Національна академія наук України

ІНСТИТУТ ФІЗИКИ КОНДЕНСОВАНИХ СИСТЕМ

ICMP–03–24E

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ZERO-TEMPERATURE PHASE TRANSITIONS
IN QUANTUM SPIN CHAINS

ЛЬВІВ

УДК: 538.9

PACS: 75.10.-b

Фазові переходи при нульовій температурі у квантових спінових ланцюжках

Олег Держко

Анотація. Ми обговорюємо вплив регулярної змінності параметрів гамільтоніана на квантовий фазовий перехід (при нульовій температурі), притаманний спін-$\frac{1}{2}$ ланцюжку Ізинга у поперечному полі. Ми показуємо, що для заданого періоду регулярної зміни число точок квантових фазових переходів сильно залежить від конкретних значень параметрів гамільтоніана. Критична поведінка залишається такою ж як у однорідному ланцюжку. Однак, можлива поява і слабких сингулярностей. Ми починаємо з вступу до теорії квантових фазових переходів, а також приводимо деякі деталі виконаних обчислень.
Це є лекція, прочитана на семінарі з теоретичної фізики (Медзев, Словаччина, 2-4 вересня 2003 року).

Zero-temperature phase transitions in quantum spin chains

Oleg Derzhko

Abstract. We discuss the effects of the regularly alternating Hamiltonian parameters on the quantum (zero-temperature) phase transition inherent in the spin-$\frac{1}{2}$ transverse Ising chain. We demonstrate that for a given period of alternation the number of quantum phase transition points is strongly parameter dependent. The critical behavior remains as that of the uniform chain. However, weak singularities may occur as well. We also provide a pedagogical introduction to the quantum phase transition theory as well as present some details of the calculations performed.
This is the lecture given at the 5th Small Triangle Meeting on Theoretical Physics (Medzev, Slovakia, September 2-4, 2003).

The present paper is related to some basic concepts of the quantum phase transition theory. Quantum phase transitions are the phase transitions which are driven by entirely quantum rather than temperature fluctuations. The quantum phase transitions occur in the ground state, i.e., at zero temperature, under the change of some parameters (external field, pressure, concentration etc.). In fact, the quantum phase transitions have been known since early 70s. However, they have become the subject of intensive research since early 90s attempting to understand the properties of high-temperature superconductors and other strongly correlated materials. Obviously, this is a very broad field nowadays which contains a lot of important findings (the relevant references can be found in numerous review papers and monographes, e.g., [1–4], to name just a few). Of course, the present paper is not a complete review of the subject. In what follows I have restricted myself to a particular problem which has been recently examined by Johannes Richter (Universität Magdeburg), Taras Krokhmalskii (ICMP NASU, L'viv), Oles' Zaburannyi (ICMP NASU, L'viv) and by the present author [5]. Before explaining our results I shall remind some generally known ideas. Thus, I start with recalling common wisdoms from statistical physics concerning phase transitions (Section 1). Then I discuss the famous experiment by D. Bitko, T. F. Rosenbaum and G. Aeppli [6] demonstrating that a phase transition may be driven in the ground state by quantum fluctuations (Section 2). Possibly the simplest relevant statistical mechanics model which describes such a phenomena is the Ising chain in a transverse field (Section 2). The main goal of the paper is to show what happens with this generic model of quantum phase transitions if we slightly modify it assuming the Hamiltonian parameters (i.e., the intersite Ising exchange interactions and the on-site transverse fields) to be given by a regularly varying sequence (Section 3). Finally, I present some technical details of the performed calculations which are based on the Jordan-Wigner transformation [7] and exploit the continued fractions [8] (Section 4).

1. Classical (temperature-driven) phase transitions

One of the purposes of statistical physics is to describe different phases of many-particle systems and the phase transitions between different phases. As a rule, we associate the changes of the properties of a substance with the temperature changes. However, such changes may be driven by other parameters (external field, pressure, concentration etc.) at a given constant (nonzero) temperature.

P. Ehrenfest suggested a classification of phase transitions. Accord-

ing to his classification 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) are discontinuous. Furthermore, we say that the phase transition is of the order two (three) if the free energy and its first (first and second) derivatives are continuous across the phase transition whereas its second (third) derivatives are discontinuous and so on.

A few years later L. Landau suggested to differ discontinuous and continuous phase transitions. The discontinuous (continuous) phase transition is characterized by a discontinuous (continuous) change in the order parameter. Since the first derivative of the free energy may play a role of the order parameter (such as magnetization) the discontinuous phase transitions are usually viewed as the first-order phase transitions whereas the continuous phase transitions are usually considered to be the second-order (or higher-order) phase transitions.

The important difference between discontinuous and continuous phase transitions is as follows. In discontinuous phase transitions the two phases coexist at the phase transition temperature. For example, ice and water coexist at the ice melting temperature. In continuous phase transitions the two phases do not coexist at the phase transition temperature. For example, ferromagnet and paramagnet do not coexist at the Curie point of a ferromagnet.

In what follows our focus will be on the continuous phase transitions only.

Statistical mechanics provides several models of continuous phase transitions within the framework of which we can follow how the short-range interparticle interactions may lead to long-range interparticle correlations at the continuous phase transition point. The most simple model was invented by E. Ising [9]. It became especially popular after L. Onsager had found an exact solution of the model in two dimensions [10]. The model consists of the magnetic moments (spins) which may have two values $\pm\frac{1}{2}$. The spins interact with the nearest neighbors on the lattice of a certain topology. Moreover, they may interact with an external field.

In one dimension the corresponding Hamiltonian is as follows:

$$H = -\sum_{n=1}^{N} J s_n^z s_{n+1}^z. \tag{1.1}$$

If $J > 0$ the parallel alignment of all the spins is favorable (ferromagnetic

exchange interaction). Using the Pauli matrix

$$\tau^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

for representation of the spin variable, $s^z = \frac{1}{2}\tau^z$, the partition function of the model (1.1) can be rewritten as follows:

$$Z = \sum_{\left\{s_n^z = \pm\frac{1}{2}\right\}} \exp\left(-\beta H\right) = \mathrm{Tr}\exp\left(-\beta H\right). \tag{1.2}$$

The trace in the r.h.s. of Eq. (1.2) can be evaluated using the transfer matrix method [11]. We can also calculate the spin correlation functions $\left\langle s_n^z s_{n+m}^z \right\rangle$,

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

It appears that for the one-dimensional Ising model the critical temperature is zero, $T_c = 0$. Moreover,

$$\left\langle s_n^z s_{n+m}^z \right\rangle = \frac{1}{4}\exp\left(-\frac{m}{\xi}\right), \quad \xi \sim \exp\left(\frac{J}{2kT}\right) \tag{1.3}$$

as $T \to T_c = 0$, i.e., the correlations (1.3) become long-range since the correlation length ξ diverges. However, real systems exhibit phase transitions at finite temperatures.

Consider further the Ising model in two dimensions. Instead of (1.1) we now have for the square-lattice topology

$$H = -\sum_{n_x=1}^{N_x}\sum_{n_y=1}^{N_y}\left(J_h s_{n_x,n_y}^z s_{n_x+1,n_y}^z + J_v s_{n_x,n_y}^z s_{n_x,n_y+1}^z\right) \tag{1.4}$$

where J_h and J_v are the exchange interactions in horizontal and vertical directions, respectively. Thanks to L. Onsager we know how to calculate the partition function of the spin model (1.4)

$$Z = \sum_{\left\{s_{n_x,n_y}^z = \pm\frac{1}{2}\right\}} \exp\left(-\beta H\right) = \mathrm{Tr}\exp\left(-\beta H\right).$$

Knowing the spin correlations $\left\langle s_{n_x,n_y}^z s_{m_x,m_y}^z \right\rangle$ we can calculate the magnetization per site

$$m^z = \frac{1}{N_x N_y}\sum_{i_x=1}^{N_x}\sum_{i_y=1}^{N_y}\left\langle s_{i_x,i_y}^z \right\rangle.$$

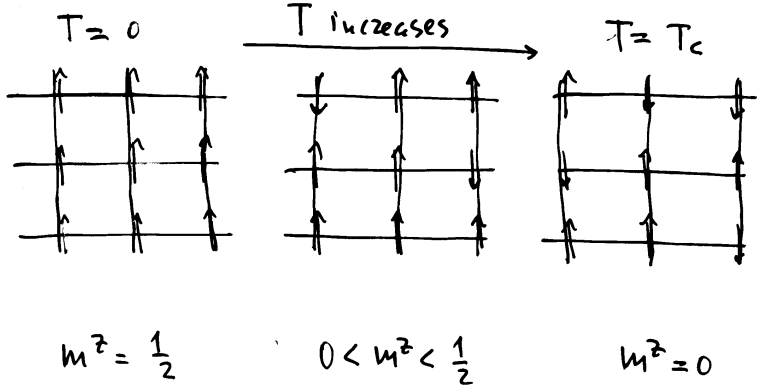

Figure 1. Temperature fluctuations of magnetization m^z. The order, which is present at zero temperature, $m^z = \frac{1}{2}$, becomes completely destroyed owing to the thermal fluctuations at the Curie temperature T_c, $m^z = 0$.

