The spin-$\frac{1}{2}$ transverse $XX$ chain
with regularly alternating bonds and fields

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Abstract

We use continued fractions for a study of the thermodynamic properties of the periodic nonuniform spin-$\frac{1}{2}$ isotropic $XY$ chain in a non–random/random (Lorentzian) transverse field. The obtained results permit to examine the influence of a magnetic field and randomness on the spin–Peierls dimerization.

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Spin-$1/2$ XY chains provide an excellent ground for a rigorous study of different properties of low–dimensional quantum magnetic systems. By means of the Jordan–Wigner transformation such spin models can be mapped onto noninteracting spinless fermions and many statistical mechanics calculations can be performed exactly. In the present Letter we shall exploit the spin-$1/2$ isotropic XY chain in a transverse field (the transverse XX chain) for an analysis of the effects of periodic nonuniformity on the thermodynamic properties.

Starting from the late 60s a number of authors considered the spin-$1/2$ XY chain in a transverse field on two sublattices. Later it was found that the XX chain (without transverse field) represents a simple system with a spin–Peierls instability. Some further studies of the spin–Peierls instability in the spin-$1/2$ XY chains can be found in Refs. 5, 6 (within the adiabatic limit) and Ref. 7 (within the non–adiabatic limit). In what follows we want to emphasize that the thermodynamic properties of the periodic nonuniform transverse XX chains can be examined in a very general fashion including into consideration even regularly alternating randomness. Such an approach is based on the continued–fraction representation of the (random–averaged) diagonal one–fermion Green functions. The involved continued fractions can be calculated exactly for any finite period of regular nonuniformity, that immediately yields rigorous explicit expressions for the diagonal one–fermion Green functions, the density of magnon states, and hence for the thermodynamic quantities. We show that the periodic nonuniformity may induce a number of interesting properties, e.g. plateaus in the low–temperature magnetization vs field dependence or a nonzero magnetization in the zero average field. As an example we consider in some detail the chain with the random Lorentzian transverse field in the case of the period 2. The obtained density of states for such a chain permits us to extend the consideration of the influence of an external field on the stability of the spin–Peierls dimerized phase discussing in more detail the non–random case and reporting for the first time the effects of randomness. The interest in the properties of the spin–Peierls systems considerably increased since the discovery of the inorganic spin–Peierls compound CuGeO$_3$. The behaviour of the spin–Peierls systems in the presence of an external field or randomness attracts much interest both from the experimental and theoretical viewpoints. We believe that the discussed possibility to analyse rigorously the influence of non–random/random field within the frames of the simple model may be of interest for the theory of spin–Peierls compounds.
We consider $N \to \infty$ spins $\frac{1}{2}$ on a circle with the Hamiltonian of the nonuniform transverse $XX$ model

$$H = \sum_{n=1}^{N} \Omega_n s_n^x + 2 \sum_{n=1}^{N} I_n (s_n^x s_{n+1}^x + s_n^y s_{n+1}^y)$$

where the transverse fields $\Omega_n$ are assumed to be independent Lorentzian random variables each with the probability distribution $p(\Omega_n) = \frac{1}{\pi (\Gamma_n - \Omega_{0n}) + \Gamma_n}$. We assume regular nonuniformity, i.e. the mean value of the transverse field $\Omega_{0n}$ at site $n$, the width of its distribution $\Gamma_n$, as well as the exchange coupling $I_n$ between neighbouring sites $n$ and $n+1$ vary regularly from site to site with a period $p$, i.e. the sequence of parameters is $\Omega_{01} \Gamma_1 \Omega_{02} \Gamma_2 I_2 \ldots \Omega_{0p} \Gamma_p \Omega_{01} \Gamma_1 \Omega_{02} \Gamma_2 \ldots \Omega_{0p} \Gamma_p I_p \ldots$.

