CHAPTER 1

QUANTUM PHASE TRANSITIONS
IN ALTERNATING TRANSVERSE ISING CHAINS

Oleg Derzhko

Institute for Condensed Matter Physics
of the National Academy of Sciences of Ukraine
1 Svientsitskii Street, L’viv-11, 79011, Ukraine
E-mail: derzhko@icmp.lviv.ua

This chapter is devoted to a discussion of quantum phase transitions in regularly alternating spin-$\frac{1}{2}$ Ising chain in a transverse field. After recalling some generally-known topics of the classical (temperature-driven) phase transition theory and some basic concepts of the quantum phase transition theory I pass to the statistical mechanics calculations for a one-dimensional spin-$\frac{1}{2}$ Ising model in a transverse field, which is the simplest possible system exhibiting the continuous quantum phase transition. The essential tool for these calculations is the Jordan-Wigner fermionization. The latter technique being completed by the continued fraction approach permits to obtain analytically the thermodynamic quantities for a “slightly complicated” model in which the intersite exchange interactions and on-site fields vary regularly along a chain. Rigorous analytical results for the ground-state and thermodynamic quantities, as well as exact numerical data for the spin correlations computed for long chains (up to a few thousand sites) demonstrate how the regularly alternating bonds/fields effect the quantum phase transition. I discuss in detail the case of period 2, swiftly sketch the case of period 3 and finally summarize emphasizing the effects of periodically modulated Hamiltonian parameters on quantum phase transitions in the transverse Ising chain and in some related models.

1. Classical and Quantum Phase Transitions

In this chapter I consider the effects of regular alternation of the Hamiltonian parameters on the quantum phase transition inherent in a one-dimensional spin-$\frac{1}{2}$ Ising model in a transverse field. Before starting to discuss this issue let me recall some common wisdoms from statistical physics.
One of the aims of statistical physics is to describe different phases which may occur in many-particle systems and the transitions between different phases, i.e., the phase transitions. We often face phase transitions in everyday life. Melting of ice, boiling of water or vanishing of the magnetic properties of iron after heating are well-known phenomena for everyone. Normally we associate the changes in properties of a substance as the temperature varies. However, such changes may occur at a fixed finite temperature while some other parameter (such as pressure) varies.

P. Ehrenfest proposed a classification of phase transitions. In the Ehrenfest classification of phase transitions we say that the phase transition is of the order one if the free energy is continuous across the phase transition whereas its first derivatives with respect to temperature and other variables (for example, pressure) are discontinuous. Similarly, we say that the phase transition is of the order two (three) if the free energy and its first derivatives (first two derivatives) are continuous across the phase transition whereas the second (third) derivatives are discontinuous. A few years later L. Landau proposed to consider discontinuous or continuous phase transitions. In the Landau sense the discontinuous (continuous) phase transition is characterized by a discontinuous (continuous) change in the order parameter and, therefore, it is usually viewed as of the first- (second- or higher-) order. In the first-order phase transitions the two phases coexist at the phase transition temperature. Thus, if ice is melting one observes two phases, i.e., liquid and solid, which coexist at the temperature of phase transition. This is an example of discontinuous phase transition. In the second-order (and higher-order) phase transitions the two phases do not coexist. An example is the Curie point of a ferromagnet above which the magnetic moment of a material vanishes. Below the Curie temperature $T_c$ we can observe only the ferromagnetic phase which continuously disappears at $T_c$. Above $T_c$ we can observe only the paramagnetic phase. Some phase transitions are not in accord with the naively applied classification rules. Thus, the Bose-Einstein condensation in an ideal Bose gas is accompanied by a kink in the temperature dependence of specific heat at the Bose-Einstein condensation temperature but is viewed as a first-order phase transition. In what follows our focus will be on the continuous phase transitions which were studied very intensively in the last century, especially in the last four decades.

Statistical mechanics provides some microscopic models of the continuous phase transitions. One of such models was invented by E. Ising about 80 years ago. It became especially well-known after L. Onsager had found an exact solution of the model in two dimensions. Let me introduce the Ising
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model and fix the notations. The model consists of magnetic moments or spins which may have two values $-\frac{1}{2}$ and $\frac{1}{2}$ and which interact with the nearest neighbors. The Hamiltonian of the model on a square lattice of $N_x N_y = N$ sites can be written in the form

$$H = - \sum_{i_x=1}^{N_x} \sum_{i_y=1}^{N_y} \left( J_h s^z_{i_x,i_y} s^z_{i_x+1,i_y} + J_v s^z_{i_x,i_y} s^z_{i_x,i_y+1} \right)$$

(1)

where $s^z_{i_x,i_y}$ is the spin variable attached to the site $i_x, i_y$, and $J_h$ and $J_v$ are the exchange interactions in horizontal and vertical directions, respectively. If the exchange interaction in (1) is positive, the same value of spin variables at neighboring sites is favorable, i.e. the exchange interaction is ferromagnetic. The spin variable $s^z$ may be presented by a half of the Pauli matrix

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and the canonical partition function which determines the thermodynamics of the model reads

$$Z = \sum_{\{s^z_{i_x,i_y} = \pm \frac{1}{2} \}} \exp(-\beta H) = \text{Tr} \exp(-\beta H),$$

(2)

where $\beta = \frac{1}{kT}$ is the inverse temperature. We are also interested in the spin correlation functions $\langle s^z_{i_x,i_y} s^z_{j_x,j_y} \rangle$, where the canonical average means

$$\langle (\ldots) \rangle = \frac{1}{Z} \text{Tr} \left( \exp(-\beta H) (\ldots) \right).$$

The spin correlation functions in the limit of infinitely large intersite distances yield the magnetization per site

$$m^z = \frac{1}{N_x N_y} \sum_{i_x=1}^{N_x} \sum_{i_y=1}^{N_y} \langle s^z_{i_x,i_y} \rangle$$

(3)

which plays the role of the order parameter. Due to the seminal study of L. Onsager we understand in great detail the properties of the two-dimensional Ising model.

At zero temperature $T = 0$ all spins have the same value, say, $\frac{1}{2}$, and $m^z = \frac{1}{2}$. As the temperature becomes nonzero some of spin variables due to temperature fluctuations have the value $-\frac{1}{2}$, and thus $m^z$ becomes smaller.
Quantitatively the temperature fluctuations of magnetic moment can be characterized by

$$\left\langle \left( \sum_{i_x=1}^{N_x} \sum_{i_y=1}^{N_y} (s_{i_x,i_y}^z - m_z^z) \right)^2 \right\rangle.$$

At the critical temperature $T_c$ the temperature fluctuations completely destroy the order: the average numbers of spins having the values $\frac{1}{2}$ and $-\frac{1}{2}$ are the same and $m_z^z = 0$. Above $T_c$ the average numbers of spins having the values $\frac{1}{2}$ and $-\frac{1}{2}$ remain the same and $m_z^z = 0$. Analytical calculations predict the logarithmic singularity of the specific heat in the vicinity of $T_c$

$$c \sim \ln |T - T_c|,$$

and the vanishing of the order parameter $m_z^z$ while $T_c - T \to +0$ as

$$m_z^z \sim (T_c - T)^{\frac{1}{8}}.$$

The correlation length $\xi$ which characterizes the long-distance behavior of spin correlations,

$$\langle s_i^z s_j^z \rangle \sim \exp \left( -\frac{|i - j|}{\xi} \right), \quad |i - j| \to \infty,$$

diverges in the vicinity of $T_c$ as

$$\xi \sim |T - T_c|^{-1}.$$

In one dimension $T_c = 0$. At any infinitesimally small temperature the temperature fluctuations destroy the long-range order which exists only at zero temperature. The exact solution\footnote{The exact solution is given by the Bethe ansatz method.} for the two-point spin correlation functions reads

$$\langle s_j^z s_{j+n}^z \rangle = \frac{1}{4} \left( \tanh \frac{\beta J}{4} \right)^n = \frac{1}{4} \exp \left( -\frac{n}{\xi} \right), \quad \frac{1}{\xi} = \ln \coth \frac{\beta J}{4},$$

and hence the correlation length $\xi$ diverges while $T \to T_c = 0$ as

$$\xi \sim \exp \frac{J}{2kT}.$$

We do not know the exact solution of the Ising model in three dimensions although qualitatively the briefly sketched picture for a two-dimensional case remains valid.
Numerous experimental studies of different substances in the vicinity of the continuous phase transition points show that the critical behavior is characterized by a set of exponents which may be identical for different substances. This remarkable result of universality urged the researchers to proceed elaborating scaling concepts, establishing scaling relations and developing renormalization ideas and many systematic renormalization-group schemes in order to calculate critical exponents. These issues constitute a basic course in the theory of classical (i.e. temperature-driven) continuous phase transitions.\textsuperscript{5,6}

In what follows I shall not speak about temperature-driven continuous phase transitions. I wish to focus on the quantum continuous phase transitions. Let me start from a brief discussion of the experiment performed by D. Bitko, T. F. Rosenbaum and G. Aeppli\textsuperscript{7} which demonstrates how a phase transition may be driven by entirely quantum rather than temperature fluctuations. D. Bitko et al carried out their measurements for a model magnet lithium holmium fluoride LiHoF\textsubscript{4} in the external field \(H_t\), which turns out to be the experimental realization of the Ising magnet in a transverse magnetic field. At low temperatures (below 2 K), the magnetic properties arise owing to the magnetic dipolar interaction of the spins of neighboring holmium ions Ho\textsuperscript{3+}. These spins prefer to be directed either up or down with respect to a certain crystalline axis and present the three-dimensional ferromagnetic Ising model. D. Bitko et al investigated the behavior of LiHoF\textsubscript{4} as a function of temperature \(T\) and an external magnetic field \(H_t\) applied normally to the Ising axis. For this purpose they measured the real and the imaginary parts of the magnetic susceptibility along the Ising axis at different temperatures establishing \(T_c\) or \(H^{\text{i}}_c\). Their findings are summarized in Fig. 1.

Let us discuss the experimentally measured phase diagram (Fig. 1) of the system which is described by the Hamiltonian of the Ising magnet in a transverse magnetic field

\[
H = \sum_{i,j} J_{ij} s_i^x s_j^x - \Omega \sum_i s_i^z, \tag{10}
\]

where \(s^\alpha, \alpha = x, y, z\) are halves of the Pauli matrices

\[
\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{11}
\]

\(J_{ij}\)s are the Ising exchange couplings and \(\Omega\) is a transverse field. Consider the behavior of the system as temperature increases at \(H_t = 0\) (the horizontal axis in Fig. 1). At \(T = 0\), all spins are pointed, say, up (i.e.,
fully polarized ferromagnetic state). As the temperature becomes nonzero, the temperature fluctuations cause some spins of the ground-state configuration to flip, i.e. some spins become pointed down. As the temperature increases, the number of flipped spins increases and, at $T_c = 1.53$ K, the numbers of up and down spins become equal. The numbers of spin up and spin down are the same for all temperatures above $T_c$. This is a scenario of the conventional temperature-driven continuous phase transition from the ferromagnetic to the paramagnetic phase with the Curie temperature $T_c = 1.53$ K.

