The ground state properties
of the spin–$\frac{1}{2}$ transverse Ising chain
with periodically varying bonds and fields

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Abstract

Using continued fractions we study the ground state properties of the spin–$\frac{1}{2}$ Ising chain in a transverse field with periodically varying interaction strengths and external fields. We consider in detail the chain having the period of modulation of interactions equals 2 and compare the results obtained with those corresponding to the spin–$\frac{1}{2}$ isotropic $XY$ chain in a transverse field. In contrast to the behaviour of the transverse $XY$ chain, the transverse Ising chain does not exhibit a step–like magnetization vs. field dependence caused by the alternation of bonds, its susceptibility exhibits a logarithmic singularity at the field determined by interaction strengths, and it is stable with respect to spin–Peierls dimerization.

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Spin–$\frac{1}{2}$ XY chains provide an excellent ground for a rigorous study of different properties of the low-dimensional quantum magnetic systems due to the fact that with the help of the Jordan–Wigner transformation such spin models can be mapped onto noninteracting spinless fermions and as a result many statistical mechanics calculations can be performed exactly. In what follows we shall consider the periodic alternating XY chain in a transverse field with extremely anisotropic spin coupling (in short called here the transverse Ising chain) in order to study the generic effects induced by regular alternation of the nearest neighbour interaction strengths and the external fields. The periodic alternating chain can be viewed as a chain having several sublattices. There are few papers dealing with the statistical mechanics properties of XY chains on two sublattices. We want to emphasize that in the above mentioned limit of the transverse Ising chain the calculation of the thermodynamic quantities can be performed in a rather general manner covering all chains with an arbitrary period of alternation. The present paper can be viewed as a nontrivial extension of the recent study of the thermodynamics of the spin–$\frac{1}{2}$ isotropic XY chain in a transverse field (called here the transverse XY chain) with regularly alternating fields and bonds. In particular, we compare below the zero temperature dependences transverse magnetization vs. transverse field and static transverse susceptibility vs. transverse field for the regularly alternating transverse Ising and XY chains. On the other hand, it is known that the transverse XY chain is a simple system exhibiting a spin–Peierls instability. An analysis of the ground state energy of the periodic alternating transverse Ising chain of period 2 allows one to examine a spin–Peierls instability of that chain with respect to dimerization. We find that the transverse Ising chain is stable with respect to dimerization which demonstrates a role of the anisotropy in spin coupling for a spin–Peierls instability.

We consider the $N \to \infty$ spins $\frac{1}{2}$ on a ring with the Hamiltonian of the nonuniform transverse Ising model

$$H = \sum_{n=1}^{N} \Omega_n s^n_z + 2 \sum_{n=1}^{N} I_n s^n_z s_{n+1}^z, \quad s^z_{N+1} = s^z_1.$$  

We assume regular nonuniformity in (1), i.e. the transverse field $\Omega_n$ at the site $n$ as well as the exchange coupling $I_n$ between the neighbouring sites $n$ and $n + 1$ vary regularly from site to site with period $p$, i.e. we have a sequence of parameters $\Omega_1 I_1 \Omega_2 I_2 \ldots \Omega_p I_p \Omega_1 I_1 \Omega_2 I_2 \ldots \Omega_p I_p \ldots$.

Our goal is to examine the thermodynamic quantities of spin model (1). In order to do this, we shall first express the Hamiltonian in terms of fermion operators. This can be done in the usual way by applying the Jordan–Wigner transformation. As a result one gets a model of spinless fermions on a ring described by the Hamiltonian

$$H = \sum_{n=1}^{N} \Omega_n \left( c_n^t c_n - \frac{1}{2} \right) + \frac{1}{2} \sum_{n=1}^{N} I_n \left( c_n^t c_{n+1}^t + c_n^t c_{n+1} - c_n c_{n+1}^t - c_n c_{n+1} \right), \quad c_{N+1}^t = c_1^t, \quad c_{N+1} = c_1$$

