Metamagnetism in the *XXZ* model with next-to-nearest-neighbor coupling

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We investigate ground-state energies and magnetization curves in the one-dimensional XXZ model with next-to-nearest neighbor coupling $\alpha>0$ and anisotropy Δ $(-1\leqslant\Delta\leqslant1)$ at $T=0$. In between the familiar ferro- and antiferromagnetic phase we find a transition region—called the metamagnetic phase—where the magnetization curve is discontinuous at a critical field $B_c(\alpha,\Delta)$. [S0163-1829(98)01718-4]

I. INTRODUCTION

Experimental results for the magnetization curves of $Fe_xMn_{1-x}TiO_3$, $GdNi_2Sb_2$, $GdCu_2Sb_2$, or $Tb_{1-x}Sc_xMn_2$ show a rapid increase (or discontinuity) if the applied B field exceeds a critical value B_c. For $B>B_c$ the substance is almost fully magnetized. This phenomenon is called ''spin-flip'' or ''metamagnetic'' transition.[1–3] There have been various attempts made to explain the ''metamagnetic'' transition in the context of Ising-like Hamiltonians. It is the purpose of this paper to show that discontinuities in the magnetization curve can be seen as well in the one-dimensional spin-$\frac{1}{2}$ XXZ model with next-to-nearest-neighbor (NNN) coupling

$$H(\alpha,\Delta,B)=J_1\sum_{i=1}^{N} S_i^xS_{i+1}^x+S_i^yS_{i+1}^y+\Delta S_i^zS_{i+1}^z +J_2(S_i^xS_{i+2}^x+S_i^yS_{i+2}^y+\Delta S_i^zS_{i+2}^z)+BS_i^z \tag{1.1}$$

in the presence of a uniform external field B. We chose the next-nearest- (NN) neighbor coupling J_1 to be antiferromagnetic ($J_1>0$) and use the notation $\alpha=J_2/J_1$. In the $\alpha-\Delta$ plane, we will primarily concentrate on the regime $\alpha\geqslant0$, $-1\leqslant\Delta\leqslant1$.

The isotropic model with $\Delta=1$ and NNN coupling α has been investigated by many authors.[4–8] Most of these investigations focused on the transition[9] from the ''spin fluid phase'' $\alpha<\alpha_c$ to the dimer phase $\alpha>\alpha_c$. The transition point $\alpha_c=0.2411\ldots$ has recently been determined with high precision[6,10] by means of conformal field theory and renormalization group techniques.

The Hamiltonian with $\alpha=1/2$, $\Delta=1$ has been studied first by Majumdar and Ghosh.[11–13] They found that the ''dimer states''

$$|\psi\rangle=\frac{1}{2^{N/4}}[1,2][3,4]\cdots[N-1,N], \tag{1.2}$$

$$|\phi\rangle=\frac{1}{2^{N/4}}[2,3][4,5]\cdots[N,1] \tag{1.3}$$

are eigenstates of $H(\alpha=1/2,\Delta=1,B=0)$. Here

$$[i,i+1]=\frac{1}{\sqrt{2}}[\chi_+(i)\chi_-(i+1)-\chi_-(i)\chi_+(i+1)] \tag{1.4}$$

are nearest-neighbor (NN) valence bond states with total spin zero, called dimers. van den Broek[14] proved that the dimer states are indeed ground states of the Hamiltonian at the ''Majumdar-Ghosh'' point $(\alpha=1/2,\Delta=1)$. Affleck, Kennedy, Lieb, and Tasaki[15,16] were able to show that the dimer states are the only ground states and that there is a finite gap to the first excited state.

Hamada, Kane, Nakagawa, and Natsume[17] discussed uniformly distributed resonating valence bonds (UDRVB) in the generalized railroad trestle model, which is equivalent to the isotropic linear Heisenberg chain with NN and NNN interactions. They found that for negative J_1 and $J_2=-1/4J_1$ the UDRVB is the ground state which is degenerate with the fully magnetized state with total spin $S=S_z=N/2$. As we will show later this phenomenon also occurs for positive values of J_1 if the parameters α and Δ are properly chosen in the Hamiltonian (1.1).

Shastry and Sutherland discussed the frustrated model with different interaction strengths in x,y, and z direction.[18] The critical properties of the anisotropic model ($\Delta\neq1$) in the absence of an external field B have been elaborated by Nomura and Okamoto.[19] They confirmed that this model and the quantum sine-Gordon model belong to the same universality class. Tonegawa and Harada[20] have studied Hamiltonian (1.1) with ferromagnetic NN and antiferromagnetic NNN interactions for positive Δ.

