x)\delta S_A^z(k_x)\delta S_B^z(-k_x) \tag{7}$$
$$-\frac{1}{2}I\sum_{k_x}\left(\delta S_A^z(k_x)\delta S_A^z(-k_x) + \delta S_B^z(k_x)\delta S_B^z(-k_x)\right),$$

here $J_{AB} = -J$. Rewriting H_{int} (7) in the matrix form:

$$H_{\text{int}} = -\frac{1}{2}\sum_{\alpha,\mu,\mu',k_x} \mathrm{J}_{\mu\mu'}^{\alpha}(k_x)\delta S_{\mu}^{\alpha}(k_x)\delta S_{\mu'}^{\alpha}(-k_x), \tag{8}$$

here $\mathrm{J}_{\mu\mu'}^{\alpha}(k_x)$ is an element of the symmetric second-order matrix $\mathrm{J}^{\alpha}(k_x)$ of the second order due to two spins in each unit cell:

$$\mathrm{J}^{x,y}(k_x) = \begin{bmatrix} 0 & \frac{J_{AB}}{\cos\varphi}(k_x) \\ \frac{J_{AB}}{\cos\varphi}(k_x) & 0 \end{bmatrix} \tag{9}$$

and

$$\mathrm{J}^z(k_x) = \begin{bmatrix} I & J_{AB}(k_x) \\ J_{AB}(k_x) & I \end{bmatrix}. \tag{10}$$

Using the functional integral method (see the detailed calculations in [1, 18, 22]) to calculate the free energy $F = -\frac{1}{\beta}\ln\left(\mathrm{Tr}\left[e^{-\beta H_0}\right]\right) - \frac{1}{\beta}\ln\left\langle \exp(-\beta H_{\text{int}})\right\rangle_0$, the specific expression for the free energy of the AFM spin chain is obtained:

$$F = NJ_{AB}b(y_A)b(y_B)$$
$$-\frac{N}{2\beta}\left(\ln\frac{\mathrm{sh}(S+1/2)y_A}{\mathrm{sh}(y_A/2)} + \ln\frac{\mathrm{sh}(S+1/2)y_B}{\mathrm{sh}(y_B/2)}\right)$$
$$+\frac{1}{2\beta}\sum_{k_x}\ln\left(\det\left[\mathrm{E}\text{-}\mathrm{M}^Z(k_x)\right]\right) \tag{11}$$
$$+\frac{1}{\beta}\sum_{k_x,\omega}\ln\left(\det\left[\mathrm{E}\text{-}\mathrm{M}^{x,y}(k_x,\omega)\right]\right),$$

here E is the unit matrix. $\mathrm{M}^z(k_x)$, $\mathrm{M}^{x,y}(k_x,\omega)$ and E are the matrices which have the same size as the matrix $\mathrm{J}^{\alpha}(k_x)$ in (9) and (10). $\mathrm{M}^{x,y}(k_x,\omega)$ and $\mathrm{M}^z(k_x)$ relate to the transverse spin fluctuations and the longitudinal spin fluctuations, respectively:

$$\mathrm{M}^{x,y}(k_x,\omega)=\begin{bmatrix} 0 & \dfrac{\frac{\beta J_{AB}}{\cos\varphi}(k_x)b(y_B)}{y_B-i\beta\omega} \\ \dfrac{\frac{\beta J_{AB}}{\cos\varphi}(k_x)b(y_A)}{y_A-i\beta\omega} & 0 \end{bmatrix}, \quad (12)$$

$$\mathrm{M}^{z}(k_x)=\begin{bmatrix} \beta I b'(y_A) & \beta J_{AB}(k_x)b'(y_B) \\ \beta J_{AB}(k_x)b'(y_A) & \beta I b'(y_B) \end{bmatrix}, \quad (13)$$

with $b(y_{A(B)})$ is the Brillouin function, $b'(y_{A(B)})$ is its 1st derivative and y_A, y_B are the total fields (including the external magnetic field and the mean field) acting on the spins *A* and the spins *B*:

$$y_{A(B)}=\beta g\mu_B h+2\beta J_{AB}b(y_{B(A)})+\beta I b(y_{A(B)}). \quad (14)$$