Consider further what happens while we are moving along the vertical axis in Fig. 1, i.e. while we increase the transverse field $H_t$ at zero temperature $T = 0$. We immediately observe that the existing order at zero temperature may be destroyed in a completely different manner even at $T = 0$. Applying transverse field $H_t$ we allow tunneling between spin-down and spin-up states. And if $H_t > H^t_c$, the ground state becomes paramagnetic even at $T = 0$. Hence, the quantum fluctuations destroy the order. In other words, the phase transition between ferromagnetic and paramagnetic phases described by the order parameter $\frac{1}{N} \sum_i \langle s_i^z \rangle$ is driven entirely by quantum fluctuations. For both $T$ and $H_t$ nonzero, D. Bitko et al found experimentally a line of continuous phase transitions which separates the ferromagnetic phase (lower region in Fig. 1) from the paramagnetic phase (upper region in Fig. 1). For example, at $T = 0.100$ K they found
$H^c_t = 49.3$ kOe. Thus, the classical phase transition at $H_t^1 = 0$ and the quantum phase transition at $T = 0$ are connected by a line of continuous phase transitions. To develop a correct theoretical description of the equally important quantum and temperature fluctuations in this region has been a focus of many recent studies.

For further discussions on this issue as well as for other examples of quantum phase transitions see the review article for a general science audience and the book of S. Sachdev.

2. Spin-$\frac{1}{2}$ Ising Chain in a Transverse Field as the Simplest Model for the Quantum Phase Transition Theory

In early sixties of the last century E. Lieb, T. Schultz and D. Mattis (see also the paper by S. Katsura) suggested a new exactly solvable model, the so-called, spin-$\frac{1}{2}$ XY chain. In particular case it transforms into the one-dimensional spin-$\frac{1}{2}$ Ising model in a transverse field; this case was examined in detail several years later by P. Pfeuty. The long-known results for the Ising chain in a transverse field may be viewed in the context of the quantum phase transition theory. The transverse Ising chain is apparently the simplest model exhibiting the continuous quantum phase transition which can be studied in much detail since many statistical mechanics quantities for that model are amenable for rigorous calculations.

I begin to discuss these results introducing the model. It consists of $N \to \infty$ spins $\frac{1}{2}$ (which are represented by halves of the Pauli matrices) which are arranged in a row. Only the neighboring spins interact via the Ising exchange interaction. Moreover, the spins interact with an external transverse field. The Hamiltonian of the model may be written as follows:

$$H = \sum_{n=1}^{N} \Omega s_n^z + \sum_{n=1}^{N} J s_n^x s_{n+1}^x. \quad (12)$$

We may impose periodic (cyclic) boundary conditions assuming $s_{N+1}^\alpha = s_1^\alpha$ or open (free) boundary conditions assuming the last term in the second sum in (12) to be zero. The Ising chain without transverse field, $\Omega = 0$, exhibits the long-range order at zero temperature $T = 0$ with the order parameter $\langle s^z \rangle = \frac{1}{N} \sum_i \langle s_i^z \rangle$ which equals, say, $\frac{1}{2}$ (we assume the exchange interaction in (12) to be ferromagnetic, $J < 0$). The long-range order is immediately destroyed, i.e. $\langle s^z \rangle = 0$, for any nonzero temperature $T > 0$. However, the Ising magnetization $\langle s^z \rangle$ can be destroyed at $T = 0$ by quantum fluctuations, when we switch on in (12) the transverse field $\Omega \neq 0$. 
Small values of $\Omega$ reduce the transverse magnetizations $\langle s^x \rangle$ and after $\Omega$ exceeds the critical value $\Omega_c = \frac{|J|}{2}$ the Ising magnetization becomes zero. That is the scenario which was discussed above in connection with the low-temperature properties of LiHoF$_4$. The advantage of the introduced model (12) is a possibility to follow in great detail the quantum phase transition tuned by $\Omega$.

Just after introducing the spin-$\frac{1}{2}$ $XY$ chains it was recognized that there was an intimate connection between the transverse Ising chain and the square-lattice Ising model (see, for example, a redirection of the Onsager solution using the Jordan-Wigner fermionization). The relationship between these models was demonstrated explicitly by M. Suzuki. Consider the square-lattice Ising model (1) with the strength of horizontal interactions $J_h > 0$ and with the strength of vertical interactions $J_v > 0$ and the transverse Ising chain (12) with the exchange interaction $J < 0$ and with the transverse field $\Omega$. The thermodynamic properties of the square-lattice Ising model are equivalent to the ground-state properties of the transverse Ising chain under the relations

$$ J_h \rightarrow 0, \quad J_v \rightarrow \infty, \quad \exp \left( \frac{-J_h}{2kT} \right) = \frac{\Omega}{|J|} \quad (13) $$

Moreover, the temperature-driven continuous phase transition in the square-lattice Ising model corresponds to the transverse field-driven continuous phase transition at $T = 0$ in the transverse Ising chain. The critical temperature $T_c$ corresponds to the critical transverse field $\Omega_c$. The dependences such as the Helmholtz free energy, entropy, and specific heat against temperature $T$ correspond to the dependences such as the ground-state energy, transverse magnetization, and static transverse susceptibility against transverse field $\Omega$. Finally, the correlation length $\xi$ corresponds to the inverse energy gap $\Delta$, $\xi \sim \Delta^{-1}$. The behavior of some ground-state quantities found by P. Pfeuty is reported in Table 1 and Fig. 2.

| square-lattice Ising model | transverse Ising chain |
|---------------------------|------------------------|
| $m^z \sim (T_c - T)^{\frac{1}{2}}$ | $\langle s^z \rangle \sim (\Omega_c - \Omega)^{\frac{x}{2}}$ |
| $c \sim \ln |T - T_c|$ | $\chi^z \sim \ln |\Omega - \Omega_c|$ |
| $\xi \sim |T - T_c|^{-1}$ | $\Delta \sim |\Omega - \Omega_c|$ |
Fig. 2. The ground-state dependences of the transverse magnetization \( m^z \) (a), the static transverse susceptibility \( \chi^z \) (b), and the longitudinal magnetization \( m^x \) (c) on the transverse field \( \Omega \) for the transverse Ising chain (12) \((J = -2)\).

Now I wish to explain briefly how can the statistical mechanics calculations for the transverse Ising chain be carried out without making any approximation. In terms of the spin raising and lowering operators \( s_n^\pm = s_n^x \pm is_n^y \) the Hamiltonian of the transverse Ising chain becomes as follows:

\[
H = \sum_n \Omega_n \left( s_n^+ s_n^- - \frac{1}{2} \right) + \sum_n \frac{J_n}{2} \left( s_n^+ s_{n+1}^- + s_n^- s_{n+1}^+ + s_n^+ s_{n+1}^+ + s_n^- s_{n+1}^- \right). \tag{14}
\]

Bearing in mind a case of regularly alternating chain we consider a model more general than (12) assuming that the Hamiltonian parameters are site-dependent, \( \Omega \rightarrow \Omega_n, \ J \rightarrow J_n = 2I_n \). Although (14) is a bilinear form in terms of \( s_n^\pm \) operators, further calculations appear to be complicated because of the commutation relations which are of the Fermi type at the same site

\[
\{ s_n^-, s_n^+ \} = 1, \quad \{ s_n^-, s_m^- \} = \{ s_n^+, s_m^+ \} = 0 \tag{15}
\]

and of the Bose type at different sites

\[
[ s_n^-, s_m^+ ] = [ s_n^-, s_m^- ] = [ s_n^+, s_m^+ ] = 0, \quad n \neq m. \tag{16}
\]

We may use the Jordan-Wigner transformation\(^a\) to introduce the Fermi operators according to the following formulas:

\[
c_n = (-2s_1^\pm)(-2s_2^\pm) \cdots (-2s_{n-1}^\pm) s_n^-; \tag{17}
\]

\(^a\)The Jordan-Wigner transformation of the spin operators to spinless fermions is also described in Chapter ? (see Eq. (3) of that Chapter).
\[ c_n^+ = (-2s_1^z)(-2s_2^z)\cdots(-2s_{n-1}^z)s_n^+ . \] (18)

Really, the introduced operators always satisfy the Fermi commutation relations
\[ \{ c_n, c_m^+ \} = \delta_{nm}, \quad \{ c_n, c_m \} = \{ c_n^+, c_m^+ \} = 0. \] (19)

Moreover, the Hamiltonian (14) in terms of the Fermi operators (17), (18) remains to be a bilinear form. Namely,
\[ H = \sum_n \Omega_n \left( c_n^+ c_n - \frac{1}{2} \right) \]
\[ + \sum_n \frac{I_n}{2} \left( c_n^+ c_{n+1}^+ + c_n^+ c_{n+1} - c_n c_{n+1}^+ - c_n c_{n+1} \right) \]
\[ = -\frac{1}{2} \sum_n \Omega_n + \sum_{n,m} \left( c_n^+ A_{nm} c_m + \frac{1}{2} (c_n^+ B_{nm} c_m - c_n B_{nm} c_m) \right) \] (20)

where
\[ A_{nm} = \Omega_n \delta_{nm} + \frac{1}{2} I_n \delta_{m,n+1} + \frac{1}{2} I_{n-1} \delta_{m,n-1} = A_{mn}, \] (21)
\[ B_{nm} = \frac{1}{2} I_n \delta_{m,n+1} - \frac{1}{2} I_{n-1} \delta_{m,n-1} = -B_{mn} . \] (22)

For periodic boundary conditions imposed on (14), the transformed Hamiltonian (20) should also contain the so-called boundary term which is omitted since we send \( N \) to infinity.