Our task is to examine the thermodynamic quantities of the spin model. Making use of the Jordan–Wigner transformation one gets a tight-binding model of spinless fermions on a circle. Introducing the temperature double–time one–fermion Green functions and averaging a set of equations for the Green functions (because of the Lorentzian probability distribution this can be done exactly) one can further make use of the continued–fraction representation for the diagonal Green functions exploited earlier for similar models by a number of authors. For any finite period of varying the mean value of the transverse field, the width of its distribution and the exchange coupling the involved continued fractions are periodic and can be evaluated by solving quadratic equations. Thus one gets rigorously the diagonal Green functions and therefore the density of magnon states $\rho(E)$ (a bar denotes the random–averaged quantity), which yields the thermodynamic quantities for the spin model. Some examples of such calculations can be found in Ref. 15. Let us present the result for the density of states of a chain having period 2 that will be used afterwards

$$\rho(E) = \frac{1}{2\pi} \frac{|Y(E)|}{B(E)},$$

$$Y(E) = (\Gamma_1 + \Gamma_2)\sqrt{\frac{B(E) + B'(E)}{2} - \text{sgn}(B''(E)) (2E - \Omega_{01} - \Omega_{02})\sqrt{\frac{B(E) - B'(E)}{2}}} ,$$

$$B'(E) = \left[ (E - \Omega_{01})(E - \Omega_{02}) - \Gamma_1 \Gamma_2 - I_1^2 - I_2^2 \right]^2 - \left[ (E - \Omega_{01})\Gamma_2 + (E - \Omega_{02})\Gamma_1 \right]^2 - 4I_1 I_2 ,$$

$$B''(E) = 2 \left[ (E - \Omega_{01})(E - \Omega_{02}) - \Gamma_1 \Gamma_2 - I_1^2 - I_2^2 \right] \left[ (E - \Omega_{01})\Gamma_2 + (E - \Omega_{02})\Gamma_1 \right] .$$

In the non–random case $\Gamma_1 = \Gamma_2 = 0$ Eq. 2 yields a nonzero value of the density of states $\rho(E) = \frac{1}{2\pi} \frac{|2E - \Omega_{01} - \Omega_{02}|}{\sqrt{-B'(E)}}$ only for $-B'(E) = 4I_1^2 I_2^2 - \left[ (E - \Omega_{01})(E - \Omega_{02}) - I_1^2 - I_2^2 \right]^2 > 0$ (two subband magnon en-
ergy spectrum). In the uniform case $\Omega_{01} = \Omega_{02} = \Omega_0$, $\Gamma_1 = \Gamma_2 = \Gamma$, $I_1 = I_2 = I$. Eq. (2) may be rewritten as 

$$\rho(E) = \mp \frac{1}{\pi} \text{Im} \frac{1}{\sqrt{(E - \Omega_0 \pm iF)^2 - 4I^2}}$$

that coincides with the result reported in Ref. 16.

Let us briefly discuss some special properties of spin model (1) induced by regular nonuniformity. Consider at first the non–random case $\Gamma_n = 0$. The main result of introducing the periodic nonuniformity is a splitting of the initial magnon band into several subbands. The number of subbands does not exceed the period of the nonuniformity. The splitting of the magnon band into subbands has several remarkable consequences for the thermodynamic properties. For example, the dependence of the transverse magnetization $m_z = -\frac{1}{2} \int_{-\infty}^{\infty} dE \rho(E) \tanh \frac{E}{2kT}$ on the transverse field $\Omega_0$ ($\Omega_{0n} = \Omega_0 + \Omega'_0$, $\Omega'_{0n}$ are fixed) at low temperatures is composed of sharply increasing parts separated by plateaus, the number of which is determined by the number of subbands. This can be nicely seen in Figs. 1a, 1b for the case of a chain with $p = 4$.

One of the interesting magnetic properties of the periodic nonuniform spin-$\frac{1}{2}$ transverse $XX$ chain is a possibility of a nonzero transverse magnetization $m_z$ at zero average transverse field $\sum_{n=1}^{N} \Omega_{0n} = 0$. A similar property was found for the spin-$\frac{1}{2}$ transverse $XX$ chain with correlated disorder. To illustrate this let us consider a chain having the period 4 in which the site $n+1$ with the transverse field $\Omega'_{02} < 0$ is surrounded by the strong couplings $I_1 = I_2$, whereas the site $n+3$ with the transverse field $-\Omega'_{02} > 0$ is surrounded by the weak couplings $I_3 = I_4 = 0$. The transverse fields at site $n$ and site $n+2$ are assumed to be zero, i.e. $\Omega'_{01} = \Omega'_{03} = 0$. Naively reasoning one may expect that the local transverse magnetization at site $n+1$ has smaller value and opposite direction with respect to the local transverse magnetization at site $n+3$ and therefore a nonzero total transverse magnetization at zero average transverse field may be anticipated. The explicit expression for the density of states for such a chain reads

$$\rho(E) = \frac{1}{4} \left[ \delta \left( E - \frac{1}{2} (\Omega_{02} - \sqrt{\Omega_{02}^2 + 8I_1^2}) \right) + \delta \left( E - \frac{1}{2} (\Omega_{02} + \sqrt{\Omega_{02}^2 + 8I_1^2}) \right) + \delta \left( E - \frac{1}{2} (\Omega_{02} + \sqrt{\Omega_{02}^2 + 8I_1^2}) \right) + \delta \left( E + \Omega_{02} \right) \right]$$

