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THERMODYNAMIC PROPERTIES OF SPIN-$\frac{1}{2}$ TRANSVERSE XX CHAIN WITH DZYALOSHINSKII-MORIYA INTERACTION: EXACT SOLUTION FOR CORRELATED LORENTZIAN DISORDER

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Термодинамічні властивості спін-$\frac{1}{2}$ поперечного XX ланцюжка з взаємодією Дзялошинського-Морія: Точний розв'язок для скорельованого лоренцового безладу

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Анотація. Ми розширюємо розгляд спін-$\frac{1}{2}$ поперечного XX ланцюжка з скорельованим лоренцовим безладом (Phys. Rev. B **55,** 14298 (1997)) на випадок присутності додаткової міжспінової взаємодії Дзялошинського-Морія. Показано, як усереднена щільність станів може бути обчислена точно. Результати приведено для щільності станів і поперечної намагніченості.

Thermodynamic properties of spin-$\frac{1}{2}$ transverse XX chain with Dzyaloshinskii-Moriya interaction: Exact solution for correlated Lorentzian disorder

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Abstract. We extend the consideration of the spin-$\frac{1}{2}$ transverse XX chain with correlated Lorentzian disorder (Phys. Rev. B **55,** 14298 (1997)) for the case of additional Dzyaloshinskii-Moriya interspin interaction. It is shown how the averaged density of states can be calculated exactly. Results are presented for the density of states and the transverse magnetization.

Recently the spin-$\frac{1}{2}$ XX chain with random Lorentzian exchange coupling J_n and a transverse field Ω_n that depends linearly on the surrounding exchange couplings J_{n-1} and J_n has been examined [1]. Obviously, due to the relation between the transverse field and the random exchange couplings we have a model of correlated disorder. The Jordan-Wigner method [2] and the method elaborated by John and Schreiber [3] permitted to derive exactly the averaged density of states for such a model and as a result to study its thermodynamic properties. Apparently the most interesting result of introducing the correlated disorder is the appearance of the nonzero averaged transverse magnetization at zero averaged transverse field. Later this effect was checked numerically [4,5]. In the present communication we shall extend the model introducing additional Dzyaloshinskii-Moriya interspin interaction. Spin-$\frac{1}{2}$ XY chains with Dzyaloshinskii-Moriya interaction were studied in several papers [6–10] in which it was shown that they exhibit some interesting thermodynamic and dynamic properties, which may be of interest for the understanding of the properties of some quasi-one-dimensional compounds (e.g. $CsCuCl_3$). It will be shown below that the Dzyaloshinskii-Moriya interaction may influence in specific manner the thermodynamic properties of a magnetic chain conditioned by correlated disorder.

Hereafter we consider XX chain in a magnetic field along z axis consisting of N spins $\frac{1}{2}$. The Hamiltonian is defined by

$$H=\sum_{n=1}^{N}\Omega_n s_n^z+\sum_{n=1}^{N}J_n(s_n^x s_{n+1}^x+s_n^y s_{n+1}^y)+\sum_{n=1}^{N}D_n(s_n^x s_{n+1}^y-s_n^y s_{n+1}^x),\qquad s_{n+N}^{\alpha}=s_n^{\alpha}. \tag{1}$$

Besides the exchange coupling J_n between the neighbouring sites n and $n+1$ an additional Dzyaloshinskii-Moriya interaction D_n between these sites is introduced, i.e. a more general case than in Ref. [1] is considered.

In what follows we consider two models.

Model (i) — We assume the Dzyaloshinskii-Moriya interaction to be ordered, i.e. $D_n=D$, whereas the exchange couplings J_n are independent random Lorentzian variables with the probability distribution

$$p(J_n)=\frac{1}{\pi}\frac{\Gamma}{(J_n-J_0)^2+\Gamma^2}. \tag{2}$$

The on-site transverse fields are determined by the formula

$$\Omega_n-\Omega_0=\frac{a}{2}(J_{n-1}+J_n-2J_0) \tag{3}$$

where a is real and $\mid a\mid\geq 1$. Note that after putting $D=0$ one obtains the model considered in Ref. [1].

