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LETTER TO THE EDITOR

The Dzyaloshinskii–Moriya interaction in spin–Peierls systems

Zhiguo Yang, Zhiguo Wang and Hong Chen

Pohl Institute of Solid Physics, Tongji University, 200092, Shanghai, People's Republic of China

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Abstract

The influence of Dzyaloshinskii–Moriya (DM) interaction on the spin–Peierls systems is studied by use of theoretical analysis and the Lanczos numerical method. The ground state of the spin–Peierls system is still a dimerized phase when DM interaction is present. The results show that the uniform DM interaction is always against dimerization but the staggered DM interaction may act in favour of or against dimerization. There exists a critical point where the staggered DM interaction has no influence on dimerization.

Since the first inorganic spin–Peierls compound CuGeO_3 [1] was found in 1993, it has attracted much attention in condensed matter physics. Various methods have been applied to obtain an accurate description of its phase diagram. In general, this compound is considered as a linear Heisenberg antiferromagnetic chain along the c -axis with the exchange interaction dependence on the intersite distance. Recently, several electron paramagnetic resonance investigations have revealed that there exists Dzyaloshinskii–Moriya (DM) interaction [2,3] in CuGeO_3 [4–6]. The DM interaction is found nowadays to be present in a number of quasi-one-dimensional and two-dimensional magnetic systems. For example it is found that the DM interaction plays a central role in the magnetic properties of $\text{BaCu}_2\text{M}_2\text{O}_7$ ($M = \text{Si}$ and Ge) [7, 8] and has been used to interpret an anomalous magnetic behaviour in the YVO_3 – SrVO_3 system [9].

The DM interaction is an antisymmetric spin exchange interaction between two spins s_1, s_2 , described as $\mathbf{D} \cdot (s_1 \times s_2)$. In a chain, vector \mathbf{D} may spatially vary in both direction and magnitude. However, the symmetry arguments usually rule out most of the possibilities and the theoretical discussions focus mainly on two principal cases. One is the uniform DM interaction [10], the other is the staggered DM interaction [11]. The influence of the uniform or staggered DM interaction on the ground state properties of the Heisenberg one-dimensional model has been reported in [12, 13]. In the uniform case the model can be reduced to the XXZ spin exchange model, and then solved exactly. Recently, a model of the XY spin chain with a ternary DM interaction has also been introduced and solved [14]. For both Heisenberg and XY models with DM interaction, the spin–spin correlation function possess an incommensurate structure [15].

For the spin–Peierls system, using numerical calculation, Derzhko and his co-workers [16] analysed the ground-state energy of the dimerized spin- $\frac{1}{2}$ transverse XX and Heisenberg chains with DM interaction to study the influence of the latter interaction on the spin–Peierls instability. They found that uniform DM interaction may act against the dimerization but staggered DM interaction may act in favour of the dimerization. However, whether the staggered DM interaction always enhances the dimerization has not been clearly answered. In this letter, we use theoretical analysis and a numerical method to study the effect of the staggered DM interaction on the dimerization. After a canonical transformation, the previous results will become clear. Furthermore, we find that whether the staggered DM interaction enhances the dimerization depends on the dependence of DM interaction on the distortion amplitude and there exists a critical point where DM interaction has no influence on dimerization. If the dependence of staggered DM interaction on the distortion amplitude is weak DM interaction will weaken the dimerization; when its dependence is large enough DM interaction will enhance the dimerization.

We deal mainly with uniform and staggered DM interaction in the spin–Peierls–Heisenberg chain, and study the effect of DM interaction on dimerization in detail. The spin–Peierls–Heisenberg chain Hamiltonian we consider has the form

$$H = \sum_n [J_n (\mathbf{s}_n \cdot \mathbf{s}_{n+1}) + \mathbf{D}_n \cdot (\mathbf{s}_n \times \mathbf{s}_{n+1})] + \frac{1}{2} K \sum_n (u_n - u_{n+1})^2, \quad (1)$$

where n denotes the sites of a chain with total site number N_0 and $\mathbf{s}_n (s_n^x, s_n^y, s_n^z)$ are $s = 1/2$ spin operators. The first term in the Hamiltonian (1) is the isotropic exchange interaction with spin–Peierls coupling $J_n = J[1 + \alpha(u_n - u_{n+1})]$; the second term represents the antisymmetric anisotropic exchange interaction or DM interaction between the neighbouring sites n and $n + 1$. The last term is the elastic energy, with u_n the displacements of magnetic ions. Without DM interaction the ground state of Hamiltonian (1) is in general in the dimerized phase, i.e. $u_n - u_{n+1} = (-1)^n u_0$, and in the following we denote the dimerization parameter by $\delta = \alpha u_0$.

