One variation on Lloyd’s theme

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Abstract

One random spin-$\frac{1}{2}$ XY chain that after Jordan-Wigner fermionization reduces to the extended Lloyd’s model is considered. The random-averaged one-fermion Green functions have been calculated exactly that yields thermodynamics of the spin model.

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An idea to exploit Lloyd’s model [1] for examining the thermodynamical properties of random spin-$\frac{1}{2}$ XY chains belongs to H.Nishimori [2]. He noted that after Jordan-Wigner trick [3] the Hamiltonian of isotropic XY model with random lorentzian transverse field describes tight-binding spinless fermions with diagonal lorentzian disorder. Since the random-averaged one-fermion Green functions for such model were found exactly by P.Lloyd, one can obtain the thermodynamics of random spin system via the averaged density of states. Later the treatment presented in [2] was generalized for the cases of alternating bonds [4] and additional intersite Dzyaloshinskii-Moriya interaction [5].

On the other hand, W.John and J.Schreiber suggested an extension of Lloyd’s method to off-diagonal disorder [6] that was successfully used in the study of disordered systems [7-11]. The idea of the present communication is to exploit Lloyd’s model with off-diagonal disorder for analysis of thermodynamics of the corresponding random spin-$\frac{1}{2}$ XY chain. Similarly to [2] we were able to calculate exactly various thermodynamical quantities, although found somewhat different results of influence of randomness on these functions.

We consider $N$ spins $\frac{1}{2}$ arranged in a circle with the Hamiltonian

$$H = \sum_{n=1}^{N} \Omega_n s^z_n + \sum_{n=1}^{N} J_n \left( s^x_n s^x_{n+1} + s^y_n s^y_{n+1} \right), \quad s^\alpha_{n+N} = s^\alpha_n, \quad (1)$$

where $\Omega_n$ is a transverse field at site $n$ and $J_n$ is the interaction between the sites $n$ and $n + 1$. The latter are taken to be random with a probability distribution density

$$p(J_1, \ldots, J_N) = \prod_{n=1}^{N} \frac{1}{\pi} \frac{\Gamma}{(J_n - J_0)^2 + \Gamma^2}, \quad (2)$$

that is the product of lorentzian distribution densities at sites that are centered at $J_0$ with the width $\Gamma$. In order to treat the model (1), (2) in exact manner the transverse field $\Omega_n$
at each site must depend on surrounding intersite interactions in the following way

\[ \Omega_n - \Omega_0 = a \left( \frac{J_{n-1} - J_0}{2} + \frac{J_n - J_0}{2} \right), \quad a \text{ is real, } |a| \geq 1, \quad (3) \]

where \( \Omega_0 \) is the averaged transverse field at site.

Really, by Jordan-Wigner transformation from operators
\[ s_j^+ \equiv s_j^x \pm is_j^y \]
to Fermi operators \( c_j, c_j^+ \) the Hamiltonian (1) becomes

\[ H = H^- + BP^+, \]

\[ H^- \equiv -\frac{1}{2} \sum_{n=1}^N \Omega_n + \sum_{n=1}^N \Omega_n c_n^+ c_n + \sum_{n=1}^N \frac{J_n}{2} \left( c_n^+ c_{n+1}^+ - c_n c_{n+1}^+ \right), \quad c_{n+N} = c_n, \quad c_{n+N}^+ = c_n^+, \]

\[ B \equiv -J_N \left( c_N^+ c_1 - c_N c_1^+ \right), \quad P^+ \equiv \frac{1 + P}{2}, \quad P \equiv \prod_{n=1}^N (-2s_n^z). \quad (4) \]

For calculation of thermodynamical properties of the model (1) one can omit the boundary term \( B \) [14], and hence one faces with one-dimensional version of Anderson’s model with the off-diagonal disorder considered by W.John and J.Schreiber.