The square-lattice Ising model exhibits a phase transition at a nonzero temperature, $T_c \neq 0$. At zero temperature all spins are aligned in the same direction, having, for example, the value of $\frac{1}{2}$ (see the left panel in Fig. 1). As temperature increases some spins owing to temperature fluctuations flip and become oriented in the opposite direction. As a result the magnetization per site m^z reduces and becomes smaller than its saturation value $\frac{1}{2}$. Finally, as temperature achieves the value T_c the numbers of spin-up and spin-down are the same and the magnetization is zero (see the right panel in Fig. 1). The temperature fluctuations completely destroy the ferromagnetic order. At the critical temperature T_c the spin correlations become long-range. Specifically, for $|\mathbf{i}-\mathbf{j}| \to \infty$

$$\left\langle s_{\mathbf{i}}^z s_{\mathbf{j}}^z \right\rangle \sim \exp\left(-\frac{|\mathbf{i}-\mathbf{j}|}{\xi}\right), \quad \xi \sim \frac{1}{|T-T_c|} \tag{1.5}$$

as $T \to T_c$. Moreover, the thermodynamic quantities have peculiarities at T_c (Fig. 2). For instance, the specific heat exhibits a logarithmic singularity (lower panel in Fig. 2).

We do not know the exact solution of the Ising model in three dimensions. However, qualitatively the picture remains the same. Thus, the magnetization decays according to a power law with exponent $\beta \approx 0.312$ (instead of $\beta = 0.125$ in two dimensions), the specific heat exhibits a power-law singularity with exponent $\alpha \approx 0.013$, the correlation length ξ

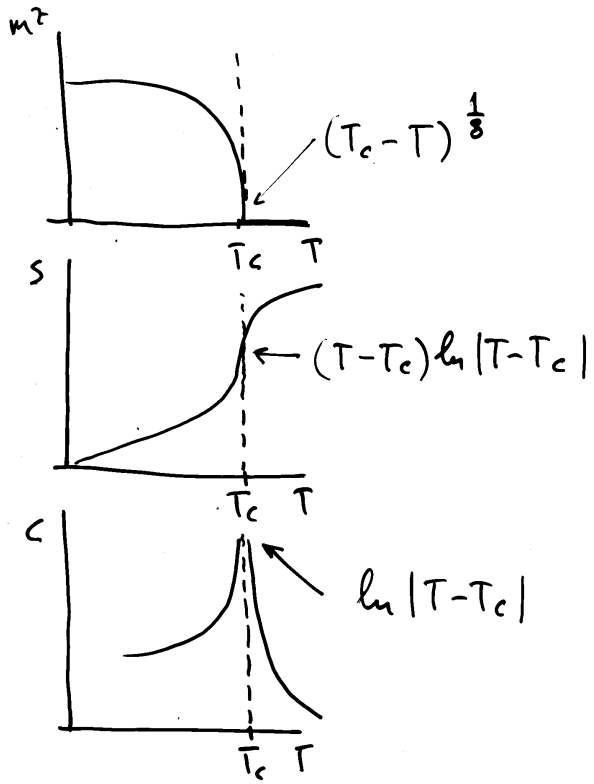

Figure 2. Square-lattice Ising model: The behavior of thermodynamic quantities in the vicinity of the phase transition temperature. From top to bottom: magnetization m^z, entropy s, specific heat c.

diverges according to a power law with exponent $\nu \approx 0.638$ (instead of $\nu = 1$ in two dimensions, Eq. (1.5)).

Statistical mechanics provides other models of continuous phase transitions (for example, the spherical model); some examples can be found in Ref. [11]. Still ongoing numerous experimental studies of different substances in the vicinity of the continuous phase transition points have shown that such a point is characterized by a set of exponents which may be identical for different substances. As a result, scaling concepts have emerged, renormalization-group ideas have appeared, many renormalization-group schemes for calculation of the critical exponents have been elaborated. This material is presented in standard text-books

on temperature-driven continuous phase transitions (see, for example, Ref. [12]). In what follows we shall not discuss thermal phase transitions any more.

2. Quantum (zero-temperature) phase transitions

We turn to a discussion of the zero-temperature (ground-state) properties of many-particle systems when there are no thermal fluctuations. Nevertheless, the order may be destroyed due to the quantum fluctuations.

We start with the famous experiment by D. Bitko, T. F. Rosenbaum and G. Aeppli [6] demonstrating how quantum fluctuations suppress the ferromagnetic order in a model magnet lithium holmium fluoride. The magnetic properties of $LiHoF_4$ at $T < 2$K arise owing to the magnetic interaction of the spins of neighboring holmium ions Ho^{3+}; the spins prefer to be directed up/down with respect to a certain crystalline axis; this compound is a three-dimensional ferromagnetic Ising model. The authors examined the ferromagnetic transition in $LiHoF_4$ in the presence of an external magnetic field H^t applied perpendicularly to the Ising axis. For this purpose they measured the real and imaginary parts of the magnetic susceptibility along the Ising axis at different temperatures. Their findings can be seen in Fig. 3.

Let us consider these results more closely. Note, that the considered system can be described by the model Hamiltonian

$$H = \sum_{i,j} J_{i,j} s_i^z s_j^z - \Omega \sum_i s_i^x \tag{2.1}$$

where

$$s^x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad s^y = \frac{1}{2}\begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad s^z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Let us first move along the horizontal axis of the phase diagram shown in Fig. 3, i.e., $H^t = 0$. We recognize a familiar picture (recall Fig. 1). As temperature deviates from zero the temperature fluctuations cause the flip of some spins from the ordered ground-state configuration which reduces magnetization. As temperature achieves the value $T_c \approx 1.53$K (the Curie temperature) the magnetization becomes zero and for higher temperatures we are in the paramagnetic phase. That is a conventional phase transition driven by temperature fluctuations. However, we can destroy the order at zero temperature in a completely different way. Really, let us move along the vertical axis of the phase diagram shown in

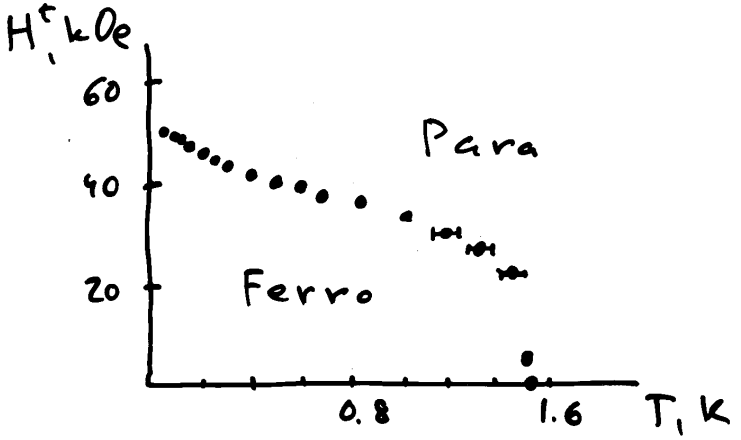

Figure 3. Experimental data for the ferromagnetic transitions in lithium holmium fluoride in the external magnetic field H^t (see [6]). $LiHoF_4$ is a three-dimensional Ising ferromagnet.

Fig. 3, i.e., assume $T = 0$ (see Fig. 4). If H^t (Ω in Eq. (2.1)) is zero all spins are, say, in the up state. However, if the transverse field deviates from zero, tunneling between the up and down states is permitted and consequently the magnetization is reduced despite the system being at zero temperature. If H^t achieves the critical value H^t_c the order is completely destroyed and the Ising magnetization becomes zero. Moreover, at that field, $H^t = H^t_c$, the spin correlations become long-range. Thus, the quantum fluctuations at zero temperature have suppressed the order. Obviously, as both T and H^t have nonzero values both thermal and quantum fluctuations occur. In Fig. 5 we indicate in the plane temperature – transverse field the classical phase transition point, the quantum phase transition point, the line of phase transitions separating ferromagnetic and paramagnetic phases, as well as the regions where quantum/temperature fluctuations should be taken into account.