For simplification, we choose the vector \mathbf{D}_n to be directed along the z -axis, $\mathbf{D}_n = |D_n^z| \hat{z}$. It has been argued that the directions of \mathbf{D}_n are not changed by the dimerization [6]; however, the dependence of the isotropic exchange interaction and DM interaction on the intersite distance may be different [3]. Therefore, two kinds of DM interaction, i.e. uniform and staggered interaction described by $D_n^z = D[1 + (-1)^n \beta \delta]$, will be studied. The parameter β is introduced to describe the effect of different DM interaction dependence on the intersite distance. If $\beta = 0$ the DM interaction does not depend on the lattice distortion, i.e. DM interaction is uniform, whereas for $\beta = 1$ the dependence of DM interaction on the lattice distortion is the same as that for the isotropic exchange interaction J_n .

We observe that the Hamiltonian (1) can be simplified by a canonical transformation [13]

$$H = e^{-iU} H e^{iU} \quad (2)$$

with

$$U = \sum_{n=1}^{N_0} \alpha_n s_n^z, \quad \alpha_n = \sum_{i=1}^{n-1} \tan^{-1}(D_i^z / J_i) \quad (3)$$

and $\alpha_1 = 0$. It should be noted that this transformation was applied to open chains. Periodic boundary conditions require $\alpha_{N_0} = 0 \pmod{2\pi}$, which is not generally satisfied. However, the thermodynamic properties of the initial and transformed Hamiltonian are identical since in the thermodynamic limit $N_0 \rightarrow \infty$ the influence of boundary conditions can be neglected.

After the transformation, the Hamiltonian has the form

$$\tilde{H} = \sum_n \left[\sqrt{J_n^2 + D_n^{z2}} (s_n^x s_{n+1}^x + s_n^y s_{n+1}^y) + J_n (s_n^z s_{n+1}^z) \right] + \frac{N_0}{2} K \left(\frac{\delta}{\alpha} \right)^2. \quad (4)$$

We notice that $\sqrt{J_n^2 + D_n^{z^2}}$ can be written as $J'(1 + (-1)^n \delta')$ with

$$J' = J \left[\frac{\sqrt{\rho + \sigma}}{2} + \frac{\sqrt{\rho - \sigma}}{2} \right] \quad (5)$$

and

$$\delta' = \frac{\sigma}{\rho + \rho \sqrt{1 - \left(\frac{\sigma}{\rho}\right)^2}} \quad (6)$$

where we have set

$$\rho = 1 + \delta^2 + (D/J)^2 + (\beta\delta D/J)^2 \quad (7)$$

and

$$\sigma = 2(1 + (D/J)^2\beta)\delta. \quad (8)$$

Now it is clear that the above Hamiltonian can be reexpressed as a new spin–Peierls Hamiltonian

$$\tilde{H} = \sum_n [J(1 + (-1)^n \delta')(s_n^x s_{n+1}^x + s_n^y s_{n+1}^y) + J'_n(s_n^z s_{n+1}^z)] + \frac{N_0}{2} K' \delta'^2. \quad (9)$$

This implies that the introducing of DM interaction induces the varying of parameters J'_n and K' , i.e. exchange coupling and elastic coefficient. In the special cases of $\beta = 0, 1$, we obtain

$$K'|_{\beta=0} \simeq (1 + (D/J)^2)^{\frac{3}{2}} K, \quad (10)$$

and

$$K'|_{\beta=1} \simeq (1 + (D/J)^2)^{-\frac{1}{2}} K. \quad (11)$$

It is evident that when the uniform DM interaction is included the dimerization parameter δ of the spin–Peierls system will decrease due to the increasing elastic coefficient, while the staggered DM interaction with $D_n^z = D[1 + (-1)^n \delta]$ will enhance the dimerization due to the decreasing elastic coefficient.

In the above, we study the influence of DM interaction on the dimerization qualitatively. This analysis is consistent with the conclusion of previous works on the XX model [16]. Since the DM interaction will induce anisotropy in the exchange coupling parameter, the above discussion is not rigorous. In the following, we use the numerical method to study it exactly.

