Influence of Dzyaloshinskii-Moriya and Kaplan-Shekhtman-Entinwohlman-Aharony superexchange interactions on ground state properties of the one-dimensional spin-Peilers model in open chain*

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The effects of the Dzyaloshinskii–Moriya (DM) and the Kaplan–Shekhtman–Entinwohlman–Aharony (KSEA) superexchange interactions on the ground state properties of the one-dimensional spin-Peilers system in open chain are studied by using the Lanczos numerical method. The study concentrates mainly on the influence of systemic dimerisation in open chain. The results show that systemic ground state energy density varies with dimerisation parameter δ in different DM interactions, and there exists a special point δ_c where the DM interaction has no influence on the systemic dimerisation, no matter whether the DM interaction is relative or irrelative to systemic dimerisation ($\eta = 1$ or $\eta = 0$). The KSEA interaction has no fixed special point, but the points of intersection are dense relatively in a certain numberical value range, and sparse in other numberical value ranges. So we can conclude that the antisymmetric anisotropy DM interaction differs from the symmetric anisotropy KSEA interaction, but they are analogous in the sense of the influence of systemic dimerisation in open chain.

Keywords: dimerisation, Dzyaloshinskii–Moriya interaction, Kaplan–Shekhtman–Entinwohlman–Aharony interaction, open chain

PACC: 7540F, 7550E, 7530G

1. Introduction

The one-dimensional antiferromagnetic $s = 1/2$ chain has been extensively investigated both theoretically and experimentally. However, many experiments on higher-dimensional compounds indicated that the isotropic exchange interaction was not sufficient to describe magnetic properties such as weak ferromagnetism in many systems.[1−5] Many years ago, Dzyaloshinsky[6] pointed out that a term of the form $\boldsymbol{D}\cdot(\boldsymbol{S}_1\times\boldsymbol{S}_2)$ favoured a canted spin arrangement over the antiferromagnetic arrangement and a weak ferromagnetic moment. Later, this term was derived by Moriya[7] and Anderson.[8] The calculation of Moriya showed that besides the Dzyaloshinskii–Moriya (DM) term, a symmetric anisotropy term in the form of $\boldsymbol{S}\cdot\boldsymbol{A}\cdot\boldsymbol{S}$ was also obtained, but was assumed to be negligible compared with the antisymmetric term. However, this assumption is incorrect if the underlying microscopic model has SU(2) spin symmetry,[9−11] since the effective spin–spin interaction has the same SU(2) invariance. As the DM term alone breaks SU(2) symmetry, the symmetric term compensates exactly spin anisotropy induced by the DM term. For this kind of system, the Kaplan–Shekhtman–Entinwohlman–Aharony (KSEA) term is tuned in such a way that SU(2) symmetry is recovered.[9−11] In some conditions, the KSEA interaction can be much larger in the Hubbard model with spin–orbit coupling.[10] A clear experimental evidence of the presence of a KSEA interaction superimposed on the DM interaction comes from neutron diffraction and inelastic neutron scattering experiments on $Ba_2CuGe_2O_7$.[3] In recent years, the effects of the DM and the KSEA superexchange interactions on the systemic ground state properties of the one-dimensional spin-Peilers model in periodic

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chain have been studied.[12,13]

At the present time, the ground-state properties of a spin-Peierls system with the DM and the KSEA interactions are not clear in one-dimensional open chain yet. In the following, we will discuss them in detail, which can be conducive to the understanding of the characteristics of the DM and the KSEA interactions deeply.

2. Hamiltonian

The Hamiltonian of one-dimensional spin-Peierls model is

$$H = \sum_{n=1}^{N}[J_n(\boldsymbol{S}_n \cdot \boldsymbol{S}_{n+1}) + \boldsymbol{D}_n \cdot (\boldsymbol{S}_n \times \boldsymbol{S}_{n+1}) + \boldsymbol{S}_n \cdot \boldsymbol{A} \cdot \boldsymbol{S}_{n+1}] + \frac{1}{2}KN\delta^2, \quad (1)$$

where $J_{\rm n} = J_0[1 + (-1)^n\delta]$, is the general spin-Peierls interaction parameter; $\boldsymbol{D}_n = \boldsymbol{D}_0\,[1 + (-1)^n\eta\delta]$, with $\boldsymbol{D}_n$ being the antisymmetric anisotropy DM interaction parameter; the third term on the right-hand side describes KSEA interaction, with $\boldsymbol{A}$ being the symmetric anisotropy KSEA interaction tensor; δ is the dimerisation displacement of lattice aberration; K is the elastic coefficient of lattice aberration; N is the lattice point number. This Hamiltonian is for a normal spin-Peierls model in the absence of the DM and the KSEA interactions.[14−22] Generally, in a system having full SU(2) symmetry, such as in $Ba_2CuGe_2O_7$,[3] DM and KSEA interactions are not independent.[11] In order to simplify the problem, we use the quantisation axis $\hat{z}$ for the spins such that $\boldsymbol{D}_n = (0,\ \ 0,\ \ D_0)$, the anisotropy tensor $|\boldsymbol{A}_n| = A_0$, and all other components are zero.

