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Spin–Peierls instability in a quantum spin chain with Dzyaloshinskii–Moriya interaction

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Abstract. We analysed the ground-state energy of some dimerized spin-1/2 transverse XX and Heisenberg chains with Dzyaloshinskii–Moriya (DM) interaction to study the influence of the latter interaction on the spin–Peierls instability. We found that DM interaction may act either in favour of the dimerization or against it. The actual result depends on the dependence of the DM interaction on the distortion amplitude in comparison with such dependence for the isotropic exchange interaction.

The spin–Peierls instability is known as a magnetic analogue of the conventional Peierls instability in electron–phonon systems. A uniform quantum spin chain at low temperatures may become unstable towards dimerization owing to the interaction with lattice degrees of freedom. This occurs because the dimerized lattice distortion lowers the magnetic energy by a greater amount than the increase in the elastic energy due to deformation. Starting in the 1970s with organic compounds exhibiting spin–Peierls transition, the interest in the spin–Peierls instability of quantum spin chains was renewed with the discovery of the inorganic spin–Peierls compound CuGeO_3 in 1993 [1, 2]. To model appropriately the spin degrees of freedom of the spin–Peierls compounds, the pure Heisenberg chain as well as its modifications, which include frustration or interchain interaction, are considered. As a rule, since those models represent quantum many-body systems, only approximate results can be obtained. However, some generic features of the spin–Peierls systems can be illustrated in a simplified but exactly solvable quantum spin model, namely, the transverse XX chain [3–6].

In the present paper we discuss the influence of the Dzyaloshinskii–Moriya (DM) interaction [7] on the spin–Peierls dimerization in the adiabatic limit. The presence of DM interaction for CuGeO_3 was proposed in references [8–10] in order to explain the EPR and ESR experimental data. The structure of the DM interaction in the cuprates was examined in references [11, 12]. The influence of this interaction on the ground-state properties of the one-dimensional and two-dimensional Heisenberg models was studied in references [13–15]. Also,

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the multisublattice transverse XX chain with DM interaction was introduced in reference [16]; however, the spin–Peierls instability was discussed only for one limiting case (see below) in the absence of an external field. DM interaction was found to be present in a number of quasi-one-dimensional magnets (see, e.g., [17, 18] and also [19] in which $\text{RbCoCl}_3 \cdot 2\text{H}_2\text{O}$ is described as a pure DM chain) and a study of one-dimensional DM Hamiltonians seems to be of great importance.

Several mechanisms which may destroy the dimerized phase in the Heisenberg chain were discussed in the literature—in particular, an external field or an Ising anisotropy. XX anisotropy also suppresses the dimerized phase although it does not destroy it completely. Therefore, initially one may expect that the appearance of an anisotropy in the form of the DM interaction could act against dimerization. Although we shall find that the Heisenberg chain, with increase of the DM interaction, may become similar to the XX chain, both enhancement and suppression of the dimerized phase are possible, depending on the details of the distortion dependence of the DM interaction.

In our study we follow the idea of reference [3] and compare the total ground-state energies of the dimerized and uniform chains in the presence of DM interaction. First we demonstrate that in some cases the DM interaction can be eliminated by a spin coordinate transformation resulting in a model with an anisotropic exchange interaction. This observation permits us to study rigorously the influence of DM interaction on the spin–Peierls instability in the transverse XX chain using the exact results for thermodynamic quantities of the regularly alternating transverse XX chain obtained recently with the help of continued fractions [20]. (The approach exploiting continued fractions, in contrast to the approaches used in previous works [3–6, 16], allows one to consider in a similar way not only the dimerized lattice but also more complicated lattice distortions.) Further, we discuss the case of the Heisenberg chain with DM interaction using exact diagonalization of finite chains. The exact analytical findings for the XX chain are helpful for the interpretation of the finite-chain results for the more realistic Heisenberg chain. In the present study we are interested in describing the generic features originated by DM interaction, and therefore no compound-specific parameters are considered.

To begin with, we consider a nonuniform chain of $N \rightarrow \infty$ spins $\frac{1}{2}$ governed by the isotropic Heisenberg Hamiltonian with DM interaction

$$H = \sum_n \Omega_n s_n^z + \sum_n (J_n (s_n \cdot s_{n+1}) + D_n \cdot [s_n \times s_{n+1}]). \quad (1)$$

Here Ω_n is an external field at site n , and J_n and D_n are the isotropic exchange interaction and the antisymmetric anisotropic exchange interaction or DM interaction between the neighbouring sites n and $n + 1$, respectively.