In order to study thermodynamics one should diagonalize the bilinear in Fermi operators form \( H^- \) (4) by canonical transformation \( \eta_k = \sum_{n=1}^N g_{kn} c_n \) with real \( g_{kn} \) that satisfy the equations

\[ \Lambda_k g_{kn} = \sum_{i=1}^N g_{ki} A_{in} \quad \text{with} \quad A_{ij} \equiv \Omega_i \delta_{ij} + \frac{1}{2} J_i \delta_{j,i+1} + \frac{1}{2} J_{i-1} \delta_{j,i-1}, \]

and

\[ \sum_{i=1}^N g_{ki} g_{pi} = \delta_{kp}, \quad \sum_{p=1}^N g_{pi} g_{pj} = \delta_{ij} \]

obtaining in result \( H^- = \sum_{p=1}^N \Lambda_p (\eta_p^+ \eta_p - \frac{1}{2}) \). The density of states \( \rho(E) \equiv \frac{1}{N} \sum_{p=1}^N \delta(E - \Lambda_p) \) determines thermodynamics for certain realization of random intersite interactions. For example, the Helmholtz free energy per site is given by

\[ f = -\frac{1}{\beta} \int dE \rho(E) \ln(2\text{ch} \beta E/2). \]

The Helmholtz free energy averaged over random realizations is given by the same formula only with the random-averaged density of states \( \overline{\rho(E)} \), where the averaging is defined by \( \overline{(...)} \equiv \int dJ_1 ... dJ_N \rho(J_1, ..., J_N)(...) \).

On the other hand, the temperature double-time Green functions \( \Gamma_{pq}^\pm (t) \equiv \mp it (\pm t) < \{ \eta_p(t), \eta_q^+ \} >, \quad \Gamma_{pq}^\pm (t) = \frac{1}{2\pi} \int_{-\infty}^\infty dE e^{-iEt} \Gamma_{pq}^\pm (E \pm i\varepsilon), \quad \varepsilon \to +0 \) yield the density of states
for a certain random realization: 
\[ \rho(E) = \frac{1}{N} \sum_{p=1}^{N} \left[ \mp \frac{1}{\pi} \text{Im} \Gamma_{pp}^{\mp}(E \pm \imath \varepsilon) \right] . \]
\( \rho(E) \) can be rewritten in terms of Green functions 
\[ G_{nm}^{\pm}(t) \equiv \mp i \theta(\pm t) < \{ c_n(t), c_m^+ \} > \]
as 
\[ \rho(E) = \mp \frac{1}{\pi} \sum_{j=1}^{N} \text{Im} G_{jj}^{\mp}(E \pm \imath \varepsilon) \text{ since } \Gamma_{pq}^{\mp}(t) = \sum_{i=1}^{N} \sum_{j=1}^{N} g_{pi} g_{qj} G_{ij}^{\mp}(t) . \]
In result the averaged density of states is determined by the averaged Green functions 
\[ \overline{G}_{nm}^{\pm}(E) \] via the relation
\[ \overline{\rho(E)} = \mp \frac{1}{\pi} \text{Im} \overline{G}_{nm}^{\pm}(E) . \]

Finally, following [6] one can derive the exact expression for 
\[ \overline{G}_{nm}^{\pm}(E) \]. First it is necessary to write a set of equations for 
\[ G_{nm}^{\pm}(E \pm \imath \varepsilon) \] that follows from equations of motion
for \( G_{nm}^{\pm}(t) \) and then to average these equations using contour integration in complex
planes of \( J_n \)s. Under the imposed condition (3) on the basis of Gershgorin criterion one
can state that for \( a \geq 1 \) the retarded (advanced) Green function cannot have a pole in
lower (upper) half-planes of \( J_n \)s, whereas for \( a \leq -1 \) in upper (lower) half-planes of \( J_n \).
Therefore, every contour of integration should be closed in the half-plane where there
is only the pole originated from lorentzian distribution, and after trivial use of residues
one gets a set of equations for the averaged Green functions that possess already the
translational symmetry and hence may be solved in a standard way. The final result for
the averaged Green functions reads
\[ \overline{G}_{nm}^{\pm}(E) = \left( \frac{\sqrt{x^2 - y^2} - x}{y} \right)^{|n-m|} \]
with 
\[ x \equiv E - \Omega_0 \pm i \mid a \mid \Gamma, \ y \equiv J_0 \mp \text{sgn}(a) \Gamma . \]

The obtained averaged Green functions (5) permit to study thermodynamics of spin
model (1)-(3). Really, the required averaged density of states that follows from (5) reads
\[ \overline{\rho(E)} = \mp \frac{1}{\pi} \text{Im} \frac{1}{\sqrt{(E - \Omega_0 \pm i \mid a \mid \Gamma)^2 - (J_0 \mp \text{sgn}(a) \Gamma)^2}} . \]
\[ A \equiv (E - \Omega_0)^2 + (1 - |a|^2)\Gamma^2 - J_0^2, \quad B \equiv 2\Gamma |a| (E - \Omega_0) + \text{sgn}(a)J_0. \]  

(6)