Model (ii) — We assume the exchange coupling to be ordered, i.e. $J_n=J$, whereas the D_n are independent random Lorentzian variables with the probability distribution

$$p(D_n)=\frac{1}{\pi}\frac{\Gamma}{(D_n-D_0)^2+\Gamma^2}. \tag{4}$$

The on-site transverse fields are determined by the formula

$$\Omega_n-\Omega_0=\frac{a}{2}(D_{n-1}+D_n-2D_0) \tag{5}$$

where a is real and $\mid a\mid\geq 1$.

With the help of the Jordan-Wigner transformation the Hamiltonian (1) can be rewritten as a Hamiltonian of non-interacting spinless fermions

$$H=\sum_{n=1}^{N}\Omega_n\left(c_n^+c_n-\frac{1}{2}\right)+\sum_{n=1}^{N}\left(\frac{J_n+\mathrm{i}D_n}{2}c_n^+c_{n+1}-\frac{J_n-\mathrm{i}D_n}{2}c_nc_{n+1}^+\right) \tag{6}$$

with cyclic boundary conditions. We omitted in (6) the boundary term that is not essential for the calculation of the thermodynamic properties [11]. Let us introduce the retarded and advanced temperature double-time Green functions $G_{nm}^{\mp}(t)=\mp\mathrm{i}\theta(\pm t)\langle\{c_n(t),c_m^+\}\rangle$, $G_{nm}^{\mp}(t)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega\mathrm{e}^{-\mathrm{i}\omega t}G_{nm}^{\mp}(\omega\pm\mathrm{i}\epsilon)$ that satisfy the set of equations

$$(\omega\pm\mathrm{i}\epsilon-\Omega_n)G_{nm}^{\mp}(\omega\pm\mathrm{i}\epsilon)-\left[\frac{J_{n-1}-\mathrm{i}D_{n-1}}{2}G_{n-1,m}^{\mp}(\omega\pm\mathrm{i}\epsilon)+\frac{J_n+\mathrm{i}D_n}{2}G_{n+1,m}^{\mp}(\omega\pm\mathrm{i}\epsilon)\right]=\delta_{nm}. \tag{7}$$

Our task is to evaluate the random-averaged Green functions since they yield the random-averaged density of states through the relation

$$\overline{\rho(E)}=\mp\frac{1}{\pi}\mathrm{Im}\overline{G_{nn}^{\mp}(E\pm\mathrm{i}\epsilon)}. \tag{8}$$

Having the independent Lorentzian random variables one may try to perform the random averaging of Eq. (7) with the help of contour integrals. However one must know the positions of the singularities of the Green functions in the planes of complex random variables. The latter information can be derived for the defined models on the basis of the Gershgorin criterion [12].

Consider at first spin model (i) described by Eqs. (1) - (3). Suppose that exchange couplings J_n (and hence the transverse fields Ω_n) are complex variables. As it follows from (7) the singularities of the matrix $\mathbf{G}^{\mp} = \parallel G^{\mp}_{nm}(\omega \pm \mathrm{i}\epsilon) \parallel$ are determined by the zeros of the determinant of the matrix $\mathbf{A} \pm \mathrm{i}\mathbf{B}^{\mp}$

$$\det\begin{pmatrix} \omega \pm \mathrm{i}\epsilon - \Omega_1 & -\frac{J_1+\mathrm{i}D}{2} & 0 & \dots & -\frac{J_N-\mathrm{i}D}{2} \\ -\frac{J_1-\mathrm{i}D}{2} & \omega \pm \mathrm{i}\epsilon - \Omega_2 & -\frac{J_2+\mathrm{i}D}{2} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ -\frac{J_N+\mathrm{i}D}{2} & 0 & 0 & \dots & \omega \pm \mathrm{i}\epsilon - \Omega_N \end{pmatrix} = 0 \quad (9)$$