Extending the spin coordinate transformation used in reference [21] for models with nonuniform J_n and D_n , first we show how the terms with cross products can be eliminated from Hamiltonian (1) in special cases. If D_n has only one nonzero component D_n^z , one may perform local rotations about the z -axis, introducing the new spin operators $s_n^{x'} = s_n^x \cos \phi_n + s_n^y \sin \phi_n$, $s_n^{y'} = -s_n^x \sin \phi_n + s_n^y \cos \phi_n$, $\phi_n = \phi_1 + \dots + \phi_{n-1}$, $\tan \phi_m = D_m^z / J_m$ in terms of which (1) becomes [22]

$$H = \sum_n \Omega_n s_n^{z'} + \sum_n (\sqrt{J_n^2 + D_n^{z2}} (s_n^{x'} s_{n+1}^{x'} + s_n^{y'} s_{n+1}^{y'}) + J_n s_n^{z'} s_{n+1}^{z'}). \quad (2)$$

Note that such transformation can be also applied to the transverse XX chain in which the spin z -components do not interact. Assume further that D_n has only one nonzero component D_n^x . Then the local rotations must be performed about the x -axis, i.e. $s_n^{y'} = s_n^y \cos \phi_n + s_n^z \sin \phi_n$,

$s_n^{z'} = -s_n^y \sin \phi_n + s_n^z \cos \phi_n$ with $\tan \phi_n = D_n^x/J_m$, resulting in

$$H = \sum_n \Omega_n (\sin \phi_n s_n^{y'} + \cos \phi_n s_n^{z'}) + \sum_n (J_n s_n^{x'} s_{n+1}^{x'} + \sqrt{J_n^2 + D_n^{x2}} (s_n^{y'} s_{n+1}^{y'} + s_n^{z'} s_{n+1}^{z'})). \quad (3)$$

Proceeding similarly for $\mathbf{D}_n = (0, D_n^y, 0)$, one finds that the transformed Hamiltonian is given by (3) with the replacements $D_n^x \rightarrow D_n^y$, $s^{x'} \rightarrow s^{y'}$, $s^{y'} \rightarrow -s^{x'}$. In the case where \mathbf{D}_n has more than one nonzero component, the above-described elimination can be performed if the orientation of \mathbf{D}_n (but not necessarily its value $D_n = \sqrt{[D_n^{x2} + D_n^{y2} + D_n^{z2}]}$) is site independent, i.e. D_n^x/D_n , D_n^y/D_n , D_n^z/D_n do not depend on n . (Obviously, the particular site-independent orientations of \mathbf{D}_n reproduce the cases discussed above.) Really, in such a case we start from the global transformation of the coordinate system with the Eulerian angles ϕ, θ, ψ , putting $\tan \phi = D_n^y/D_n^x$, $\theta = \pi/2$, $\tan \psi = D_n^z/\sqrt{[D_n^{x2} + D_n^{y2}]}$, and then perform the above-mentioned local rotations about the x -axis with $\tan \phi_n = D_n^x/J_m$, finding as a result

$$H = \sum_n \Omega_n \left(\frac{D_n^z}{D_n} s_n^{x'} + \frac{\sqrt{D_n^{x2} + D_n^{y2}}}{D_n} (\cos \phi_n s_n^{y'} - \sin \phi_n s_n^{z'}) \right) + \sum_n (J_n s_n^{x'} s_{n+1}^{x'} + \sqrt{J_n^2 + D_n^2} (s_n^{y'} s_{n+1}^{y'} + s_n^{z'} s_{n+1}^{z'})). \quad (4)$$

It should be noted that the above-described transformations were applied to open chains. For cyclic chains, they yield the above-presented expressions (2)–(4) at least up to the boundary term. Evidently, the thermodynamic properties of the initial and transformed Hamiltonians are identical. Due to these transformations (equations (2)–(4)), one is able to exploit the broad knowledge on anisotropic Heisenberg chains and XX chains. In what follows we shall use the thermodynamic equivalence of the initial and transformed Hamiltonians both in the analytical treatment and in the numerical computations.