(solid curve in Fig. 1a) and for $T = 0$ one gets $m_z = -\frac{1}{8} \neq 0$ at $\sum_{n=1}^{N} \Omega_{0n} = 0$ (solid curves in Figs. 1b, 1c). The picture becomes more complicated if the weak couplings $I_3 = I_4$ have small but nonzero value (see Fig. 1). In that case for $T = 0$ we have $m_z = 0$ at $\sum_{n=1}^{N} \Omega_{0n} = 0$, however, the position of the magnon subbands provides an interesting dependence of $m_z$ on temperature (dashed curve in Fig. 1c). The latter dependence reminds the ‘order from disorder’ phenomenon, i.e. increasing of order with increasing temperature.

The main effect of the diagonal Lorentzian disorder is a smearing out of the band structure. The details of
the smoothed magnon subbands may be essentially different in the case of the uniform disorder (all $\Gamma_n$ are the same) and the nonuniform disorder ($\Gamma_n$ are different). In the latter case one may observe a different degree of smearing out of the different subbands that results in a different degree of smoothing of the different ‘steps’ in the step–like dependence of \( \overline{\mathcal{E}} \) on $\Omega_0$.

Finally, let us discuss the dependence $\overline{\mathcal{E}}(\delta) - \overline{\mathcal{E}}(0)$ in the presence of non–random/random field following Ref. 4. For this purpose we introduce the dimerization parameter $\delta$, $0 \leq \delta \leq 1$ assuming that $|I_1| = |I|(1 + \delta)$, $|I_2| = |I|(1 - \delta)$. The magnetic ground state energy per site immediately follows from the derived density of states (5) $\overline{\epsilon_0(\delta)} = -\frac{1}{\pi} \int_{-\infty}^{\infty} dE \rho(E)|E|$, the elastic energy per site is $\alpha \delta^2$ and hence the total energy is $\overline{\mathcal{E}}(\delta) = \overline{\epsilon_0(\delta)} + \alpha \delta^2$. We shall study the change of the total energy $\overline{\mathcal{E}}(\delta) - \overline{\mathcal{E}}(0)$ as a function of the dimerization parameter $\delta$ revealing in such a way the instability of the chain with respect to dimerization. For the non–random case $\epsilon_0(\delta)$ can be expressed through the elliptic integral of the second kind $\text{E}(\psi, a^2) \equiv \int_0^\psi d\varphi \sqrt{1 - a^2 \sin^2 \varphi}$, namely,

$$e_0(\delta) = -\frac{\sqrt{(\Omega_0 - \Omega_2)^2 + 16I^2}}{2\pi} \text{E} \left( \psi, \frac{16I^2(1 - \delta^2)}{(\Omega_0 - \Omega_2)^2 + 16I^2} \right) - |\Omega_0 + \Omega_2| \left( \frac{1}{4} - \frac{\psi}{\pi} \right),$$

$$\psi = \begin{cases} 0, & \text{if} \quad \sqrt{(\Omega_0 - \Omega_2)^2 + 16I^2} \leq |\Omega_0 + \Omega_2|, \\ \arcsin \sqrt{\frac{(\Omega_0 - \Omega_2)^2 + 16I^2}{4\pi^2(1 - \delta^2)}}, & \text{if} \quad \sqrt{(\Omega_0 - \Omega_2)^2 + 16I^2\delta^2} \leq |\Omega_0 + \Omega_2| < \sqrt{(\Omega_0 - \Omega_2)^2 + 16I^2}, \\ \frac{\pi}{2}, & \text{if} \quad |\Omega_0 + \Omega_2| < \sqrt{(\Omega_0 - \Omega_2)^2 + 16I^2\delta^2}. \end{cases}$$ (3)

