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The symmetric and antisymmetric superexchange interactions in spin-Peierls system*

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The influences of Dzyaloshinskii–Moriya (DM) interaction and Kaplan–Shekhtman–Entinwohlman–Aharony (KSEA) interaction on the dimerization of a spin-Peierls system are investigated theoretically by using the Lanczos numerical method. The ground state of the spin-Peierls system is still dimerized phase when both of the DM and the KSEA interactions have the same value with Heisenberg interaction. It is found that the KSEA interaction and uniform DM interaction are always against systemic dimerization, but the staggered DM interaction acts in favour of dimerization. Furthermore, the influences of the DM and the KSEA interactions are also studied in terms of the ground state index rate and the energy gap index rate of the dimerized Heisenberg system. The results show that the DM interaction makes the index rates larger, while the KSEA interaction makes them smaller.

Keywords: dimerization, Dzyaloshinskii–Moriya interaction, Kaplan–Shekhtman–Entinwohlman-Aharony interaction
PACC: 7540F, 7550E, 7530G

1. Introduction

Low-dimensional quantum-spin system is a topic of basic and applied interest due to its fascinating properties. The one-dimensional (1D) antiferromagnetic $s = 1/2$ chain has been extensively investigated both theoretically and experimentally. However, many experiments on higher-dimensional compounds indicate that the isotropic exchange interaction is not sufficient to describe magnetic properties such as weak ferromagnetism in many systems.[1−5] Many years ago, Dzyaloshinskii pointed out that a term of the form $\boldsymbol{D} \cdot (\boldsymbol{S}_1 \times \boldsymbol{S}_2)$,[6] where $\boldsymbol{D}$ is Dzyaloshinskii vector and $\boldsymbol{S}_{1,2}$ are the sublattice magnetizations, favours a canted spin arrangement over the antiferromagnetic one and a weak ferromagnetic moment. This term is later derived by Moriya.[7,8] The calculation of Moriya showed that besides the Dzyaloshinskii–Moriya (DM) term, a symmetric anisotropy term of the form $\boldsymbol{S} \cdot \mathbf{A} \cdot \boldsymbol{S}$ was also obtained, but was assumed to be negligible compared with the antisymmetric one. 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 has to be such that it compensates exactly spin anisotropy induced by the DM term. For this kind of system, the symmetric anisotropy term is called the Kaplan–Shekhtman–Entinwohlman–Aharony (KSEA) term and it 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 KSEA interaction superimposed on the DM interaction comes from neutron diffraction and inelastic neutron scattering experiments on $Ba_2CuGe_2O_7$.[3]

The ground state properties of the spin-Peierls system with the DM and the KSEA interactions have ever been studied.[12] But how the DM and the KSEA interactions affect the 1D dimerized Heisenberg system ground state index rate and the energy gap index rate is not clear. Here, we will discuss them in detail.

2. The model

The Hamiltonian of 1D dimerized Heisenberg chain with the DM and the KSEA interactions is

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

where J_n is a general spin-Peierls interaction parameter, i.e. it is intrachain Heisenberg interaction parameter, $\boldsymbol{D}_n$ is the antisymmetric anisotropy DM interaction parameter between the spins along the chain, the third term describes symmetric anisotropy KSEA interaction, where $\mathbf{A}$ is KSEA interaction tensor. In the absence of the KSEA interaction, the model with DM interaction describes the physical materials $CuGeO_3$ very well.[13−15] Generally, in a system having full $SU(2)$ symmetry, such as $Ba_2CuGe_2O_7$,[3] $\boldsymbol{D}$ and $\mathbf{A}$ are not independent of each other.[11] For the convenience of discussion, we use the quantization axis $\hat{z}$ for the spins, such that $\boldsymbol{D}=D_0(1+\eta(-1)^n\delta)\hat{z}$, and the anisotropy tensor $\mathbf{A}$ reduces to $A_{zz}=A_0$ and all other components become zero.

The Hamiltonian (1) can be simplified by a canonical transformation[16]

$$H=\mathrm{e}^{-\mathrm{i}U}H\mathrm{e}^{\mathrm{i}U} \quad (2)$$

with

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

It should be noted that this transformation is applied to open chains. The periodic boundary condition requires $\alpha_N=0\mathrm{mod}\,2\pi$, which is not generally satisfied. However, the thermodynamic properties of the initial and transformed Hamiltonian are identical since in the thermodynamic limit $N\to\infty$, the influence of boundary conditions can be neglected.