(2)

(the boundary term, that is unimportant as far as the thermodynamics is concerned, has been omitted). Unlike, in Ref. 6, we cannot proceed directly by using a continued fraction representation for the diagonal one–fermion Green functions of the tight–binding spinless fermions since the Hamiltonian (2) contains the products of two creation (annihilation) operators. However, it is well known (see, e.g., 1,11,12) that after introducing new

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operators $\eta_k = \sum_{i=1}^{N} (g_{ki} c_i + h_{ki} c_i^+)$, $\eta_k^+ = \sum_{i=1}^{N} (h_{ki} c_i + g_{ki} c_i^+)$ the Hamiltonian (2) transforms into

$$H = \sum_{k=1}^{N} \Lambda_k \left( \eta_k^+ \eta_k - \frac{1}{2} \right), \quad \{ \eta_k^+ , \eta_q \} = \delta_{kq}, \quad \{ \eta_k , \eta_q \} = \{ \eta_k^+ , \eta_q^+ \} = 0$$

(3)

if the unknown coefficients $g_{ki} = \frac{1}{2} (\Phi_{ki} + \Psi_{ki})$, $h_{ki} = \frac{1}{2} (\Phi_{ki} - \Psi_{ki})$ are determined from the following equations

$$\Omega_{n-1} I_{n-1} \Phi_{k,n-1} + (\Omega_n^2 + I_n^2 - \Lambda_k^2) \Phi_{kn} + \Omega_n I_n \Phi_{k,n+1} = 0, \quad \Phi_{k0} = \Phi_{kN}, \quad \Phi_{k,N+1} = \Phi_{k1};$$

$$\Omega_n I_{n-1} \Psi_{k,n-1} + (\Omega_n^2 + I_n^2 - \Lambda_k^2) \Psi_{kn} + \Omega_n I_n \Psi_{k,n+1} = 0, \quad \Psi_{k0} = \Psi_{kN}, \quad \Psi_{k,N+1} = \Psi_{k1}.$$  

(4)

Eqs. (4) formally coincide with those describing displacements of particles in a nonuniform harmonic chain with nearest neighbour interactions. To find the distribution of the squares of “phonon” (magnetic excitation) frequencies $R(E^2) = \frac{1}{\pi N} \sum_{n=1}^{N} \delta (E^2 - \Delta_n^2)$ we may use the Green function approach. Consider, for example, the Green functions $G_{nm} \equiv G_{nm}(E^2)$ that satisfy the set of equations

$$(E^2 - \Omega_n^2 - I_n^2) G_{nm} - \Omega_{n-1} I_{n-1} G_{n-1,m} - \Omega_n I_n G_{n+1,m} = \delta_{nm}$$

(5)

with periodic boundary conditions implied. Knowing $G_{nm}$ one immediately finds the density of states $R(E^2)$ through the relation

$$R(E^2) = \pm \frac{1}{\pi N} \sum_{n=1}^{N} \text{Im} G_{nn}(E^2 \pm i\epsilon), \quad \epsilon \to +0.$$  

(6)

As follows from (4) all the thermodynamic quantities can be expressed through $R(E^2)$. For example, the Helmholtz free energy per site is given by

$$f = -\frac{2}{\beta} \int_{0}^{\infty} dE R(E^2) \ln \left( 2 \cosh \frac{\beta E}{2} \right).$$

(7)

Obviously, $R(E^2)$ can be obtained with the help of the Green functions introduced on the basis of the set of equations for the coefficients $\Psi_{kn}$ (4). We have performed such a calculation and found the same result for $R(E^2)$ in the cases considered below (Eqs. (8) and (11)).