Statistical mechanics provides a simple model which, on the one hand, exhibits a quantum phase transition, and, on the other hand, can be solved exactly. This is the so-called transverse Ising chain, i.e., the one-dimensional Ising model in a transverse field. The Hamiltonian of the model reads

$$H = \sum_{n=1}^{N} J s_n^x s_{n+1}^x + \sum_{n=1}^{N} \Omega s_n^z. \tag{2.2}$$

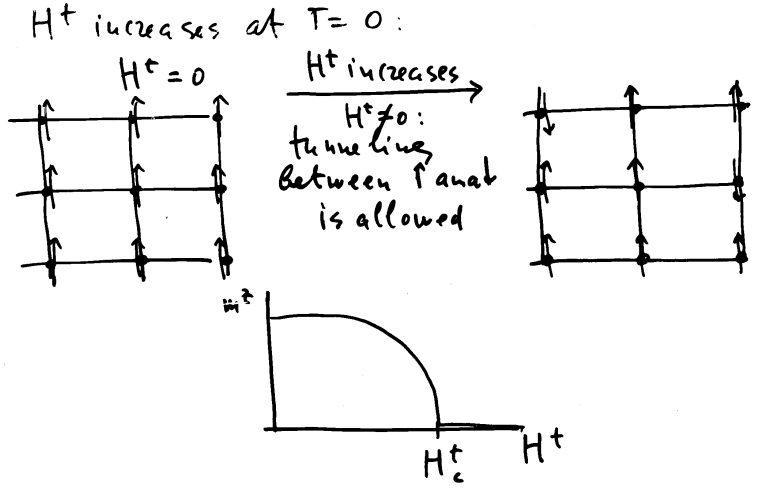

Figure 4. Quantum fluctuations of the Ising magnetization m^z at zero temperature. Tunneling between up and down states is allowed if H^t (Ω in Eq. (2.1)) is nonzero.

I have rotated the spin axes in comparison with the specification used in Eq. (1.1) (and Eq. (2.1)); besides now $J = 2I < 0$ corresponds to the ferromagnetic exchange interaction. The introduced model (2.2) can be solved rigorously (i.e., without making any simplifying approximations) using the Jordan-Wigner transformation [7,13] (some details are given in Section 4 for convenience). From this solution we know how the system behaves in the ground state as Ω increases. If Ω becomes nonzero the Ising magnetization $m^x = \frac{1}{N}\sum_{i=1}^{N} \langle s_i^x \rangle$ becomes less than $\frac{1}{2}$; the Ising magnetization m^x tends to zero as Ω approaches $\Omega_c = |I|$. This is in accordance with what we have discussed above explaining the phase diagram of $LiHoF_4$. Moreover, we know the behavior of different ground-state quantities. Thus, in the vicinity of Ω_c

$$m^x \sim (\Omega - \Omega_c)^{\frac{1}{8}}, \tag{2.3}$$

$$m^z = \frac{1}{N}\sum_{i=1}^{N} \langle s_i^z \rangle \sim (\Omega - \Omega_c) \ln|\Omega - \Omega_c|, \tag{2.4}$$

$$\chi^z = \frac{\partial m^z}{\partial \Omega} \sim \ln|\Omega - \Omega_c|. \tag{2.5}$$

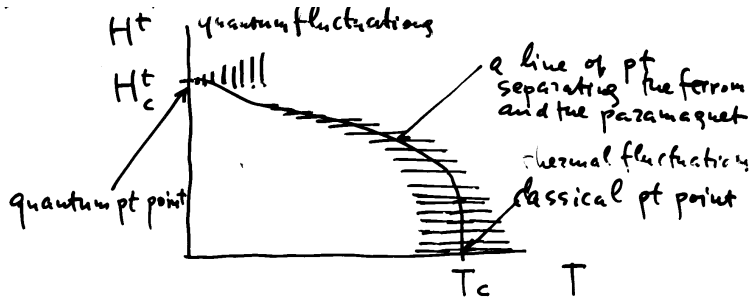

Figure 5. Phase diagram in the plane temperature – transverse field.

Moreover, the quantum phase transition is accompanied by vanishing of the energy gap Δ,

$$\Delta \sim |\Omega - \Omega_c| \,. \tag{2.6}$$

It should be stressed that the discussed zero-temperature phase transition is a pure quantum effect due to noncommutativity of the spin variables. It is not observed in the classical counterpart of the model. Really, consider a classical spin chain in which the spin is presented as a 3-component vector

$$\mathbf{s} = (s\sin\theta\cos\phi, s\sin\theta\sin\phi, s\cos\theta)$$

(hereafter the length of spin $s = \frac{1}{2}$) with the Hamiltonian

$$H = \sum_{n=1}^{N} 2Is^2 \sin\theta_n \sin\theta_{n+1}\cos\phi_n\cos\phi_{n+1} + \sum_{n=1}^{N}\Omega s\cos\theta_n. \tag{2.7}$$

The ground-state energy ansatz for (2.7) reads

$$E_0(\theta) = -\frac{1}{2}N|I|\sin^2\theta + \frac{1}{2}N\Omega\cos\theta \tag{2.8}$$

where the angle θ is determined from the equation

$$\frac{\partial E_0(\theta)}{\partial\theta} = 0. \tag{2.9}$$

From Eqs. (2.8), (2.9) one immediately finds

$$\cos\theta = \begin{cases} 1, & \text{if } \frac{\Omega}{2|I|} < -1, \\ -\frac{\Omega}{2|I|}, & \text{if } -1 \le \frac{\Omega}{2|I|} < 1, \\ -1, & \text{if } 1 \le \frac{\Omega}{2|I|}. \end{cases} \tag{2.10}$$

Table 1. Towards the correspondence between the thermodynamic properties of the square-lattice Ising model and the ground-state properties of the transverse Ising chain (under the relations (2.12)).

square-lattice Ising model	transverse Ising chain
$m^z \sim (T_c - T)^{\frac{1}{8}}$	$m^x \sim (\Omega_c - \Omega)^{\frac{1}{8}}$
$c \sim \ln\|T - T_c\|$	$\chi^z \sim \ln\|\Omega - \Omega_c\|$
$\xi \sim \|T - T_c\|^{-1}$	$\Delta \sim \|\Omega - \Omega_c\|$

Now, using this result (2.10), we get the ground-state energy per site, the Ising magnetization $m^x = s\sin\theta$, the transverse magnetization $m^z = s\cos\theta$ and the transverse susceptibility

$$\chi^z = \frac{\partial m^z}{\partial\Omega} = \begin{cases} 0, & \text{if } \frac{\Omega}{2|I|} < -1, \\ -\frac{1}{4|I|}, & \text{if } -1 \le \frac{\Omega}{2|I|} < 1, \\ 0, & \text{if } 1 \le \frac{\Omega}{2|I|}. \end{cases} \tag{2.11}$$

Obviously, χ^z (2.11) does not become singular at $\Omega = \Omega_c$ as χ^z (2.5) does.

Finally, comparing Eqs. (2.3) – (2.5) with the critical behavior of the square-lattice Ising model (Fig. 2) one can notice a similarity which was found explicitly by M. Suzuki [14]. Namely, considering the square-lattice Ising model with the exchange interactions in horizontal and vertical directions J_h and J_v, respectively, and the transverse Ising chain with the Ising interaction and transverse field J and Ω, respectively, M. Suzuki found that in the limit

$$J_h \to 0, \quad J_v \to \infty, \quad \frac{\exp\left(-\frac{J_v}{2kT}\right)}{\frac{J_h}{2kT}} = \frac{\Omega}{|J|} \tag{2.12}$$

the thermodynamic properties of the square-lattice Ising model are equivalent to the ground-state properties of the transverse Ising chain. We compare the corresponding dependences in Table 1.

3. Spin-$\frac{1}{2}$ transverse Ising chain with regularly alternating bonds/fields

Now I turn to a discussion of the effects of the regularly alternating Hamiltonian parameters on the quantum phase transition inherent in

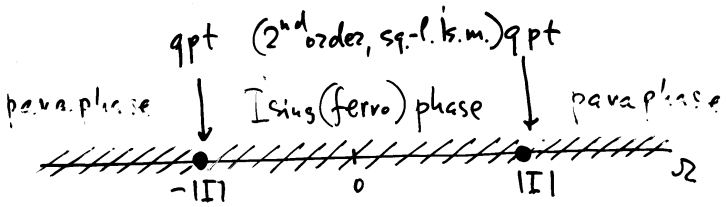

Figure 6. The ground-state phases and phase transitions tuned by the transverse field for the uniform chain ($p = 1$).

the transverse Ising chain. It is quite natural to introduce some modifications into the basic model and to see what the consequences of these changes are. In fact, there were numerous studies of the 'modified' transverse Ising chains. For example, an analysis of the critical behavior of the chain with an aperiodic sequence of interactions was performed in Ref. [15], an extensive real-space renormalization-group treatment of the random chains was reported in Ref. [16], a renormalization-group study of the aperiodic chain was presented in Ref. [17]. However, a simpler case of the transverse Ising chain with regularly alternating bonds/fields apparently was overlooked. Nevertheless, as we shall see below, the regularly alternating Hamiltonian parameters may have intriguing effects on the quantum phase transition points and critical behavior.