where $\mathbf{A}$ and $\mathbf{B}^{\mp}$ are the Hermitian matrices given by

$$\mathbf{A} = \begin{pmatrix} \omega - \mathrm{Re}\Omega_1 & -\frac{1}{2}\mathrm{Re}J_1 - \frac{\mathrm{i}}{2}D & \dots & -\frac{1}{2}\mathrm{Re}J_N + \frac{\mathrm{i}}{2}D \\ -\frac{1}{2}\mathrm{Re}J_1 + \frac{\mathrm{i}}{2}D & \omega - \mathrm{Re}\Omega_2 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ -\frac{1}{2}\mathrm{Re}J_N - \frac{\mathrm{i}}{2}D & 0 & \dots & \omega - \mathrm{Re}\Omega_N \end{pmatrix} \quad (10)$$

and

$$\mathbf{B}^{\mp} = \begin{pmatrix} \epsilon \mp \mathrm{Im}\Omega_1 & \mp\frac{1}{2}\mathrm{Im}J_1 & 0 & \dots & \mp\frac{1}{2}\mathrm{Im}J_N \\ \mp\frac{1}{2}\mathrm{Im}J_1 & \epsilon \mp \mathrm{Im}\Omega_2 & \mp\frac{1}{2}\mathrm{Im}J_2 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \mp\frac{1}{2}\mathrm{Im}J_N & 0 & 0 & \dots & \epsilon \mp \mathrm{Im}\Omega_N \end{pmatrix}, \quad (11)$$

respectively. John and Schreiber noticed that if all eigenvalues of $\mathbf{B}^{\mp}$ are positive then $\det(\mathbf{A} \pm \mathrm{i}\mathbf{B}^{\mp}) \neq 0$ [3]. On the other hand for any eigenvalue λ of the matrix $\mathbf{B}^{\mp}$ (11) the Gershgorin criterion guarantees that at least one of the inequalities

$$|\epsilon \mp \mathrm{Im}\Omega_n - \lambda| \le \left|\mp\frac{1}{2}\mathrm{Im}J_{n-1}\right| + \left|\mp\frac{1}{2}\mathrm{Im}J_n\right|, \quad n = 1, \dots, N \quad (12)$$

is satisfied. Using Eq. (3) we can transform Eq. (12) into

$$\left|\epsilon \mp \frac{a}{2}\left(\mathrm{Im}J_{n-1} + \mathrm{Im}J_n\right) - \lambda\right| \le \frac{1}{2}\left|\mathrm{Im}J_{n-1}\right| + \frac{1}{2}\left|\mathrm{Im}J_n\right|,$$
$$\mid a \mid \ge 1, \quad n = 1, \dots, N. \quad (13)$$

From (13) it immediately follows that the retarded (advanced) Green function does not have poles for $\mathrm{Im}J_n < 0$ ($\mathrm{Im}J_n > 0$) if $a \ge 1$ and for $\mathrm{Im}J_n > 0$ ($\mathrm{Im}J_n < 0$) if $a \le -1$. Noting that $\overline{F(\dots, \Omega_n, J_n, \dots)} = F(\dots, \Omega_0 - \mathrm{i}a\Gamma, J_0 - \mathrm{i}\Gamma, \dots)$ if $F(\dots, \Omega_n, J_n, \dots)$ does not have poles in lower half-planes J_n and $\overline{F(\dots, \Omega_n, J_n, \dots)} = F(\dots, \Omega_0 + \mathrm{i}a\Gamma, J_0 + \mathrm{i}\Gamma, \dots)$ if $F(\dots, \Omega_n, J_n, \dots)$ does not have poles in upper half-planes J_n one finds the following result of averaging the set of equations (7)

$$(\omega - \Omega_0 \pm \mathrm{i} \mid a \mid \Gamma)\overline{G^{\mp}_{nm}(\omega)}$$
$$- \left[\frac{J_0 - \mathrm{i}D \mp \mathrm{i}\ \mathrm{sgn}(a)\ \Gamma}{2}\overline{G^{\mp}_{n-1,m}(\omega)}\right.$$
$$\left. + \frac{J_0 + \mathrm{i}D \mp \mathrm{i}\ \mathrm{sgn}(a)\ \Gamma}{2}\overline{G^{\mp}_{n+1,m}(\omega)}\right] = \delta_{nm}. \quad (14)$$

