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2000 J. Phys. A: Math. Gen. 33 8627

(http://iopscience.iop.org/0305-4470/33/48/303)

J. Phys. A: Math. Gen. **33** (2000) 8627–8634. Printed in the UK PII: S0305-4470(00)13682-0

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

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Received 2 May 2000, in final form 26 September 2000

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

Spin-$\frac{1}{2}$ XY chains provide an excellent ground for a rigorous study of different properties of low-dimensional quantum magnetic systems due to the fact that with the help of the Jordan–Wigner transformation such spin models can be mapped onto noninteracting spinless fermions and as a result many statistical mechanics calculations can be performed exactly [1]. In what follows we shall consider the periodic alternating XY chain in a transverse field with *extremely anisotropic* spin coupling (for short called here the transverse Ising chain) in order to study the generic effects induced by regular alternation of the nearest-neighbour interaction strengths and the external fields. The periodic alternating chain can be viewed as a chain having several sublattices. There are few papers dealing with the statistical mechanics properties of XY chains on two sublattices [2–5]. We want to emphasize that in the above-mentioned limit of the transverse Ising chain the calculation of the thermodynamic quantities can be performed in a rather general manner covering all chains with an arbitrary period of alternation. This paper can be viewed as a nontrivial extension of the recent study of the thermodynamics of the spin-$\frac{1}{2}$ *isotropic* XY chain in a transverse field (called here the transverse XY chain) with regularly alternating fields and bonds [6]. In particular, we compare below the zero-temperature dependences of transverse magnetization on the transverse field and static transverse susceptibility on the transverse field for the regularly alternating transverse Ising and XY chains. On the other hand, it is known that the transverse XY chain is a simple system exhibiting a spin-Peierls instability [7–10]. An analysis of the ground state energy of

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0305-4470/00/488627+08$30.00

the periodic alternating transverse Ising chain of period 2 allows one to examine a spin-Peierls instability of that chain with respect to dimerization. We find that the transverse Ising chain is stable with respect to dimerization, which demonstrates a role of the anisotropy in spin coupling for a spin-Peierls instability.

We consider a ring of $N(\to \infty)$ spins described by the $S = \frac{1}{2}$ Hamiltonian of the nonuniform transverse Ising model

$$H = \sum_{n=1}^{N} \Omega_n s_n^z + 2 \sum_{n=1}^{N} I_n s_n^x s_{n+1}^x \qquad s_{N+1}^{\alpha} = s_1^{\alpha}. \tag{1}$$

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

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

$$\begin{aligned} &H = \sum_{n=1}^{N} \Omega_n (c_n^+ c_n - \tfrac{1}{2}) + \tfrac{1}{2} \sum_{n=1}^{N} I_n (c_n^+ c_{n+1}^+ + c_n^+ c_{n+1} - c_n c_{n+1}^+ - c_n c_{n+1}) \\ &c_{N+1}^+ = c_1^+ \quad c_{N+1} = c_1 \end{aligned} \tag{2}$$

(the boundary term, that is unimportant as far as the thermodynamics is concerned, has been omitted). Unlike the case in [6], we cannot proceed directly by using a continued fraction representation for the diagonal one-fermion Green functions of the tight-binding spinless fermions since the Hamiltonian (2) contains the products of two creation (annihilation) operators. However, it is well known (see, e.g., [1,11,12]) that after introducing new operators $\eta_k = \sum_{i=1}^{N} (g_{ki} c_i + h_{ki} c_i^+)$ and $\eta_k^+ = \sum_{i=1}^{N} (h_{ki} c_i + g_{ki} c_i^+)$ the Hamiltonian (2) transforms into

$$H = \sum_{k=1}^{N} \Lambda_k (\eta_k^+ \eta_k - \tfrac{1}{2}) \qquad \{\eta_k^+, \eta_q\} = \delta_{kq} \quad \{\eta_k, \eta_q\} = \{\eta_k^+, \eta_q^+\} = 0 \tag{3}$$

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

$$\begin{aligned} &\Omega_{n-1} I_{n-1} \Phi_{k,n-1} + (\Omega_n^2 + I_{n-1}^2 - \Lambda_k^2) \Phi_{kn} + \Omega_n I_n \Phi_{k,n+1} = 0 \\ &\Phi_{k0} = \Phi_{kN} \quad \Phi_{k,N+1} = \Phi_{k1} \\ &\Omega_n I_{n-1} \Psi_{k,n-1} + (\Omega_n^2 + I_n^2 - \Lambda_k^2) \Psi_{kn} + \Omega_{n+1} I_n \Psi_{k,n+1} = 0 \\ &\Psi_{k0} = \Psi_{kN} \quad \Psi_{k,N+1} = \Psi_{k1}. \end{aligned} \tag{4}$$