Specifically, we consider a chain of quantum spins $\frac{1}{2}$ with the Hamiltonian

$$H = \sum_n 2I_n s_n^x s_{n+1}^x + \sum_n \Omega_n s_n^z \tag{3.1}$$

and assume that a sequence of parameters in (3.1) has a period p, i.e.,

$$I_1\Omega_1 I_2\Omega_2 \ldots I_p\Omega_p I_1\Omega_1 I_2\Omega_2 \ldots I_p\Omega_p \ldots .$$

Of course, the above considered uniform case corresponds to $p = 1$. However, we can perform rigorous analytical calculations of the thermodynamic quantities for any finite (in practice not too long) period of alternation [8,5]. In what follows I discuss the cases $p = 2$ and $p = 3$ in some detail.

Let us consider the changes in the ground-state properties owing to regular alternation as the tranverse field varies. I start recalling what we already know about the uniform case $p = 1$ (Fig. 6). If the transverse field is small the system exhibits the Ising magnetization $m^x \neq 0$, which

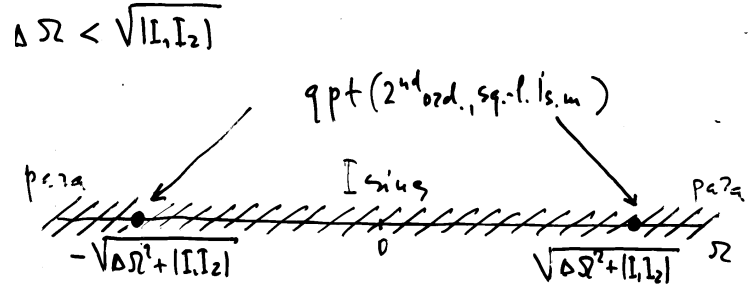

Figure 7. The ground-state phases and phase transitions for the regularly alternating transverse Ising chain of period 2 with $\Omega_{1,2} = \Omega \pm \Delta\Omega$, $\Delta\Omega < \sqrt{|I_1 I_2|}$.

plays a role of the order parameter, and its nonzero value indicates the Ising (ferromagnetic) phase. When a value of the transverse field exceeds the critical one ($\Omega_c = |I|$) the Ising magnetization becomes zero and the system is in the paramagnetic phase. The transition between the ferromagnetic and paramagnetic phases occurs according to the second-order quantum phase transition scenario and belongs to the square-lattice Ising model universality class.

Now we pass to a chain of period 2. Assume that

$$\Omega_{1,2} = \Omega \pm \Delta\Omega, \quad \Delta\Omega > 0$$

and let us see what happens to the quantum phase transitions tuned by Ω. It appears that the answer strongly depends on the strength of nonuniformity controlled by $\Delta\Omega$. If the strength of nonuniformity is weak,

$$\Delta\Omega < \sqrt{|I_1 I_2|},$$

only quantitative changes in comparison with the uniform case take place (compare Fig. 7 and Fig. 6). Namely, the system may exhibit either the ferromagnetic order (in weak transverse fields) or the paramagnetic order (in strong transverse fields). The positions of the quantum phase transition points between these phases are as follows:

$$\pm\sqrt{\Delta\Omega^2 + |I_1 I_2|}. \tag{3.2}$$

The critical behavior remains as in the uniform chain, i.e., it is of the square-lattice Ising model universality class. Further, if

$$\Delta\Omega = \sqrt{|I_1 I_2|}$$

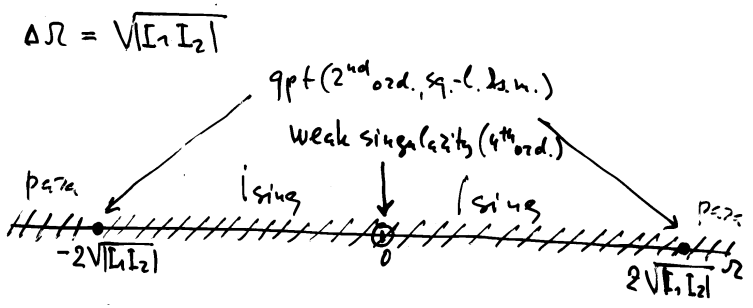

Figure 8. The ground-state phases and phase transitions for the regularly alternating transverse Ising chain of period 2 with $\Omega_{1,2} = \Omega \pm \Delta\Omega$, $\Delta\Omega = \sqrt{|I_1 I_2|}$.

in addition to the changes of the critical field values in accordance with (3.2) a point of weak singularities in the ground-state quantities appears at $\Omega_c = 0$ (Fig. 8). The critical behavior in the vicinity of this point is like the fourth-order phase transition in Ehrenfest's sense: that is, the static transverse susceptibility χ^z remains finite and only its second derivative with respect to field, $\frac{\partial^2 \chi^z}{\partial \Omega^2}$, exhibits a logarithmic singularity. Finally, if the strength of nonuniformity is strong,

$$\Delta\Omega > \sqrt{|I_1 I_2|},$$

a number of quantum phase transitions tuned by varying Ω increases (Fig. 9). The critical fields are as follows:

$$\pm\sqrt{\Delta\Omega^2 \pm |I_1 I_2|}; \tag{3.3}$$

the system exhibits the low-field (if $|\Omega| < \sqrt{\Delta\Omega^2 - |I_1 I_2|}$) and the high-field (if $\sqrt{\Delta\Omega^2 + |I_1 I_2|} < |\Omega|$) paramagnetic phases and the ferromagnetic phase (if $\sqrt{\Delta\Omega^2 - |I_1 I_2|} < |\Omega| < \sqrt{\Delta\Omega^2 + |I_1 I_2|}$); all phase transitions belong to the square-lattice Ising model universality class.

Postponing an explanation of how these findings can be derived till the last Section let us discuss the dependence of energy gap on Ω in all three cases (Figs. 10, 11, 12). The energy gap Δ may play a role of the order parameter and the vanishing energy gap indicates a quantum phase transition point. As can be seen in Figs. 10, 11, 12 the considered regularly alternating transverse Ising chain may exhibit either two, or

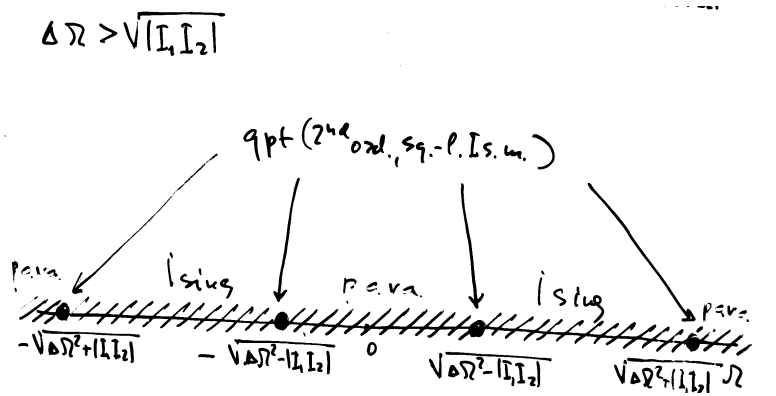

Figure 9. The ground-state phases and phase transitions for the regularly alternating transverse Ising chain of period 2 with $\Omega_{1,2} = \Omega \pm \Delta\Omega$, $\Delta\Omega > \sqrt{|I_1 I_2|}$.

three, or four quantum phase transition points. The actual number of quantum phase transition points depends on a relation between $\Delta\Omega$ and $\sqrt{|I_1 I_2|}$. Moreover, the energy gap may vanish either linearly (second-order quantum phase transition) or proportionally to a deviation from the critical point squared (fourth-order quantum phase transition).