We use the Lanczos method [18, 19] to calculate the low-lying energy spectrum of Hamiltonian (4) with finite size. Through comparing the total ground-state energy of the dimerized chain with the uniform case in the presence of DM interaction on dimerization, we can analyse the influence of DM interaction on dimerization. In calculation, it should be noted that the system always has gaps due to the finite-size effect, so the system does not have conformal invariance. In order to extract the finite-size effect, we use the following extrapolated formula to obtain the results of the infinite-length chain:

$$\varepsilon_0(J, D, \beta, \delta, N) = \varepsilon_0(J, D, \beta, \delta) + \frac{\rho}{N} + \frac{\lambda}{N^2}, \quad (12)$$

where the parameters ρ and λ will be determined by fitting the numerical data. The energy density $\varepsilon_0(\delta)$ of the ground state was calculated for δ varying from 0 to 1. $\varepsilon_0(\delta)$ consists of the magnetic part and the elastic part. In figure 1, $\varepsilon_0(\delta) - \varepsilon_0(0)$ versus N^{-1} was plotted for $\delta = 0.2$, $D = 0.8$, $\beta = 1$, $K = 0.85$ as an example to verify our finite scaling law equation (12). Therefore, from the numerical results and the scaling law, we can obtain the ground-state energy $\varepsilon_0(\delta)$ of an infinite-length chain, and study its dependence on the model parameters. The derivative of $\varepsilon_0(\delta)$ versus δ is considered for various cases of DM interaction.

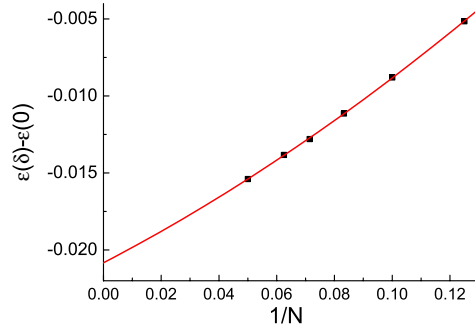


Figure 1. The dependence of the ground-state energy on the lattice number. The solid curve in the figure is the function $-0.0283 + 0.09752/N + 0.22466/N^2$.

(This figure is in colour only in the electronic version)

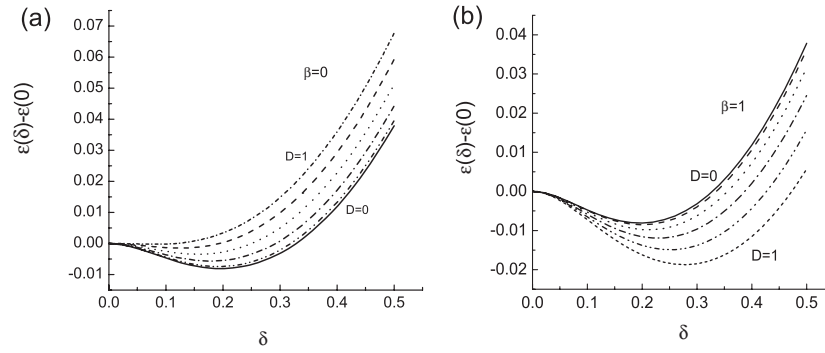


Figure 2. Dependence of $\varepsilon(\delta) - \varepsilon(0)$ on δ for the spin-Peierls chain with DM interaction. $J = 1$, $Ka^2 = 0.85$; (a) is for the case of uniform DM interaction ($\beta = 0$); (b) is for the case of staggered DM interaction ($\beta = 1$).

The condition $(\partial\varepsilon_0(\delta))/\partial\delta = 0$ always has a nonzero solution δ^* . Because δ^* is a function of parameters D , β and K , we can discuss the influences of DM interaction on the dimerization. In figure 2 we show the relationship between $\varepsilon_0(\delta) - \varepsilon_0(0)$ and δ with $\beta = 0, 1$ for D varying from 0 to 1. It is evident that for $\beta = 1$ DM interaction acts in favour of dimerization, whereas against it for $\beta = 0$. This result is similar to that of [16].

From the above result, we can deduce that there should exist a critical value of β between $\beta = 0$ and 1 where the staggered DM interaction has no effect on dimerization. We study the effect of varying parameter β with a definite value of K . For definite K we find that there exists a unique critical value of $\beta = \beta^*$: when $\beta > \beta^*$ the DM interaction will enhance the dimerization; otherwise the DM interaction will lower the dimerization. This result is plotted in figure 3. Furthermore, we obtain the relation between elastic coefficient K and critical value β^* . If the elastic coefficient K increases, the parameter β^* increases too. The relationship of $K-\beta^*$ is shown in figure 4.