So, the form of Eq.(1) can be written as

$$H=\sum_{n=1}^{N}\{[A+(-1)^nB](S_n^x\cdot S_{n+1}^x+S_n^y\cdot S_{n+1}^y)+\{J_0[1+(-1)^n\delta]+A_0\}S_n^z\cdot S_{n+1}^z\}+\frac{1}{2}KN\delta^2,$$
$$A=\frac{\sqrt{J_0^2(1+\delta)^2+D_0^2(1+\eta\delta)^2}+\sqrt{J_0^2(1-\delta)^2+D_0^2(1-\eta\delta)^2}}{2},$$
$$B=\frac{\sqrt{J_0^2(1+\delta)^2+D_0^2(1+\eta\delta)^2}-\sqrt{J_0^2(1-\delta)^2+D_0^2(1-\eta\delta)^2}}{2}. \quad (3)$$

3. Numerical calculation and result analysis

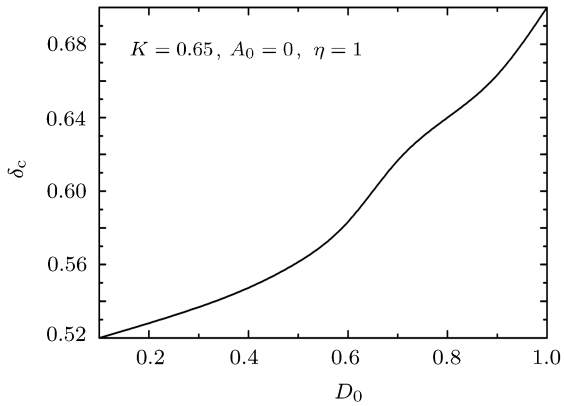


Fig.1. Variation of dimerization displacement δ_c with parameter D_0, for $\eta=1$.

In the following, we first study the influences of Heisenberg, DM and KSEA interactions on systemic dimerization, respectively, then the influences of DM, KSEA interactions on the dimerized Heisenberg system ground state index rate and the energy gap index rate. The lattice number in calculation is 30. To obtain dimerization displacement of systemic ground state, we look for the mini-point of ground state energy density $\varepsilon(\delta)-\varepsilon(0)$ which varies with dimerization displacement parameter δ. In all the calculations, we set systemic lattice aberration elastic coefficient $K=0.65$ and $J_0=1$ according to the concrete properties of materials and the parameter of NMR experimental result, where $J_0=1$ acts as energy units.

The variation of dimerization displacement with $D_0(\eta=1)$ is described in Fig.1. We find that the dimerization displacement δ_c increases gradually with increasing DM interaction, which is related with the mini-point of systemic ground state energy density. It implies that DM interaction ($\eta=1$) acts in favour of dimerization. The change of dimerization displacement δ_c with D_0 ($\eta=0$) is shown in Fig.2. While the change of dimerization displacement δ_c with A_0 is de-

scribed in Fig.3. Here, systemic steady ground state dimerization parameter δ_c will decrease with increasing DM ($\eta = 0$) and KSEA interaction. These results imply that DM ($\eta = 0$) interaction and KSEA interaction are both against systemic dimerization. That is to say, the staggered DM interaction favours systemic dimerization, whereas the uniform DM interaction is against it, but KSEA interaction is always against systemic dimerization.

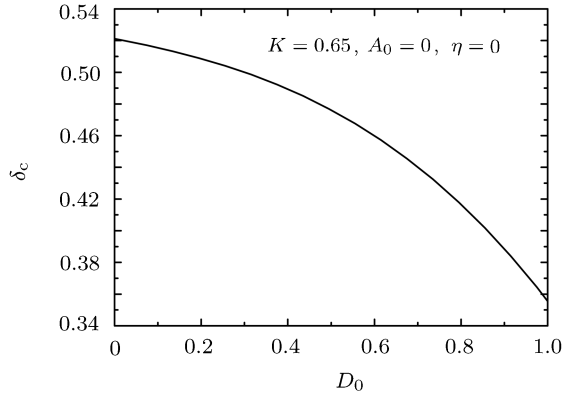


Fig.2. Variation of dimerization displacement δ_c with parameter D_0, for $\eta = 0$.