We proceed by considering the transverse XX chain with DM interaction having only a z -component:

$$H = \sum_n \Omega_n s_n^z + \sum_n J_n (s_n^x s_{n+1}^x + s_n^y s_{n+1}^y) + \sum_n D_n^z (s_n^x s_{n+1}^y - s_n^y s_{n+1}^x). \quad (5)$$

For the Hamiltonian (5) we are able to perform rigorous analytical calculations, since after the Jordan–Wigner transformation it reduces to noninteracting spinless fermions. As has been already mentioned, the thermodynamics of the model given by (5) is the same as that of the transverse XX chain (without DM interaction) with exchange interaction $\sqrt{[J_n^2 + D_n^{z2}]}$. The thermodynamic properties of the latter model with regular alternation in bonds and fields having finite period p have been examined recently with the help of continued fractions [20]. To study the spin–Peierls dimerization in the adiabatic limit we need the ground-state energy of a spin chain with period $p = 2$, i.e. with the sequence of parameters $\Omega_1 J_1 D_1^z \Omega_2 J_2 D_2^z \Omega_1 J_1 D_1^z \Omega_2 J_2 D_2^z \dots$. Moreover, we assume the following reasonable dimerization *ansatz*: $J_1 = J(1 + \delta)$, $J_2 = J(1 - \delta)$, $D_1^z = D^z(1 + k\delta)$, $D_2^z = D^z(1 - k\delta)$, where $0 \leq \delta \leq 1$ is the dimerization parameter. It is argued that the directions of \mathbf{D} -vectors are not changed by the dimerization [10]†. From reference [7] we know that the dependences on the intersite distance of the isotropic exchange interaction and DM interaction may be different. This effect is described by the parameter k . Putting $k = 0$, one has a chain in which D^z does not depend on the lattice distortion, whereas for $k = 1$, the dependence of D^z on the lattice distortion is the same as that for the isotropic exchange

† Note, however, that according to references [8, 10], \mathbf{D} -vectors in CuGeO_3 are parallel to one another along the \mathbf{a} -axis and they are alternating along the \mathbf{b} -axis.

interaction J . The latter case with $\Omega_n = 0$ was considered in [16]. Also, we bear in mind that, as a rule, the value of the DM interaction is significantly smaller than the value of the isotropic exchange interaction [7].

Further, we consider the case of zero temperature and look for the total energy per site $\mathcal{E}(\delta)$ which consists of the magnetic part $e_0(\delta)$ and the elastic part $\alpha\delta^2$, $\alpha > 0$. From reference [20] we know the exact expression for the magnetic ground-state energy:

$$e_0(\delta) = -\frac{1}{\pi} b_1 E\left(\psi, \frac{b_1^2 - b_2^2}{b_1^2}\right) - \frac{1}{2} |\Omega_1 + \Omega_2| \left(\frac{1}{2} - \frac{\psi}{\pi}\right) \quad (6)$$

$$b_{1,2} = \frac{1}{2} \sqrt{(\Omega_1 - \Omega_2)^2 + (I_1 \pm I_2)^2}$$

$$I_{1,2} = \sqrt{J^2(1 \pm \delta)^2 + D^2(1 \pm k\delta)^2}$$

$$\psi = \begin{cases} 0 & \text{if } b_1 \leq \frac{1}{2} |\Omega_1 + \Omega_2| \\ \arcsin \sqrt{\frac{b_1^2 - \frac{1}{4}(\Omega_1 + \Omega_2)^2}{b_1^2 - b_2^2}} & \text{if } b_2 \leq \frac{1}{2} |\Omega_1 + \Omega_2| < b_1 \\ \frac{\pi}{2} & \text{if } \frac{1}{2} |\Omega_1 + \Omega_2| < b_2 \end{cases}$$

where

$$E(\psi, a^2) \equiv \int_0^\psi d\phi \sqrt{1 - a^2 \sin^2 \phi}$$

is the elliptic integral of the second kind. We also seek for a nonzero solution $\delta^* \neq 0$ of the equation $\partial\mathcal{E}(\delta)/\partial\delta = 0$ that can be easily derived from (6). In what follows we consider the case of a uniform transverse field $\Omega_1 = \Omega_2 = \Omega_0 \geq 0$. In the limit $\delta \ll 1$ valid for hard lattices (having large values of α and corresponding to the experimental situation), one finds $b_1 = I$, $b_2 = I\aleph\delta$ with $I = \sqrt{J^2 + D^2}$ and

$$\aleph = \frac{J^2 + kD^2}{J^2 + D^2}.$$

Instead of equation (6), one then has

$$e_0(\delta) = -\frac{I}{\pi} E(\psi, 1 - \aleph^2 \delta^2) - \Omega_0 \left(\frac{1}{2} - \frac{\psi}{\pi}\right) \quad (7)$$