We have now to calculate the diagonal Green functions $G_{nn}$. Let us use the continued fraction representation for $G_{nn}$ that follows from (4)

$$G_{nn} = \frac{1}{E^2 - \Omega_n^2 - I_n^2 - \Delta_n^+ - \Delta_n^-},$$

$$\Delta_n^+ = \frac{\Omega_n^2 I_n^2}{E^2 - \Omega_n^2 - I_n^2 - \frac{\Omega_{n+1}^2 I_{n+1}^2}{E^2 - \Omega_{n+1}^2 - I_{n+1}^2 - \frac{\Omega_{n+2}^2 I_{n+2}^2}{E^2 - \Omega_{n+2}^2 - I_{n+2}^2 - \ldots}}},$$

$$\Delta_n^- = \frac{\Omega_n^2 I_n^2}{E^2 - \Omega_n^2 - I_n^2 - \frac{\Omega_{n-1}^2 I_{n-1}^2}{E^2 - \Omega_{n-1}^2 - I_{n-1}^2 - \frac{\Omega_{n-2}^2 I_{n-2}^2}{E^2 - \Omega_{n-2}^2 - I_{n-2}^2 - \ldots}}}. $$

(8)

For any finite period of varying $\Omega_n$ and $I_n$ the continued fractions in (8) become periodic (evidently, the limit $N \to \infty$ is hinted) and can be easily calculated by solving quadratic equations. As a result we get rigorous results for the Green functions, density of states (4) and thermodynamic quantities (3) of the periodic alternating spin
model \([1]\). Note that the thermodynamic quantities are not sensitive to the signs of \(\Omega_n\) and \(I_n\). Therefore, one may assume \(\Omega_n \geq 0, I_n \geq 0\) without loss of generality.

It should be remarked at this point that the possibility of obtaining \(R(E^2)\) exactly in the manner described above exists only for the transverse Ising chain. For the transverse \(XY\) chain with an arbitrary anisotropic exchange coupling one arrives at a set of five diagonal coupled equations (not three, as above), corresponding to a nonuniform harmonic chain with nearest and next nearest neighbour interactions.\(^{1,12}\) Hence, one cannot proceed as above.

To illustrate how the method works we begin with the uniform case, namely, the periodic alternating chain having period 1. For such a case,

\[
\Delta_n^+ = \Delta_n^- = \frac{1}{2}(E^2 - \Omega^2 - I^2) \pm \sqrt{(E^2 - \Omega^2 - I^2)^2 - 4\Omega^2 I^2},
\]

and therefore

\[
R(E^2) = \begin{cases} 
\frac{1}{\pi} \sqrt{\frac{1}{E^2 - a_1(E^2 - a_2)}}, & \text{if } a_1 < E^2 < a_2, \\
0, & \text{otherwise,}
\end{cases}
\]

with \(a_1 = (\Omega - I)^2, a_2 = (\Omega + I)^2\). From Eq. \([3]\), the ground state energy per site, \(e_0 = -\int_0^\infty dE^2 R(E^2)\), is

\[
e_0 = -\frac{1}{\pi} \int_{\text{a_1}}^{a_2} \frac{dE^2}{\sqrt{-(E^2 - a_1)(E^2 - a_2)}},
\]

which after the change of variable \(E = \sqrt{a_2 - (a_2 - a_1)\sin^2 \phi} \), leads to the known\(^{13}\) expression

\[
e_0 I = -\frac{1}{\pi} \int_0^{\pi} d\phi \sqrt{(1 + \lambda)^2 - 4\lambda \sin^2 \phi}, \quad \lambda = \frac{\Omega}{I}.
\]