The dimer states (1.2), (1.3) are eigenstates of the anisotropic model along the whole line $\alpha=\frac{1}{2}$, $-\infty<\Delta<\infty$ as will be shown explicitly in Sec. II. However, the eigenvalues

$$E_D\left(\alpha=\frac{1}{2},\Delta\right)=-N\left(\frac{1}{4}+\frac{\Delta}{8}\right) \tag{1.5}$$

are ground-state energies only for $\Delta>-\frac{1}{2}$. For $\Delta<-\frac{1}{2}$ the ground state $|F\pm\rangle$ with energy

$$E_F\left(\alpha=\frac{1}{2},\Delta\right)=-\frac{3}{8}\Delta N \tag{1.6}$$

is found in the ferromagnetic sector where all spins are down or up. This is a first hint, that the model (1.1) is particularly suited to study the transition from antiferromagnetism to ferromagnetism.

The outline of the paper is as follows. In Sec. II we report on the quantum numbers and the finite size effects of the ground states as they depend on α,Δ and the magnetization $M=S_z/N$. Section III is devoted to an analysis of the magnetic properties of the model (1.1). Three phases can be found in the $\alpha-\Delta$ plane: the ferromagnetic, the antiferromagnetic, and the metamagnetic phase.

The Hamiltonians with $\alpha=0$, $\Delta=-1$ and $\alpha=0.5$, $\Delta=-0.5$ are special in the sense that the ground state is highly degenerate — namely with respect to $S_z=0,\pm1,\pm2,\ldots,\pm N/2$. This feature is discussed in Sec. IV.

II. QUANTUM NUMBERS AND FINITE SIZE EFFECTS IN THE GROUND STATE

Let us start with the ground-state properties of the Hamiltonian (1.1) in the strip

$$0\leqslant\alpha\leqslant\frac{1}{2}. \tag{2.1}$$

In the absence of a magnetic field, the ground state is found in the sector with total spin $S_z=0$ and momentum p_0 ($p_0=0, N=2n, n$ even, $p_0=\pi, N=2n, n$ odd). We obtain the ground-state energies $E(S_z,\alpha,\Delta,N)$ on finite systems up to $N=30$ through a direct Lanczos diagonalization, making use of the translational invariance of Hamiltonian (1.1). This reduces the dimension of the Hilbert space approximately by a factor of N. We choose a set of base states as proposed in Ref. 21 by Takahashi. This choice results in a real Hamiltonian matrix even for momenta $p\neq0,\pi$. Hence we obtain the proper ground state of the model even if its momentum is not $p=0$ or $p=\pi$.

Along the line $\alpha=\frac{1}{2},\Delta>-\frac{1}{2}$ the ground state is twofold degenerate; the two states are just the dimer states (1.2), (1.3). The proof of this statement follows the arguments of van den Broek.[14] The Hamiltonian

$$H\left(\alpha=\frac{1}{2},\Delta,B=0\right)=\sum_i H(i,i+1,i+2,\Delta) \tag{2.2}$$

is expressed in terms of three spin Hamiltonians:

$$\begin{aligned}H(i,i+1,i+2,\Delta)=&\frac{1}{4}(S_i^+S_{i+1}^-+S_i^-S_{i+1}^++S_{i+1}^+S_{i+2}^-\\&+S_{i+1}^-S_{i+2}^++S_i^+S_{i+2}^-+S_i^-S_{i+2}^+)\\&+\frac{\Delta}{2}(S_i^zS_{i+1}^z+S_{i+1}^zS_{i+2}^z+S_i^zS_{i+2}^z).\end{aligned} \tag{2.3}$$

The dimer states (1.2), (1.3) turn out to be eigenstates of $H(i,i+1,i+2,\Delta)$ with eigenvalue $\epsilon_0(\Delta)=-(\frac{1}{4}+\Delta/8)$. One can easily prove that this is the lowest eigenvalue of the three spin Hamiltonian for $\Delta>-\frac{1}{2}$. However, this is not the case for $\Delta<-\frac{1}{2}$, where the lowest eigenvalue of the three spin Hamiltonian is given by $\epsilon_1(\Delta)=-3\Delta/8$. The corresponding eigenstate has all three spins pointing in the same direction [cf. (1.6)].