Since the transverse Ising chain is, as a matter of fact, the system of free fermions (see Section 4, Eq. (4.19)) its Helmholtz free energy per site can be written as

$$\begin{aligned} f &= -kT \int_{-\infty}^{\infty} \mathrm{d}E \rho(E) \ln\left(2\cosh\frac{E}{2kT}\right) \\ &= -2kT \int_{0}^{\infty} \mathrm{d}E E R(E^2) \ln\left(2\cosh\frac{E}{2kT}\right) \end{aligned} \tag{3.4}$$

where the density of states $\rho(E)$ ($R(E^2)$) describes the distribution of the elementary excitation energies (the distribution of the squares of elementary excitation energies, see Eqs. (4.20), (4.22)). The gapless chain has the zero-energy elementary excitation that implies

$$R(E^2) \sim \frac{1}{\sqrt{E^2}} \tag{3.5}$$

as $E \to 0$. On the other hand, using (3.4) one gets the specific heat

$$\frac{c}{k} = 2\int_{0}^{\infty} \mathrm{d}E E R(E^2) \left(\frac{\frac{E}{2kT}}{\cosh\frac{E}{2kT}}\right)^2. \tag{3.6}$$

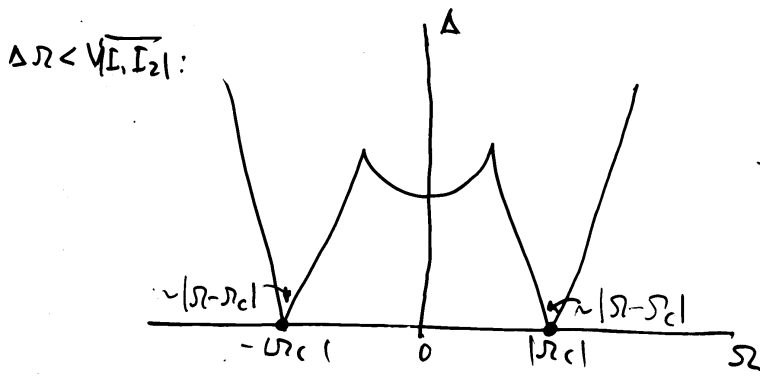

Figure 10. A transverse Ising chain of period 2 with $\Omega_{1,2} = \Omega \pm \Delta\Omega$, $\Delta\Omega < \sqrt{|I_1 I_2|}$: Energy gap Δ versus transverse field Ω.

From Eqs. (3.6), (3.5) it can be read off that the vanishing energy gap produces a linear low-temperature dependence of the specific heat on temperature. Really, splitting the interval of integration in (3.6) and expanding the integrand in the first integral in which $E < kT$,

$$\frac{c}{k} = 2\int_0^{kT} \mathrm{d}E E \frac{C}{\sqrt{E^2}} \left(\frac{E}{2kT}\right)^2 + 2\int_{kT}^{\infty} \mathrm{d}E E R(E^2) \left(\frac{\frac{E}{2kT}}{\cosh\frac{E}{2kT}}\right)^2, \quad (3.7)$$

one notes that the second integrand (for which $E > kT$) tends to zero as $T \to 0$ whereas the first integral in (3.7) after a rescaling of the variable, $\frac{1}{2}CkT\int_0^1 \mathrm{d}x x^2$, appears to be proportional to temperature. Exact analytical calculations of the specific heat [5] are in complete agreement with the results on the energy gap clearly indicating the quantum phase transition points (3.2), (3.3) seen in Figs. 10, 11, 12.

Unfortunately, we cannot analytically calculate the spin correlation functions in a regularly alternating transverse Ising chain. However, they can be computed numerically for very long chains of a few thousand sites (see, for example, [18]). Knowing the two-site correlation function of x spin components we can find the Ising magnetization m^x looking for a limiting value of the square-root of such correlation function as the interspin distance goes to infinity. The behavior of the ground-state Ising magnetization versus the transverse field confirms the above discussed effects of regularly alternating transverse field on the quantum phase transition. Again, if $\Delta\Omega < \sqrt{|I_1 I_2|}$ we may observe paramagnetic phase (the x magnetization equals to zero) and ferromagnetic phase (nonzero

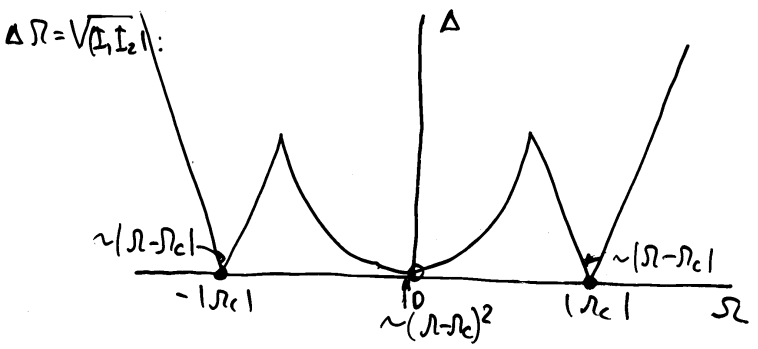

Figure 11. A transverse Ising chain of period 2 with $\Omega_{1,2} = \Omega \pm \Delta\Omega$, $\Delta\Omega = \sqrt{|I_1 I_2|}$: Energy gap Δ versus transverse field Ω.

values of the x magnetization); if $\Delta\Omega = \sqrt{|I_1 I_2|}$ the x magnetization tends to zero in the ferromagnetic phase if $\Omega = 0$; if $\Delta\Omega > \sqrt{|I_1 I_2|}$ we may observe high-field and low-field paramagnetic phases (the x magnetization equals to zero) and ferromagnetic phase at moderate fields (nonzero values of the x magnetization). The appearance of the paramagnetic phase ($m^x = 0$) at weak fields Ω can be associated with a classical picture when owing to the regular alternation of the on-site transverse fields,

$$(\Omega + \Delta\Omega)(\Omega - \Delta\Omega)(\Omega + \Delta\Omega)(\Omega - \Delta\Omega)\ldots,$$

$\Delta\Omega$ large, all on-site magnetizations are directed parallel/antiparallel to the z-axis in spin space. Naturally, this picture may play only an auxiliary role for the considered quantum system.

The results concerning the quantum phase transitions tuned by the transverse field Ω in the regularly alternating transverse Ising chain of period 2 with $\Omega_{1,2} = \Omega \pm \Delta\Omega$ can be summarized as follows. If $\Delta\Omega < \sqrt{|I_1 I_2|}$ the system shows two quantum phase transitions; if $\Delta\Omega > \sqrt{|I_1 I_2|}$ the system shows four quantum phase transitions; at the boundary between these regions, i.e., if $\Delta\Omega = \sqrt{|I_1 I_2|}$, the system shows two quantum phase transitions and a point of weak singularities.

What happens when we increase the period of alternation? More specifically, we consider a transverse Ising chain of period 3 assuming

$$\Omega_{1,2,3} = \Omega + \Delta\Omega_{1,2,3}, \quad \Delta\Omega_1 + \Delta\Omega_2 + \Delta\Omega_3 = 0, \quad |I_1 I_2 I_3| = 1.$$

A possible number of phase transition points for such a chain is shown in Fig. 13. Thus, as far as the transverse field Ω varies such a chain may

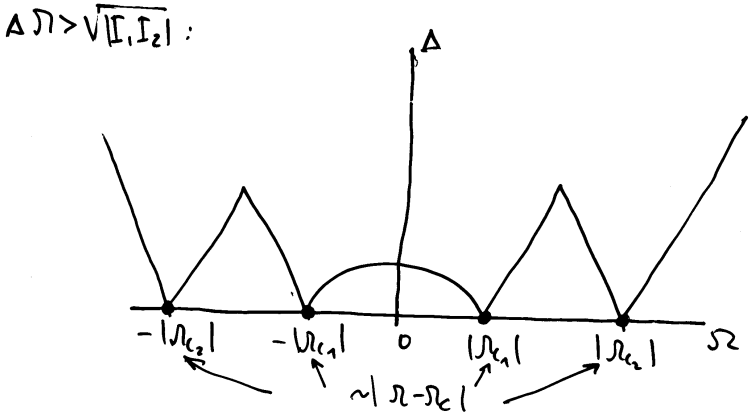

Figure 12. A transverse Ising chain of period 2 with $\Omega_{1,2} = \Omega \pm \Delta\Omega$, $\Delta\Omega > \sqrt{|I_1 I_2|}$: Energy gap Δ versus transverse field Ω.

show either two, or four, or six second-order quantum phase transitions. Moreover, for special relations between parameters weak singularities may additionally occur in the Ising phases.

What about an arbitrary period of alternation? Quantum phase transition points follow from the condition

$$\Omega_1 \Omega_2 \dots \Omega_p = \pm I_1 I_2 \dots I_p \tag{3.8}$$

which was obtained long ago by P. Pfeuty [19] (note, however, that Eq. (6) in this paper does not contain two signs as Eq. (3.8) does; the minus sign immediately follows by symmetry after simple spin axes rotations). The number of quantum phase transitions, i.e., the number of critical transverse fields Ω_c which satisfy (3.8), strongly depends on a concrete set of the Hamiltonian parameters. However, it cannot exceed $2p$ where p is the period of alternation. The critical behavior is similar to the square-lattice Ising model, i.e.,

$$\Delta \sim |\Omega - \Omega_c|, \quad \chi^z \sim \ln|\Omega - \Omega_c|, \quad \xi \sim \frac{1}{|\Omega - \Omega_c|}, \quad m^x \sim (\Omega_c - \Omega)^{\frac{1}{8}}$$

as $\Omega \to \Omega_c$. However, for some sets of parameters a weak singularity may occur as well, i.e.,

$$\Delta \sim |\Omega - \Omega_c|^2, \quad \frac{\partial^2 \chi^z}{\partial \Omega^2} \sim \ln|\Omega - \Omega_c|, \quad \xi \sim \frac{1}{|\Omega - \Omega_c|^2}$$

as $\Omega \to \Omega_c$. For further details see Ref. [5].