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

$$(E^2 - \Omega_n^2 - I_{n-1}^2) G_{nm} - \Omega_{n-1} I_{n-1} G_{n-1,m} - \Omega_n I_n G_{n+1,m} = \delta_{nm} \tag{5}$$

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

$$R(E^2) = \mp \frac{1}{\pi N} \sum_{n=1}^{N} \operatorname{Im} G_{nn}(E^2 \pm \mathrm{i}\epsilon) \qquad \epsilon \to +0. \tag{6}$$

As follows from (3) all the thermodynamic quantities can be expressed through $R(E^2)$. For example, the Helmholtz free energy per site is given by

$$f = -\frac{2}{\beta}\int_0^\infty \mathrm{d}E\, E R(E^2) \ln\left(2\cosh\frac{\beta E}{2}\right). \tag{7}$$

Obviously, $R(E^2)$ can be obtained with the help of the Green functions introduced on the basis of the set of equations for the coefficients Ψ_{kn} (4). We have performed such a calculation and found the same result for $R(E^2)$ in the cases considered below (equations (9) and (11)).

We have now to calculate the diagonal Green functions G_{nn}. Let us use the continued fraction representation for G_{nn} that follows from (5):

$$\begin{aligned} G_{nn} &= \frac{1}{E^2 - \Omega_n^2 - I_{n-1}^2 - \Delta_n^- - \Delta_n^+} \\ \Delta_n^- &= \cfrac{\Omega_{n-1}^2 I_{n-1}^2}{E^2 - \Omega_{n-1}^2 - I_{n-2}^2 - \cfrac{\Omega_{n-2}^2 I_{n-2}^2}{E^2 - \Omega_{n-2}^2 - I_{n-3}^2 - \ddots}} \\ \Delta_n^+ &= \cfrac{\Omega_n^2 I_n^2}{E^2 - \Omega_{n+1}^2 - I_n^2 - \cfrac{\Omega_{n+1}^2 I_{n+1}^2}{E^2 - \Omega_{n+2}^2 - I_{n+1}^2 - \ddots}}. \end{aligned} \tag{8}$$

For any finite period of varying Ω_n and I_n the continued fractions in (8) become periodic (evidently, the limit $N \to \infty$ is hinted at) and can be easily calculated by solving quadratic equations. As a result we obtain rigorous results for the Green functions, density of states (6) and thermodynamic quantities (7) of the periodic alternating spin model (1). Note that the thermodynamic quantities are not sensitive to the signs of Ω_n and I_n. Therefore, one may assume $\Omega_n \geqslant 0$ and $I_n \geqslant 0$ without loss of generality.

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

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

$$\begin{aligned} \Delta_n^- = \Delta_n^+ &= \tfrac{1}{2}\left(E^2 - \Omega^2 - I^2 \pm \sqrt{(E^2 - \Omega^2 - I^2)^2 - 4\Omega^2 I^2}\right) \\ G_{nn} &= \mp\frac{1}{\sqrt{(E^2 - \Omega^2 - I^2)^2 - 4\Omega^2 I^2}} \end{aligned}$$

and therefore

$$R(E^2) = \begin{cases} \dfrac{1}{\pi}\dfrac{1}{\sqrt{-(E^2 - a_1)(E^2 - a_2)}} & \text{if} \quad a_1 < E^2 < a_2 \\ 0 & \text{otherwise} \end{cases} \tag{9}$$

with $a_1 = (\Omega - I)^2$ and $a_2 = (\Omega + I)^2$. From equation (9), the ground state energy per site, $e_0 = -\int_0^\infty \mathrm{d}E\, E^2 R(E^2)$, is

$$e_0 = -\frac{1}{\pi}\int_{\sqrt{a_1}}^{\sqrt{a_2}} \frac{\mathrm{d}E\, E^2}{\sqrt{-(E^2 - a_1)(E^2 - a_2)}}$$

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

$$\frac{e_0}{I} = -\frac{1}{\pi}\int_0^{\frac{\pi}{2}} \mathrm{d}\phi \sqrt{(1+\lambda)^2 - 4\lambda\sin^2\phi} \qquad \lambda = \frac{\Omega}{I}. \tag{10}$$