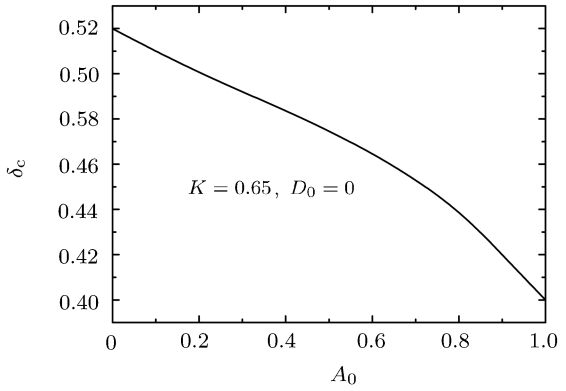


Fig.3. Variation of dimerization displacement δ_c with parameter A_0.

Now that the staggered DM interaction（that is $\boldsymbol{D} = D_0(1 + (-1)^n\delta)\hat{z}$) is in favour of systemic dimerization, while the KSEA interaction always acts against systemic dimerization, so that we can find some points on which the systemic dimerization raised by the staggered DM interaction will be killed by the KSEA interaction, as shown in Fig.4. Here, systemic dimerization is unchangeable. Otherwise, in Fig.5, the ground state energy density varying with dimerization is also studied when the DM ($\eta = 0$) and the KSEA interactions have the same value as the Heisenberg interaction has. The result shows that the systemic dimerization is still present, and that the DM and the KSEA interactions are much smaller than the Heisenberg interaction in usual cases.

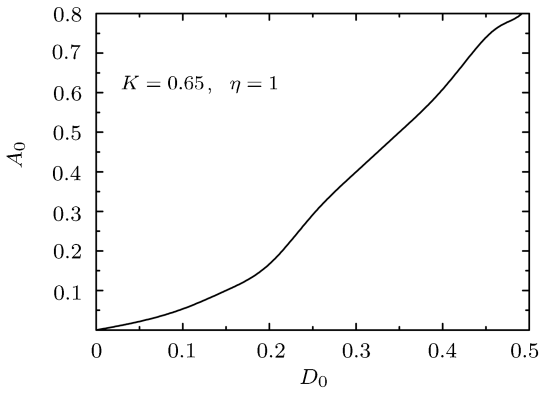


Fig.4. The influences of both the DM and the KSEA interactions on systemic dimerization, with $\eta = 1$ (systemic dimerization is invariable in this figure).

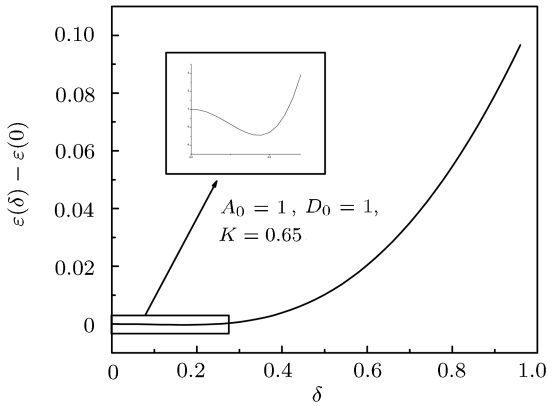


Fig.5. The system dimerization energy density versus dimerization parameter δ, with $\eta = 0$, $J_0 = 1$ and $D_0 = A_0 = 1$ (in order to make the DM and the KSEA interactions take the same value as Heisenberg interaction).

However, the systemic dimerization will decrease to zero when the DM ($\eta = 0$) and the KSEA interactions are large enough as shown in Fig.6.

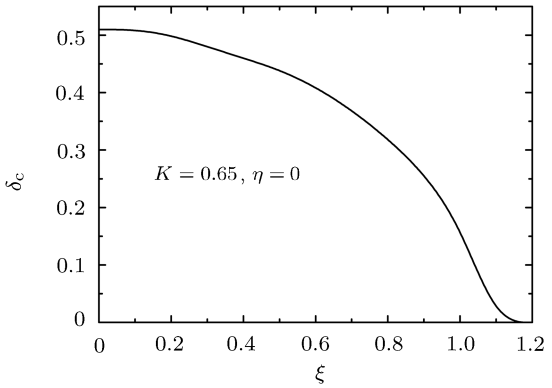


Fig.6. The systemic dimerization parameter $\delta_c$versus parameter ξ, with $D_0 = A_0 = \xi$. DM interaction is of the form $\boldsymbol{D} = D_0\hat{z}$.