$$\psi = \begin{cases} 0 & \text{if } I < \Omega_0 \\ \arcsin \sqrt{\frac{I^2 - \Omega_0^2}{I^2(1 - \aleph^2 \delta^2)}} & \text{if } I\aleph\delta \leq \Omega_0 < I \\ \frac{\pi}{2} & \text{if } \Omega_0 < I\aleph\delta \end{cases}$$

whereas the equation for δ^* reads

$$\frac{2\pi\alpha}{I} = \frac{\aleph^2}{1 - \aleph^2 \delta^{*2}} (F(\psi, 1 - \aleph^2 \delta^{*2}) - E(\psi, 1 - \aleph^2 \delta^{*2})) \quad (8)$$

where

$$F(\psi, a^2) \equiv \int_0^\psi \frac{d\phi}{\sqrt{1 - a^2 \sin^2 \phi}}$$

is the elliptic integral of the first kind.

Consider at first the case $\Omega_0 = 0$. After rescaling: $I \rightarrow J$, $\alpha/\aleph^2 \rightarrow \alpha$, $\aleph\delta^* \rightarrow \delta^*$, one finds that equation (8) is exactly the same as that considered in reference [3], and thus

$$\delta^* \sim \frac{1}{\aleph} \exp\left(-\frac{2\pi\alpha}{I\aleph^2}\right).$$

Thus for $k = 1$ ($\aleph = 1$), nonzero D^z leads to an increasing of the dimerization parameter δ^* , whereas for $k = 0$ ($\aleph \leq 1$), nonzero D^z leads to a decreasing of δ^* . Let us pass to the case $0 < \Omega_0 < I$. Varying δ^* in the r.h.s. of equation (8) from 0 to 1, one calculates a lattice parameter α for which the value taken for δ^* realizes an extremum of $\mathcal{E}(\delta)$, equation (7). One immediately observes that for $\Omega_0/(I\aleph) \leq \delta^*$, the dependence of α versus δ^* remains the same as that in the absence of the field, whereas for $0 \leq \delta^* < \Omega_0/(I\aleph)$ the calculated quantity α starts to decrease. From this, one concludes that the field

$$\frac{\Omega_0}{I} = \exp\left(-\frac{2\pi\alpha}{I\aleph^2}\right)$$

makes the dimerization unstable against the uniform phase. The latter relation tells us that nonzero D^z increases the value of that field for $k = 1$ and decreases it for $k = 0$. It is known [2] that the increasing of the external field leads to a transition from the dimerized phase to the incommensurate phase rather than to the uniform phase. However, the former phase cannot appear within the framework of the adopted *ansatz* for the lattice distortions $\delta_1\delta_2\delta_1\delta_2\cdots$, $\delta_1 + \delta_2 = 0$.

Following on from the discussion of the limit $\delta \ll 1$, we now present the results for arbitrary $0 \leq \delta \leq 1$ based on (6). In figures 1, 2 we plot the changes of the total energy $\mathcal{E}(\delta) - \mathcal{E}(0)$, equation (6), versus δ and the nonzero solution δ^* of the equation $\partial\mathcal{E}(\delta)/\partial\delta = 0$ versus α , respectively, for various strengths of DM interaction. These results confirm that for $k = 1$, the DM interaction D^z acts in favour of dimerization, whereas for $k = 0$ it acts against it. To understand the validity of the data obtained by exact diagonalization of finite chains

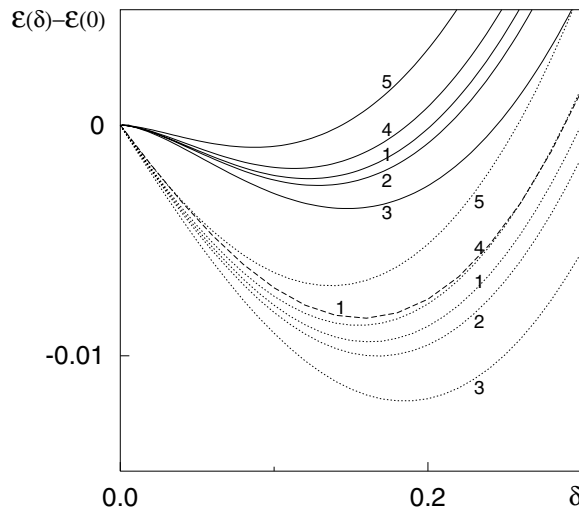


Figure 1. The dependence of $\mathcal{E}(\delta) - \mathcal{E}(0)$, equation (6), versus δ for the transverse XX chain with DM interaction. $J = 2$, $\Omega_0 = 0$, $\alpha = 0.8$, $D^z = 0$ (curve 1), $D^z = 0.4, 0.8$ for $k = 1$ (curves 2 and 3, respectively), and $k = 0$ (curves 4 and 5, respectively). Solid curves correspond to analytical calculations ($N \rightarrow \infty$), whereas dotted ones correspond to exact-diagonalization results ($N = 24$). The dashed curve corresponds to the numerical results for $N = 28$.