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

$$R(E^2) = \begin{cases} \dfrac{1}{2\pi}\dfrac{|2E^2 - \Omega_1^2 - \Omega_2^2 - I_1^2 - I_2^2|}{\sqrt{\mathcal{B}(E^2)}} & \text{if} \quad \mathcal{B}(E^2) > 0 \\ 0 & \text{otherwise} \end{cases}$$

$$\begin{aligned} \mathcal{B}(E^2) &= 4\Omega_1^2\Omega_2^2 I_1^2 I_2^2 - (E^4 - (\Omega_1^2 + \Omega_2^2 + I_1^2 + I_2^2)E^2 + \Omega_1^2\Omega_2^2 + I_1^2 I_2^2)^2 \\ &= -(E^2 - b_1)(E^2 - b_2)(E^2 - b_3)(E^2 - b_4) \end{aligned} \tag{11}$$

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

Obviously, (11) recovers the result for the uniform chain (9) if $\Omega_1 = \Omega_2 = \Omega$, $I_1 = I_2 = I$. The resulting density of states $R(E^2)$ (11) yields all thermodynamic quantities of the regularly alternating transverse Ising chain $\Omega_1 I_1 \Omega_2 I_2 \Omega_1 I_1 \Omega_2 I_2, \ldots$.

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

$$\begin{aligned} &\frac{e_0(\delta)}{I} = -\frac{1}{2\pi}\int_0^{\frac{\pi}{2}} \mathrm{d}\phi \left(\sqrt{1 + \lambda^2 + \delta^2 + 2\sqrt{W}} + \sqrt{1 + \lambda^2 + \delta^2 - 2\sqrt{W}} \right) \\ &W = \lambda^2 + \delta^2 - \lambda^2(1 - \delta^2)\sin^2\phi. \end{aligned} \tag{12}$$

If $\delta = 0$ (12) transforms into the ground state energy of the uniform chain (10).

Further, we calculate the zero-temperature transverse magnetization $m_z = \frac{\partial e_0}{\partial \Omega}$ by differentiating the rhs of equation (12) with respect to λ. In figure 1 the obtained dependence of the transverse magnetization on the transverse field for several values of the dimerization parameter δ is plotted. As one can see from figure 1 the transverse Ising chain with regularly alternating bonds does not exhibit a step-like dependence of magnetization on field and the magnetization profile only smoothly deforms with the increasing δ. This behaviour is in contrast to that of the transverse XY chain (for which the Hamiltonian (1) would contain $s_n^x s_{n+1}^x + s_n^y s_{n+1}^y$ instead of $s_n^x s_{n+1}^x$), since the latter model does show a step-like dependence of magnetization on field (i.e. a plateau at $m_z = 0$) for regularly alternating bonds [6] (the light curves in figure 1). The dissimilarity is conditioned by the different symmetries of these models, since $\sum_{n=1}^{N} s_n^z$ does not commute with the Hamiltonian of the transverse Ising chain but it does commute with the Hamiltonian of the transverse XY chain. In addition, it is worth considering both models in the limit $\delta = 1$ when the chain splits into noninteracting clusters consisting of two sites. The zero-temperature transverse magnetization follows from the formula $m_z = \frac{1}{2}\langle GS|s_1^z + s_2^z|GS\rangle$ where $|GS\rangle$ is the ground state eigenvector of the two-site cluster Hamiltonian. For the transverse Ising model $|GS\rangle$ smoothly varies with increasing Ω. Moreover, $\langle GS|s_1^z + s_2^z|GS\rangle = 0$ if $\Omega = 0$ and $\langle GS|s_1^z + s_2^z|GS\rangle \to -1$ if $\Omega \to \infty$. Unlike the case for the transverse XY model the ground state is a singlet (and thus $\langle GS|s_1^z + s_2^z|GS\rangle = 0$) if $0 \leqslant \Omega < 2I$. However, if Ω exceeds $2I$ the ground state becomes a triplet and $\langle GS|s_1^z + s_2^z|GS\rangle$ abruptly changes to -1.

The ground state static transverse susceptibility $\chi_{zz} = \frac{\partial m_z}{\partial \Omega} = \frac{1}{I}\frac{\partial^2}{\partial \lambda^2}\frac{e_0(\delta)}{I}$ follows straightforwardly from equation (12). In the left panel in figure 2 the obtained dependence

