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SPIN-$\frac{1}{2}$ PERIODIC NONUNIFORM XX CHAINS AND THE SPIN-PEIERLS INSTABILITY

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Using continued fractions we obtained the exact result for the density of magnon states of the regularly alternating spin-$\frac{1}{2}$ XX chain with the Dzyaloshinskii–Moriya interaction. We examined the stability of the magnetic chain with respect to the spin-Peierls dimerization.

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Since the discovery of the inorganic spin-Peierls compound $CuGeO_3$ the interest in the properties of spin-Peierls systems considerably increased [1]. The models that can be examined exactly play an important role in clarifying the generic features of such systems. An example of such a model is the spin-$\frac{1}{2}$ XX chain that was studied in several papers [2–4] (note, however, that in the non-adiabatic limit such a spin chain does not permit exact analysis [5]). The aim of the present study is to examine the influence of an additional Dzyaloshinskii–Moriya coupling on the spin-Peierls dimerization. The presence of such a term for $CuGeO_3$ was proposed in [6, 7]. The multisublattice spin-$\frac{1}{2}$ XX chain with the Dzyaloshinskii–Moriya interaction was introduced in [8]. In our study we follow the idea of [2] and compare the total ground state energy of the dimerized and uniform chains. However, in contrast to previous works [2–4, 8] we use the continued-fraction representation for the one-fermion Green functions [9] that allows a natural extension of the calculations for more complicated lattice distortions having finite period.

We consider $N \to \infty$ spins $\frac{1}{2}$ on a circle with the Hamiltonian

$$H = \sum_n \Omega_n s_n^z + 2\sum_n I_n \left(s_n^x s_{n+1}^x + s_n^y s_{n+1}^y\right)$$
$$+2\sum_n D_n \left(s_n^x s_{n+1}^y - s_n^y s_{n+1}^x\right). \tag{1}$$

After the Jordan–Wigner transformation one comes to tight-binding spinless fermions on a circle with complex hopping integrals. We introduce the temperature double-time one-fermion Green functions that yield the density of magnon states $\rho(E)=\mp\frac{1}{\pi N}\sum_n \mathrm{Im}G^{\mp}_{nn}$, $G^{\mp}_{nm}\equiv G^{\mp}_{nm}(E\pm \mathrm{i}\epsilon)$. We further make use of the continued-fraction representation for the required diagonal Green functions

$$G^{\mp}_{nn}=\frac{1}{E\pm\mathrm{i}\epsilon-\Omega_n-\Delta^-_n-\Delta^+_n},$$

$$\Delta^-_n=\frac{I^2_{n-1}+D^2_{n-1}}{E\pm\mathrm{i}\epsilon-\Omega_{n-1}-\frac{I^2_{n-2}+D^2_{n-2}}{E\pm\mathrm{i}\epsilon-\Omega_{n-2}-\ddots}},$$

$$\Delta^+_n=\frac{I^2_{n}+D^2_{n}}{E\pm\mathrm{i}\epsilon-\Omega_{n+1}-\frac{I^2_{n+1}+D^2_{n+1}}{E\pm\mathrm{i}\epsilon-\Omega_{n+2}-\ddots}}. \tag{2}$$

One immediately notes that for any finite period of varying Ω_n, I_n, D_n the continued fractions Δ^-_n, Δ^+_n involved into $G^{\mp}_{nn}$ (2) become periodic and thus can be calculated exactly yielding the exact result for the density of states and hence for the thermodynamic quantities of spin model (1). For example, for the periodic chain having period 2 $\Omega_1I_1D_1\Omega_2I_2D_2\Omega_1I_1D_1\Omega_2I_2D_2\ldots$ the described scheme gives

$$\rho(E)=\begin{cases}0, & \text{if} \quad E\le b_4,\ b_3\le E\le b_2,\ b_1\le E,\\ \frac{1}{2\pi}\frac{|2E-\Omega_1-\Omega_2|}{\sqrt{\mathcal{B}(E)}}, & \text{if} \quad b_4<E<b_3,\ b_2<E<b_1,\end{cases}$$