The obtained equations possess translational symmetry and proceeding further in standard manner one obtains

$$\overline{\rho(E)} = \frac{1}{\pi}\sqrt{\frac{\sqrt{A^2 + B^2} - A}{2(A^2 + B^2)}},$$
$$A = (E - \Omega_0)^2 + (1 - \mid a \mid^2)\Gamma^2 - J_0^2 - D^2,$$
$$B = 2\Gamma[\mid a \mid (E - \Omega_0) + \mathrm{sgn}(a)\ J_0]. \quad (15)$$

Consider now spin model (ii) described by Eqs. (1), (4), (5). Assuming that D_n (and hence Ω_n) are complex variables we are again examining the conditions under which $\det(\mathbf{A} \pm \mathrm{i}\mathbf{B}^{\mp}) \neq 0$ where

$$\mathbf{A} = \begin{pmatrix} \omega - \mathrm{Re}\Omega_1 & -\frac{1}{2}J - \frac{\mathrm{i}}{2}\mathrm{Re}D_1 & \dots & -\frac{1}{2}J + \frac{\mathrm{i}}{2}\mathrm{Re}D_N \\ -\frac{1}{2}J + \frac{\mathrm{i}}{2}\mathrm{Re}D_1 & \omega - \mathrm{Re}\Omega_2 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ -\frac{1}{2}J - \frac{\mathrm{i}}{2}\mathrm{Re}D_N & 0 & \dots & \omega - \mathrm{Re}\Omega_N \end{pmatrix} \quad (16)$$

and

$$\mathbf{B}^{\mp} = \begin{pmatrix} \epsilon \mp \mathrm{Im}\Omega_1 & \mp\frac{\mathrm{i}}{2}\mathrm{Im}D_1 & 0 & \dots & \pm\frac{\mathrm{i}}{2}\mathrm{Im}D_N \\ \pm\frac{\mathrm{i}}{2}\mathrm{Im}D_1 & \epsilon \mp \mathrm{Im}\Omega_2 & \mp\frac{\mathrm{i}}{2}\mathrm{Im}D_2 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \mp\frac{\mathrm{i}}{2}\mathrm{Im}D_N & 0 & 0 & \dots & \epsilon \mp \mathrm{Im}\Omega_N \end{pmatrix}. \quad (17)$$

In accordance with [3] we are seeking for the conditions under which all eigenvalues λ of the matrix $\mathbf{B}^{\mp}$ (17) are positive using for this purpose the Gershgorin criterion. On the basis of this criterion and relation (5) one finds that for any λ at least one of the following inequalities

$$\left|\epsilon \mp \frac{a}{2}\left(\mathrm{Im}D_{n-1}+\mathrm{Im}D_n\right)-\lambda\right| \leq \frac{1}{2}\left|\mathrm{Im}D_{n-1}\right|+\frac{1}{2}\left|\mathrm{Im}D_n\right|,$$
$$\mid a \mid \geq 1, \quad n=1,\ldots,N \qquad (18)$$

must be satisfied. Eq. (18) immediately yields that the retarded (advanced) Green function does not have poles for $\mathrm{Im}D_n<0$ ($\mathrm{Im}D_n>0$) if $a\geq 1$ and for $\mathrm{Im}D_n>0$ ($\mathrm{Im}D_n<0$) if $a\leq -1$. This observation permits to average Eq. (7) with the result

$$(\omega-\Omega_0\pm \mathrm{i}\mid a\mid\Gamma)\overline{G^{\mp}_{nm}(\omega)}$$
$$-\left[\frac{J-\mathrm{i}D_0\mp\mathrm{sgn}(a)\,\Gamma}{2}\overline{G^{\mp}_{n-1,m}(\omega)}\right.$$
$$\left.+\frac{J+\mathrm{i}D_0\pm\mathrm{sgn}(a)\,\Gamma}{2}\overline{G^{\mp}_{n+1,m}(\omega)}\right]=\delta_{nm}. \qquad (19)$$