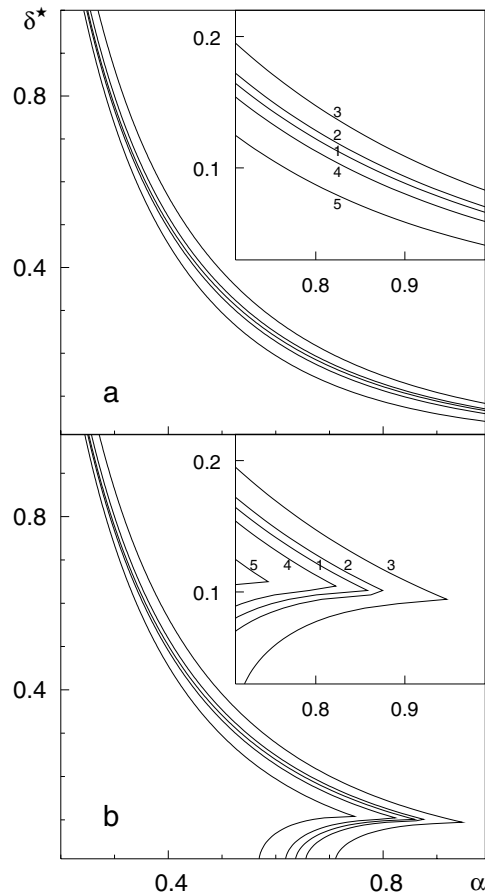


Figure 2. The dependence of δ^* versus α for the transverse XX chain with DM interaction. $J = 2$, $\alpha = 0.8$, $\Omega_0 = 0$ (a), $\Omega_0 = 0.2$ (b), $D^z = 0$ (curve 1), $D^z = 0.4, 0.8$ for $k = 1$ (curves 2 and 3, respectively), and $k = 0$ (curves 4 and 5, respectively).

that will be used below for the Heisenberg chain, we present in figure 1 also the numerical results for $\mathcal{E}(\delta) - \mathcal{E}(0)$ versus δ for $N = 24$ spins (open boundary conditions). Note that although the finite-chain results for $N = 24$ still noticeably overestimate the value of δ^* and the depth $\mathcal{E}(\delta^*) - \mathcal{E}(0)$, they nonetheless—and this is most important—reproduce qualitatively correctly the influence of D^z in both cases $k = 1$ and $k = 0$. The possible influences of D^z are reproduced correctly even for shorter chains of $N = 16, 20$ spins. Moreover, with increasing the chain length from $N = 16$ to 24 , the numerical data approach the analytical ones valid for $N \rightarrow \infty$. This expected tendency can also be seen by comparison of curves 1 for $N = 24$, $N = 28$ (the computation in this case has already become very time consuming) and $N \rightarrow \infty$ in figure 1.

Let us turn to the Heisenberg chain with DM interaction. Assume that the vectors \mathbf{D}_n have the same orientation at all sites, e.g. in the z -direction. (The assumption that $\mathbf{D}_n = (0, 0, D_n^z)$ does not lead to a loss of generality if $\Omega_0 = 0$.) In such a case, the influence of DM interaction on the thermodynamics follows from a study of the thermodynamic properties of the Heisenberg chain with anisotropic exchange interaction (2). We immediately find the appearance of XX anisotropy, since the interaction between the x - and y -components of the