Let us now turn to the periodic alternating chain having period 2. Following the procedure above, one finds

\[
R(E^2) = \begin{cases} 
\frac{1}{4\pi} \frac{|2E^2 - \Omega^2 - I_1^2 - I_2^2|}{\sqrt{B(E^2)}}, & \text{if } B(E^2) > 0, \\
0, & \text{otherwise,}
\end{cases}
\]

\[
B(E^2) = 4\Omega_1^2 \Omega_2^2 I_1^2 I_2^2 - (E^4 - (\Omega_1^2 + \Omega_2^2 + I_1^2 + I_2^2) E^2 + \Omega_1^2 \Omega_2^2 + I_1^2 I_2^2)^2
\]

\[
= -(E^2 - b_1)(E^2 - b_2)(E^2 - b_3)(E^2 - b_4),
\]

\[
\{b_j\} = \left\{ \frac{1}{2} \left( \Omega_1^2 + \Omega_2^2 + I_1^2 + I_2^2 \pm \sqrt{(\Omega_1^2 + \Omega_2^2 + I_1^2 + I_2^2)^2 - 4(\Omega_1 \Omega_2 \pm I_1 I_2)^2} \right) \right\}.
\]

Obviously, \([11]\) recovers the result for the uniform chain \([3]\) if \(\Omega_1 = \Omega_2 = \Omega, I_1 = I_2 = I\). The resulting density of states \(R(E^2)\) \([11]\) yields all thermodynamic quantities of the regularly alternating transverse Ising chain \(\Omega_1 I_1 \Omega_2 I_2 \Omega_3 I_3 \Omega_4 I_4 \ldots\).

Consider further, in some detail, the alternating transverse Ising chain with \(p = 2\) with the dimerization ansatz \(\Omega_1 = \Omega_2 = \Omega, I_1 = I(1 + \delta), I_2 = I(1 - \delta)\) in mind, where \(0 \leq \delta \leq 1\) is the dimerization parameter. For such a chain the ground state energy according to \([11]\) can be written as

\[
e_0(\delta) I = -\frac{1}{2\pi} \int_0^{\pi} d\phi \left( \sqrt{1 + \lambda^2 + \delta^2 + 2\sqrt{W}} + \sqrt{1 + \lambda^2 + \delta^2 - 2\sqrt{W}} \right),
\]

\[
W = \lambda^2 + \delta^2 - \lambda^2(1 - \delta^2) \sin^2 \phi.
\]

\([12]\)
If \( \delta = 0 \) (12) transforms into the ground state energy of the uniform chain (11).

Further, we calculate the zero temperature transverse magnetization \( m_z = \frac{\partial m_z}{\partial I} \) by differentiating the r.h.s of Eq. (12) with respect to \( \lambda \). In Fig. 1 the obtained dependence of the transverse magnetization on the transverse field for several values of the dimerization parameter \( \delta \) is plotted. As one can see from Fig. 1 the transverse Ising chain with regularly alternating bonds does not exhibit a step-like dependence of magnetization vs. field and the magnetization profile only smoothly deforms with the increasing \( \delta \). This behaviour is contrary to that of the transverse XY chain (for which the Hamiltonian (11) would contain \( s_n^x s_{n+1}^x + s_n^y s_{n+1}^y \) instead of \( s_n^x s_{n+1}^x \)), since the latter model does show a step-like dependence of magnetization vs. field (i.e. a plateau at \( m_z = 0 \)) for regularly alternating bonds\(^6\) (the light curves in Fig. 1). The dissimilarity is conditioned by the different symmetries of these models, since \( \sum_{n=1}^{N} s_n^z \) does not commute with the Hamiltonian of the transverse Ising chain but it does commute with the Hamiltonian of the transverse XY chain. It is worth to consider in addition both models in the limit \( \delta = 1 \) when the chain splits into noninteracting clusters consisting of two sites. The zero temperature transverse magnetization follows from the formula \( m_z = \frac{1}{2} | GS \rangle | s_1^x + s_2^x \rangle \) where \( | GS \rangle \) is the ground state eigenvector of the two-site cluster Hamiltonian. For the transverse Ising model \( | GS \rangle \) smoothly varies with increasing \( \Omega \). Moreover, \( \langle GS | s_1^x + s_2^x | GS \rangle = 0 \) if \( \Omega = 0 \) and \( \langle GS | s_1^x + s_2^x | GS \rangle \rightarrow -1 \) if \( \Omega \rightarrow \infty \). Unlike, for the transverse XY model the ground state is singlet (and thus \( \langle GS | s_1^x + s_2^x | GS \rangle = 0 \) if \( 0 \leq \Omega < 2J \)). However, if \( \Omega \) exceeds \( 2J \) the ground state becomes triplet and \( \langle GS | s_1^x + s_2^x | GS \rangle \) abruptly changes to \(-1\).