Eq. (3) in the uniform limit $\Omega_0 = \Omega_2 = \Omega_0$ yields the result obtained in Ref. 5. We shall also consider the solution $\delta^*$ of the equation $\frac{\partial \overline{\mathcal{E}}(\delta)}{\partial \delta} = 0$ that may have a nonzero solution $\delta^* \neq 0$. In the non–random case the latter solution may arise as a solution of the equation

$$\alpha = \frac{\sqrt{(\Omega_0 - \Omega_2)^2 + 16I^2}}{4\pi(1 - \delta^2)} \left( \text{F} \left( \psi, \frac{16I^2(1 - \delta^2)}{(\Omega_0 - \Omega_2)^2 + 16I^2} \right) - \text{E} \left( \psi, \frac{16I^2(1 - \delta^2)}{(\Omega_0 - \Omega_2)^2 + 16I^2} \right) \right)$$ (4)

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

Let us discuss the dependence $\overline{\mathcal{E}}(\delta) - \overline{\mathcal{E}}(0)$ vs $\delta$ which manifests the spin–Peierls dimerization. We restrict our discussion to the uniform case $\Omega_0 = \Omega_2 = \Omega_0$, $\Gamma_1 = \Gamma_2 = \Gamma$. Consider at first the non–random case. Note that for strong transverse fields $|\Omega_0| \geq 2|I|$ from Eq. (3) it immediately follows that $\mathcal{E}(\delta) = -\frac{1}{2}|\Omega_0| + \alpha \delta^2$ and hence $\mathcal{E}(\delta) - \mathcal{E}(0)$ exhibits a minimum only at $\delta^* = 0$. This tells us that in strong enough field the uniformed state is energetically favoured over the dimerized one. Consider further weaker fields $|\Omega_0| < 2|I|$. From Eq. (3)
it follows that $E(\delta)$ is influenced by the field for $0 \leq \delta < \frac{|\Omega_0|}{2\gamma I}$ but $E(\delta)$ does not feel the presence of the field for $\frac{|\Omega_0|}{2\gamma I} \leq \delta \leq 1$. On the other hand one can calculate the r.h.s. of Eq. (1) varying $\delta$ from 0 to 1 finding in such a way the values of the dimerization parameter at which the total energy for a certain lattice (characterized by $\alpha$) exhibits an extremum. As it follows from Eq. (1) $\frac{\alpha}{2\gamma I} \to \frac{1}{8}$ as $\delta \to 1$ that means that for $\frac{\alpha}{2\gamma I} < \frac{1}{8}$ the total energy $E(\delta)$ does not have the extremum of interest for $0 \leq \delta \leq 1$. Hence, we shall exclude the soft lattices having small $\alpha$ from further consideration. The dependence $E(\delta) - E(0)$ vs $\delta$ at different $\Omega_0$ is shown in Fig. 2a. One finds that at $\Omega_0 = 0$ the quantity $E(\delta) - E(0)$ exhibits a minimum at $\delta^* \neq 0$. The position of this minimum does not change switching on the field. However, after a certain value of the transverse field (for which Eq. (1) has an additional solution $\delta^* = 0$) an additional local minimum in $E(\delta) - E(0)$ appears at $\delta^* = 0$. The two minima are separated by a maximum at an intermediate value of the dimerization parameter. With further increasing of $\Omega_0$ the depths of the minima become the same at a certain value of the transverse field and then the minimum at $\delta^* = 0$ becomes the global one. Finally at a certain field (for which Eq. (1) has the solution $\delta^* = \frac{|\Omega_0|}{2\gamma I}$) the minimum at the nonzero value of the dimerization parameter abruptly disappears that means a complete suppression of the dimerization by the field. The above sketched picture represents a typical scenario of a first order phase transition and is illustrated by the phase diagram in the $\Omega_0 - \alpha$ plane shown in Fig. 3a.

The dependences of $E(\delta) - E(0)$ vs $\delta$ in the presence of randomness at $\Omega_0 = 0$ and $\Omega_0 \neq 0$ are shown in Figs. 2b, 2c. In the case $\Omega_0 = 0$ with increasing of $\Gamma$ the position and the depth of the minimum at $\delta^* \neq 0$ continuously decrease and for a certain value of the strength of disorder the minimum occurs already at $\delta^* = 0$. That mean, that a random field with zero mean value can suppress the dimerization, too. However, the dimerization parameter $\delta^*$ vanishes according to a second order phase transition scenario in contrast to the transition in a non–random field. The influence of the randomness on the dependence $E(\delta) - E(0)$ at $\Omega_0 \neq 0$ can be traced in Fig. 2c. The phase diagrams in the plane $\Gamma - \alpha$ are shown in Figs. 3b, 3c.