3 Numerical Results and Discussion

In the numerical calculations, the exchange parameter ***J*** is used as a new scale of energy and then the reduced external magnetic field is $\mathrm{h_r}=g\mu_B h/J$; the reduced temperature is $\tau_{\mathrm{r}}=k_B T/J$; and $m_{A(B)}=-\dfrac{1}{Ng\mu_B}\dfrac{\partial F}{\partial h_{A(B)}}$ denotes the magnetization per site *A* or *B*. However, we will analyze the effects of the magnetic field and the DMI through two quantities describing the magnetic order and the phase transition of the AFM spin chain, they are total magnetization $(\mathrm{m_T})$ and staggered magnetization $(\mathrm{m_S})$ [17], which are given as below:

$$\mathrm{m_T}=\frac{1}{2}\left(m_A-|m_B|\right) \quad (15)$$

and

$$\mathrm{m_S}=\frac{1}{2}\left(m_A+|m_B|\right) \quad (16)$$

Fig. 1(a) shows the behaviour of the staggered magnetization $\mathrm{m_S}$ as a function of the reduced temperature for various values of the DM parameter without the magnetic field and in this case $m_A=|m_B|$, so $\mathrm{m_T}=0$. As mentioned in [18], a small single-ion anisotropic parameter need to be taken into consideration to suppress the thermal fluctuations and thus prevent a disruption of the AFM order in the spin chain due to the size effect according to the Mermin-Wagner theorem [20]. From Fig. 1(a), one can see that the DM parameter reduces the AFM order of the system. This result was also indicated by the MFA [17]. However here we insist on the role of the transverse spin fluctuations produced by the DMI, which are ignored in the MFA. The increase of the DMI causes the increase of the transverse thermal fluctuations $\delta\mathrm{m_S^{x,y}}$ (see Fig. 1(b)), which makes the magnitude of the staggered magnetization $\mathrm{m_S}$ reduced even at $\tau_{\mathrm{r}}\approx 0$ and the AFM order breakable with an enough large value of the DM parameter (see the inset in Fig. 1(b)).

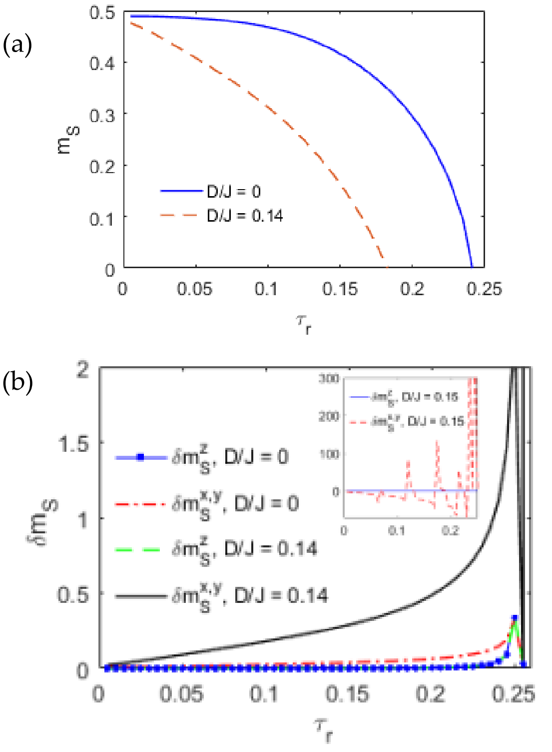

Fig. 1. The dependence on the reduced temperature with various values of the DM parameter of (a) the staggered magnetization and (b) the thermal spin fluctuations, the inset shows ones for $D/J=0.15$. Here $\mathrm{h_r}=0$, $I/J=0.01$ and $S=0.5$.

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From the discussion above, the dependence of the staggered magnetization on the DM parameter is considered in Fig. 2 to see more clearly the significant influence of the DM interaction on the AFM order of the spin chain. From the Fig. 1 and Fig. 2, one can see that there exists a critical value $(D_J)_{cr}$ which is the boundary between the stable range $(D/J < (D_J)_{cr})$ and the unstable range $(D/J > (D_J)_{cr})$, which indicates that there is a magnetic phase transition occurring at this point.