To diagonalize a bilinear in Fermi operators form (20) we perform the linear canonical transformation with real coefficients
\[ \eta_k = \sum_n \left( g_{kn} c_n + h_{kn} c_n^+ \right), \]
\[ \eta_k^+ = \sum_n \left( g_{kn} c_n^+ + h_{kn} c_n \right). \] (23)

The resulting Hamiltonian becomes as follows:
\[ H = \sum_{k=1}^N \Lambda_k \left( \eta_k^+ \eta_k - \frac{1}{2} \right), \]
\[ \{ \eta_k^+, \eta_{k'}^{+} \} = \delta_{kk'}, \quad \{ \eta_k^+, \eta_{k'} \} = \{ \eta_k^+, \eta_{k'}^+ \} = 0 \] (24)

if the coefficients \( g_{kn}, h_{kn} \) or, more precisely, their linear combinations
\[ \Phi_{kn} = g_{kn} + h_{kn}, \]
\[ \Psi_{kn} = g_{kn} - h_{kn} \] (25)
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satisfy the set of equations
\[
\Lambda_k^2 \Phi_{kn} = \sum_j \Phi_{kj} ((A - B)(A + B))_{jn},
\]
\[
\Lambda_k^2 \Psi_{kn} = \sum_j \Psi_{kj} ((A + B)(A - B))_{jn}.
\]  

Eqs. (26) explicitly read
\[
\Omega_n - I_n - 1 \Phi_{kn} - 1 + (I_n^2 - \Omega^2_n - \Lambda_k^2) \Phi_{kn} + \Omega_n I_n \Phi_{kn+1} = 0,
\]
\[
\Omega_n I_n - 1 \Psi_{kn} - 1 + (I_n^2 + \Omega^2_n - \Lambda_k^2) \Psi_{kn} + \Omega_n I_n \Psi_{kn+1} = 0,
\]  

with periodic or open boundary conditions implied. Eqs. (27), (25) determine the coefficients \(g_{kn}, h_{kn}\) in (23) and the elementary excitation energies \(\Lambda_k\) in (24).

For the uniform transverse Ising chain, \(\Omega_n = \Omega, I_n = I\), the bilinear in Fermi operators form (20) becomes diagonal after performing: i) the Fourier transformation
\[
c_j = \frac{1}{\sqrt{N}} \sum_\kappa \exp \left(-i\kappa j\right) c_\kappa,
\]
\[
c_j^+ = \frac{1}{\sqrt{N}} \sum_\kappa \exp \left(i\kappa j\right) c_\kappa^+.
\]  

with \(\kappa = \frac{2\pi}{N} n\) and \(n = -\frac{N}{2}, -\frac{N}{2} + 1, \ldots, \frac{N}{2} - 1\) if \(N\) is even or \(n = -\frac{N-1}{2}, -\frac{N-1}{2} + 1, \ldots, \frac{N-1}{2}\) if \(N\) is odd and ii) the Bogolyubov transformation
\[
\eta_\kappa = x_\kappa c_\kappa + y_\kappa c^+_{-\kappa},
\]
\[
\eta^+_{-\kappa} = y^*_\kappa c_\kappa + x^*_{-\kappa} c^+_{-\kappa}
\]  

with
\[
x_\kappa = \frac{iI \sin \kappa}{\sqrt{2\Lambda_\kappa (\Lambda_\kappa - \epsilon_\kappa)}},
\]
\[
y_\kappa = \sqrt{\frac{\Lambda_\kappa - \epsilon_\kappa}{2\Lambda_\kappa}}
\]  

and
\[
\Lambda_\kappa = \sqrt{\epsilon_\kappa^2 + I^2 \sin^2 \kappa},
\]
\[
\epsilon_\kappa = \Omega + I \cos \kappa.
\]
Knowing the energies of noninteracting fermions $\Lambda_k$ in (24) we immediately obtain the Helmholtz free energy per site (and hence all thermodynamic quantities),

$$f = -\frac{1}{N\beta} \ln \text{Tr} \exp (-\beta H)$$

$$= -\frac{1}{N\beta} \ln \prod_{k=1}^{N} \left( \exp \left( \frac{\beta \Lambda_k}{2} \right) + \exp \left( -\frac{\beta \Lambda_k}{2} \right) \right)$$

$$= -\frac{1}{N\beta} \sum_{k=1}^{N} \ln \left( 2 \cosh \frac{\beta \Lambda_k}{2} \right)$$

$$= -\frac{1}{2\pi\beta} \int_{-\pi}^{\pi} d\kappa \ln \left( 2 \cosh \frac{\beta \Lambda_\kappa}{2} \right) \quad (32)$$

(the last line in (32) refers to the uniform case (31)). Note, that we can obtain all thermodynamic quantities knowing the distributions of the energies of elementary excitations,

$$\rho(E) = \frac{1}{N} \sum_{k=1}^{N} \delta (E - \Lambda_k) ,$$

$$\int_{-\infty}^{\infty} dE \rho(E) = 1, \quad (33)$$
or the distribution of the squared energies of elementary excitations

$$R(E^2) = \frac{1}{N} \sum_{k=1}^{N} \delta (E^2 - \Lambda_k^2) ,$$

$$\int_{0}^{\infty} dE^2 R(E^2) = 1. \quad (34)$$

Really, the density of states $\rho(E)$ (33) or the density of states $R(E^2)$ (34) immediately yields

$$f = -\frac{1}{\beta} \int_{-\infty}^{\infty} dE \rho(E) \ln \left( 2 \cosh \frac{\beta E}{2} \right)$$

$$= -\frac{2}{\beta} \int_{0}^{\infty} dE^2 \rho(E^2) \ln \left( 2 \cosh \frac{\beta E}{2} \right). \quad (35)$$

The calculation of the spin correlation functions in the fermionic picture looks as follows. First we write down the relations between the spin and Fermi operators. We have

$$s_n^z = c_n^+ c_n - \frac{1}{2} = -\frac{1}{2} (c_n^+ + c_n) (c_n^+ - c_n) = -\frac{1}{2} \phi_n^+ \phi_n^- \quad (36)$$
where we have introduced the operators $\varphi^\pm_n = c^+_n \pm c^-_n$. Further,

$$s^x_n = \frac{1}{2} \varphi^+_1 \varphi^-_1 \cdots \varphi^+_{n-1} \varphi^-_{n-1} \varphi^+_n,$$

(37)

$$s^y_n = \frac{1}{2i} \varphi^+_1 \varphi^-_1 \cdots \varphi^+_{n-1} \varphi^-_{n-1} \varphi^-_n.$$

(38)

Note that the relations between the operators $s^x_n$, $s^y_n$ and the Fermi operators are nonlocal since the r.h.s. in Eqs. (37), (38) involve the Fermi operators attached to all previous sites. That is in contrast to the similar relation (36) for the operator $s^z_n$, the r.h.s. of which contains only the Fermi operators attached to the same site $n$.

Now we can rewrite the spin correlation functions in fermionic language. For example,

$$\langle s^z_n s^z_{n+m} \rangle = \frac{1}{4} \langle \varphi^+_n \varphi^-_n \varphi^+_n \varphi^-_{n+m} \rangle,$$

(39)

$$\langle s^x_n s^x_{n+m} \rangle = \frac{1}{4} \langle \varphi^-_n \varphi^+_{n+1} \varphi^-_{n+1} \cdots \varphi^+_{n+m} \varphi^-_{n+m} \rangle.$$

(40)

To get the latter result we use the relations

$$\{ \varphi^+_n, \varphi^+_m \} = - \{ \varphi^-_n, \varphi^-_m \} = 2 \delta_{nm}, \quad \{ \varphi^+_n, \varphi^-_m \} = 0.$$

(41)

The operators $\varphi^\pm_n$ are linear combinations of operators $\eta_k$, $\bar{\eta}_k$ involved into (24),

$$\varphi^+_n = \sum_{p=1}^N \Phi_{pn} (\eta^+_p + \eta^-_p),$$

(42)

$$\varphi^-_n = \sum_{p=1}^N \Psi_{pn} (\eta^+_p - \eta^-_p),$$

or for the uniform chain

$$\varphi^+_n = \frac{1}{\sqrt{N}} \sum_{\kappa} \exp (i\kappa n) (x_\kappa + y_\kappa) (\eta^+_\kappa + \eta^{-}_\kappa),$$

$$\varphi^-_n = \frac{1}{\sqrt{N}} \sum_{\kappa} \exp (i\kappa n) (x_\kappa - y_\kappa) (\eta^+_\kappa - \eta^{-}_\kappa).$$

(43)

\[ b \] The operators $\varphi^\pm$ are related to the Clifford operators $\Gamma^1$, $\Gamma^2$ (Chapter ?, Eq. (5)) as follows: $\varphi^+_n = \Gamma^1_n$, $\varphi^-_n = -i \Gamma^2_n$. 
Therefore, we calculate (39), (40) using the Wick-Bloch-de Dominicis theorem. Namely,

\[
4\langle s_n^z s_{n+m}^z \rangle = \langle \varphi^+_n \varphi^-_{n+m} \varphi^-_{n+m} \rangle = \langle \varphi^+_n \varphi^-_{n+m} \rangle \langle \varphi^+_n \varphi^-_{n+m} \rangle - \langle \varphi^+_n \varphi^-_{n+m} \rangle \langle \varphi^-_{n+m} \varphi^-_{n+m} \rangle + \langle \varphi^+_n \varphi^-_{n+m} \rangle \langle \varphi^-_{n+m} \varphi^-_{n+m} \rangle.
\]

(44)

The r.h.s. of Eq. (44) may be compactly written as the Pfaffian of the 4 \times 4 antisymmetric matrix

\[
4\langle s_n^z s_{n+m}^z \rangle = \text{Pf}\begin{pmatrix}
0 & \langle \varphi^+_n \varphi^-_{n+m} \rangle & \langle \varphi^+_n \varphi^+_{n+m} \rangle & \langle \varphi^+_n \varphi^-_{n+m} \rangle \\
-\langle \varphi^+_n \varphi^-_{n+m} \rangle & 0 & \langle \varphi^-_{n+m} \varphi^-_{n+m} \rangle & \langle \varphi^-_{n+m} \varphi^+_{n+m} \rangle \\
-\langle \varphi^-_{n+m} \varphi^+_{n+m} \rangle & -\langle \varphi^-_{n+m} \varphi^-_{n+m} \rangle & 0 & \langle \varphi^-_{n+m} \varphi^+_{n+m} \rangle \\
-\langle \varphi^-_{n+m} \varphi^+_{n+m} \rangle & -\langle \varphi^-_{n+m} \varphi^-_{n+m} \rangle & -\langle \varphi^-_{n+m} \varphi^+_{n+m} \rangle & 0 \\
\end{pmatrix}.
\]

(45)