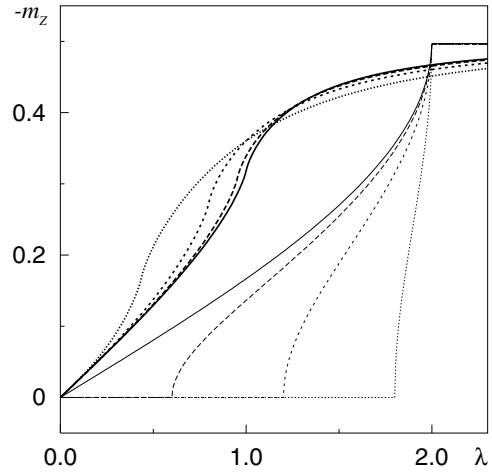

Figure 1. The ground state transverse magnetization versus transverse field for the transverse Ising chain with regularly alternating bonds with period 2. $\delta = 0$ (uniform chain), 0.3, 0.6 and 0.9 correspond to solid, long-dashed, short-dashed and dotted bold curves, respectively. For comparison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

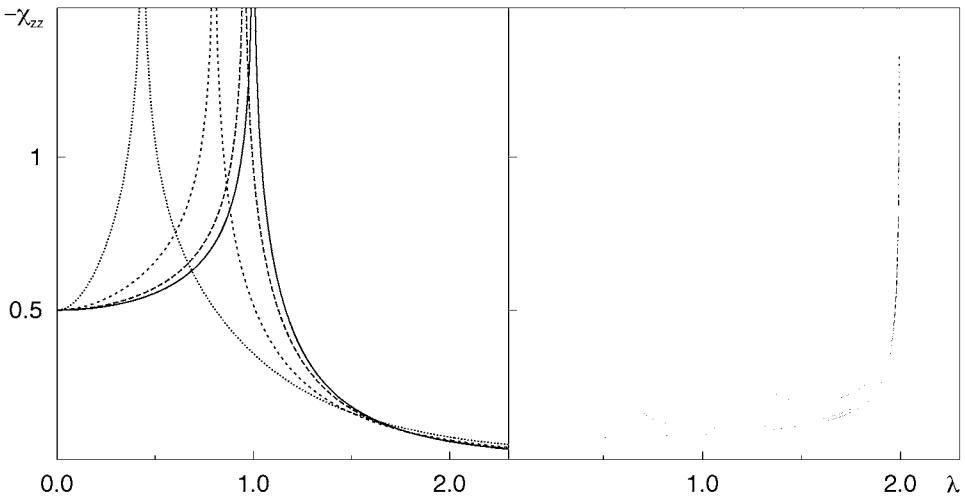

Figure 2. The ground state static transverse susceptibility versus transverse field for the transverse Ising chain (left panel) and the transverse XY chain (right panel) with regularly alternating bonds with period 2. $\delta = 0$ (uniform chain), 0.3, 0.6 and 0.9 correspond to solid, long-dashed, short-dashed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

of the static transverse susceptibility on the transverse field for several δ is plotted. Using equation (12) it is easy to show that χ_{zz} for the dimerized chain consists of a finite part and a singular part

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

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

To discuss a spin-Peierls dimerization in the adiabatic limit one must examine the dependence of the total energy $\mathcal{E}(\delta) = e_0(\delta) + \alpha\delta^2$, which consists of the magnetic part

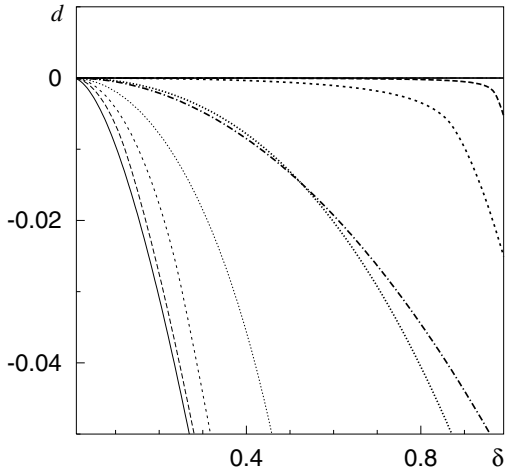

Figure 3. The change of the ground state magnetic energy $d = \frac{e_0(\delta)}{I} - \frac{e_0(0)}{I}$ versus δ for the transverse Ising chain for $\lambda = 0, 0.25, 0.5, 1$ and 2 (solid, long-dashed, short-dashed, dotted and dashed–dotted bold curves, respectively). For comparison the corresponding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