Let us next turn to the finite size effects of the ground-state energy. Within the strip $0\leqslant\alpha\leqslant\frac{1}{2},\Delta>-\frac{1}{2}$, they turn out to be monotonically increasing with N. Finite size effects vanish on the ‘‘dimerline’’ $\alpha=\frac{1}{2},\Delta\geqslant-\frac{1}{2}$, where the ground state is completely dimerized and degenerate. Right to the dimerline, i.e., for $\alpha>\frac{1}{2},\Delta\geqslant-\frac{1}{2}$, the ground-state properties—with respect to its momentum quantum numbers—change and the monotonic behavior of the finite size effects is lost.

In the presence of a uniform magnetic field B with magnetization $M(B)=S_z/N$ the ground state of the isotropic model ($\Delta=1$) is found in the sector with total spin $S_z=S$. A rule for the momenta p_s of these states can be deduced from Marshall's sign rule:[22]

$$\begin{aligned}p_s&=0 \quad \text{for} \quad 2S+N=4n,\\ p_s&=\pi \quad \text{for} \quad 2S+N=4n+2.\end{aligned} \tag{2.4}$$

This rule has been proven[4,8] to be correct in the unfrustrated case, however it turned out to be valid in a larger M-dependent domain in the $\alpha-\Delta$ plane. For example, in the isotropic case ($\Delta=1$) we found[8] that the momentum rule (2.4) is satisfied for $\alpha<\alpha_0(M)$, i.e., below some curve $\alpha_0(M)$, which starts at the Majumdar-Ghosh point

$$\alpha_0(M=0,\Delta=1)=\frac{1}{2} \tag{2.5}$$

and ends at

$$\alpha_0\left(M=\frac{1}{2},\Delta=1\right)=\frac{1}{4}. \tag{2.6}$$

The ground state is degenerate along the curve $\alpha_0(M,\Delta)$. The two states differ in their momenta; the first one follows (2.4). A rule for the momentum of the second state has not yet been found.

In Fig. 1 we have plotted numerical results of the curves $\alpha_0(M,\Delta)$ for various values of the anisotropy parameter $\Delta=1.0,0.4,0.1,-0.2$. The data for $\alpha_0(M,\Delta)$ mark those points in the $\alpha-M$ plane, where the ground states with energy $\epsilon(M,\alpha_0(M,\Delta),\Delta,N)$, $N=12,\ldots,18$ are twofold degenerate. Finite size effects of $\alpha_0(M,\Delta)$ are visible at $M=1/4$ and $M=1/6,1/3$ where systems of size $N=12,16$ and $N=12,18$, respectively, are realized. In spite of the finite size effects we think that the finite system results shown in Fig. 1 reproduce the qualitative features of the curves $\alpha_0(M,\Delta)$ in the thermodynamical limit: 1. All curves start and end at the points (2.5) and (2.6). 2. $\alpha_0(M,\Delta=1)$ has a pronounced maximum around $M=0.2$ with rather large finite size effects. For decreasing values of Δ the height of the maximum is reduced and its position is shifted to smaller values of M.

Beyond the curve $\alpha_0(M,\Delta)$ — i.e., for $\alpha>\alpha_0(M,\Delta)$ — the ground-state momenta deviate from the rule (2.4) and we therefore expect a change in the ground-state properties.

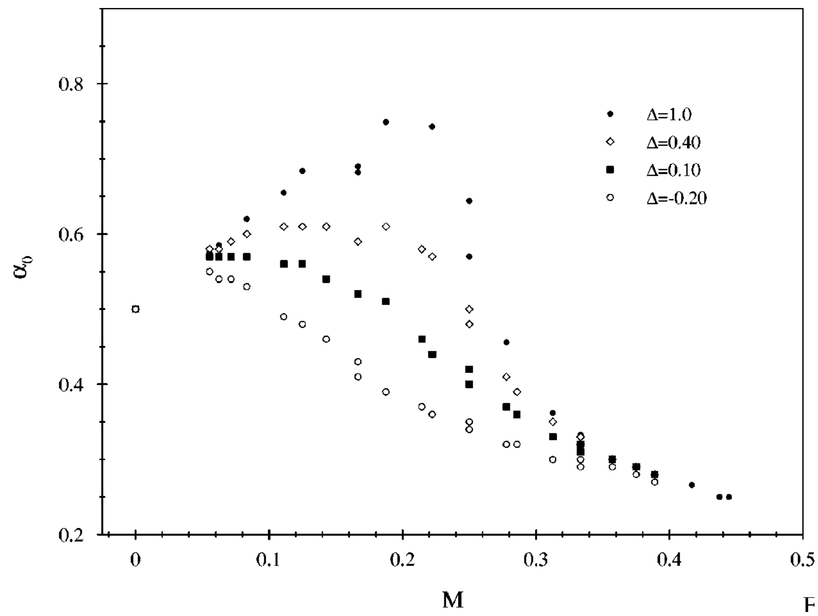

FIG. 1. The ground states of the Hamiltonian (1.1) are degenerate along the curves $\alpha_0(M,\Delta)$. The numerical data points were obtained on finite system calculations with $N=12,14,16$, and 18 and are shown for $\Delta=1.0,0.4,0.1$, and -0.2.