The entropy and specific heat can be calculated by formulae

\[ s = \int dE \bar{\rho}(E) \left[ \ln \left( \frac{2\text{ch} \beta E}{2} \right) - \frac{\beta E}{2} \text{th} \frac{\beta E}{2} \right], \quad (7) \]

\[ c = \int dE \bar{\rho}(E) \left( \frac{\beta E}{2} \right)^2 \left( \frac{\text{ch} \beta E}{2} \right)^2. \quad (8) \]

Due to the noteworthy property of (6) \[ \frac{\partial}{\partial \Omega_0} \rho(E) = -\frac{\partial}{\partial E} \rho(E) \] one can express transverse magnetization and static transverse linear susceptibility through the density of states

\[ m_z \equiv < \frac{1}{N} \sum_{n=1}^{N} s_n^z > = -\frac{1}{2} \int dE \bar{\rho}(E) \text{th} \frac{\beta E}{2}, \quad (9) \]

\[ \chi_{zz} \equiv \frac{\partial m_z}{\partial \Omega_0} = -\beta \int dE \bar{\rho}(E) \frac{1}{(2\text{ch} \beta E)^2}. \quad (10) \]

Let us discuss the obtained results. In the absence of randomness (\( \Gamma = 0 \)) (6) reduces to the well-known result: \( \bar{\rho}(E) = \frac{1}{\pi} \frac{1}{\sqrt{J_0^2 - (E - \Omega_0)^2}} \) if \( | E - \Omega_0 | \leq | J_0 | \) and \( \bar{\rho}(E) = 0 \) otherwise.

The isotropic XY model in random lorentzian transverse field treated by H.Nishimori may be obtained in the limit \( \Gamma \to 0, \ |a| \ |\Gamma = \text{const} = \Gamma_N \). The model in question (1)-(3) essentially differs from that model: the density of states (6) in contrast to the case of diagonal disorder is not symmetric with respect to the change \( E - \Omega_0 \to -(E - \Omega_0) \).

However, it remains the same after the replacement \( E - \Omega_0 \to -(E - \Omega_0), \ a \to -a, \) or \( E - \Omega_0 \to -(E - \Omega_0), \ J_0 \to -J_0 \), since the simultaneous change of signs of \( J_0 \) and \( a \) in (6) does not affect \( \bar{\rho}(E) \). For convenience hereafter will be put \( J_0 = 1 \). The above-mentioned symmetry of the density of states can be seen in Fig.1, where the averaged density of states (6) for \( \Gamma = 1 \) is displayed. The density of states for non-random case is depicted in
Fig.1 by dashed lines. For large $|a|$ due to disorder the edges of the zone are completely smeared out; for $|a| \approx 1$ the disorder results in smearing out mainly of one edge of the zone. Some consequences induced by this dependence of $\rho(E)$ on $a$ for $\Gamma \neq 0$ will be seen in the behaviour of thermodynamical quantities.

The results of numerical calculations of thermodynamical quantities for $\Gamma = 1$ and few values of $a$ are presented in Figs.2-5, namely, the temperature dependences of entropy (7) (Fig.2), specific heat (8) (Fig.3) and static transverse linear susceptibility (10) (Fig.5) and the dependence on averaged transverse field at low temperatures of the transverse magnetization (9) (Fig.4); the curves that correspond to non-random case are depicted in these figures by dashed lines. The influence of randomness on thermodynamics is mainly rather typical. It leads to weak deformation of the curve entropy versus temperature with decreasing of entropy at high temperatures (Fig.2), broadening and decreasing of the peak in dependence specific heat versus temperature (Fig.3), smearing out of the cast in the $m_z$ versus $\Omega_0$ curve at $T = 0$ for $\Omega_0 = J_0$ and nonsaturated transverse magnetization at any finite transverse field (Fig.4), suppressing of static transverse linear susceptibility versus temperature curve (Fig.5). However, as can be seen in Figs.2-5 the influence of disorder, especially for small $a$, essentially depends on the sign of $a$. Particularly interesting is the case of strong asymmetry in the density of states $\overline{\rho(E)}$ when $|a| \approx 1$. From mathematical point of view the dependence of computed quantities on temperature and averaged transverse field and the well-pronounced difference between the cases $a \approx -1$ and $a \approx 1$ can be understood while bear in mind that these quantities according to (7)-(10) are the integrals over $E$ of the products of $\overline{\rho(E)}$ depicted in Fig.1 by the functions with evident dependence on $E$ at different $\beta$. It is interesting to note that for some
Hamiltonian parameters and temperatures even the large randomness (controlled by $\Gamma$) almost does not affect the observable thermodynamical quantities. This can be nicely seen in Figs. 2-5.