Hamiltonian (1) can be simplified by a canonical transformation[23]

$$H = {\rm e}^{-{\rm i}u} H\, {\rm e}^{{\rm i}u}, \quad (2)$$

with $U = \sum_{n=1}^{N_0} \alpha_n s_n^z, \alpha_n = \sum_{i=1}^{n-1} \tan^{-1}(D_i^z/J_i)$, and $\alpha_1 = 0$.

At a result, we can turn Hamiltonian (1) into the form

$$H = \sum_{n=1}^{N} \left\{[A + (-1)^n\, B]\left(S_n^x \cdot S_{n+1}^x + S_n^y \cdot S_{n+1}^y\right) + \{J_0\,[1 + (-1)^n\,\delta] + A_0\}\, S_n^z \cdot S_{n+1}^z\right\} + \frac{1}{2}KN\delta^2,$$

$$A = \frac{\sqrt{J_0^2\,(1+\delta)^2 + D_0^2(1+\eta\delta)^2} + \sqrt{J_0^2\,(1-\delta)^2 + D_0^2(1-\eta\delta)^2}}{2}\,,$$

$$B = \frac{\sqrt{J_0^2\,(1+\delta)^2 + D_0^2(1+\eta\delta)^2} - \sqrt{J_0^2\,(1-\delta)^2 + D_0^2(1-\eta\delta)^2}}{2}\,. \quad (3)$$

3. Calculation and analysis

Lattice point number in calculation is 30. In all the calculations, we set systemic lattice aberration elastic coefficient $K = 0.65$ and $J_0 = 1$ according to concrete properties of materials and parameter of NMR experimental result, where $J_0 = 1$ acts as energy unit.

First, we study the influence of the DM superexchange interactions on the systemic ground state properties of the one-dimensional spin-Peilers model in open chain. When DM interaction depends on dimerisation ($(\eta = 1)$, the result is given in Fig. 1. The systemic ground state energy density varies with dimerisation parameter δ in different DM interactions. Obviously, there is a special point $\delta_{\rm c}$ where the DM interaction has no influence on the systemic dimerisation. It acts against systemic dimerisation in $\delta < \delta_{\rm c}$, but favours systemic dimerisation in $\delta > \delta_{\rm c}$.

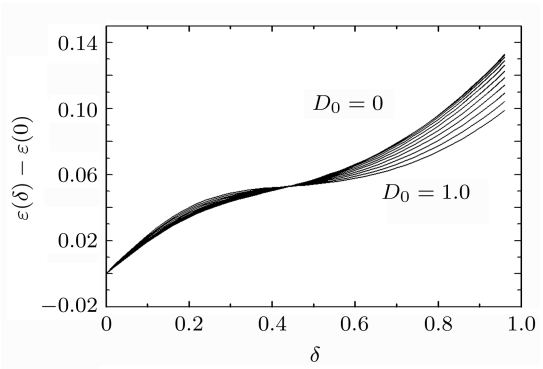


Fig. 1. Variations of dimerisation energy density with parameter δ in different DM interactions ($\eta = 1$) in open chain, with $J_0 = 1, A_0 = 0$.

When the DM interaction is irrelative to systemic dimerisation ((η = 0), the result is shown in Fig. 2. The systemic ground state energy densities vary with dimerisation parameter δ at different DM interactions. Apparently, there is a similar special point δ_c where the DM interaction has no influence on the systemic dimerisation, either. Here, the DM interaction favours systemic dimerisation in $\delta < \delta_c$, whereas the DM interaction acts against systemic dimerisation in $\delta > \delta_c$. It is just contrary to the case of $\eta = 1$.

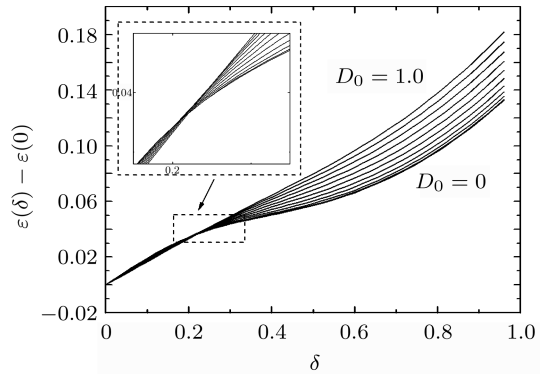


Fig. 2. Variations of dimerisation energy density with parameter δ in different DM interactions (η = 0) in open chain, with $J_0 = 1$, and $A_0 = 0$.