Similarly to the previous case (see Appendix) we find that the random-averaged density of states again is given by Eq. (15), however with

$$A=(E-\Omega_0)^2+(1-\mid a\mid^2)\Gamma^2-J^2-D_0^2,$$
$$B=2\Gamma[\mid a\mid(E-\Omega_0)+\mathrm{sgn}(a)\,D_0]. \qquad (20)$$

Let us discuss the obtained densities of magnon states for the spin models considered. First of all note that after replacement $J_0\to D_0$, $D\to J$ the density of states (15) transforms into the density of states (20). Therefore it is sufficient in what follows to consider only one spin model, for instance, model (i) defined by (1) - (3). It can be straightforwardly checked that (15) covers in the particular case $D=0$ the result derived in Ref. [1]. In the limit of diagonal disorder $\Gamma\to 0$, $\mid a\mid\Gamma=\gamma=\mathrm{const}$ Eq. (15) reproduces the density of states for spin-$\frac{1}{2}$ XX chain with Dzyaloshinskii-Moriya interaction in a random Lorentzian transverse field with the mean value Ω_0 and the width of distribution γ [10]. The density of states (15) remains the same after the simultaneous change of signs of J_0 and a; hereafter we choose $J_0>0$.

Let us remind how the density of states is influenced by correlated disorder in case of $D=0$ (for details see [1]). For $\mid a\mid\approx 1$ the disorder causes a smearing out of mainly one edge of the magnon band (which one depends on the sign of a). As a result we have $\int_{-\infty}^{0}\mathrm{d}E\overline{\rho(E)}\neq\int_{0}^{\infty}\mathrm{d}E\overline{\rho(E)}$ at $\Omega_0=0$ that leads to the appearance of a nonzero averaged transverse magnetization $\overline{m_z}=-\frac{1}{2}\int_{-\infty}^{\infty}\mathrm{d}E\overline{\rho(E)}\tanh\frac{\beta E}{2}$ at zero averaged

transverse field Ω_0. With an increase of $\mid a\mid$ the symmetry of the non-random case is recovered, i.e., both edges of the magnon band become smeared out in a symmetric way, the numbers of states $\int_{-\infty}^{0}\mathrm{d}E\overline{\rho(E)}$ and $\int_{0}^{\infty}\mathrm{d}E\overline{\rho(E)}$ at $\Omega_0=0$ become equal to each other, and $\overline{m_z}=0$ at $\Omega_0=0$.

Figs. 1a, 1b demonstrate the changes in the behaviour of the averaged density of states $\overline{\rho(E)}$ versus $E-\Omega_0$ for $\Gamma=1$, $a=\pm 1.01$, $J_0=1$ for three different strengths of the Dzyaloshinskii-Moriya interaction $D=0$, $D=1$, $D=2$. It can be seen that an additional Dzyaloshinskii-Moriya interspin interaction 1) increases the width of the smoothed magnon band; 2) leads to the recovering of the symmetry with respect to the change $E-\Omega_0\to-(E-\Omega_0)$. Thus the increase of the Dzyaloshinskii-Moriya interaction leads to the decrease of the nonzero value of $\overline{m_z}$ at $\Omega_0=0$ (Figs. 1c, 1d).

In Fig. 2 we depicted the influence of an increase of the averaged exchange coupling J_0 at fixed $D=0$. Similarly to the previous case one observes an increasing of the band width, however, in contrast to the previous case the density of states remains not symmetric with respect to the change $E-\Omega_0\to-(E-\Omega_0)$ (Figs. 2a, 2b) and as a result the model exhibits a noticeable nonzero value of $\overline{m_z}$ at $\Omega_0=0$ (Figs. 2c, 2d). The difference in the behaviour of the density of states with increasing D or J_0 is not surprising since J_0 and D enter in a different way into (15).

To summarize, we have studied the spin-$\frac{1}{2}$ transverse XX chain in the presence of correlated Lorentzian disorder. Going beyond the results given in Ref. [1] we include in the model the Dzyaloshinskii-Moriya interaction. The assumption of correlated disorder allows the exact calculation of the averaged density of states $\overline{\rho(E)}$. The exact formulae (15) and (20) for $\overline{\rho(E)}$ are the main results of the paper. Based on these formulae one can calculate in a simple way exactly the thermodynamic properties like entropy, specific heat, transverse magnetization and static transverse linear susceptibility (see for details [1]). In that sense the presented random quantum spin model may serve as a reference model to study the interplay of disorder and quantum effects. In particular, it may be used to test approximations and/or calculations for finite systems. As an example we present results for the density of states and the transverse magnetization. In particular, we find that the Dzyaloshinskii-Moriya interaction may lead to a decrease of the nonzero averaged transverse magnetization at zero averaged transverse field that appears due to correlated disorder. It is known [6–9] that in the non-random case the Dzyaloshinskii-Moriya interaction leads to spectacular changes in the spin correlations and their

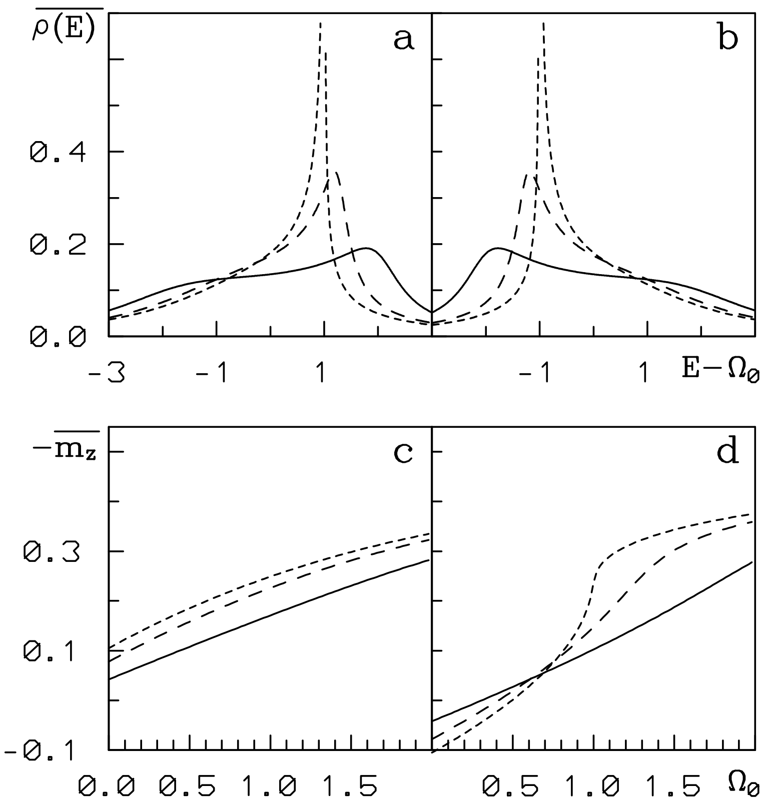

Figure 1. The density of states (described by Eq. (15)) (Figs. 1a, 1b) and the transverse magnetization $-\overline{m_z}$ versus Ω_0 at $\beta = 1000$ (Figs. 1c, 1d) at fixed $J_0 = 1$, $\Gamma = 1$ and $a = -1.01$ (Figs. 1a, 1c) or $a = 1.01$ (Figs. 1b, 1d). The short-dashed curves correspond to $D = 0$, long-dashed curves to $D = 1$ and the solid curves to $D = 2$.