Similarly,

\[
4\langle s_n^z s_{n+m}^z \rangle = \text{Pf}\begin{pmatrix}
0 & \langle \varphi^+_n \varphi^-_{n+1} \rangle & \langle \varphi^-_{n+1} \varphi^-_{n+1} \rangle & \cdots & \langle \varphi^-_{n+1} \varphi^+_{n+1} \rangle \\
-\langle \varphi^-_{n+1} \varphi^+_{n+1} \rangle & 0 & \langle \varphi^+_{n+1} \varphi^-_{n+1} \rangle & \cdots & \langle \varphi^+_{n+1} \varphi^+_{n+1} \rangle \\
-\langle \varphi^-_{n+1} \varphi^+_{n+1} \rangle & -\langle \varphi^-_{n+1} \varphi^-_{n+1} \rangle & 0 & \cdots & \langle \varphi^-_{n+1} \varphi^+_{n+1} \rangle \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
-\langle \varphi^-_{n+1} \varphi^+_{n+1} \rangle & -\langle \varphi^-_{n+1} \varphi^-_{n+1} \rangle & -\langle \varphi^-_{n+1} \varphi^+_{n+1} \rangle & \cdots & 0 \\
\end{pmatrix}.
\]

(46)

The elementary contractions involved into (45), (46) read

\[
\langle \varphi^+_n \varphi^-_{n+m} \rangle = \sum_{k=1}^{N} \Phi_{kn} \Phi_{km} = \delta_{nm},
\]

\[
\langle \varphi^+_n \varphi^-_{n+1} \rangle = \sum_{k=1}^{N} \Phi_{kn} \Psi_{km} \tanh \frac{\beta \Lambda_n}{2},
\]

\[
\langle \varphi^-_{n+1} \varphi^-_{n+1} \rangle = -\sum_{k=1}^{N} \Psi_{kn} \Phi_{km} \tanh \frac{\beta \Lambda_{n+1}}{2},
\]

\[
\langle \varphi^+_n \varphi^+_{n+m} \rangle = -\sum_{k=1}^{N} \Psi_{kn} \Psi_{km} = -\delta_{nm}.
\]

(47)

\[\text{See also Section 3.1.2 in Chapter ?.}\]
In the uniform case, instead of (47) we have

\[ \langle \varphi_n^+ \varphi_m^- \rangle = \frac{1}{N} \sum_{\kappa} \exp(i\kappa(n-m)) \frac{\Omega + I \exp(-i\kappa)}{\Lambda_\kappa} \tanh \frac{\beta \Lambda_\kappa}{2}, \]

\[ \langle \varphi_n^- \varphi_m^+ \rangle = -\frac{1}{N} \sum_{\kappa} \exp(-i\kappa(n-m)) \frac{\Omega + I \exp(-i\kappa)}{\Lambda_\kappa} \tanh \frac{\beta \Lambda_\kappa}{2}. \] (48)

It is worthy to recall some properties of the Pfaffians which are used in calculating them. In the first numerical studies the authors used the relation

\[ (\text{PfA})^2 = \det A \] (49)

and computed numerically the determinants which gave the values of Pfaffians. On the other hand, the Pfaffian may be computed directly noting that

\[ \text{Pf} \left( U^T A U \right) = \det U \text{ Pf} A \] (50)

and that

\[
\text{Pf}
\begin{pmatrix}
0 & R_{12} & 0 & 0 & \ldots & 0 \\
-R_{12} & 0 & 0 & 0 & \ldots & 0 \\
0 & 0 & 0 & R_{34} & \ldots & 0 \\
0 & 0 & -R_{34} & 0 & \ldots & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & 0 & \ldots & 0
\end{pmatrix} = R_{12} R_{34} \ldots .
\] (51)

Let me finally show how the results for the transverse Ising chain obtained by P. Pfeuty [12] arise in the described approach. Recalling Eq. (24) (or Eq. (32)) it is not hard to see that the ground-state energy per site can be written as

\[
e_0 = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\kappa \left( -\frac{\Lambda_\kappa}{2} \right)
\]

\[= -\frac{1}{4\pi} \int_{-\pi}^{\pi} d\kappa \sqrt{\Omega^2 + 2\Omega I \cos \kappa + I^2}
\]

\[= -\frac{I}{4\pi} \int_{-\pi}^{\pi} d\kappa \sqrt{\lambda^2 + 2\lambda \cos \kappa + 1}
\]

\[= -\frac{I(1+\lambda)}{\pi} \int_{0}^{\pi} d\phi \sqrt{1 - \left( \frac{2\sqrt{\lambda}}{1+\lambda} \right)^2 \sin^2 \phi}
\]

\[= -\frac{I(1+\lambda)}{\pi} E \left( \frac{\pi}{2}, \frac{2\sqrt{\lambda}}{1+\lambda} \right) . \] (52)
where \( \lambda = \frac{\Omega}{I} \) and

\[
E\left(\frac{\pi}{2}, a\right) = \int_{0}^{\frac{\pi}{2}} d\phi \sqrt{1 - a^2 \sin^2 \phi}
\]

is the complete elliptic integral of the second kind. In the vicinity of \( a = 1 \)

\[
E\left(\frac{\pi}{2}, a\right) \sim 1 + \frac{1 - a^2}{4} \ln \frac{16}{1 - a^2}
\]

(53)

(see Ref. [20] and therefore in the vicinity of \( \lambda_c = 1 \) the ground-state energy (52) contains the nonanalytic contribution

\[
e_0 \sim (\lambda - \lambda_c)^2 \ln |\lambda - \lambda_c| .
\]

(54)

As a result the ground-state transverse magnetization contains the nonanalytic contribution

\[
m^z \sim (\lambda - \lambda_c) \ln |\lambda - \lambda_c|
\]

and the ground-state static transverse susceptibility exhibits a logarithmic singularity

\[
\chi^z \sim \ln |\lambda - \lambda_c| .
\]

(56)

At \( \lambda_c = 1 \) the energy spectrum is gapless, i.e. there is a zero-energy elementary excitation. In the vicinity of \( \lambda_c = 1 \) the energy gap is given by the smallest value of \( \Lambda_\kappa = \sqrt{\Omega^2 + 2\Omega I \cos \kappa + I^2} \) and hence

\[
\Delta \sim |\lambda - \lambda_c| .
\]

(57)

To end up the discussion of the ground-state properties of the transverse Ising chain, let me emphasize that the quantum phase transition appears since the spin variables are the q-numbers rather than the c-numbers. To demonstrate this explicitly we may consider spin-vector (instead of spin-matrix) transverse Ising chain. The model consists of \( N \to \infty \) 3-componet vectors

\[
s = (s^x, s^y, s^z) = (s \sin \theta \cos \phi, s \sin \theta \sin \phi, s \cos \theta)
\]

which are governed by the Hamiltonian

\[
H = \sum_n \Omega s \cos \theta_n + \sum_n 2I s^2 \sin \theta_n \sin \theta_{n+1} \cos \phi_n \cos \phi_{n+1} .
\]

(58)

Here \( s \) is the value of the spin which plays only a quantitative role and further is put \( s = \frac{1}{2} \). To obtain the ground-state energy we should place all spins in \( xz \) plane putting \( \phi_n = 0 \) (\( I < 0 \)). Moreover, the angles \( \theta_n \) must
minimize the sum of contributions due to the interaction with the field and due to the intersite interaction. Thus, the ground-state energy ansatz reads

\[ E_0(\theta) = \frac{1}{2} N \Omega \cos \theta - \frac{1}{2} N |I| \sin^2 \theta \]  \hspace{1cm} (59)

where \( \theta \) is determined to minimize \( E_0(\theta) \) \hspace{1cm} (59). Obviously

\[ \cos \theta = \begin{cases} 1, & \text{if } \Omega < -2|I|, \\ -\frac{\Omega}{2|I|}, & \text{if } -2|I| \leq \Omega < 2|I|, \\ -1, & \text{if } 2|I| \leq \Omega. \end{cases} \]  \hspace{1cm} (60)

As a result, we find that the ground-state energy per site is given by

\[ e_0 = \begin{cases} \Omega, & \text{if } \Omega < -2|I|, \\ \frac{|I|}{2} \left(1 + \frac{\Omega^2}{4|I|^2}\right), & \text{if } -2|I| \leq \Omega < 2|I|, \\ -\Omega, & \text{if } 2|I| \leq \Omega. \end{cases} \]  \hspace{1cm} (61)

Moreover, the \( x \)- and \( z \)-magnetizations which can be obtained after inserting (60) into the formulas \( m^x = s \sin \theta \) and \( m^z = s \cos \theta \), respectively, behave as

\[ m^x = \begin{cases} 0, & \text{if } \Omega < -2|I|, \\ \frac{1}{2} \sqrt{1 - \frac{\Omega^2}{4|I|^2}}, & \text{if } -2|I| \leq \Omega < 2|I|, \\ 0, & \text{if } 2|I| \leq \Omega. \end{cases} \]  \hspace{1cm} (62)

and

\[ m^z = \begin{cases} \frac{1}{\sqrt{2}}, & \text{if } \Omega < -2|I|, \\ -\frac{\Omega}{4|I|}, & \text{if } -2|I| \leq \Omega < 2|I|, \\ -\frac{1}{\sqrt{2}}, & \text{if } 2|I| \leq \Omega. \end{cases} \]  \hspace{1cm} (63)

respectively. Evidently, there is no singularity in the ground-state dependence of the static transverse susceptibility \( \chi^z = \frac{\partial m^z}{\partial \Omega} \) on the transverse field \( \Omega \). As the transverse field increases from zero to \( 2|I| \), the on-site magnetic moments smoothly change their direction from \( x \)- to \( z \)-axis. The quantum phase transition appears only due to the quantum fluctuations which arise when the spin components do not commute and no phase transition occurs when the spin components are classical variables (compare Fig. 2 and Fig. 3).

3. Spin-\( \frac{1}{2} \) Ising Chain in a Transverse Field with Regularly Alternating Hamiltonian Parameters: Continued

Fraction Approach

We are turning to a discussion of the effects of regularly alternating exchange interactions and fields on the quantum phase transition inherent in
the transverse Ising chain. Note, that there was a great deal of work done examining the effects of different modifications of the skeleton model on the quantum phase transition. Thus, J. M. Luck\(^{21}\) analyzed the critical behavior of the chain with an aperiodic sequence of interactions, D. S. Fisher\(^{22}\) performed an extensive real-space renormalization group study of random chains, F. Iglói et al.\(^{23}\) reported a renormalization-group study of aperiodic chains. However, a simpler case of regularly alternating transverse Ising chain still contains a good deal of unexplored physics. It appears possible to obtain analytically exact results for thermodynamic quantities of such models using the Jordan-Wigner fermionization and the continued fraction approach.\(^{24,25}\) Moreover, for certain sets of the Hamiltonian parameters the exact results may be obtained for the spin correlation functions.\(^{26}\) In all other cases, spin correlations may be explored numerically at a high precision level considering sufficiently long chains up to a few thousand sites.\(^{20,27}\) It is appropriate to mention here the old studies,\(^{28,29}\) referring to the chains of period 2 which were extended further to the one-dimensional anisotropic XY model on superlattices.\(^{30,31}\) The quantum critical points in the anisotropic XY chains in a transverse field with periodically varying intersite interactions (having periods 2 and 3) have been determined recently\(^{32}\) using the transfer matrix method.