It should be noted that the critical value $(D_J)_{cr}$ depends on other factors such as the anisotropy and the magnetic field, for example, with $I/J \approx 0.01$ and $h_r = 0$ we have $(D_J)_{cr} \approx 0.15$ (see the inset in Fig. 1(b)), or with $I/J \approx 0.01$ and $h_r = 0.05$, $(D_J)_{cr} \approx 0.10$ (see Fig. 3(a)). Because the DM term is only about a few per cent of the Heisenberg exchange one without the single anisotropy [10, 11] and only produces a small canting of the spins, this result is quite suitable. When $D/J < (D_J)_{cr}$, the plot of m_S vs D/J is smooth, stable and magnitude of m_S decreases when increasing the DM parameter, the system is now in the AFM phase. When $D/J > (D_J)_{cr}$, this curve goes up and down chaotically, which shows that the spin chain is in another complicated magnetic phase due to an abnormal arrangement of the spins when increasing D/J. To see more clearly this phase transition point, the dependence on D/J of the derivative dm_S/dD is shown in Fig. 2(b), where one can observe a sharp peak at $D/J = (D_J)_{cr}$ corresponding to the phase transition point in the plot of the dependence on D/J of the staggered magnetization.

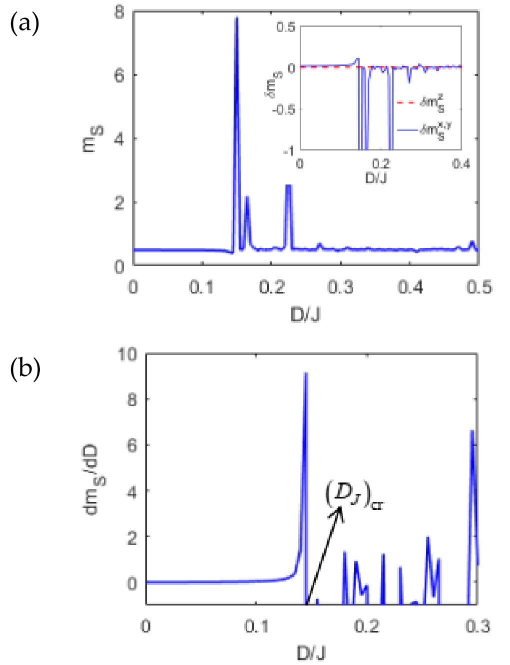

Fig. 2. The dependence on the DM parameter of (a) the staggered magnetization and (b) the derivative dm_S/dD, here $h_r = 0$, $\tau_r = 0.005$, $S = 0.5$ and $I/J = 0.01$. The inset in Fig. 2(a) shows the thermal spin fluctuations.

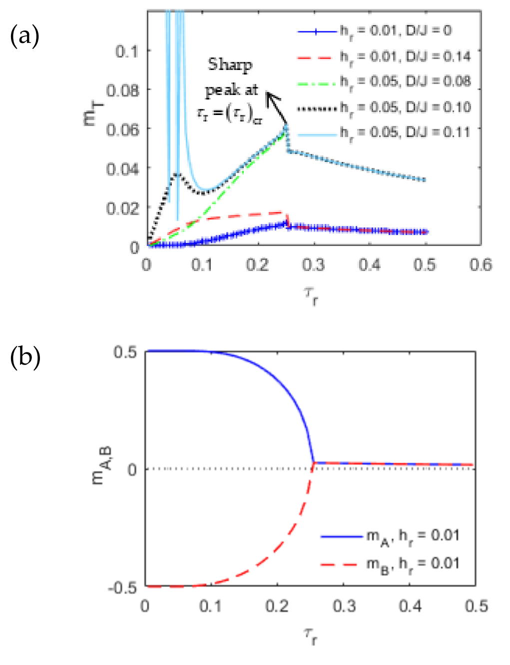

Fig. 3. The dependence on the reduced temperature of (a) the total magnetization with various values of the magnetic field and the DM parameter; and (b) the sublattice magnetizations with $h_r = 0.01$, $D/J = 0$. Here $I/J = 0.01$ and $S = 0.5$.