In the following, the influences of the DM and the KSEA interactions on ground state index rate and the energy gap index rate of the dimerized Heisenberg system will be studied. Naturally, the systemic elastic energy is not considered. Firstly, we calculate the influence of the DM ($\eta = 1$) interaction on the systemic energy gap index rate. The result is given in Fig.7.

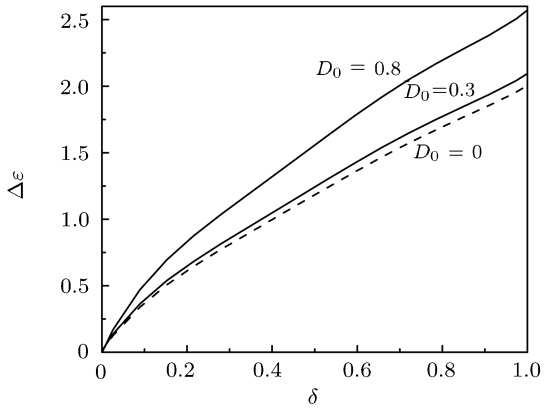


Fig.7. Spin-energy-gap versus dimerization δ, for different values of DM.

It is clear that the systemic energy gap varying with dimerization parameter δ is different for different intensity of DM interaction. The dashed line demonstrates the energy gap index rate, and it shows that the DM interaction makes the energy gap index rate larger. The influence of KSEA interaction on systemic energy gap index rate is given in Fig.8.

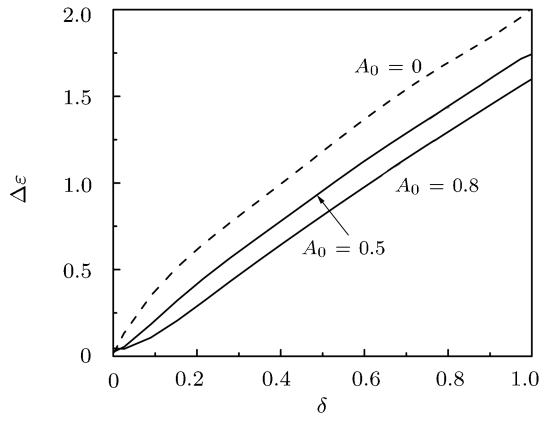


Fig.8. Spin-energy-gap as a function of dimerization δ, for different values of KSEA interaction.

It is clear that the KSEA interaction makes it smaller. Furthermore, we give the influence of the DM and the KSEA interactions on the ground state index rate in Fig.9. The dashed line demonstrates the ground state index rate. The results show that the DM interaction makes it larger, and the KSEA interaction makes it smaller.

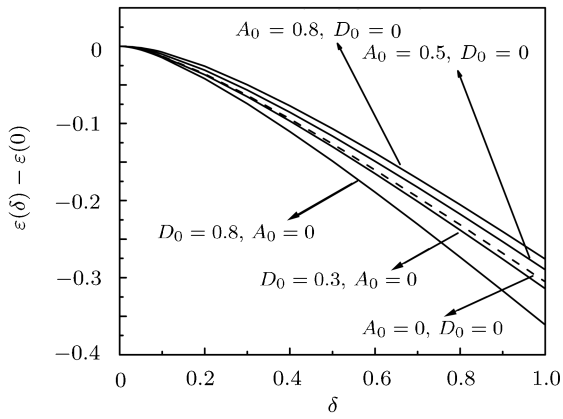


Fig.9. Systemic ground state energy density versus dimerization parameter δ, for different values of the DM and the KSEA interactions.

4. Conclusion

In this paper, the influences of the DM and the KSEA interactions on the dimerization of 1D spin-Peierls system have been studied by use of the Lanczos numerical method. It is shown that the DM interaction acts against dimerization when the DM interaction is irrelative to the dimerization. On the other hand, the DM interaction is favourable for dimerization when the DM interaction depends on the dimerization. However, the KSEA interaction is always against dimerization. The KSEA interaction affects the contribution of the DM interaction to the dimerization, and even offsets the effect of the DM interaction. The dimerization vanishes when the DM and the KSEA interactions are large enough in some special conditions. Otherwise, the ground state of spin-Peierls system is still a dimerized phase when the DM and the KSEA interactions take the same value as the Heisenberg interaction. At the same time, the influences of the DM and the KSEA interactions on the 1D dimerized Heisenberg system ground state index rate and the energy gap index rate are also studied. The results show that the DM interaction will raise them, whereas the KSEA interaction will decrease them.

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