I begin with explaining how the thermodynamic quantities can be derived using continued fractions. For this purpose let me recall that the energies of the Jordan-Wigner fermions which determine the thermodynamic properties of a spin chain are involved into Eqs. (27). Consider, for example, the first set of equations in (27) which can be rewritten in the matrix form.
as follows:

\[
(H - \Lambda_k^2 1) \begin{pmatrix} \phi_{k1} \\ \phi_{k2} \\ \phi_{k3} \\ \vdots \\ \phi_{kN} \end{pmatrix} = 0 \tag{64}
\]

where

\[
H = \begin{pmatrix}
\vdots & \vdots & \vdots & \vdots & \vdots \\
\Omega_{n-2} I_{n-2} + \Omega_{n-1}^2 & I_{n-2}^2 & \Omega_{n-1} I_{n-1} & 0 & 0 & \ldots \\
\Omega_{n-1} I_{n-1} & I_{n-1}^2 + \Omega_n^2 & \Omega_n I_n & 0 & 0 & \ldots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\end{pmatrix}
\tag{65}
\]

and 1 denotes the unit matrix. Thus, all \( \Lambda_k^2 \) are the eigenvalues of the \( N \times N \) matrix \( (65) \) entering \( (64) \). To find their distribution \( R(E^2) \) \( (34) \) we may use the Green function approach. Consider a matrix \( G \) composed of the elements \( G_{nm} = G_{nm}(E^2) \) which is introduced by the equation

\[
(E^2 1 - H) G = 1. \tag{66}
\]

Having composed a matrix \( U^+ \) of the eigenvectors of the matrix \( H \) \( (65) \), i.e.

\[
U H U^+ = \begin{pmatrix}
\Lambda_1^2 & 0 & \ldots & 0 \\
0 & \Lambda_2^2 & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & \Lambda_N^2
\end{pmatrix}, \tag{67}
\]

one finds that

\[
\begin{pmatrix}
E^2 - \Lambda_1^2 & 0 & \ldots & 0 \\
0 & E^2 - \Lambda_2^2 & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & E^2 - \Lambda_N^2
\end{pmatrix} U G U^+ = 1. \tag{68}
\]

As a result

\[
\text{Tr} G = \sum_{k=1}^{N} (U G U^+)_k = \sum_{k=1}^{N} \frac{1}{E^2 - \Lambda_k^2}. \tag{69}
\]
Making the substitution

\[ E^2 \rightarrow E^2 \pm \epsilon, \quad \epsilon \rightarrow +0 \]  

(70)

and using the symbolic identity

\[ \frac{1}{E^2 - \Lambda_k^2 \pm i\epsilon} = \mathcal{P} \frac{1}{E^2 - \Lambda_k^2} \mp i\pi \delta(E^2 - \Lambda_k^2), \quad \epsilon \rightarrow +0 \]  

(71)

one arrives at the relation

\[ \mp \frac{1}{N\pi} \sum_{n=1}^{N} \Im G_{nn}(E^2 \pm \epsilon) = \frac{1}{N} \sum_{n=1}^{N} \delta(E^2 - \Lambda_n^2) = R(E^2). \]  

(72)

Thus, our task is to find the diagonal Green functions \( G_{nn} \) defined by Eqs. (66), (65).

Considering the equation for \( G_{nn} \),

\[(E^2 - \Omega_n^2 - I_{n-1}^2) G_{nn} - \Omega_{n-1} I_{n-1} G_{n-1,n} - \Omega_n I_n G_{n+1,n} = 1, \]  

(73)

and then the equations

\[
(E^2 - \Omega_{n-1}^2 - I_{n-2}^2) G_{n-1,n} - \Omega_{n-2} I_{n-2} G_{n-2,n} - \Omega_{n-1} I_{n-1} G_{n,n} = 0, \\
(E^2 - \Omega_{n-2}^2 - I_{n-3}^2) G_{n-2,n} - \Omega_{n-3} I_{n-3} G_{n-3,n} - \Omega_{n-2} I_{n-2} G_{n,n} = 0 
\]

(74)

etc. to determine \( G_{n+1,n}, G_{n+2,n}, \) etc., and the equations

\[
(E^2 - \Omega_{n+1}^2 - I_{n}^2) G_{n+1,n} - \Omega_n I_n G_{n+1,n} - \Omega_{n+1} I_{n+1} G_{n+2,n} = 0, \\
(E^2 - \Omega_{n+2}^2 - I_{n+1}^2) G_{n+2,n} - \Omega_{n+1} I_{n+1} G_{n+1,n} - \Omega_{n+2} I_{n+2} G_{n+3,n} = 0 
\]

(75)

e.tc. to determine \( G_{n+1,n}, G_{n+2,n}, \) etc., we easily find the following continued fraction representation for the diagonal Green functions

\[
G_{nn} = \frac{1}{E^2 - \Omega_n^2 - I_{n-1}^2 - \Delta_n^+ - \Delta_n^-}, \\
\Delta_n^- = \frac{\Omega_{n-1}^2 I_{n-1}^2}{E^2 - \Omega_{n-2}^2 - I_{n-2}^2 - \ldots}, \\
\Delta_n^+ = \frac{\Omega_n^2 I_n^2}{E^2 - \Omega_{n+1}^2 - I_{n+1}^2 - \ldots}. 
\]

(76)
A crucial simplification occurs if a sequence of the Hamiltonian parameters is periodic,

\[ \Omega_1 I_1, \Omega_2 I_2, \ldots, \Omega_p I_p, \Omega_1 I_1, \Omega_2 I_2, \ldots, \Omega_p I_p, \ldots \]

Then the continued fractions in (76) become periodic and can be evaluated exactly by solving a square equation. Consider, for example, the case \( p = 1 \), i.e. the uniform chain. Then \( \Delta_n = \Delta_n = \Delta \) (do not confuse with the energy gap \( \Delta \)) and \( \Delta \) satisfies the following equation

\[ \Delta = \frac{\Omega^2 I^2}{E^2 - \Omega^2 - I^2 - \Delta} \]  \( (77) \)

The solution of Eq. (77),

\[ \Delta = \frac{1}{2} \left( E^2 - \Omega^2 - I^2 \pm \sqrt{(E^2 - \Omega^2 - I^2)^2 - 4\Omega^2 I^2} \right), \]  \( (78) \)

yields

\[ G_{nn} = \pm \frac{1}{\sqrt{(E^2 - \Omega^2 - I^2)^2 - 4\Omega^2 I^2}} \]  \( (79) \)

and hence in accordance with (72)

\[ R(E^2) = \left\{ \begin{array}{ll}
\frac{1}{\pi \sqrt{-4\Omega^2 I^2 - (E^2 - \Omega^2 - I^2)^2}} & \text{if } \ (\Omega - I)^2 < E^2 < (\Omega + I)^2, \\
0, & \text{otherwise.}
\end{array} \right. \]  \( (80) \)

We may easily repeat the calculations for \( p = 2 \) or \( p = 3 \). The desired density of states in these cases is given by

\[ R(E^2) = \left\{ \begin{array}{ll}
\frac{|Z_{p-1}(E^2)|}{\pi \sqrt{A_{2p}(E^2)}} & \text{if } A_{2p}(E^2) > 0, \\
0, & \text{otherwise,}
\end{array} \right. \]  \( (81) \)

where \( Z_{p-1}(E^2) \) and \( A_{2p}(E^2) = -\prod_{j=1}^{2p} (E^2 - a_j) \) are polynomials of the order \( p - 1 \) and \( 2p \), respectively, and \( a_j \geq 0 \) are the roots of \( A_{2p}(E^2) \). Explicitly,

\[ Z_1(E^2) = 2E^2 - \Omega_1^2 - \Omega_2^2 - I_1^2 - I_2^2, \]

\[ A_4(E^2) = 4\Omega_1^2 \Omega_2^2 I_1^2 I_2^2 \]

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

\[ = -(E^2 - a_1)(E^2 - a_2)(E^2 - a_3)(E^2 - a_4), \]

\[ \{a_j\} = \left\{ \frac{1}{2} (\Omega_1^2 + \Omega_2^2 + I_1^2 + I_2^2} \right\}; \]  \( (82) \)
\[ Z_2(E^2) = 3E^4 - 2 \left( \Omega_1^2 + \Omega_2^2 + \Omega_3^2 + I_1^2 + I_2^2 + I_3^2 \right) E^2 \]
\[ + \Omega_1^2 \Omega_2^2 + \Omega_1^2 I_2^2 + I_1^2 I_2^2 + \Omega_2^2 \Omega_3^2 + \Omega_2^2 I_3^2 + I_2^2 I_3^2 \]
\[ + \Omega_3^2 I_1^2 + \Omega_3^2 I_1^2 + I_3^2 I_1^2, \]
\[ A_6(E^2) = 4 \sum_{n=1}^{6} \Omega_n^2 \sum_{m=1}^{3} I_m^2 \]
\[ - \left( E^6 - \left( \Omega_1^2 + \Omega_2^2 + \Omega_3^2 + I_1^2 + I_2^2 + I_3^2 \right) E^4 \right) \]
\[ + \left( \Omega_1^2 \Omega_2^2 + \Omega_1^2 I_2^2 + I_1^2 I_2^2 + \Omega_2^2 \Omega_3^2 + \Omega_2^2 I_3^2 + I_2^2 I_3^2 \right) E^2 \]
\[ + \Omega_3^2 I_1^2 + \Omega_3^2 I_1^2 + I_3^2 I_1^2 \]
\[ - \Omega_1^2 \Omega_3^2 - I_1^2 I_3^2 \]^2
\[ = -(E^2 - a_1)(E^2 - a_2)(E^2 - a_3)(E^2 - a_4)(E^2 - a_5)(E^2 - a_6), \] (83)

where \( a_1, \ldots, a_6 \) are the solutions of two cubic equations which follow from the equation \( A_6(E^2) = 0 \).