It is worth to underline that the asymmetry of $\rho(E)$ leads to the appearance of nonzero transverse magnetization $m_z$ at zero averaged transverse field $\Omega_0$. As it can be seen from (9) $m_z = 0$ at $T = 0$, $\Omega_0 = 0$ if $\int_{-\infty}^{0} dE \rho(E) = \int_{0}^{\infty} dE \rho(E)$. This is evidently true for a symmetric density of states $\rho(E)$ (as in the case considered by H. Nishimori) but is not obvious in the case in question (6). The difference between the integrals $\int_{-\infty}^{0} dE \rho(E)$ and $\int_{0}^{\infty} dE \rho(E)$ can be clearly demonstrated by numerical finite-chain calculations [13] as a difference between the numbers of negative and positive eigenvalues of $N \times N$ matrix $\Lambda_p$, denoted by $\mathcal{N}_-$ and $\mathcal{N}_+$ respectively, for certain realization of random model (1)-(3). For a realization of random chain (1)-(3) of 1000 spins with $\Omega_0 = 0$, $J_0 = 1$, $\Gamma = 1$ that gives $\frac{1}{N} \sum_{n=1}^{N} J_n = 1.009$ we found that for $a = -5$ $\mathcal{N}_- = 495$, $\mathcal{N}_+ = 505$, for $a = -2$ $\mathcal{N}_- = 470$, $\mathcal{N}_+ = 530$, for $a = -1.01$ $\mathcal{N}_- = 402$, $\mathcal{N}_+ = 598$. Another random realization of this chain with $\frac{1}{N} \sum_{n=1}^{N} J_n = 0.986$ yields for $a = -5$ $\mathcal{N}_- = 503$, $\mathcal{N}_+ = 497$, for $a = -2$ $\mathcal{N}_- = 471$, $\mathcal{N}_+ = 529$, for $a = -1.01$ $\mathcal{N}_- = 408$, $\mathcal{N}_+ = 592$. The transverse magnetization for certain realization at $T = 0$ is given by $m_z = \frac{\mathcal{N}_- - \mathcal{N}_+}{2N}$ and one finds a good agreement of calculated in such a manner $-m_z$ with the results depicted in Fig. 4.

To summarize, this paper is devoted to thermodynamics of spin-$\frac{1}{2}$ isotropic XY chain with random lorentzian intersite interaction and transverse field that depends linearly on the surrounding intersite interactions (1)-(3). The derived exact expressions for the averaged density of states (6) and thermodynamical quantities (7)-(10) seems to be interesting from academic point of view since they permit to understand the disorder effects and from
applied point of view since they may be used as a testing ground for approximate methods of spin systems with off-diagonal disorder.

Unfortunately, the obtained results do not permit to calculate exactly the averaged spin correlation functions because such calculation requires the knowledge of averaged many-particle fermion Green functions. Spin correlations and their dynamics may be examined using exact finite-chain calculations developed in \[14, 15\].

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\[ \rho(E) \]

\[ E - \Omega_0 \]

\[ a = -1.01 \]

\[ a = -2 \]

\[ a = -5 \]

\[ a = 1.01 \]

\[ a = 2 \]

\[ a = 5 \]
\[
a = -1.01
\]
\[
a = -2
\]
\[
a = -5
\]
\[
a = 1.01
\]
\[
a = 2
\]
\[
a = 5
\]
$-\chi_{zz}$

$\chi_{zz} = 1.01$

$a = -1.01$
$a = -2$
$a = -5$

$\frac{1}{\beta}$

$-\chi_{zz}$

$a = 1.0$
$a = 2$
$a = 5$
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Fig.1. The averaged density of states (6) \( \rho(E) \) vs. \( E - \Omega_0 \).

Fig.2. The entropy \( S \) (7) vs. temperature \( \frac{1}{\beta} \).

Fig.3. The specific heat \( c \) (8) vs. temperature \( \frac{1}{\beta} \).

Fig.4. The transverse magnetization \( -m_z \) (9) vs. transverse field \( \Omega_0 \) at low temperature \( (\frac{1}{\beta} = 0.001) \).

Fig.5. The static transverse linear susceptibility \( -\chi_{zz} \) (10) vs. temperature \( \frac{1}{\beta} \) at \( \Omega_0 = 0.5 \).