$$\mathcal{B}(E)=4\mathcal{I}_1^2\mathcal{I}_2^2-\left[(E-\Omega_1)(E-\Omega_2)-\mathcal{I}_1^2-\mathcal{I}_2^2\right]^2$$

$$=-(E-b_4)(E-b_3)(E-b_2)(E-b_1),$$

$$\{b_4\le b_3\le b_2\le b_1\}=\left\{\frac{1}{2}(\Omega_1+\Omega_2)\pm b_1,\frac{1}{2}(\Omega_1+\Omega_2)\pm b_2\right\},$$

$$b_1=\frac{1}{2}\sqrt{(\Omega_1-\Omega_2)^2+4\left(|\mathcal{I}_1|+|\mathcal{I}_2|\right)^2},$$

$$b_2=\frac{1}{2}\sqrt{(\Omega_1-\Omega_2)^2+4\left(|\mathcal{I}_1|-|\mathcal{I}_2|\right)^2}, \tag{3}$$

where $\mathcal{I}_n^2=I_n^2+D_n^2$.

To examine the instability of the considered spin chain with respect to dimerization we may assume $|I_1|=|I|(1+\delta)$, $|D_1|=|D|(1+\delta)$, $|I_2|=|I|(1-\delta)$, $|D_2|=|D|(1-\delta)$, $0\le\delta\le 1$ restricting ourselves to a case of the uniform transverse field $\Omega_1=\Omega_2=\Omega_0$. The total energy per site $\mathcal{E}(\delta)$ consists of the magnetic part $e_0(\delta)$ that follows from (3)

$$e_0(\delta)=-\frac{1}{2}\int_{-\infty}^{\infty}\mathrm{d}E\rho(E)|E|=-\frac{2|\mathcal{I}|}{\pi}E(\psi,1-\delta^2)-|\Omega_0|\left(\frac{1}{2}-\frac{\psi}{\pi}\right), \tag{4}$$

where the effective interspin coupling $|\mathcal{I}|=\sqrt{I^2+D^2}$ has been introduced, $E(\psi,a^2)\equiv\int_0^{\psi}\mathrm{d}\phi\sqrt{1-a^2\sin^2\phi}$ is the elliptic integral of the second kind,

$\psi = 0$ if $2|\mathcal{I}| \le |\Omega_0|$, $\psi = \arcsin\sqrt{\frac{4\mathcal{I}^2-\Omega_0^2}{4\mathcal{I}^2(1-\delta^2)}}$ if $2\delta|\mathcal{I}| \le |\Omega_0| < 2|\mathcal{I}|$, $\psi = \pi/2$ if $|\Omega_0| < 2\delta|\mathcal{I}|$, and the elastic part $\alpha\delta^2$. Besides the trivial solution $\delta^* = 0$ the equation $\partial\mathcal{E}(\delta)/\partial\delta = 0$ may have a nonzero one $\delta^* \neq 0$ at moderate and weak fields (i.e. $|\Omega_0| < 2|\mathcal{I}|$). This nontrivial δ^* comes from the equation that follows from (4)

$$\frac{\pi\alpha}{|\mathcal{I}|} = \frac{1}{1-\delta^2}\left[F(\psi, 1-\delta^2) - E(\psi, 1-\delta^2)\right], \tag{5}$$

where $F(\psi, a^2) \equiv \int_0^\psi \mathrm{d}\phi/\sqrt{1-a^2\sin^2\phi}$ is the elliptic integral of the first kind.

Let us consider the case $\Omega_0 = 0$. Looking for a solution of Eq. (5) that satisfies the inequality $\delta \ll 1$ (that is the limit interesting for applications) one observes that the right hand side (r.h.s.) of Eq. (5) can be rewritten approximately as $\int_0^1 \mathrm{d}x/\sqrt{\delta^2+x^2}$ ($x = \cos\phi$) that yields $\delta^* \sim \exp(-\pi\alpha/|\mathcal{I}|)$. A posteriori we conclude that the small dimerization parameters δ^* occur for hard lattices having large values of $\alpha/|\mathcal{I}|$. One also notes that the obtained result coincides with the one reported in [2] up to a renormalization of the effective interspin coupling $|I| \to |\mathcal{I}| = \sqrt{I^2+D^2}$. Thus the Dzyaloshinskii–Moriya interaction leads to the increase in the dimerization parameter δ^* characterizing the dimerized phase.