As a conclusion, in this letter, we employ the Lanczos method to study the influence of DM interaction on the spin-Peierls instability in detail. The result shows that for a definite elastic coefficient whether DM interaction is in favour of or against dimerization is determined by the dependence on the intersite distance of DM interaction. When $\beta = \beta^*$, the DM interaction has no effect on dimerization, and β^* increases with increasing elastic coefficient.

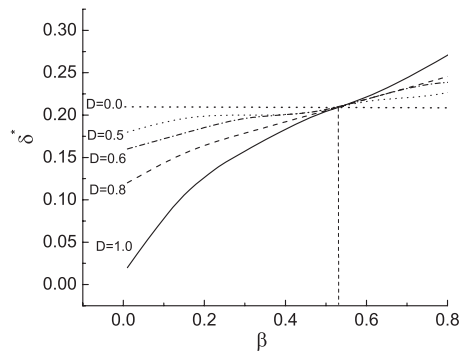


Figure 3. The relationship between the displacements of magnetic ions and the dependence on the intersite distance of DM interaction.

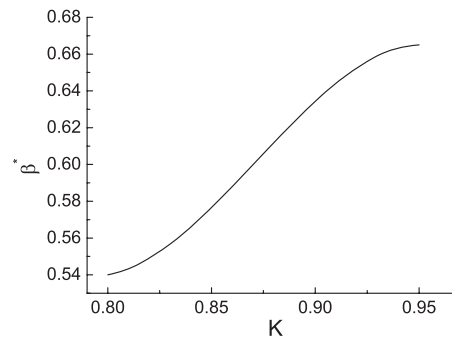


Figure 4. The influence of elastic coefficient K on the critical value of parameter β^* .

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References

- [1] Hase M, Terasak I and Uchinokura K 1993 *Phys. Rev. Lett.* **70** 3651
- [2] Dzyaloshinsky I 1958 *J. Phys. Chem. Solids* **4** 241
- [3] Moriya T 1960 *Phys. Rev.* **120** 91
- [4] Yamada I, Nishi M and Akimitsu J 1996 *J. Phys.: Condens. Matter* **8** 2625
- [5] Glazkov V N, Smirnov A I, Petrenko O A, Paul D M, Vetkin A G and Eremina R M 1998 *J. Phys.: Condens. Matter* **10** 7879
- [6] Nojiri H, Ohta H, Okubo S, Fujita O, Akimitsu J and Motokawa M 1999 *J. Phys. Soc. Japan* **68** 3417
- [7] Tsukada I *et al* 1999 *Phys. Rev. B* **60** 6601
Zheludev A *et al* 2000 *Phys. Rev. Lett.* **85** 4799
Kenzelmann M *et al* 2001 *Phys. Rev. B* **64** 054422
- [8] Tsukada I *et al* 2000 *Phys. Rev. B* **62** R6061
- [9] Sakai K, Migita S, Yamada K, Shindo T, Fujii H and Murakami H 1999 *Physica C* **317-18** 464-70
- [10] Schotte U, Kelnberger A and Stusser N 1998 *J. Phys.: Condens. Matter* **10** 6391
- [11] Ian Affleck and Oshikawa M 1999 *Phys. Rev. B* **60** 1038
Ian Affleck and Oshikawa M 1997 *Phys. Rev. Lett.* **79** 2883
- [12] Alcaraz F C and Wreszinski W F 1990 *J. Stat. Phys.* **58** 45
- [13] Aristov D N and Maleyev S V 2001 *Physica B* **297** 78
- [14] Gottlieb D and Rossler J 1999 *Phys. Rev. B* **60** 9232
- [15] Kontorovich V M and Tsukernik V M 1967 *Zh. Eksp. Teor. Fiz.* **52** 1446
- [16] Derzhko O, Richter J and Zaburannyi O 2000 *J. Phys.: Condens. Matter* **12** 8661
- [17] Aristov D N and Maleyev S V 2000 *Phys. Rev. B* **62** R751
- [18] Wang Z G, Zhang H Y and Xu B W 1999 *Commun. Theor. Phys.* **32** 313
- [19] Roomany H H, Wyld H W and Holloway L E 1980 *Phys. Rev. D* **26** 1558
- [20] Pincus P 1971 *Solid State Commun.* **9** 1971
Beni G and Pincus P 1972 *J. Chem. Phys.* **57** 3531