The ground state static transverse susceptibility \( \chi_{zz} = \frac{\partial m_z}{\partial I} = \frac{1}{2} \frac{\partial^2 c_0(\delta)}{\partial \lambda^2} \) follows straightforwardly from Eq. (12). In the left panel in Fig. 2 the obtained dependence of the static transverse susceptibility on the transverse field for several \( \delta \) is plotted. Using Eq. (12) it is easy to show that \( \chi_{zz} \) for the dimerized chain consists of a finite part and a singular part

\[
\chi_{zz} = \text{finite term} - \frac{\lambda^2}{2\pi} \int_0^{\pi} d\phi \frac{(1 - (1 - \delta^2) \sin^2 \phi)^2}{W^{\frac{3}{2}} \sqrt{1 + \lambda^2 + \delta^2 - 2\sqrt{W}}} \quad (13)
\]

As it follows from (13) the ground state static transverse susceptibility exhibits a logarithmic singularity at \( \lambda = \lambda^* = \sqrt{1 - \delta^2} \), i.e. \( \chi_{zz} \sim \ln |\lambda - \lambda^*|, \lambda \to \lambda^* \). It should be noted, that \( \chi_{zz} \) for the corresponding dimerized XY chain exhibits two square root singularities at \( \lambda_1^* = 2\delta \) and \( \lambda_2^* = 2 \) (right panel in Fig. 2, see also Ref. 6).

To discuss a spin–Peierls dimerization in the adiabatic limit one must examine the dependence of the total energy \( E(\delta) = c_0(\delta) + \alpha\delta^2 \), which consists of the magnetic part \( c_0(\delta) \) (12) and the elastic part \( \alpha\delta^2 \), \( \alpha > 0 \), on the dimerization parameter \( \delta \). In Fig. 3 one can see the dependence of the magnetic energy (12) on \( \delta \) for different values of the transverse field. From these plots one concludes that the magnetic energy as a rule decreases with the increase of \( \delta \) (except for \( \lambda = 0 \) and \( \lambda \to \infty \) when \( c_0(\delta) \) (12) does not depend on \( \delta \) and equals \(-\frac{1}{2} \) and \(-\frac{1}{2} \), respectively) that is a necessary condition for the existence of the dimerized phase. However, the magnetic energy decreases too slowly in comparison with the increase of the elastic energy that provides stability of the chain with respect to dimerization. To demonstrate this, we calculate \( a = -\frac{\partial}{\partial \delta^2} c_0(\delta) \) by differentiating the r.h.s. of Eq. (12) with respect to \( \delta^2 \), and display the dependence of this quantity on \( \delta \) for several values of the transverse field in Fig. 4. These plots show that \( E(\delta) \) may exhibit a maximum (but not a minimum) at the
nonzero value of dimerization parameter for lattices having small $\frac{a}{I}$ as the slope of the curves $a = -\frac{\partial}{\partial \delta} \frac{\epsilon_0(\delta)}{I}$ vs. $\delta$ manifests. Hence, the uniform chain with $\delta = 0$ is favourable. On the contrary, for the $XY$ chain the ground state energy decreases sufficiently rapidly to provide a stability of the dimerized phase. In Fig. 4 we also display the dependence of $a = -\frac{\partial}{\partial \delta} \frac{\epsilon_0(\delta)}{I}$ on $\delta$ for the transverse $XY$ chain (light curves) (see also Ref. 6) emphasizing explicitly the difference between those two spin models.