Knowing the density of states \( R(E^2) \) (81) we immediately obtain all quantities of interest. Thus, the gap in the energy spectrum of the spin model is given by the square root of the smallest root of the polynomial \( A_{2p}(E^2) \). Further, the ground-state energy per site is given by
\[ e_0 = - \int_0^\infty dE E^2 R(E^2). \] (84)

Recalling Eq. (85) for the Helmholtz free energy per site we find that the specific heat per site is given by
\[ \frac{c}{k} = 2 \int_0^\infty dE E R(E^2) \left( \frac{\beta E}{\cosh \beta E} \right)^2 . \] (85)

We assume that \( \Omega_n = \Omega + \Delta \Omega_n \) and define the transverse magnetization per site and the static transverse susceptibility per site as follows:
\[ m^z = \frac{\partial f}{\partial \Omega} \] (86)
and
\[ \chi^z = \frac{\partial m^z}{\partial \Omega}. \] (87)

Unfortunately, the elaborated approach yields only the density of states (34) and thus is restricted to the thermodynamic quantities. To obtain the spin correlation functions \( \langle s_j^\alpha s_{j+n}^\alpha \rangle, \alpha = x, z \) of the regularly alternating transverse Ising chain (45), (46), (47) we use the numerical
The on-site magnetizations can be calculated from the spin correlation functions using the relation
\[ m^\alpha_{j_1} m^\alpha_{j_2} = \lim_{r \to \infty} \langle s^\alpha_{j_1} s^\alpha_{j_2+rp} \rangle, \]
where \( 1 \ll j_1 \ll N \) is one of the \( p \) consecutive numbers taken sufficiently far from the ends of the chain and \( j_2 - j_1 = 0, 1, \ldots, p - 1 \). Assuming that
\[ \langle s^\alpha_j s^\alpha_{j+rp} \rangle - \langle s^\alpha_j \rangle \langle s^\alpha_{j+rp} \rangle \sim \exp \left( -rp/\xi^\alpha \right) \]
for large \( r \) \((1 \ll j, j+rp \ll N)\) we can determine the correlation length \( \xi^\alpha \).

4. Effects of Regularly Alternating Bonds/Fields on the Quantum Phase Transition

Now we shall use the analytical results for the ground-state and thermodynamic quantities and the numerical data for the spin correlation functions to discuss the effects of regularly alternating Hamiltonian parameters on the quantum phase transition inherent in the transverse Ising chain.

We start with the energy gap \( \Delta \). The quantum phase transition point is determined by the condition \( \Delta = 0 \). The density of states \( R(E^2) \) permits us to find the energy gap \( \Delta \) since, as it was mentioned before, the smallest root of the polynomial \( A_{2p}(E^2) \) (see (81)) is the smallest elementary excitation energy squared. Therefore, the energy spectrum becomes gapless when
\[ A_{2p}(0) = 0. \]
In the case of period 2 the condition \( A_4(0) = 0 \), yields
\[ \Omega_1 \Omega_2 = \pm I_1 I_2. \]
In the case of period 3 the condition \( A_6(0) = 0 \), yields
\[ \Omega_1 \Omega_2 \Omega_3 = \pm I_1 I_2 I_3. \]

It should be emphasized here that we have rederived the long-known condition of the zero-energy elementary excitations obtained by P. Pfeuty. P. Pfeuty showed that a nonuniform transverse Ising chain becomes gapless if
\[ \Omega_1 \Omega_2 \Omega_3 \ldots \Omega_N = \pm I_1 I_2 I_3 \ldots I_N. \]
(In fact, Eq. (6) of the P. Pfeuty’s paper does not contain two signs; minus immediately follows from symmetry arguments (after performing simple rotations of spin axes) and is important for what follows.)
Analysing the conditions for quantum phase transition points (91), (92), we immediately observe that a number of quantum phase transition points for a given period of nonuniformity is strongly conditioned by specific values of the Hamiltonian parameters. Consider, for example, the case $p = 2$ and assume $\Omega_1, \Omega_2 = \Omega \pm \Delta \Omega$, $\Delta \Omega > 0$. Then, for a small strength of transverse-field nonuniformity $\Delta \Omega < \sqrt{|I_1 I_2|}$ the system exhibits two quantum phase transition points $\Omega_c = \pm \sqrt{\Delta \Omega^2 + |I_1 I_2|}$. Moreover, the ferromagnetic phase occurs for $|\Omega| < \sqrt{\Delta \Omega^2 + |I_1 I_2|}$ whereas the paramagnetic phase occurs for $\sqrt{\Delta \Omega^2 + |I_1 I_2|} < |\Omega|$. If a strength of transverse-field nonuniformity is large enough, $\Delta \Omega > \sqrt{|I_1 I_2|}$, the system exhibits four quantum phase transition points $\Omega_c = \pm \sqrt{\Delta \Omega^2 \pm |I_1 I_2|}$. Moreover, the ferromagnetic phase occurs for $\sqrt{\Delta \Omega^2 - |I_1 I_2|} < |\Omega| < \sqrt{\Delta \Omega^2 + |I_1 I_2|}$ whereas the paramagnetic phase occurs for low fields, $|\Omega| < \sqrt{\Delta \Omega^2 - |I_1 I_2|}$, and for strong fields, $\sqrt{\Delta \Omega^2 + |I_1 I_2|} < |\Omega|$. In the case $\Delta \Omega = \sqrt{|I_1 I_2|}$ we get three quantum phase transition points, $\Omega_c = \pm \sqrt{2} |I_1 I_2|, 0$. The fields $\pm \sqrt{2} |I_1 I_2|$ correspond to the transition between ferromagnetic and paramagnetic phases. At $\Omega = 0$ only a weak singularity occurs. We shall motivate the statements about the phases which occur as $\Omega$ varies considering the dependence of the ground-state Ising magnetization on $\Omega$ (see below). The important message which follows from this simple analysis is that the number of quantum phase transitions in the regularly alternating transverse Ising chain of a certain period strongly depends on a specific set of the Hamiltonian parameters.

Let us note that in our treatment we assume $\Omega_n = \Omega + \Delta \Omega_n$, fix $\Delta \Omega_n$ and $I_n$, and consider the changes in the ground-state properties as $\Omega$ varies, thus, breaking a symmetry between the transverse fields and the exchange interactions. Alternatively, we may assume $I_n = I + \Delta I_n$, fix $\Omega_n$ and $\Delta I_n$, and assume $I$ to be a free parameter. In this case the quantum phase transition is tuned by varying $I$. Naturally, in general, the quantum phase transition conditions (91), (92) may be tuned by some parameter(s) effecting the on-site fields and the intersite interactions.

Let us consider a critical behavior of the system in question. To get the behavior of the ground-state properties in the vicinity of the critical fields we start with expanding the smallest root of the polynomial $A_{2p}(E^2)$ with respect to deviation of the field from its critical value $\epsilon = \Omega - \Omega_c$. For $p = 2$
with $\Omega_{1,2} = \Omega \pm \Delta \Omega$ and $\Omega_c = \pm \sqrt{\Delta \Omega^2 \pm |I_1 I_2|}$ we have

$$a_1 = \Omega^2 + \Delta \Omega^2 + \frac{1}{2} (I_1^2 + I_2^2)$$

$$- \sqrt{\left( \Omega^2 + \Delta \Omega^2 + \frac{1}{2} (I_1^2 + I_2^2) \right)^2 - (\Omega^2 - \Omega_c^2)^2} \approx \frac{(\Omega^2 - \Omega_c^2)^2}{2 (\Omega^2 + \Delta \Omega^2 + \frac{1}{2} (I_1^2 + I_2^2))}. \quad (94)$$

As a result, the energy gap $\Delta = \sqrt{a_1}$ decays linearly

$$\Delta \sim |\epsilon| \quad (95)$$

if $\Omega_c \neq 0$ and as

$$\Delta \sim \epsilon^2 \quad (96)$$

if $\Omega_c = 0$. The latter case occurs when $\Delta \Omega = \sqrt{|I_1 I_2|}$.

Now we can evaluate the ground-state energy in the vicinity of the critical point. The nonanalytic contribution in the r.h.s. of Eq. (94) is coming from the energy interval between $\sqrt{a_1}$ (which is proportional either to $|\epsilon|$ or to $\epsilon^2$) and $\sqrt{a_2}$ ($a_1 < a_2 < a_3 < \ldots$); all the other intervals of energies yield only analytical contributions to the ground-state energy $e_0$ with respect to $\epsilon$. Therefore, we have

$$e_0 = -\frac{1}{2\pi} \int_{\sqrt{a_1}}^{\sqrt{a_2}} dE \frac{E^2 f(E^2)}{\sqrt{E^2 - a_1}} + \text{analytical with respect to } \epsilon^2 \text{ terms}$$

$$\sim \epsilon^2 \ln |\epsilon| + \text{analytical with respect to } \epsilon^2 \text{ terms}. \quad (97)$$

(Here $f(E^2)$, $f(0) \neq 0$ is some function the explicit expression of which is not important for deriving the asymptotic behavior.) Eq. (97) is valid for $\Omega_c \neq 0$ when $\sqrt{a_1} \sim |\epsilon|$. As a result

$$m^2 \sim \epsilon \ln |\epsilon| + \text{analytical with respect to } \epsilon^2 \text{ terms}, \quad (98)$$

and

$$\chi^2 \sim \ln |\epsilon| + \text{analytical with respect to } \epsilon^2 \text{ terms}. \quad (99)$$

Thus, the critical behavior remains unchanged in comparison with that of the uniform chain (compare with (54), (55), (56), (57)). This can be also nicely seen in Fig. 4 where some results referring to the chains of period 2 with $I_1 = I_2 = 1$ and $\Delta \Omega = 0.5$ and $\Delta \Omega = 1.5$ are collected.
Towards the ground-state properties of the transverse Ising chain of period 2, \( I_1 = I_2 = 1 \), \( \Omega_1, 2 = \Omega \pm \Delta \Omega \), \( \Delta \Omega = 0.5 \) \( (\Omega_c = \pm \sqrt{1.25}) \) (a - c), \( \Delta \Omega = 1.5 \) \( (\Omega_c = \pm \sqrt{1.25}, \pm \sqrt{3.25}) \) (d - f). The dependences of energy gap (dotted curves in (a), (d)), transverse magnetization \( m_z \) (solid curves in (a), (d)), static transverse susceptibility \( \chi_z \) (dashed curves in (a), (d)), longitudinal sublattice magnetizations \( |m_x| \) (solid curves with up and down triangles in (b), (e) which are obtained from the data for \( N = 600 \)), and correlation length \( \xi = \) (triangles and squares in (c), (f) correspond to the data for \( N = 300 \) and \( N = 600 \), respectively), on the transverse field \( \Omega \).
Let us turn now to the case $\Omega_c = 0$ which occurs for the chain of period 2 with $\Delta \Omega = \sqrt{|I_1 I_2|}$. In this case the smallest root $a_1$ tends to zero proportionally to $\epsilon^4$ as $\Omega$ approaches $\Omega_c$ and as a result

$$e_0 \sim \epsilon^4 \ln |\epsilon| + \text{analytical terms} \quad (100)$$

and, therefore,

$$m^z \sim \epsilon^3 \ln |\epsilon| + \text{analytical terms} \quad (101)$$

and

$$\chi^z \sim \epsilon^2 \ln |\epsilon| + \text{analytical terms}. \quad (102)$$

Thus, the transverse susceptibility $\chi^z$ is finite in the critical point $\Omega_c = 0$ and only its second derivative with respect to the field $\frac{\partial^2 \chi^z}{\partial \Omega^2}$ exhibits a logarithmic singularity. This weak singularity may be called the fourth-order quantum phase transition in the Ehrenfest sense.