III. THE PHASE DIAGRAM IN THE PRESENCE OF A MAGNETIC FIELD

In this section we will present numerical results for the ground-state energy per site $\epsilon(M,\alpha,\Delta,N)=(1/N)E(S_z,\alpha,\Delta,N)$. We are in particular interested in the changes of the M dependence of these energies with α and Δ since they indicate a change in the ground-state ordering. The following situations have been found.

Ferromagnetic phase. Here the free energy

$$f(M,\alpha,\Delta)=\epsilon(M,\alpha,\Delta)-BM \tag{3.1}$$

is minimized by the states $|F\pm\rangle$, where all spins are up $(+)$ or down $(-)$, respectively. It turns out that the boundary of the ferromagnetic phase $\Delta<\Delta_f(\alpha)$ is characterized by the degeneracy

$$\epsilon(M=0,\alpha,\Delta_f(\alpha),N)=\epsilon\left(M=\frac{1}{2},\alpha,\Delta_f(\alpha),N\right) \tag{3.2}$$

of the lowest energy eigenvalues in the sectors with $S_z=0$ and $S_z=N/2$.

Antiferromagnetic phase. The minimum of the free energy is found for $0\leqslant M\leqslant\frac{1}{2}$ at

$$\frac{d\epsilon}{dM}-B=0, \tag{3.3}$$

$$\frac{d^2\epsilon}{dM^2}>0. \tag{3.4}$$

This means that $\epsilon(M,\alpha,\Delta,N)$ is monotonically increasing and convex for $0\leqslant M\leqslant\frac{1}{2}$. The saturating field

$$\frac{d\epsilon}{dM}\Big|_{M=1/2}=B\left(M=\frac{1}{2},\alpha,\Delta\right), \tag{3.5}$$

which is needed to align all spins in the system, can be computed from the one magnon states:

$$\left|p,S_z=\frac{N}{2}-1\right\rangle=\frac{1}{\sqrt{N}}\sum_x e^{ipx}|x\rangle, \tag{3.6}$$

where $|x\rangle$ denotes the state with one spin down at site x and all other spins up. The energy of this state is

$$E\left(S_z=\frac{N}{2}-1,\alpha,\Delta,N\right)=\cos p+\alpha\cos 2p+\Delta(1-\alpha)\left(\frac{N}{4}-1\right) \tag{3.7}$$

and the ground-state energy is found by minimization with respect to p. For $0\leqslant\alpha\leqslant 1/4$ the minimum is found at $p=\pi$ and the saturating field is

$$B\left(M=\frac{1}{2},\alpha,\Delta\right)=\Delta(1+\alpha)+(1-\alpha). \tag{3.8}$$

For $\frac{1}{4}<\alpha\leqslant\frac{1}{2}$, the minimum energy (3.7) is found for

$$\cos p=-\frac{1}{4\alpha}, \tag{3.9}$$

which yields for the saturating field

$$B\left(M=\frac{1}{2},\alpha,\Delta\right)=\Delta(1+\alpha)+\alpha+\frac{1}{8\alpha}. \tag{3.10}$$

The boundary $\Delta_a(\alpha)$ of the antiferromagnetic phase $\Delta>\Delta_a(\alpha)$ is characterized by the condition

$$\frac{d^2\epsilon}{dM^2}(M,\alpha,\Delta_a(\alpha),N)|_{M=1/2}=0, \tag{3.11}$$

i.e., the convexity condition is lost for $\Delta<\Delta_a(\alpha)$.