spin becomes $\sqrt{[J^2(1 \pm \delta)^2 + D^2(1 \pm k\delta)^2]} (\approx \{\sqrt{[J^2 + D^2]}\}(1 \pm \aleph\delta)$ for $\delta \ll 1$), whereas between the spin z -components it remains $J(1 \pm \delta)$. Restricting consideration to small δ , we perform the redefinitions $\sqrt{[J^2 + D^2]} = J'$, $\aleph\delta = \delta'$, $\alpha/\aleph^2 = \alpha'$. As a result we come to the anisotropic alternating Heisenberg chain with xx and yy interactions $J'(1 \pm \delta')$ and zz interaction $J'\Delta(1 \pm \delta'/\aleph)$, $\Delta = J/\sqrt{[J^2 + D^2]}$ and the expression for the elastic energy per site $\alpha'\delta'^2$. Any increase of D results in an increasing of the intersite coupling J' and increasing of the XX anisotropy manifested by Δ going from 1 ($D = 0$) to 0 ($D \rightarrow \infty$). Hence, the Heisenberg chain should start to exhibit a behaviour inherent to the XX chain as D becomes large. Omitting the role of a change in the zz interaction, which becomes less important as D increases, and bearing in mind the corresponding analysis for the XX chain based on (8), we may expect that for $\Omega_0 = 0$ the dimerized phase will be enhanced for $k = 1$ (since $\alpha' = \alpha$) and will be suppressed for $k = 0$ (since $\alpha' > \alpha$). The numerical results for $\mathcal{E}(\delta) - \mathcal{E}(0)$ versus δ for the Heisenberg chain of $N = 24$ sites (open boundary conditions) shown in figure 3 confirm this expectation. As can be seen from the plots displayed, the general tendency for the changes caused by DM interaction is the same for XX and Heisenberg chains.

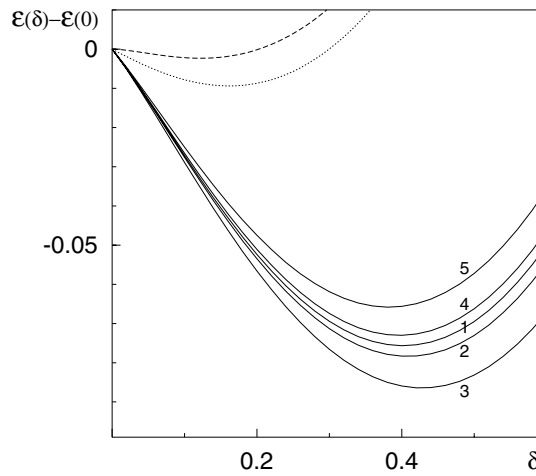


Figure 3. The dependence of $\mathcal{E}(\delta) - \mathcal{E}(0)$ versus δ for the Heisenberg chain with DM interaction obtained by exact diagonalization of finite chains. $J = 2$, $\Omega_0 = 0$, $\alpha = 0.8$, $D = 0$ (curve 1), $D = 0.4, 0.8$ for $k = 1$ (curves 2 and 3, respectively), and $k = 0$ (curves 4 and 5, respectively). We also plotted the dependence $\mathcal{E}(\delta) - \mathcal{E}(0)$ versus δ for the corresponding XX chain with $D = 0$ (i.e. curves 1 in figure 1) obtained by analytical calculation for $N \rightarrow \infty$ (dashed curve) and numerical computation for $N = 24$ (dotted curve).

To conclude, we have examined the stability of some spin- $\frac{1}{2}$ transverse XX and Heisenberg chains with respect to dimerization in the presence of DM interaction, analysing the dependence of the ground-state energy on the dimerization parameter. If the orientations of \mathbf{D}_n are the same at all sites, significant simplification occurs, i.e. the terms with cross products can be eliminated from the Hamiltonian resulting in the appearance of the anisotropy in the exchange interaction. In addition, the external field becomes more complicated, having three site-dependent components (see (4)). The transformed Hamiltonian may be more transparent and convenient for further analytical or numerical treatment. For the transverse XX chain, we have found that DM interaction having only a z -component may act either in favour of the dimerization or against it. The result of its influence depends on the dependence of the DM interaction on the amplitude of the lattice distortion in comparison with a corresponding dependence of the isotropic exchange interaction. For the Heisenberg chain, DM interaction

having the same orientation at all sites leads to XX anisotropy (and extra nonuniform on-site fields in the presence of an external field). For the Heisenberg chain without a field, we have observed qualitatively the same behaviour as in the XX chain determined by the dependence of the DM interaction on the lattice distortion.

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a preprint by Aristov and Maleyev:
Aristov D N and Maleyev S V 2000 *Preprint cond-mat/0004272* (<http://xxx.lanl.gov>)
appeared, in which a similar transformation was used in studying the influence of the DM interaction in the Heisenberg chain for the observables in polarized neutron scattering experiments.