I proceed with exact analytical results for a regularly alternating transverse Ising chain showing how the ground-state wave function $|\text{GS}\rangle$ can be obtained exactly for special sets of the Hamiltonian parameters. Let us consider the chain of period 2 with $\Omega_{1,2} = \Omega \pm \Delta \Omega$. It is obvious that

$$|\text{GS}\rangle = \ldots |\uparrow\rangle_j |\uparrow\rangle_{j+1} \ldots \quad (103)$$
as $\Omega \to -\infty$ and

$$|\text{GS}\rangle = \ldots |\downarrow\rangle_j |\downarrow\rangle_{j+1} \ldots \quad (104)$$
as $\Omega \to \infty$. We can also expect that at $\Omega = 0$

$$|\text{GS}\rangle = \ldots |\downarrow\rangle_j |\uparrow\rangle_{j+1} \ldots \quad (105)$$
if $\Delta \Omega \gg |I_1|, |I_2|$ and

$$|\text{GS}\rangle = \ldots \frac{1}{\sqrt{2}} (|\downarrow\rangle_j \pm |\uparrow\rangle_j) \frac{1}{\sqrt{2}} (|\downarrow\rangle_{j+1} \pm |\uparrow\rangle_{j+1}) \ldots \quad (106)$$
if $\Delta \Omega = 0$. Less evident is the ground-state wave function $|\text{GS}\rangle$ for $\Omega = \mp \Delta \Omega$ when $\Omega_1 = 0$, $\Omega_2 = -2\Delta \Omega$ or $\Omega_1 = 2\Delta \Omega$, $\Omega_2 = 0$. To obtain the ground-state wave functions for these values of the transverse field let us note that after performing the unitary transformations

$$U = \ldots \exp \left( i\pi s_n^x s_{n+1}^y \right) \exp \left( i\pi s_{n+1}^x s_{n+2}^y \right) \ldots \quad (107)$$

and

$$R^z = \ldots \exp \left( i\frac{\pi}{2} s_n^z \right) \exp \left( i\frac{\pi}{2} s_{n+1}^z \right) \ldots \quad (108)$$
the Hamiltonian of the transverse Ising chains with the fields \( \Omega_1 \Omega_2 \ldots \) and the interactions \( I_1 I_2 \ldots \) transforms (with the accuracy to the boundary terms) into the Hamiltonian of the transverse Ising chains with the fields \( I_1 I_2 \ldots \) and the interactions \( \Omega_1 \Omega_2 \ldots \),

\[ R^z U H U^+ R^z = \sum_j I_j s^z_j + \sum_j 2\Omega_{j+1} s_j^x s_{j+1}^x. \]  

(109)

For \( \Omega = \mp \Delta \Omega \) the Hamiltonian \( R^z U H U^+ R^z \) represents a system of noninteracting clusters which consist of two sites. We can easily find the ground-state of a two-site cluster with the Hamiltonian \( \Omega = -\Delta \Omega \)

\[ H_{12} = I_1 s^z_1 + I_2 s^z_2 - 4\Delta s^x_1 s^x_2. \]  

(110)

It reads \((I_1 I_2 > 0)\)

\[ |\text{GS}\rangle_{12} = c_1 |\downarrow\rangle_1 |\downarrow\rangle_2 + c_2 |\uparrow\rangle_1 |\uparrow\rangle_2, \]

\[ c_1 = \frac{1}{\sqrt{2}} \frac{I + \sqrt{I^2 + \Delta \Omega^2}}{\sqrt{I^2 + \Delta \Omega^2 + \Delta \Omega^2}}, \]

\[ c_2 = \frac{1}{\sqrt{2}} \frac{\Delta \Omega}{\sqrt{I^2 + \Delta \Omega^2 + \Delta \Omega^2}} \]

\[ I = \frac{1}{2} (I_1 + I_2). \]  

(111)

As a result, the desired ground-state wave function reads

\[ |\text{GS}\rangle = U^+ R^z \ldots (c_1 |\downarrow\rangle_{n+1} |\downarrow\rangle_{n+2} + c_2 |\uparrow\rangle_{n+1} |\downarrow\rangle_{n+2}) \]

\[ \cdot (c_1 |\downarrow\rangle_{n+3} |\downarrow\rangle_{n+4} + c_2 |\uparrow\rangle_{n+3} |\downarrow\rangle_{n+4}) \ldots. \]  

(112)

For \( \Omega = \Delta \Omega \), the ground-state is again given by \((112), (111)\) with the change \( n \rightarrow n - 1, \Delta \Omega \rightarrow -\Delta \Omega \).

Knowing the ground-state wave function we can easily calculate different spin correlation functions. For example, for \( \Omega = -\Delta \Omega \) according to Eq. \((112)\) we get

\[ \langle s^x_{n+1} s^x_{n+2} \rangle = \langle s^x_{n+1} s^x_{n+4} \rangle = \ldots \]

\[ = \langle s^x_{n+2} s^x_{n+3} \rangle = \langle s^x_{n+2} s^x_{n+5} \rangle = \ldots \]

\[ = \frac{1}{4} (c^2 - c^2_1), \]

\[ \langle s^x_{n+1} s^x_{n+3} \rangle = \langle s^x_{n+1} s^x_{n+5} \rangle = \ldots \]

\[ = \frac{1}{4} (c^2 - c^2_1)^2, \]

\[ \langle s^x_{n+2} s^x_{n+4} \rangle = \langle s^x_{n+2} s^x_{n+6} \rangle = \ldots = \frac{1}{4}. \]  

(113)
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\[
\langle s_z^{n+1} s_z^{n+2} \rangle = \langle s_z^{n+1} s_z^{n+4} \rangle = \ldots = \langle s_z^{n+2} s_z^{n+3} \rangle = \langle s_z^{n+2} s_z^{n+5} \rangle = \ldots
\]

\[
= \langle s_z^{n+2} s_z^{n+4} \rangle = \langle s_z^{n+2} s_z^{n+6} \rangle = \ldots = 0,
\]

\[
\langle s_z^{n+1} s_z^{n+3} \rangle = \langle s_z^{n+1} s_z^{n+5} \rangle = \ldots = (c_1 c_2)^2.
\]  

(114)

For \( \Omega = \Delta \Omega \), the correlation functions follow from (113), (114) after the change \( n \rightarrow n - 1 \).

Now we discuss the exact numerical results for finite chains presented in Figs. 4, 5. The ground-state Ising (longitudinal) sublattice magnetizations \( |m_x^j| \) and the correlation length \( \xi_\perp \) (b) against the transverse field \( \Omega \) for chains having 300, 600 and 900 sites (triangles, squares and circles).

Fig. 5. Towards the ground-state properties of the transverse Ising chain of period 2, \( l_1 = l_2 = 1 \), \( \Omega_{1,2} = \Omega \pm \Delta \Omega \), \( \Delta \Omega = 0.99 \) (open symbols), \( \Delta \Omega = 1.01 \) (full symbols). The longitudinal sublattice magnetization \( |m_x^j| \) (a) and the correlation length \( \xi_\perp \) (b) against the transverse field \( \Omega \) for chains having 300, 600 and 900 sites (triangles, squares and circles).
\[ \Delta \Omega < \sqrt{|I_1 I_2|} \] (Fig. 4a and Fig. 5a (open symbols)) and \[ \Delta \Omega > \sqrt{|I_1 I_2|} \] (Fig. 4b and Fig. 5a (full symbols)). In accordance with the analytical results for \( \Delta \), \( m^z \) and \( \chi^z \) the numerical data show the existence of either two phases (quantum Ising (ferromagnetic) phase for \( |\Omega| < \sqrt{\Delta \Omega^2 + |I_1 I_2|} \) and strong-field quantum paramagnetic phase otherwise) or three phases (low-field quantum paramagnetic phase for \( |\Omega| < \sqrt{\Delta \Omega^2 - |I_1 I_2|} \), quantum Ising (ferromagnetic) phase for \( \sqrt{\Delta \Omega^2 - |I_1 I_2|} < |\Omega| < \sqrt{\Delta \Omega^2 + |I_1 I_2|} \) and strong-field quantum paramagnetic phase otherwise). The longitudinal on-site magnetizations \( m^x_j \) are nonzero in quantum Ising phases and become strictly zero in quantum paramagnetic phases. The transverse magnetization \( m^y \) in quantum paramagnetic phases is almost constant being in the vicinity of zero in the low-field phase and of saturation value in the strong-field phase, thus producing plateau-like steps in the dependence \( m^z \) versus \( \Omega \) (see the solid curve in Fig. 4d). The correlation length \( \xi^x \) (Figs. 4c, 4f, 5b (full symbols)) illustrates that the transition between different phases is accompanied by the divergency of \( \xi^x \). Comparing the data for \( N = 600 \) and \( N = 900 \) reported in Fig. 5b one observes a strong size-dependence of the correlation length value \( \xi^x \) about the critical fields (full squares and circles in Fig. 5b) and a weak size-dependence of \( \xi^x \) for other values of \( \Omega \) (for example, open squares and circles in Fig. 5b). It is interesting to note that short chains (\( N = 20 \)) are already sufficient to reproduce a correct order-parameter behavior in the quantum Ising phase away from the quantum critical point, but not in the quantum paramagnetic phases. The chain length of up to \( N = 900 \) sites is clearly sufficient to see a sharp transition in the order parameter (Figs. 4, 5) and even to extract reliable results for \( \xi^x \) from the long-distance behavior of \( \langle s^x_j s^x_{j+n} \rangle \) as can be seen from the data presented in Figs. 4, 5 and in Fig. 5b. We also note that the numerical data for \( |m^y_j| \) and \( \xi^x \) at \( \Omega = \pm \Delta \Omega \) coincide with the exact expression (113).