Let us consider further the case $0 < |\Omega_0| < 2|\mathcal{I}|$. Varying δ in the r.h.s. of Eq. (5) from 0 to 1 one calculates a lattice parameter $\alpha/|\mathcal{I}|$ for which the taken value of δ realizes an extremum of $\mathcal{E}(\delta)$. One immediately observes that for $|\Omega_0|/2|\mathcal{I}| \le \delta \le 1$ the dependence $\alpha/|\mathcal{I}|$ versus δ remains as that in the absence of the field, whereas for $0 \le \delta < |\Omega_0|/2|\mathcal{I}|$ the quantity $\alpha/|\mathcal{I}|$ starts to decrease. From this one concludes that for hard lattices the field $|\Omega_0|/2|\mathcal{I}| = \exp(-\pi\alpha/|\mathcal{I}|)$ makes the dimerization unstable against the uniform phase. The latter relation tells us that the Dzyaloshinskii–Moriya interaction increases the value of that field.

It is generally known [1] that the increase in the external field leads to a transition from the dimerized phase to the incommensurate phase rather than to the uniform phase. Evidently, the incommensurate phase cannot appear in the presented treatment within the frames of the adopted ansatz for the lattice distortions $\delta_1\delta_2\delta_1\delta_2\ldots$, $\delta_1 + \delta_2 = 0$. To clarify a possibility of more complicated distortions the chains with longer periods should be examined.

Alternatively, we may also assume different dependences on δ for the isotropic coupling and the Dzyaloshinskii–Moriya coupling, for example, $|I_1| = |I|(1+\delta)$, $|D_1| = |D|$, $|I_2| = |I|(1-\delta)$, $|D_2| = |D|$. Supposing that $\delta \ll 1$ after simple rescaling arguments one finds that the dimerization parameter $\delta^* \sim \frac{\mathcal{I}^2}{I^2}\exp\left(-\frac{\pi}{|\mathcal{I}|}\frac{\mathcal{I}^4}{I^4}\alpha\right)$. Thus, in such a case the Dzyaloshinskii–Moriya interaction leads to a decrease in the dimerization parameter characterizing the dimerized phase. The value of the field which destroys dimerization $\frac{|\Omega_0|}{2|\mathcal{I}|} = \exp\left(-\frac{\pi}{|\mathcal{I}|}\frac{\mathcal{I}^4}{I^4}\alpha\right)$ decreases as well.

To conclude, we have analysed a stability of the spin-$\frac{1}{2}$ transverse XX chain with respect to dimerization in the presence of the Dzyaloshinskii–Moriya interaction calculating for this purpose with the help of continued fractions the ground state energy for an arbitrary value of the dimerization parameter. Assuming that the ratio of the Dzyaloshinskii–Moriya coupling to the isotropic coupling does not depend on the dimerization parameter we have found that the Dzyaloshinskii–Moriya interaction leads to an increase in the effective interspin coupling and thus to some quantitative changes, i.e. to an increase in the value of the dimerization parameter which characterizes the dimerized phase and the value of the field which destroys the dimerized phase. In the other limiting case when the Dzyaloshinskii–Moriya coupling does not depend on the dimerization parameter it has an opposite effect leading to a decrease in the value of the dimerization parameter and the value of the field which destroys dimerization. The obtained results are in agreement with some earlier studies of the thermodynamic properties of spin-$\frac{1}{2}$ transverse XX chains with Dzyaloshinskii–Moriya interaction [10]. Finally, it is known that the Dzyaloshinskii–Moriya interaction may lead to drastical changes in spin correlations [11] and a study of a relation of these changes to the spin-Peierls instability seems to be an interesting issue.

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