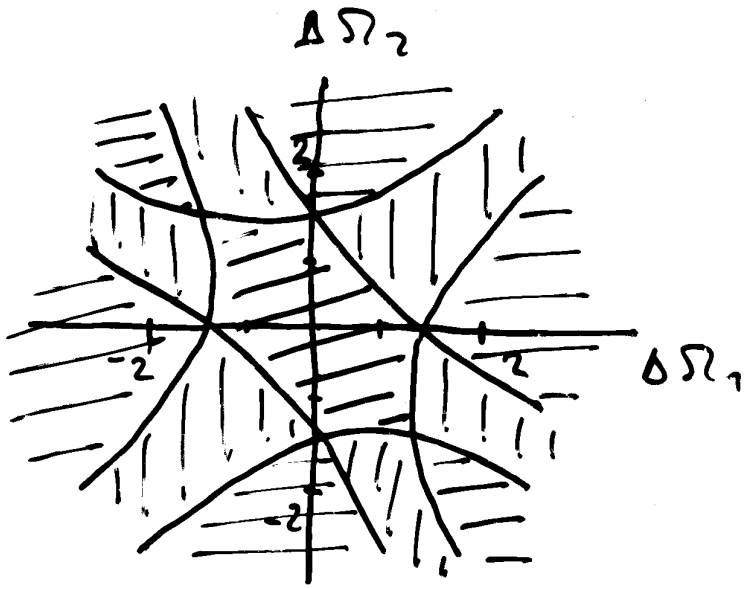

Figure 13. Towards a possible number of quantum phase transitions in the transverse Ising chain of period 3 with $\Omega_{1,2,3} = \Omega + \Delta\Omega_{1,2,3}$, $\Delta\Omega_1 + \Delta\Omega_2 + \Delta\Omega_3 = 0$, $|I_1 I_2 I_3| = 1$: the central region (two quantum phase transitions), the region denoted by vertical lines (four quantum phase transitions), the rest regions (six quantum phase transitions), weak singularities (one or two) occur for the parameters corresponding to the boundaries between different regions.

4. Technical details

In this concluding Section I briefly explain how the reported results on the uniform and regularly alternating transverse Ising chains can be obtained. The essential tool for these calculations is the Jordan-Wigner transformation which permits us to map the considered spin chains onto the spinless fermions with the Hamiltonian which is a bilinear form in terms of the creation and annihilation operators [7]. To bring this Hamiltonian into the diagonal form we perform the Bogolyubov transformation. Alternatively, for the calculation of thermodynamic quantities we may use the Green functions method which becomes extremely useful in the case of regularly alternating transverse Ising chains after being completed by the continued fraction approach.

4.1. Jordan-Wigner fermionization

We consider the spin-$\frac{1}{2}$ anisotropic XY chain in a transverse field with the Hamiltonian

$$H = \sum_n \left(2I_n^x s_n^x s_{n+1}^x + 2I_n^y s_n^y s_{n+1}^y\right) + \sum_n \Omega_n s_n^z$$
$$= \sum_n \left(\frac{I_n^x + I_n^y}{2} \left(s_n^+ s_{n+1}^- + s_n^- s_{n+1}^+\right) \right.$$
$$\left. + \frac{I_n^x - I_n^y}{2} \left(s_n^+ s_{n+1}^+ + s_n^- s_{n+1}^-\right) + \Omega_n \left(s_n^+ s_n^- - \frac{1}{2}\right)\right); \qquad (4.1)$$

here $s^\pm = s^x \pm \mathrm{i}s^y$. At first glance Eq. (4.1) seems to be very simple since it does not contain the products of four spin raising and lowering operators. However, a closer look reveals a difficulty: although the Hamiltonian (4.1) is indeed a bilinear form in terms of the spin raising and lowering operators the commutation rules they obey are of the Fermi type at one and the same site,

$$\left\{s_j^-, s_j^+\right\} = 1, \quad \left(s_j^+\right)^2 = \left(s_j^-\right)^2 = 0, \qquad (4.2)$$

and of the Bose type at different sites,

$$\left[s_n^-, s_m^+\right] = \left[s_n^+, s_m^+\right] = \left[s_n^-, s_m^-\right] = 0, \quad n \neq m. \qquad (4.3)$$

The key to a solution is to introduce the operators which satisfy the Fermi commutation relations using the Jordan-Wigner transformation

$$c_1 = s_1^-, \quad c_2 = \left(-2s_1^z\right) s_2^-, \quad \ldots,$$
$$c_n = \left(-2s_1^z\right)\left(-2s_2^z\right)\ldots\left(-2s_{n-1}^z\right) s_n^-, \quad \ldots;$$
$$c_1^+ = s_1^+, \quad c_2^+ = \left(-2s_1^z\right) s_2^+, \quad \ldots,$$
$$c_n^+ = \left(-2s_1^z\right)\left(-2s_2^z\right)\ldots\left(-2s_{n-1}^z\right) s_n^+, \quad \ldots. \qquad (4.4)$$

(Sometimes Eq. (4.4) is written with $\exp\left(\pm\mathrm{i}\pi s^+ s^-\right) = \exp\left(\pm\mathrm{i}\pi\left(s^z + \frac{1}{2}\right)\right)$ instead of $\left(-2s^z\right)$, which is, obviously, equivalent.) Let us first check whether the operators introduced by Eq. (4.4) really satisfy the Fermi commutation relations. Evidently, the commutation relations at one and the same site remain of the Fermi type. For example,

$$\left\{c_j, c_j^+\right\} = s_j^- \left(-2s_1^z\right)^2 \left(-2s_2^z\right)^2 \ldots \left(-2s_{n-1}^z\right)^2 s_j^+$$
$$+ s_j^+ \left(-2s_1^z\right)^2 \left(-2s_2^z\right)^2 \ldots \left(-2s_{n-1}^z\right)^2 s_j^- = \left\{s_j^-, s_j^+\right\} = 1 \qquad (4.5)$$

owing to (4.3) and the equality

$$\left(-2s^z\right)^2 = 1. \qquad (4.6)$$

Consider now different sites assuming for concreteness $n < m$. Using (4.3) and (4.6) we find

$$c_n^+ c_m = s_n^+ \left(-2s_n^z\right)\ldots\left(-2s_{m-1}^z\right) s_m^-;$$
$$c_m c_n^+ = s_m^- \left(-2s_n^z\right)\ldots\left(-2s_{m-1}^z\right) s_n^+. \qquad (4.7)$$

To get the lower line in the r.h.s. in (4.7) from the upper line in the r.h.s. in (4.7) one has to permute s_n^+ and s_n^z which is accompanied by the change of sign. As a result

$$c_n^+ c_m = -c_m c_n^+. \qquad (4.8)$$

Repeating calculations similar to (4.7), (4.8) for other pairs of the introduced operators we became convinced that they anticommute at different sites.

Let us rewrite the Hamiltonian (4.1) in terms of the introduced operators. We have already seen (Eq. (4.5)) that $s_n^+ s_n^- = c_n^+ c_n$. Using (4.4) and the properties of the Pauli matrices one is easily convinced that

$$c_j^+ c_{j+1}^+ = s_j^+ \left(-2s_j^z\right) s_{j+1}^+ = s_j^+ s_{j+1}^+, \quad c_j^+ c_{j+1} = s_j^+ s_{j+1}^-,$$
$$c_j c_{j+1}^+ = s_j^- \left(-2s_j^z\right) s_{j+1}^+ = -s_j^- s_{j+1}^+, \quad c_j c_{j+1} = -s_j^- s_{j+1}^- \qquad (4.9)$$

and consequently the Hamiltonian (4.1) becomes

$$H = \sum_n \left(\frac{I_n^x + I_n^y}{2} \left(c_n^+ c_{n+1} - c_n c_{n+1}^+\right) \right.$$
$$\left. + \frac{I_n^x - I_n^y}{2} \left(c_n^+ c_{n+1}^+ - c_n c_{n+1}\right) + \Omega_n \left(c_n^+ c_n - \frac{1}{2}\right)\right). \qquad (4.10)$$

(I have omitted the boundary term (which is present if periodic boundary conditions are implied in (4.1)) which is not important for the calculation of thermodynamic quantities.)