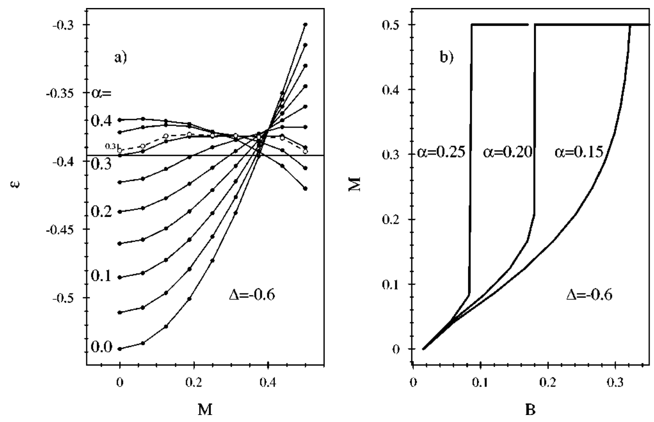

FIG. 2. (a) M dependence of the ground-state energy per site $\epsilon(M,\alpha,\Delta,N)$ with $N=16$, $\Delta=-0.6$, and $\alpha=0.0,0.1,\ldots,0.4$. (b) Magnetization curves $M(B,\alpha,\Delta)$ for $\Delta=-0.6$ as they follow from the ground-state energy per site $\epsilon(M,\alpha,\Delta,N)$ shown in (a). In the metamagnetic phase (e.g., at $\alpha=0.2,0.25$, and $\Delta=-0.6$) there is a critical field $B_c(\alpha,\Delta)$, where the system jumps into the fully magnetic state with $M=1/2$.

Metamagnetic phase. Between the ferromagnetic and the antiferromagnetic phase

$$\Delta_f(\alpha)<\Delta<\Delta_a(\alpha), \tag{3.12}$$

we find a metamagnetic phase, which is characterized by a zero in the second derivative:

$$\frac{d^2\epsilon}{dM^2}>0, \quad 0<M<M_c(\alpha,\Delta), \tag{3.13}$$

$$\frac{d^2\epsilon}{dM^2}(M,\alpha,\Delta,N)\big|_{M=M_c}=0. \tag{3.14}$$

The minimum of the free energy is found for

$$\frac{d\epsilon}{dM}=B \quad \text{for} \quad 0<M<M_c(\alpha,\Delta) \tag{3.15}$$

and at

$$M=\frac{1}{2} \quad \text{for} \quad B>B_c=\frac{d\epsilon}{dM}\bigg|_{M=M_c}. \tag{3.16}$$

Therefore, in this metamagnetic phase we have a discontinuity at $B_c(\alpha,\Delta)$ where the magnetization curve jumps from $M=M_c(\alpha,\Delta)$ to $M=\frac{1}{2}$. $B_c(\alpha,\Delta)$ decreases, if one crosses the metamagnetic phase coming from the antiferromagnetic phase and moving towards the ferromagnetic phase. An example will be given below.

For small magnetic fields $0<B<B_c$ the system looks antiferromagnetic, for $B>B_c$ ferromagnetic.

For the determination of the phase boundaries $\Delta_f(\alpha)$ and $\Delta_a(\alpha)$ of the ferromagnetic and antiferromagnetic phase, we have first computed the lowest energy densities $\epsilon(M,\alpha,\Delta,N)$ as they depend on the magnetization M and the parameters α and Δ. As an example we show in Fig. 2(a) the evolution of the M dependence for $\Delta=-0.6,\alpha=0.0,\ldots,0.40$ on a system with $N=16$ sites. One clearly observes the three phases discussed above. For small values

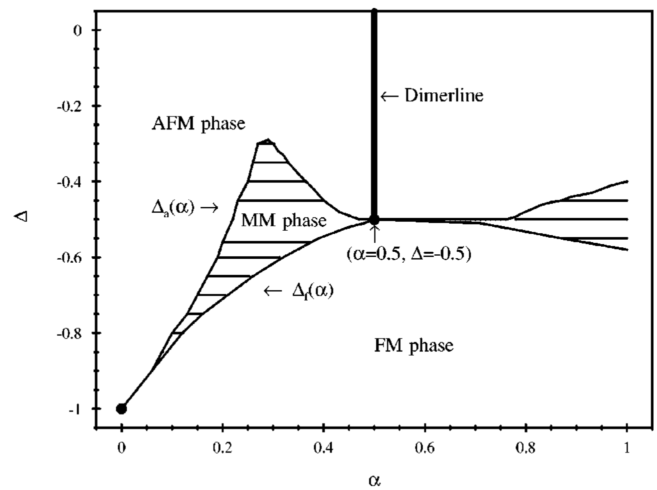

FIG. 3. The phase diagram in the $\alpha-\Delta$ plane, as it follows from the numerical evaluation of (3.2) ($N=18$) and (3.10) ($N=50$). The metamagnetic domain $\Delta_f(\alpha)<\Delta<\Delta_a(\alpha)$ is hatched.