However, the complicated behaviours of the spin chain in the $D/J > (D_J)_{cr}$ range cannot be precisely calculated and explained within the scope of this article, because the translational symmetry of the spin chain is broken and the transverse spin fluctuations become overwhelming in this range (see the inset in Fig. 2(a)). Some works have also studied the spin structures in the strong DMI range and showed the unusual spin structures, such as chiral magnetism order (by using the first principle calculations) [23] or the skyrmion formation (by using the density functional calculations) [16, 24] in some low dimensional magnetic systems.

Fig. 3(a) shows the dependence on the temperature of the total magnetization m_T for various values of the reduced magnetic field and the DM parameter. For $D=0$, the model is a simple AFM spin chain in the magnetic field and this magnetic field is parallel to the spins *A* and antiparallel to the spins *B*. Therefore, the magnetic field $h_r = \frac{g\mu_B h}{J} \neq 0$ forces the spins *B* to rotate in the field's direction from the initial orientation $(\downarrow)$ of the spins *B*, which causes the rotation of the spins *A* through the exchange interactions between the spins, so we have the non-zero total magnetization $m_T \neq 0$. In this situation, there is a competition between the thermal energy, the exchange energy, the anisotropic energy and the magnetic energy in the spin chain. When the temperature increases, the thermal energy lessens the initial magnetization (or the spontaneous magnetization) in both sublattices *A* and *B*, as shown in Fig. 3(b). As the longitudinal magnetic field is applied leading to an increase of the total magnetization with the temperature and m_T reaches to a sharp peak in the dependence on the temperature at $\tau_r = (\tau_r)_{cr}$. When $\tau_r > (\tau_r)_{cr}$ the effect of thermal energy surpasses one of the magnetic energy and then m_T decreases with the temperature. This similar behaviour in the dependence of the sublattice magnetizations on the temperature in the presence of the longitudinal magnetic field was also obtained for the AFM and ferrimagnetic systems by using the sublattice self-consistent numerical procedure [25]. As increasing the DM parameter D/J, this total magnetization is more deviated from the initial one because the DMI increases the transverse spin fluctuations (see Fig. 4). Therefore, it should be noted that the combination between the magnetic field and the DMI make the AFM order broken faster in the increment of D/J, for example, with $h_r = 0.05$ the instability starts to happen when $D/J \approx 0.10$.

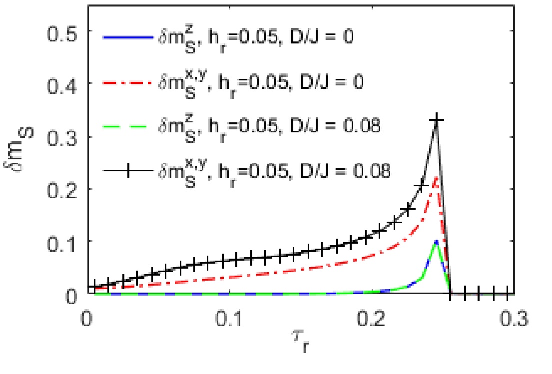

Fig. 4. The dependence on the reduced temperature of the thermal spin fluctuations with various values of the magnetic field and the DM parameter, here $I/J = 0.01$ and $S = 0.5$.

4 Conclusion

In this article, the effect of the DMI on the AFM behaviours and the phase transition of the spin chain in the presence of the longitudinal magnetic field is investigated by using the functional integral method. The spin fluctuations are taken into account through the mean field approximation and thus the role of them, namely the transverse ones, is highlighted. It can be seen that when applying a magnetic field parallel to the initial direction of the spins, it tends to rotate the spins perpendicular to the applied field.

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Therefore the combination of the DMI and the magnetic field leads to the increasing of the transverse spin fluctuations which reduces the AFM order and causes the deviation of the total magnetization from the initial one. Besides, there exists the critical value of the DMI at that the AFM order is broken and then the AFM phase of the spin chain transforms into other complicated magnetic ones. This problem cannot be solved within the scope of the current article and further calculations are required.

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