It is necessary to mention that we have considered here only the stability of the dimerized phase against the uniformed one. Though, the qualitative picture of a first order phase transition in a uniform field may be correct, we notice that both experiments and approximate analytical treatments as well as exact numerical computations (mainly for CuGeO$_3$) show a transition from the dimerized to incommensurate phase. Evidently,
assuming the simple ansatz for the lattice distortion $\delta_1 \delta_2 \delta_1 \delta_2 \ldots$, $\delta_1 + \delta_2 = 0$ we were able to compare the
ground state energies only for the dimerized and uniformed phases. To detect a transition from the dimerized
phase to the incommensurate phase with increasing of the field one must analyze the ground state energy of a
chain having sufficiently large period (say, a chain with $p = 12$, for which one can still easily obtain the density of
states$^{19}$). In the presence of random fields (or/and random exchange couplings) even more complicated lattice
distortions should be examined and the elaborated approach for the calculation of the ground state energy of
the nonuniform spin-$\frac{1}{2}$ transverse $XX$ chain provides some possibilities to perform such an analysis.

To summarize, we have suggested a general scheme for the study of thermodynamics of the regularly alternating
spin-$\frac{1}{2}$ transverse $XX$ chains. It is based on the continued–fraction representation for the diagonal
one–fermion Green functions. We have discussed briefly some magnetic properties of the periodic nonuniform
spin-$\frac{1}{2}$ transverse $XX$ chains such as plateaus in magnetization curves or a nonzero magnetization at the zero
average field, as well as the influence of (Lorentzian) randomness in the transverse field on these properties. We
have examined also the stability of spin–Peierls dimerized phase in the spin-$\frac{1}{2}$ $XX$ chain in the presence of non–
random/random (Lorentzian) transverse field using the rigorous expression for the (averaged over randomness)
ground state energy of the corresponding alternating chain.

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FIGURE 1. Magnetic properties of the chain having period 4. The local transverse fields are $\Omega_{0n} = \Omega_0 + \Omega'_{0n}$, $\Omega'_{01} = \Omega'_{03} = 0$, $\Omega'_{02} = -\Omega'_{04} = -1$, the exchange couplings are $|I_1| = |I_2| = 0.5$, $|I_3| = |I_4| = 0$ (solid curves), $|I_3| = |I_4| = 0.05$ (dashed curves), $|I_3| = |I_4| = 0.25$ (dashed–dotted curves), $|I_3| = |I_4| = 0.5$ (dotted curves). a) Density of states. b) Transverse magnetization vs transverse field $\Omega_0$ at $T = 0$. c) Transverse magnetization vs temperature at $\Omega_0 = 0$.

FIGURE 2. $\bar{E}(\delta) - \bar{E}(0)$ vs $\delta$ for a chain with $|I| = 0.5$, $\alpha = 0.5$. a) Non–random case $\Gamma = 0$, $\Omega_0 = 0$, 0.01, 0.02, 0.03, 0.04, 0.05, 0.06, 0.07, 0.08, 0.09, 0.1 (from bottom to top). b) $\Omega_0 = 0$, $\Gamma = 0$, 0.001, 0.003, 0.006, 0.01, 0.02, 0.03, 0.05 (from bottom to top). c) $\Omega_0 = 0.04$, $\Gamma = 0$, 0.001, 0.003, 0.006, 0.01, 0.02, 0.03, 0.05 (from bottom to top).

FIGURE 3. Phase diagram of the spin-$\frac{1}{2}$ transverse XX chain with $|I| = 0.5$ as it follows from the dimerization ansatz for the ground state energy. a) Non–random case $\Gamma = 0$. A — dimerized state. B$_1$, B$_2$ — both dimerized and uniformed states are possible, moreover, in B$_1$ the former one is favourable, whereas in B$_2$ the latter one is favourable; on the line that separates B$_1$ and B$_2$ the depth of both minima in $E(\delta) - E(0)$ is equal. C — uniformed state. b) Random case with mean value of the field $\Omega_0 = 0$. A — dimerized state. C — uniformed state. c) Random case with mean value of the field $\Omega_0 = 0.04$. A, B$_1$, B$_2$, C are of the same meaning as in a).
Figure 2:
Figure 3: