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

Oleg Derzhko
Institute for Condensed Matter Physics, 1 Svientsitskii Street, L'viv-11, 290011, Ukraine

Johannes Richter
Institut für Theoretische Physik, Universität Magdeburg, P.O. Box 4120, D-39016 Magdeburg, Germany

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We extend the consideration of the spin-$\frac{1}{2}$ transverse XY chain with correlated Lorentzian disorder [Phys. Rev. B **55,** 14 298 (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. [S0163-1829(99)06501-7]

Much work has been done since the famous paper by Lieb, Schultz, and Mattis[1] to derive exact results for thermodynamics and spin correlations of one-dimensional spin-$\frac{1}{2}$ XY models. Much less exact results were obtained for random versions of spin-$\frac{1}{2}$ XY chains. One can mention here a group of papers dealing with random spin-$\frac{1}{2}$ XY models using the well-known Dyson and Lloyd models of disorder.[2–4] Recently the interest in random spin-$\frac{1}{2}$ XY chains has noticebly increased since they provide a laboratory for the investigation of generic features of quantum phase transitions in disordered systems. As an example we refer to papers on renormalization group[5] and numerical[6] studies on random spin-$\frac{1}{2}$ transverse Ising chains.

In the present paper we continue the study started in Ref. 4 that concerns the spin-$\frac{1}{2}$ isotropic XY 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. Obviously, due to the relation between the transverse field and the random exchange couplings this is a model of correlated disorder. The Jordan-Wigner method[1] and the method elaborated by John and Schreiber[7] permitted us to exactly derive 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.[8,9] In the present paper we shall extend the model introducing additional Dzyaloshinskii-Moriya interspin interactions. Spin-$\frac{1}{2}$ XY chains with Dzyaloshinskii-Moriya interaction were studied in several papers[10–14] in which it was shown that they exhibit 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 the thermodynamic properties of a magnetic chain conditioned by correlated disorder in a specific manner.

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

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

$$s_{n+N}^\alpha=s_n^\alpha .$$

In addition to the exchange coupling J_n between the neighboring 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. 4 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 $|a|\geqslant 1$. Note that after putting $D=0$ one obtains the model considered in Ref. 4.

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 $|a|\geqslant 1$.

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

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

with cyclic boundary conditions. In Eq. (6) we omitted the boundary term that is not essential for the calculation of the thermodynamic properties.[15] Let us introduce the retarded and advanced temperature double-time Green functions $G_{nm}^{\mp}(t)=\mp i\theta(\pm t)\langle\{c_n(t),c_m^{+}\}\rangle$, $G_{nm}^{\mp}(t)=(1/2\pi)\int_{-\infty}^{\infty}d\omega e^{-i\omega t}G_{nm}^{\mp}(\omega\pm i\epsilon)$ that satisfy the set of equations

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

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

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

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.[16]

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 follows from Eq. (7) the singularities of the matrix $\mathbf{G}^{\mp}=||G_{nm}^{\mp}(\omega\pm i\epsilon)||$ are determined by the zeros of the determinant of the matrix $\mathbf{A}\pm i\mathbf{B}^{\mp}$, where $\mathbf{A}$ and $\mathbf{B}^{\mp}$ are the Hermitian matrices given by

$$\mathbf{A}=\begin{pmatrix}\omega-\mathrm{Re}\,\Omega_1 & -\frac{1}{2}\mathrm{Re}\,J_1-(i/2)D & 0 & \cdots & -\frac{1}{2}\mathrm{Re}\,J_N+(i/2)D\\ -\frac{1}{2}\mathrm{Re}\,J_1+(i/2)D & \omega-\mathrm{Re}\,\Omega_2 & -\frac{1}{2}\mathrm{Re}\,J_2-(i/2)D & \cdots & 0\\ \vdots & \vdots & \vdots & \vdots & \vdots\\ -\frac{1}{2}\mathrm{Re}\,J_N-(i/2)D & 0 & 0 & \cdots & \omega-\mathrm{Re}\,\Omega_N\end{pmatrix}\qquad(9)$$

and

$$\mathbf{B}^{\mp}=\begin{pmatrix}\epsilon\mp\mathrm{Im}\,\Omega_1 & \mp\frac{1}{2}\mathrm{Im}\,J_1 & 0 & \cdots & \mp\frac{1}{2}\mathrm{Im}\,J_N\\ \mp\frac{1}{2}\mathrm{Im}\,J_1 & \epsilon\mp\mathrm{Im}\,\Omega_2 & \mp\frac{1}{2}\mathrm{Im}\,J_2 & \cdots & 0\\ \vdots & \vdots & \vdots & \vdots & \vdots\\ \mp\frac{1}{2}\mathrm{Im}\,J_N & 0 & 0 & \cdots & \epsilon\mp\mathrm{Im}\,\Omega_N\end{pmatrix},\qquad(10)$$

respectively. John and Schreiber noticed that if all eigenvalues of $\mathbf{B}^{\mp}$ are positive then $\det(\mathbf{A}\pm i\mathbf{B}^{\mp})\neq 0$.[7] On the other hand, for any eigenvalue λ of the matrix $\mathbf{B}^{\mp}$ (10) the Gershgorin criterion after making use of Eq. (3) guarantees that at least one of the inequalities

$$\left|\epsilon\mp\frac{a}{2}(\mathrm{Im}\,J_{n-1}+\mathrm{Im}\,J_n)-\lambda\right|\leqslant\frac{1}{2}|\mathrm{Im}\,J_{n-1}|+\frac{1}{2}|\mathrm{Im}\,J_n|,\qquad |a|\geqslant 1,\quad n=1,\ldots,N\qquad(11)$$

is satisfied. From Eq. (11) 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 $a\geqslant 1$ and for $\mathrm{Im}\,J_n>0$ $(\mathrm{Im}\,J_n<0)$ if $a\leqslant -1$. Noting that $\overline{F(\ldots,\Omega_n,J_n,\ldots)}=F(\ldots,\Omega_0-ia\Gamma,J_0-i\Gamma,\ldots)$ if $F(\ldots,\Omega_n,J_n,\ldots)$ does not have poles in lower half planes J_n and $\overline{F(\ldots,\Omega_n,J_n,\ldots)}=F(\ldots,\Omega_0+ia\Gamma,J_0+i\Gamma,\ldots)$ if $F(\ldots,\Omega_n,J_n,\ldots)$ does not have poles in upper half planes J_n one finds the following result of averaging the set of Eqs. (7):

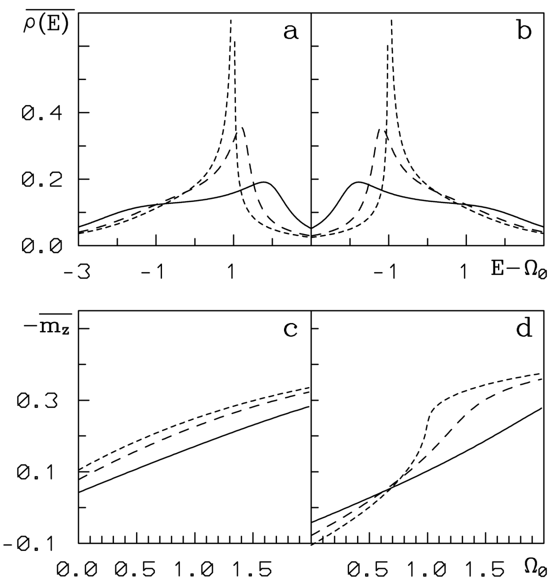

FIG. 1. The density of states [described by Eq. (13)] [(a),(b)] and the transverse magnetization $-\overline{m_z}$ versus Ω_0 at $\beta=1000$ [(c),(d)] at fixed $J_0=1$, $\Gamma=1$, and $a=-1.01$ [(a),(c)] or $a=1.01$ [(b),(d)]. The short-dashed curves correspond to $D=0$, long-dashed curves to $D=1$, and the solid curves to $D=2$.

$$(\omega-\Omega_0\pm i|a|\Gamma)\overline{G^{\mp}_{nm}(\omega)}-\left[\frac{J_0-iD\mp i\,\mathrm{sgn}(a)\,\Gamma}{2}\overline{G^{\mp}_{n-1,m}(\omega)}\right.$$
$$\left.+\frac{J_0+iD\mp i\,\mathrm{sgn}(a)\,\Gamma}{2}\overline{G^{\mp}_{n+1,m}(\omega)}\right]=\delta_{nm}. \qquad (12)$$

The obtained equations (12) possess translational symmetry and proceeding further in a standard manner one obtains

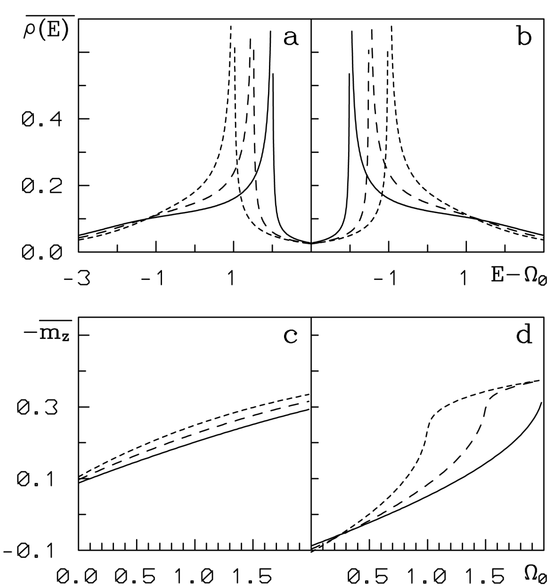

FIG. 2. The density of states [described by Eq. (13)] [(a),(b)] and the transverse magnetization $-\overline{m_z}$ versus Ω_0 at $\beta=1000$ [(c),(d)] at fixed $D=0$, $\Gamma=1$, and $a=-1.01$ [(a),(c)] or $a=1.01$ [(b),(d)]. The short-dashed curves correspond to $J_0=1$, long-dashed curves to $J_0=1.5$, and the solid curves to $J_0=2$.

$$\overline{\rho(E)}=\frac{1}{\pi}\sqrt{\frac{\sqrt{A^2+B^2}-A}{2(A^2+B^2)}},$$
$$A=(E-\Omega_0)^2+(1-|a|^2)\Gamma^2-J_0^2-D^2,$$
$$B=2\Gamma[|a|(E-\Omega_0)+\mathrm{sgn}(a)\,J_0]. \qquad (13)$$

Consider now spin model (ii) described by Eqs. (1),(4),(5). Certainly we may repeat the whole calculation once more obtaining as a result $\overline{\rho(E)}$ for this model. However, there is a relationship between models (i) and (ii) that immediately yields thermodynamics of the latter model if it is known for the former one. Namely, consider the following rotations of spin axes around the z axis:

$$(s_n^\alpha)'=\exp\left[-i\frac{\pi(n-1)}{2}s_n^z\right]s_n^\alpha\exp\left[i\frac{\pi(n-1)}{2}s_n^z\right]. \qquad (14)$$

One immediately finds that the Hamiltonian (1) arises as a result of transformations (14) applied to a Hamiltonian of form (1), however, with the exchange couplings D_n and the Dzyaloshinskii-Moriya interactions $-J_n$. Therefore it becomes evident that the density of states (13) after the replacement $J_0\to D_0$, $D^2\to J^2$ transforms into the density of states for the model (ii). Hence it is sufficient in what follows to consider only the spin model (i) defined by Eqs. (1)–(3).

Let us discuss the obtained density of magnon states (13). It can be straightforwardly checked that Eq. (13) covers in the particular case $D=0$ the result derived in Ref. 4. In the limit of diagonal disorder $\Gamma\to 0$, $|a|\Gamma=\gamma=$const, Eq. (13) reproduces the density of states for the spin-$\frac{1}{2}$ isotropic XY chain with Dzyaloshinskii-Moriya interaction in a random Lorentzian transverse field with the mean value Ω_0 and the width of distribution γ.[14] The density of states (13) remains the same after the simultaneous change of signs of J_0 and a; hereafter we choose $J_0>0$.

Let us remind the reader of how the density of states is influenced by correlated disorder in the case of $D=0$ (for details see Ref. 4). For $|a|\approx 1$ 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 $\int_{-\infty}^0 dE\overline{\rho(E)}\neq\int_0^\infty dE\overline{\rho(E)}$ at $\Omega_0=0$ that leads to the appearance of a nonzero averaged transverse magnetization $\overline{m_z}=-\frac{1}{2}\int_{-\infty}^{\infty}dE\overline{\rho(E)}\tanh(\beta E/2)$ at zero averaged transverse field Ω_0. With an increase of $|a|$ the symmetry of the nonrandom case is recovered, i.e., both edges of the magnon band become smeared out in a symmetric way, the numbers of states $\int_{-\infty}^0 dE\overline{\rho(E)}$ and $\int_0^\infty dE\overline{\rho(E)}$ at $\Omega_0=0$ become equal to each other, and $\overline{m_z}=0$ at $\Omega_0=0$.

Figures 1(a), 1(b) demonstrate the changes in the behavior 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. 1(c), 1(d)].

In Fig. 2 we depicted the influence of an increase of the averaged exchange coupling J_0 at fixed $D=0$. Similar 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 $E-\Omega_0 \rightarrow -(E-\Omega_0)$ [Figs. 2(a), 2(b)] and as a result the model exhibits a noticeable nonzero value of $\overline{m_z}$ at $\Omega_0=0$ [Figs. 2(c), 2(d)]. The difference in the behavior 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 Eq. (13).

To summarize, we have studied the spin-$\frac{1}{2}$ transverse isotropic XY chain in the presence of correlated Lorentzian disorder. Going beyond the results given in Ref. 4 we include in the model the Dzyaloshinskii-Moriya interaction. The asumption of correlated disorder allows the exact calculation of the averaged density of states $\overline{\rho(E)}$. The exact formula (13) for $\overline{\rho(E)}$ is the main result of the paper. Based on this formula one can exactly calculate in a simple way thermodynamic properties such as entropy, specific heat, transverse magnetization, and static transverse linear susceptibility (see for details Ref. 4). 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 because of the correlated disorder. It is known[10–13] that in the nonrandom case the Dzyaloshinskii-Moriya interaction leads to spectacular changes in the spin correlations and their 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.[17]

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