Secondly, the effects of the KSEA superexchange interactions on the systemic ground state properties of the one-dimensional spin-Peilers model in open chain are described in Fig. 3. Figure 3(a) shows the magnified vertical axis from point 0.039 to 0.06 and the magnified horizontal axis the abscissa from 0.21 to 0.4. Similarly, Fig. 3(b) displays the magnified vertical axis from point 0.029 to 0.039 and the magnified horizontal axis from 0.15 to 0.21; Figure 3(c) indicates the magnified vertical axis from point 0.019 to 0.029 and the magnified horizontal axis from 0.095 to 0.15; Figure 3(d) exhibits the magnified vertical axis from point 0.0105 to 0.019 and the magnified horizontal axis from 0.055 to 0.095. The results show that systemic ground state energy densities vary with dimerisation parameter δ in different KSEA superexchange interactions. The points of intersection are dense in a certain numberical value range, e.g., Fig. 3(b), and they are sparse in other numberical value ranges, e.g., Figs. 3(a), 3(c) and 3(d), though there is not a similar fixed special numberical value point. We can see that the characteristics of the antisymmetric anisotropy DM interaction and the symmetric anisotropy KSEA interaction are analogous in the sense of the contribution of systemic dimerisation in open chain.

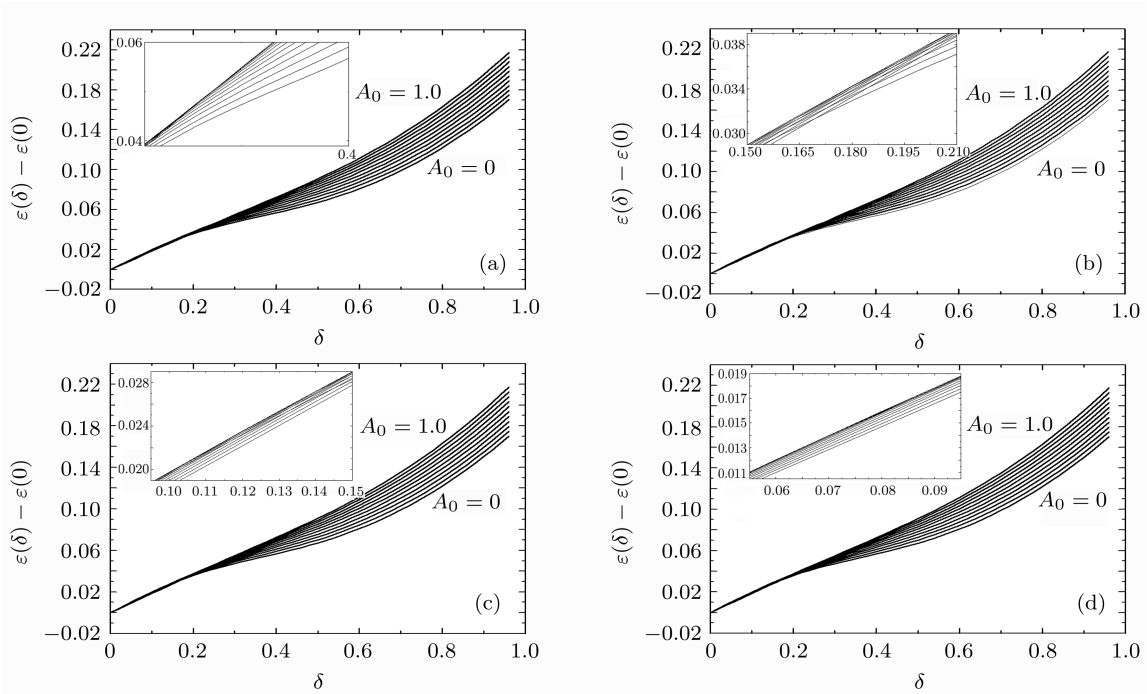


Fig. 3. Variations of dimerisation energy density with parameter δ in different KSEA interactions in open chain, with $J_0 = 1$, and $D_0 = 0$. Insets show the magnified vertical axes from points 0.039 to 0.06 (a), 0.029 to 0.039 (b), 0.019 to 0.029 (c), and 0.0105 to 0.019 (d), and the magnified horizontal axes from points 0.21 to 0.4 (a), 0.15 to 0.21(b), 0.095 to 0.15 (c), and 0.055 to 0.095 (d).

4. Conclusion

In this paper, the effects of the DM and the KSEA superexchange interactions on the systemic ground state properties of the one-dimensional spin-Peilers model in open chain have been studied by using the Lanczos numerical method. The results show that DM interaction has no effect on the systemic dimerisation at a certain fixed special numberical value point, no matter whether it is relative or irrelative to the systemic dimerisation. The KSEA interaction has no similar special numberical value point, but the points of intersection are dense relatively in a certain numberical value range, and sparse in other ranges. So we can conclude that the characteristics of the antisymmetric anisotropy DM interaction and the symmetric anisotropy KSEA interaction are analogous in the sense of contribution of systemic dimerisation in open chain, though the antisymmetric anisotropy DM interaction differs from the symmetric anisotropy KSEA interaction.

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