4.2. Diagonalization (uniform chain)

To calculate the thermodynamic quantities for the spin model we must diagonalize a bilinear form (4.10) reducing a problem to a study of thermodynamics of noninteracting (spinless) fermions. It can be easily done

in the uniform case $I_n^\alpha = I^\alpha$, $\Omega_n = \Omega$ after performing the Fourier transformation and the Bogolyubov transformation.

In detail, introducing new Fermi operators

$$c_n^+ = \frac{1}{\sqrt{N}} \sum_\kappa \exp\left(\mathrm{i}\kappa n\right) c_\kappa^+, \quad c_n = \frac{1}{\sqrt{N}} \sum_\kappa \exp\left(-\mathrm{i}\kappa n\right) c_\kappa, \qquad (4.11)$$

with $\kappa = \frac{2\pi}{N} n$, $n = -\frac{N}{2}, -\frac{N}{2}+1, \ldots, \frac{N}{2}-1$ (N is even) we can rewrite (4.10) as follows

$$\begin{aligned} H &= \sum_\kappa \left(-\frac{\Omega}{2} + \left(\Omega + (I^x + I^y)\cos\kappa\right) c_\kappa^+ c_\kappa \right. \\ &\qquad \left. -\frac{\mathrm{i}}{2}\left(I^x - I^y\right)\sin\kappa \left(c_\kappa^+ c_{-\kappa}^+ + c_\kappa c_{-\kappa}\right)\right) \\ &= \sum_\kappa{}' \left(-\Omega + \left(\Omega + (I^x + I^y)\cos\kappa\right)\left(c_\kappa^+ c_\kappa + c_{-\kappa}^+ c_{-\kappa}\right)\right. \\ &\qquad \left. -\mathrm{i}\left(I^x - I^y\right)\sin\kappa \left(c_\kappa^+ c_{-\kappa}^+ + c_\kappa c_{-\kappa}\right)\right) \\ &= \sum_\kappa{}' \begin{pmatrix} c_\kappa^+ & c_{-\kappa} \end{pmatrix} \begin{pmatrix} A & -\mathrm{i}C \\ \mathrm{i}C & -A \end{pmatrix} \begin{pmatrix} c_\kappa \\ c_{-\kappa}^+ \end{pmatrix}; \qquad (4.12) \\ A &= \Omega + (I^x + I^y)\cos\kappa, \quad C = (I^x - I^y)\sin\kappa; \end{aligned}$$

the prime denotes that in the thermodynamic limit κ varies from 0 to π. Introduce new Fermi operators

$$\begin{pmatrix} \beta_\kappa \\ \beta_{-\kappa}^+ \end{pmatrix} = \begin{pmatrix} \mathrm{i}u_\kappa & v_\kappa \\ v_\kappa & \mathrm{i}u_\kappa \end{pmatrix} \begin{pmatrix} c_\kappa \\ c_{-\kappa}^+ \end{pmatrix}; \qquad (4.13)$$

the unknown functions u_κ and v_κ are real. Moreover, $u_{-\kappa} = -u_\kappa$, $v_{-\kappa} = v_\kappa$, $u_\kappa^2 + v_\kappa^2 = 1$. The inverse to (4.13) transformation reads

$$\begin{pmatrix} c_\kappa \\ c_{-\kappa}^+ \end{pmatrix} = \begin{pmatrix} -\mathrm{i}u_\kappa & v_\kappa \\ v_\kappa & -\mathrm{i}u_\kappa \end{pmatrix} \begin{pmatrix} \beta_\kappa \\ \beta_{-\kappa}^+ \end{pmatrix}. \qquad (4.14)$$

If u_κ, v_κ satisfy the equation

$$\begin{aligned} \frac{u_\kappa}{v_\kappa} &= \frac{A}{C} \pm \sqrt{\left(\frac{A}{C}\right)^2 + 1} = \frac{A \pm \mathrm{sgn}(C)\Lambda_\kappa}{C}, \\ \Lambda_\kappa &= \sqrt{A^2 + C^2} = \sqrt{\left(\Omega + (I^x + I^y)\cos\kappa\right)^2 + \left(I^x - I^y\right)^2 \sin^2\kappa}, \qquad (4.15) \end{aligned}$$

that is, if

$$\begin{aligned} u_\kappa &= \mathrm{sgn}\left(\left(I^x - I^y\right)\sin\kappa\right) \frac{1}{\sqrt{2}} \sqrt{1 + \frac{\Omega + (I^x + I^y)\cos\kappa}{\Lambda_\kappa}}, \\ v_\kappa &= \frac{1}{\sqrt{2}} \sqrt{1 - \frac{\Omega + (I^x + I^y)\cos\kappa}{\Lambda_\kappa}}, \qquad (4.16) \end{aligned}$$

one arrives at

$$\begin{aligned} &\begin{pmatrix} \mathrm{i}u_\kappa & v_\kappa \\ v_\kappa & \mathrm{i}u_\kappa \end{pmatrix} \begin{pmatrix} A & -\mathrm{i}C \\ \mathrm{i}C & -A \end{pmatrix} \begin{pmatrix} -\mathrm{i}u_\kappa & v_\kappa \\ v_\kappa & -\mathrm{i}u_\kappa \end{pmatrix} \\ &\qquad = \begin{pmatrix} \sqrt{A^2 + C^2} & 0 \\ 0 & -\sqrt{A^2 + C^2} \end{pmatrix}. \qquad (4.17) \end{aligned}$$

Thus, after the Bogolyubov transformation (4.13), (4.16) the Hamiltonian (4.12) takes the form

$$\begin{aligned} H &= \sum_\kappa{}' \begin{pmatrix} \beta_\kappa^+ & \beta_{-\kappa} \end{pmatrix} \begin{pmatrix} \Lambda_\kappa & 0 \\ 0 & -\Lambda_\kappa \end{pmatrix} \begin{pmatrix} \beta_\kappa \\ \beta_{-\kappa}^+ \end{pmatrix} \\ &= \sum_\kappa{}' \Lambda_\kappa \left(\beta_\kappa^+ \beta_\kappa - \beta_{-\kappa}\beta_{-\kappa}^+\right) = \sum_\kappa \Lambda_\kappa \left(\beta_\kappa^+ \beta_\kappa - \frac{1}{2}\right). \qquad (4.18) \end{aligned}$$

It is now easy to calculate the partition function (and hence all thermodynamic quantities) of the spin chain. Really, for the fermions with the Hamiltonian (4.18) we have

$$Z = \prod_\kappa \left(\exp\left(\frac{\Lambda_\kappa}{2kT}\right) + \exp\left(-\frac{\Lambda_\kappa}{2kT}\right)\right) = \prod_\kappa 2\cosh\frac{\Lambda_\kappa}{2kT}. \qquad (4.19)$$

The described scheme becomes cumbersome if p exceeds 1. Namely, the size of the matrix appearing in Eq. (4.12) increases (for $p = 2$ one face the 4×4 matrix [20]) [1]. Of course, the bilinear form (4.10) can be brought to the diagonal form

$$H = \sum_{k=1}^N \Lambda_k \left(\eta_k^+ \eta_k - \frac{1}{2}\right) \qquad (4.20)$$

[1] It is interesting to mention here a recent preprint [21] in which a completely different approach for calculation of the partition function of quantum spin chains has been used. Namely, the partition function can be calculated by the combinatorial method avoiding the eigenvalue problem of the Hamiltonian. In particular, the authors have calculated the Helmholtz free energy of a period-two XY chain in a transverse field.

by a unitary transformation

$$\eta_k = \sum_i \left(g_{ki} c_i + h_{ki} c_i^+\right), \quad \eta_k^+ = \sum_i \left(h_{ki} c_i + g_{ki} c_i^+\right), \tag{4.21}$$

after imposing certain conditions on $g_{ki} = \frac{1}{2}\left(\Phi_{ki} + \Psi_{ki}\right)$ and $h_{ki} = \frac{1}{2}\left(\Phi_{ki} - \Psi_{ki}\right)$ (see [7] for the uniform chain and Eq. (4.23) for a nonuniform transverse Ising chain). However, to find the unknown functions Φ_{ki} and Ψ_{ki} and the energies Λ_k in the case of regularly alternating Hamiltonian parameters having an arbitrary period p is a difficult task. Nevertheless, if we are interested in the thermodynamic quantities only, we may proceed taking an advantage of the fact that only a set of elementary excitation energies $\{\Lambda_k\}$ is needed. Really, the Helmholtz free energy (3.4) is known if the density of states

$$R(E^2) = \frac{1}{N} \sum_{k=1}^{N} \delta\left(E^2 - \Lambda_k^2\right) \tag{4.22}$$

is known. To calculate the density of state $R(E^2)$ (4.22) we may use the Green functions approach which recovers the results obtained by diagonalization of the fermionic Hamiltonian and, what is more important, which can be extended for regularly alternating chains.