$e_0(\delta)$ (12) and an elastic part $\alpha\delta^2$, $\alpha > 0$, on the dimerization parameter δ. In figure 3 one can see the dependence of the magnetic energy (12) on δ for different values of the transverse field. From these plots one concludes that the magnetic energy as a rule decreases with the increase of δ (except for $\lambda = 0$ and $\lambda \to \infty$ when $\frac{e_0(\delta)}{I}$ (12) does not depend on δ and is equal to $-\frac{1}{2}$ and $-\frac{\lambda}{2}$, respectively) that is a necessary condition for the existence of the dimerized phase. However, the magnetic energy decreases too slowly in comparison with the increase of the elastic energy that provides stability of the chain with respect to dimerization. To demonstrate this, we calculate $a = -\frac{\partial}{\partial\delta^2}\frac{e_0(\delta)}{I}$ by differentiating the rhs of equation (12) with respect to δ^2, and display the dependence of this quantity on δ for several values of the transverse field in figure 4. These plots show that $\mathcal{E}(\delta)$ may exhibit a maximum (but not a minimum) at a nonzero value of the dimerization parameter for lattices having small $\frac{\alpha}{I}$ as the slope of the curves of $a = -\frac{\partial}{\partial\delta^2}\frac{e_0(\delta)}{I}$ against δ manifests. Hence, the uniform chain with $\delta = 0$ is favourable. In contrast, for the XY chain the ground state energy decreases sufficiently rapidly to provide stability of the dimerized phase. In figure 4 we also display the dependence of $a = -\frac{\partial}{\partial\delta^2}\frac{e_0(\delta)}{I}$ on δ for the transverse XY chain (light curves) (see also [6]) emphasizing explicitly the difference between those two spin models.

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

To conclude, we have proposed to use continued fractions for the calculation of thermodynamic quantities of regularly alternating spin-$\frac{1}{2}$ transverse Ising chains. For such a chain, in which the bonds are alternating in magnitude along the chain with period 2, we have found no plateaus in the dependence magnetization versus field. The susceptibility of the chain exhibits a logarithmic singularity at a field determined by the interaction strengths. Moreover, we have found that in the adiabatic limit the transverse Ising chain is stable with respect to a

† These arguments were suggested by an anonymous referee.

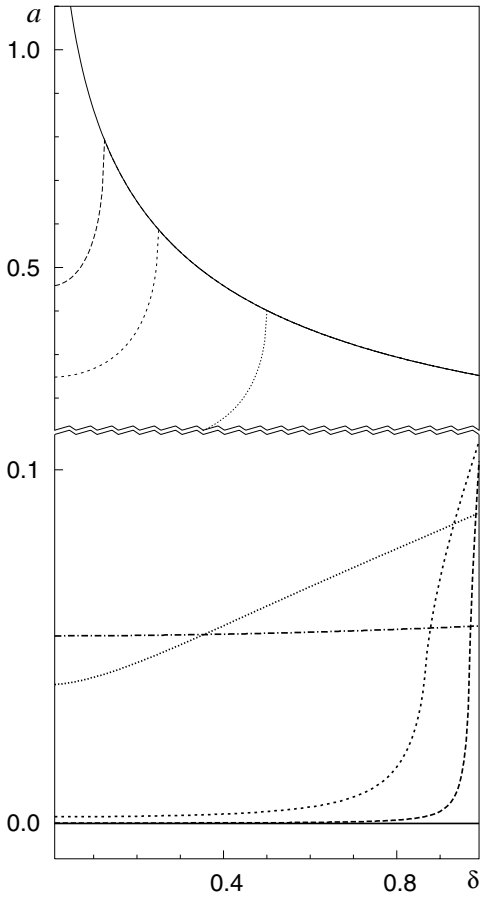

Figure 4. The dependence of $a = -\frac{\partial}{\partial\delta^2}\frac{e_0(\delta)}{J}$ on δ for the transverse Ising chain with $\lambda = 0, 0.25, 0.5, 1$ and 2 (solid, long-dashed, short-dashed, dotted and dashed–dotted bold curves, respectively). For comparison the corresponding results for the transverse XY chain are shown by light curves.

spin-Peierls dimerization. These findings differ dramatically from the corresponding results for the transverse isotropic XY chain, and therefore it would be of great interest to study the periodic alternating transverse *anisotropic* XY chain that connects both these limiting cases.

Acknowledgments

The author is grateful to the Max Planck Institute for the Physics of Complex Systems, Dresden, for hospitality at the end of 1999 when the paper was completed. The paper was presented in part at the international workshop on the theme of 'Microscopic theories of phase transitions: quantum versus thermal fluctuations' (Bad Honnef 1999). The author thanks the WE–Heraeus Foundation for hospitality and the participants for discussions and comments. He acknowledges numerous valuable discussions with J Richter, T Krokhmalskii and O Zaburannyi and expresses appreciation to J W Tucker for a critical reading of the manuscript. Finally, he thanks the referees for many useful comments and helpful suggestions.

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