In particular, the values of the longitudinal sublattice magnetizations for these fields are \( \frac{1}{2} \) and \( \frac{1}{2} |c^2_2 - c^2_1| \).

Finally, the low-temperature dependence of the specific heat \( c \) at different \( \Omega \) \( (\geq 0) \) obtained from the exact analytical expression (15) confirms the existence of either two phase transitions (Fig. 6a) or four phase transitions (Fig. 6b) depending on the relationship between \( \Delta \Omega \) and \( \sqrt{|I_1 I_2|} \). At the quantum phase transition points the spin chain becomes gapless and \( c \) depends linearly on \( T \). Really, at the quantum phase transition point as
Fig. 6. The low-temperature dependence of the specific heat for the transverse Ising chain of period 2, $I_1 = I_2 = 1$, $\Omega_{1,2} = \Omega \pm \Delta \Omega$, $\Delta \Omega = 0.5$ (a), $\Delta \Omega = 1.5$ (b).

$$T \to 0$$

$$\frac{c}{k} = 2 \int_0^{kT} dE E \frac{C}{\sqrt{E}^2} \left( \frac{E}{2kT} \right)^2 + 2 \int_{kT}^\infty dE E \left( \frac{E}{2kT} \cosh \frac{E}{2kT} \right)^2.$$

(115)

(Here $C$ is some constant the value of which is not important for deriving the asymptotic behavior.) The second term in (115) disappears in the limit $T \to 0$ ($E > kT$) and as a result

$$c \sim T.$$  

(116)

The ridges seen in Figs. 6a, 6b correspond to the maxima in the dependence $c$ versus $\Omega$ as $T$ varies. They single out the boundaries of quantum critical regions. These boundaries correspond to a relation $\Delta \sim kT$ that can be checked by comparison with the data for $\Delta$ versus $\Omega$ reported in Figs. 4a, 4d. As can be seen from Fig. 6 the $c(T)$ behavior for $\Omega$ slightly above or below $\Omega_c$ changes crossing the boundaries of quantum critical regions. Furthermore, we notice that for $\Delta \Omega = 1.5$ (Fig. 6b) an additional low-temperature peak appears in the temperature dependence of the specific heat.

To end up, let us turn to a chain of period 3 for which the analytical and the numerical calculations presented above can be repeated. The quantum phase transition points follow from the condition (92). Depending on the
parameters, either two, four, or six quantum phase transitions are possible. This behavior is illustrated in Fig. 7 for a chain of period 3 with $I_1 = I_2 = I_3 = 1$, $\Omega_n = \Omega + \Delta \Omega_n$, $\Delta \Omega_1 + \Delta \Omega_2 + \Delta \Omega_3 = 0$. The dark, gray, or light regions correspond to parameters for which the system exhibits two, four, or six quantum phase transitions, respectively. At the boundaries between different regions weak singularities occur.

$\Omega_n = \Omega + \Delta \Omega_n$, $\Delta \Omega_1 + \Delta \Omega_2 + \Delta \Omega_3 = 0$. Moreover, such chains may exhibit weak singularities. For example, for the set of parameters at the boundary between dark and gray regions there are three critical fields; at one of them a weak singularity occurs.

To summarize, I have shown how the exact results for the thermodynamics of a regularly alternating spin-$\frac{1}{2}$ Ising chain in a transverse field can be derived using the Jordan-Wigner transformation and continued fractions. Furthermore, for special parameter values the exact ground-state wave function and spin correlation functions can be obtained as well. For parameters for which the correlation functions are not accessible for rigorous analytical analysis they can be obtained from exact numerical results for finite but large systems. From these numerical data we can extract the order parameter and the correlation length in high precision. We have found, that the quantum phase transition occurring in the uniform transverse Ising chain is not suppressed by deviation from uniformity in the form of a regular al-
ternation of bonds and fields. On the contrary, field alternation may lead to the appearance of additional quantum phase transitions tuned by the field. The number of phase transitions for a given period of alternation strongly depends on the precise values of the parameters of the model. We have examined the critical behavior of the energy gap $\Delta$, the ground-state energy $e_0$, the transverse magnetization $m^z$, and the static transverse susceptibility $\chi^z$ and have found the same critical indices both for a nonuniform and uniform chain. For some sets of the Hamiltonian parameters, the ground-state quantities may exhibit a weak singularity.

5. Related Models

In the remainder of this chapter I shall discuss another simple models which, apart from the transverse Ising chain, exhibit a quantum phase transition. Namely, I consider the spin-$\frac{1}{2}$ isotropic $XY$ (i.e., $XX$) chain in a transverse field and the spin-$\frac{1}{2}$ $XYZ$ chain in an external magnetic field directed along $z$ axis focusing on the effects of regularly alternating Hamiltonian parameters on the dependence of the ground-state quantities on the external field.

The uniform transverse $XX$ chain described by the Hamiltonian

$$H = \sum_{n=1}^{N} \Omega s^z_n + \sum_{n=1}^{N} 2I \left( s^x_n s^x_{n+1} + s^y_n s^y_{n+1} \right)$$

(117)

by employing the Jordan-Wigner transformation (17), (18) can be mapped onto the system of noninteracting spinless fermions with the Hamiltonian

$$H = \sum_{n=1}^{N} \Lambda_\kappa \left( c^+_\kappa c_\kappa - \frac{1}{2} \right)$$

(118)

where the elementary excitation energies $\Lambda_\kappa$ are given by

$$\Lambda_\kappa = \Omega + 2I \cos\kappa.$$  

(119)

Alternatively, we may find the density of states $\rho(E)$ (33) which is given by

$$\rho(E) = \begin{cases} \frac{1}{\pi \sqrt{4I^2 - (E - \Omega)^2}}, & \text{if } 4I^2 - (E - \Omega)^2 > 0, \\ 0, & \text{otherwise}. \end{cases}$$

(120)

As a result, the thermodynamic properties of the spin chain (117) can be easily analyzed.

In contrast to the transverse Ising chain (and to any chain with anisotropic $XY$ interaction in a transverse field) $\sum_{n=1}^{N} s^z_n$ commutes with
the Hamiltonian describing the isotropic \( XY \) interspin interaction and, therefore, a change in the transverse field \( \Omega \) has a different effect on the ground-state quantities of the spin chain (117). As can be seen from (118), (119) the transverse field plays a role of the chemical potential controlling a filling of the fermion band. The transverse \( XX \) chain remains gapless until \(|\Omega| \leq 2|I|\). If \(|\Omega| \) exceeds \(2|I|\), the energy gap \( \Delta \) opens linearly. This produces singularities in the ground-state quantities. For example, a square-root singularity in the zero-temperature dependence of the static transverse susceptibility \( \chi_z \) on the transverse field \( \Omega \).

After introducing a regular alternation, i.e. after making a substitution in (117) \( \Omega \rightarrow \Omega_n \), \( I \rightarrow I_n \) with a periodic sequence of parameters

\[
\Omega_1 I_1 \Omega_2 I_2 \ldots \Omega_p I_p \Omega_1 \Omega_2 I_2 \ldots \Omega_p I_p \ldots,
\]

we can easily obtain with the help of continued fractions the density of states \( \rho(E) \) of the Jordan-Wigner fermions which represent the regularly alternating transverse \( XX \) chain, and hence analyze the effects of regularly alternating Hamiltonian parameters on the thermodynamic properties of the considered spin system \( \text{Ref. 34} \) (for another approach see Ref. 35). The main consequence of the introduced periodic nonuniformity is a splitting of the initial fermion band into several subbands the number of which does not exceed the period of the chain \( p \) (for special (symmetric) values of the Hamiltonian parameters one may observe a smaller than \( p \) number of subbands). The transverse field \( \Omega \) (\( \Omega_n = \Omega + \Delta \Omega_n \)) controls a filling of the fermion subbands. Again the energy gap \( \Delta \) disappears/appears linearly and the critical behavior remains as for the uniform chain. Note, that the ground-state dependence of the transverse magnetization

\[
m^z = -\frac{1}{2} \int_{-\infty}^{\infty} dE \rho(E) \tanh \frac{E}{2kT}
\]

on \( \Omega \) is composed of sharply increasing parts separated by horizontal parts (plateaus) in accordance with a famous conjecture of M. Oshikawa, M. Yamanaka and I. Affleck (see Ref. 36).

A more general situation is the case of regularly alternating \( XYZ \) chain in a magnetic field. Let us consider the Hamiltonian

\[
H = \sum_n \Omega_n s^z_n + \sum_n \left( I^x_n s^x_n s^x_{n+1} + I^y_n s^y_n s^y_{n+1} + I^z_n s^z_n s^z_{n+1} \right),
\]

\[
I^x_n = 1 + \gamma + (-1)^n \delta, \quad I^y_n = 1 - \gamma + (-1)^n \delta,
\]

which captures the interplay between an exchange interaction anisotropy \((\gamma, I^z)\), exchange interaction modulation or, more precisely, exchange in-
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interaction dimerization ($\delta$), and the uniform magnetic field ($\Omega$). Such a model has been studied recently in some details\cite{ref1,ref2,ref3} using the bosonization approach\cite{ref4,ref5} and the Lanczos diagonalization technique. Let us first discuss the free fermion case $I^z = 0$. After the Jordan-Wigner transformation (17), (18) the Hamiltonian can be readily diagonalized (see Refs.\cite{ref6,ref7,ref8}). The critical field values at which the spin system (122) becomes gapless are given by

$$\Omega_c = \pm \sqrt{\delta^2 - \gamma^2}. \quad (123)$$

At the critical field the (transverse) magnetization behaves as

$$m^z - m_c^z \sim (\Omega - \Omega_c) (\ln |\Omega - \Omega_c| - 1) \quad (124)$$

and the static (transverse) susceptibility $\chi^z$ exhibits a logarithmic singularity (compare with Eqs. (98), (99)). The bosonization approach results\cite{ref9} show that the same picture is valid for an arbitrary $I^z \neq 0$ provided $\delta$ and $\gamma$ are suitably renormalized. The results of bosonization approach elaborated for small $\gamma$ and $\delta$ may be compared with numerical findings within non-perturbative regimes. From this analysis ($0 \leq I^z \leq 1$) it was found that the critical line for $\Omega = 0$ is given by

$$\delta \sim \gamma \quad (125)$$

in accord with\cite{ref10,ref11}. For the behavior of the magnetization curves near the critical fields $\Omega_c$ ($I^z = 1$) a fair regime\cite{ref12} was obtained. These outcomes suggest that some basic features of the fully interacting system\cite{ref13} are captured by the free fermion picture.

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