4.3. Green functions, continued fractions (transverse Ising chains)

Let us consider a nonuniform transverse Ising chain ($I_n^x = I_n$, $I_n^y = 0$) for which a set of equations for unknown quantities Φ_{ki}, Ψ_{ki}, Λ_k has the following form

$$\begin{aligned} \Omega_{n-1} I_{n-1} \Phi_{k,n-1} + \left(\Omega_n^2 + I_{n-1}^2 - \Lambda_k^2\right) \Phi_{k,n} + \Omega_n I_n \Phi_{k,n+1} = 0, \\ \Omega_n I_{n-1} \Psi_{k,n-1} + \left(\Omega_n^2 + I_n^2 - \Lambda_k^2\right) \Psi_{k,n} + \Omega_{n+1} I_n \Psi_{k,n+1} = 0. \end{aligned} \tag{4.23}$$

We may rewrite Eq. (4.23) in the matrix form

$$\left(\mathbf{H} - \Lambda_k^2 \mathbf{1}\right) \begin{pmatrix} \Phi_{k,1} \\ \Phi_{k,2} \\ \vdots \\ \Phi_{k,N} \end{pmatrix} = 0 \tag{4.24}$$

with the three diagonal band matrix

$$\mathbf{H} = \begin{pmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & 0 & \Omega_{n-1} I_{n-1} & \Omega_n^2 + I_{n-1}^2 & \Omega_n I_n & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}. \tag{4.25}$$

Let us introduce the Green functions $G_{nm} = G_{nm}(E^2)$ by the following equation

$$\left(E^2 \mathbf{1} - \mathbf{H}\right) \mathbf{G} = \mathbf{1}. \tag{4.26}$$

Since the matrix $\mathbf{H}$ (4.25) can be diagonalized (see Eq. (4.24)), i.e.,

$$\mathbf{U}\mathbf{H}\mathbf{U}^+ = \begin{pmatrix} \Lambda_1^2 & 0 & \dots & 0 \\ 0 & \Lambda_2^2 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & \Lambda_N^2 \end{pmatrix},$$

from Eq. (4.26) we have

$$\mathbf{U}\mathbf{G}\mathbf{U}^+ = \begin{pmatrix} \frac{1}{E^2 - \Lambda_1^2} & 0 & \dots & 0 \\ 0 & \frac{1}{E^2 - \Lambda_2^2} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & \frac{1}{E^2 - \Lambda_N^2} \end{pmatrix},$$

and hence

$$\sum_{k=1}^{N} \frac{1}{E^2 - \Lambda_k^2} = \mathrm{Tr}\left(\mathbf{U}\mathbf{G}\mathbf{U}^+\right) = \sum_{n=1}^{N} G_{nn}(E^2). \tag{4.27}$$

Utilizing in Eq. (4.27) the famous symbolic identity

$$\frac{1}{x \pm \mathrm{i}\epsilon} = \mathcal{P}\frac{1}{x} \mp \mathrm{i}\pi\delta(x), \quad \epsilon \to +0$$

we find the relation between the diagonal Green functions defined by (4.26) and the density of states (4.22)

$$R(E^2) = \mp \frac{1}{N\pi} \sum_{n=1}^{N} \Im G_{nn}\left(E^2 \pm \mathrm{i}\epsilon\right). \tag{4.28}$$

Now our task is to find the diagonal Green functions defined by (4.26). From Eq. (4.26) one can easily obtain the following continued fraction representation for the diagonal Green functions

$$G_{nn} = \frac{1}{E^2 - \Omega_n^2 - I_{n-1}^2 - \Delta_n^- - \Delta_n^+}, \tag{4.29}$$

$$\Delta_n^- = \cfrac{\Omega_{n-1}^2 I_{n-1}^2}{E^2 - \Omega_{n-1}^2 - I_{n-2}^2 - \cfrac{\Omega_{n-2}^2 I_{n-2}^2}{E^2 - \Omega_{n-2}^2 - I_{n-3}^2 - \ddots}},$$

$$\Delta_n^+ = \cfrac{\Omega_n^2 I_n^2}{E^2 - \Omega_{n+1}^2 - I_n^2 - \cfrac{\Omega_{n+1}^2 I_{n+1}^2}{E^2 - \Omega_{n+2}^2 - I_{n+1}^2 - \ddots}}.$$

This representation becomes extremely useful for periodic sequences of the Hamiltonian parameters since the continued fractions in (4.29) become periodic and can be evaluated by solving square equations.

I illustrate how this scheme works in the simplest case $p = 1$. For the uniform case $\Delta_n^- = \Delta_n^+ = \Delta$ (do not confuse with the energy gap Δ!) and

$$\Delta = \frac{\Omega^2 I^2}{E^2 - \Omega^2 - I^2 - \Delta}. \tag{4.30}$$

Now

$$G_{nn} = \mp \frac{1}{\sqrt{\left(E^2 - \Omega^2 - I^2\right)^2 - 4\Omega^2 I^2}} \tag{4.31}$$

and the density of states has the following form

$$R(E^2) = \begin{cases} \frac{1}{\pi\sqrt{-(E^2-a_1)(E^2-a_2)}} & \text{if} \quad a_1 < E^2 < a_2, \\ 0, & \text{otherwise} \end{cases} \tag{4.32}$$

with $a_{1,2} = (\Omega \pm I)^2$. (Now it becomes clear why we adopted the square-root singularity of $R(E^2)$ in Eq. (3.5).)

4.4. Critical behavior

Finally, let us explain how the critical behavior can be derived. We start from the ground-state energy per site

$$e_0 = -\int_0^\infty \mathrm{d}E E^2 R(E^2). \tag{4.33}$$

Here the density of states has the following form (compare with (4.32))

$$R(E^2) = \begin{cases} \frac{|\mathcal{Z}_{p-1}(E^2)|}{\pi p\sqrt{\mathcal{A}_{2p}(E^2)}}, & \text{if} \quad \mathcal{A}_{2p}(E^2) > 0, \\ 0, & \text{otherwise} \end{cases} \tag{4.34}$$

where $\mathcal{Z}_{p-1}(E^2)$ and $\mathcal{A}_{2p}(E^2)$ are the polynomials of the order $p-1$ and $2p$, respectively. Moreover, $\mathcal{A}_{2p}(E^2) = -\left(E^2 - a_1\right)\left(E^2 - a_2\right)\ldots\left(E^2 - a_{2p}\right)$ where $0 \le a_1 \le a_2 \le \ldots \le a_{2p}$ are the roots of $\mathcal{A}_{2p}(E^2)$. As $|\Omega - \Omega_c| = \epsilon \to 0$ the smallest root a_1 vanishes either proportionally to ϵ^2 or proportionally to ϵ^4. As a result the nonanalytic contribution to the ground-state energy (4.33) has the following form

$$-\frac{1}{\pi p}\int_{\sqrt{a_1}}^{\sqrt{a_2}} \mathrm{d}E E^2 \frac{f(E^2)}{\sqrt{E^2 - a_1}}. \tag{4.35}$$

Using the table integral

$$\int \mathrm{d}x \frac{x^2}{\sqrt{x^2 - a^2}} = \frac{1}{2}\left(x\sqrt{x^2 - a^2} - a^2 \ln\left(x - \sqrt{x^2 - a^2}\right)\right)$$

one finds that the nonanalytic contribution to the ground-state energy (4.35) behaves either as

$$\sim \epsilon^2 \ln \epsilon \tag{4.36}$$

(if $a_1 \sim \epsilon^2$ and the energy gap $\Delta \sim \epsilon$) or as

$$\sim \epsilon^4 \ln \epsilon \tag{4.37}$$

(if $a_1 \sim \epsilon^4$ and the energy gap $\Delta \sim \epsilon^2$). Taking the derivatives with respect to Ω in (4.36) or (4.37) one immediately gets (2.4), (2.5) or the critical behavior in the vicinity of the weak singularity point.

ACKNOWLEDGMENTS - It is a pleasure to thank the Organizing Committee of the Small Triangle Meeting 2003 for kind hospitality. I am grateful to Michal Jaščur, Jozef Strečka and Taras Verkholyak for stimulating discussions in Medzev. I thank Johannes Richter for kind hospitality in the Magdeburg University in the autumn of 2003 where the paper was completed.

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Роботу отримано 5 грудня 2003 р.

Затверджено до друку Вченою радою ІФКС НАН України

Рекомендовано до друку семінаром відділу теорії модельних спінових систем

Виготовлено при ІФКС НАН України