It is worthy to note, that the absence of a spin–Peierls dimerization in the transverse Ising chain may be anticipated on the basis of the following reasoning.\footnote{14} Considering the transverse $XY$ chain one notes that for $\Omega = 0$ the ground state corresponds to a half-filled fermion band, the system is gapless and the Peierls mechanism does work. As $\Omega$ increasing becomes equal to $I$ the ground state corresponds to an empty fermion band, the system becomes gaped and the dimerized phase does not appear. The ground state of the transverse Ising chain\footnote{13} always corresponds to an empty fermion band, the system is gapped unless $\Omega = I$ and as a result no Peierls dimerization should be expected.

To conclude, we have proposed to use continued fractions for the calculation of thermodynamic quantities of regularly alternating spin–$\frac{1}{2}$ transverse Ising chains. For such a chain, in which the bonds are alternating in magnitude along the chain with period 2, we have found no plateaus in the dependence magnetization vs. field. The susceptibility of the chain exhibits a logarithmic singularity at the field determined by interaction strengths. Moreover, we have found that in the adiabatic limit the transverse Ising chain is stable with respect to a spin–Peierls dimerization. These findings differ dramatically from the corresponding results for the transverse isotropic $XY$ chain, and therefore it would be of great interest to study the periodic alternating transverse anisotropic $XY$ chain that connects both these limiting cases.

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FIGURE 1. The ground state transverse magnetization vs. transverse field for the transverse Ising chain with regularly alternating bonds with the period 2. δ = 0 (uniform chain), δ = 0.3, δ = 0.6, and δ = 0.9 correspond to solid, long–dashed, short–dashed, and dotted bold curves, respectively. For comparison the corresponding results for the transverse XY chain are shown by light curves.

FIGURE 2. The ground state static transverse susceptibility vs. transverse field for the transverse Ising chain (left panel) and the transverse XY chain (right panel) with regularly alternating bonds with the period 2. δ = 0 (uniform chain), δ = 0.3, δ = 0.6, and δ = 0.9 correspond to solid, long–dashed, short–dashed, and dotted curves, respectively.

FIGURE 3. The change of the ground state magnetic energy $d = e_0(\delta) - e_0(0)$ vs. δ for the transverse Ising chain for λ = 0, 0.25, 0.5, 1, and 2 (solid, long–dashed, short–dashed, dotted, and dashed–dotted bold curves, respectively). For comparison the corresponding results for the transverse XY chain are shown by light curves.

FIGURE 4. The dependence $a = -\frac{∂}{∂\delta} e_0(\delta)$ vs. δ for the transverse Ising chain with λ = 0, 0.25, 0.5, 1, and 2 (solid, long–dashed, short–dashed, dotted, and dashed–dotted bold curves, respectively). For comparison the corresponding results for the transverse XY chain are shown by light curves.
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Figure 3: The change of the ground state magnetic energy $d = \frac{\varepsilon_n(\delta)}{\varepsilon_n(0)} - \frac{\varepsilon_n(0)}{\varepsilon_n(0)}$ vs. $\delta$ for the transverse Ising chain for $\lambda = 0, 0.25, 0.5, 1, \text{ and } 2$ (solid, long–dashed, short–dashed, dotted, and dashed–dotted bold curves, respectively). For comparison the corresponding results for the transverse $XY$ chain are shown by light curves.
Figure 4: The dependence $a = -\frac{\partial}{\partial \delta} \sigma_{\lambda}^{(l)}$ vs. $\delta$ for the transverse Ising chain with $\lambda = 0, 0.25, 0.5, 1, \text{and } 2$ (solid, long-dashed, short-dashed, dotted, and dashed-dotted bold curves, respectively). For comparison the corresponding results for the transverse $XY$ chain are shown by light curves.