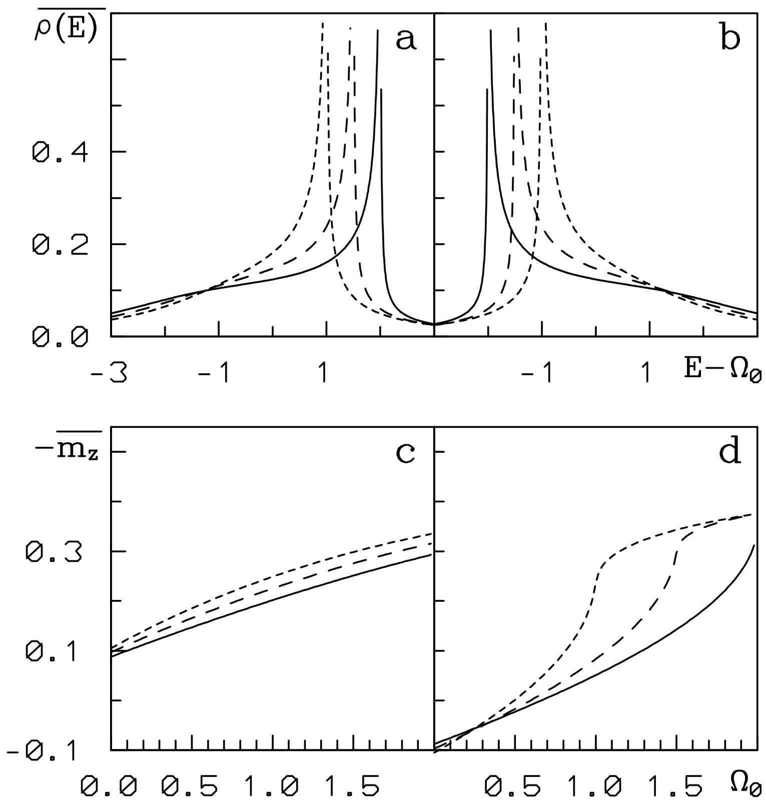

Figure 2. The density of states (described by Eq. (15)) (Figs. 2a, 2b) and the transverse magnetization $-\overline{m_z}$ versus Ω_0 at $\beta = 1000$ (Figs. 2c, 2d) at fixed $D = 0$, $\Gamma = 1$ and $a = -1.01$ (Figs. 2a, 2c) or $a = 1.01$ (Figs. 2b, 2d). The short-dashed curves correspond to $J_0 = 1$, long-dashed curves to $J_0 = 1.5$ and the solid curves to $J_0 = 2$.

dynamics. However, the rigorous consideration of correlated disorder in this paper is restricted to thermodynamic quantities based on the density of states. The effect of the Dzyaloshinskii-Moriya interaction on the spin correlations and their dynamics in the presence of correlated disorder may be studied numerically [13].

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Appendix

Usually, to solve the set of translationally invariant equations (19) one performs the Fourier transformation with respect to the site indices. However, the desired Green functions $\overline{G^{\mp}_{nn}(\omega)}$ (and hence $\overline{\rho(E)}$) can be obtained apparently in a more straightforward manner with the help of continued fractions. It is a simple matter to show on the basis of Eq. (19) that

$$\overline{G^{\mp}_{nn}(\omega)} = \frac{1}{\omega - \Omega_0 \pm \mathrm{i} \mid a \mid \Gamma - 2\Delta},$$
$$\Delta = \frac{\delta}{\omega - \Omega_0 \pm \mathrm{i} \mid a \mid \Gamma - \frac{\delta}{\omega - \Omega_0 \pm \mathrm{i} | a | \Gamma - \ddots}},$$
$$\delta = \frac{1}{4}\left(J^2 + D_0^2 - \Gamma^2 \mp 2\mathrm{i}\,\mathrm{sgn}(a)\,\Gamma D_0\right). \tag{21}$$

Since the periodic continued fraction Δ satisfies the equation $\Delta = \frac{\delta}{\omega - \Omega_0 \pm \mathrm{i}|a|\Gamma - \Delta}$ it can be easily calculated and as a result

$$\overline{G^{\mp}_{nn}(\omega)} = \frac{1}{\sqrt{\left(\omega - \Omega_0 \pm \mathrm{i} \mid a \mid \Gamma\right)^2 - 4\delta^2}}. \tag{22}$$

Substituting this result into (8) one obtains (20).

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Термодинамічні властивості спін-$\frac{1}{2}$ поперечного XX ланцюжка з взаємодією Дзялошинського-Морія: Точний розв'язок для скорельованого лоренцового безладу

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