of α, $\epsilon(M,\alpha,\Delta)$ is monotonically increasing and convex. Here, we are in the antiferromagnetic phase. At $\alpha=0.15$ the second derivative (3.14) vanishes first at $M_c=\frac{1}{2}$. The metamagnetic phase extends from $\alpha=0.15$ to $\alpha=0.305$, where the degeneracy (3.2) shows up. The behavior of the corresponding magnetization curves can be seen in Fig. 2(b). We obtain these magnetization curves by applying the method of Bonner and Fisher[23] to our finite system results. For $\alpha>0.305$ we then enter the ferromagnetic phase. The resulting phase diagram in the $\alpha-\Delta$ plane is shown in Fig. 3 . The numerical evaluation of (3.2) on finite systems does not show a significant finite size dependence. In other words, the determination of the phase boundary $\Delta_f(\alpha)$ is well under control.

The determination of the second phase boundary $\Delta_a(\alpha)$ from (3.11) turned out to be much more difficult. We numerically calculated $\epsilon(M=1/2-2/N,\alpha,\Delta,N)$—i.e., the lowest eigenvalue in the sector with two spins flipped—on rather large systems with $N=20,30,40,50$ and looked for a zero in the second derivative:

$$\epsilon\left(M=\frac{1}{2}-\frac{2}{N},\alpha,\Delta,N\right)+\epsilon\left(M=\frac{1}{2},\alpha,\Delta,N\right) -2\epsilon\left(M=\frac{1}{2}-\frac{1}{N},\alpha,\Delta,N\right)=0. \tag{3.17}$$

The resulting $\Delta_a(\alpha)$ suffers under finite size effects particularly in the vicinity of the point $\alpha=0.5$, $\Delta=-0.5$. The curve $\Delta_a(\alpha)$ plotted in the phase diagram (Fig. 3) represents the result of (3.17) for the largest system size $N=50$.

The points $\alpha=0,\Delta=-1$ and $\alpha=\frac{1}{2},\Delta=-\frac{1}{2}$ are special in the sense that the boundaries $\Delta_a(\alpha),\Delta_f(\alpha)$ for the antiferromagnetic and ferromagnetic phase meet. Therefore, we have no metamagnetic phase between the ferro- and antiferromagnetic phase at these points. This can also be clearly seen in Figs. 4(a) and 4(b), where we have plotted the M and Δ dependence of $\epsilon(M,\alpha=0,\Delta)$ and $\epsilon(M,\alpha=1/2,\Delta)$, respectively. These energies turn out to be convex for $\Delta>-1$, ($\alpha=0$) and $\Delta>-\frac{1}{2}$, ($\alpha=0.5$) and concave for $\Delta<-1$, ($\alpha=0$), $\Delta<-\frac{1}{2}$, ($\alpha=0.5$), respectively. At $\Delta=-1,\alpha=0$ and

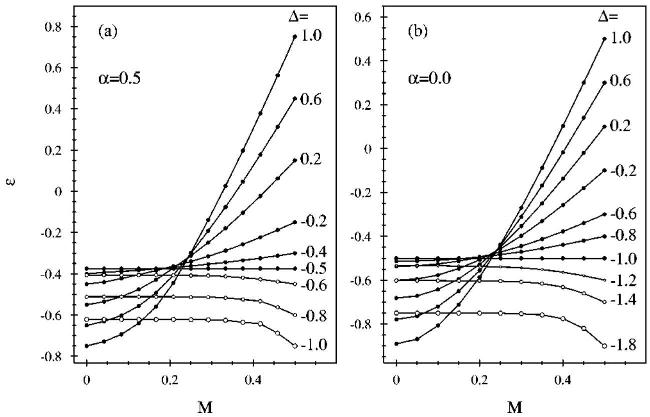

FIG. 4. Ground-state energies $\epsilon(M,\alpha,\Delta,N=20,24)$ along the lines (a) $\alpha=0.5$, $\Delta=1.0,0.6,\ldots,-1.0$, and (b) $\alpha=0.0$, $\Delta=1.0,\ldots,-1.8$. The ground-state degeneracy is clearly visible for $\alpha=0.5$, $\Delta=-0.5$ and $\alpha=0$, $\Delta=-1$, where the direct transition from antiferromagnetism to ferromagnetism occurs.

$\Delta=-\frac{1}{2},\alpha=\frac{1}{2}$, the ground-state energies $\epsilon(M,\alpha,\Delta,N)$ are all degenerate with respect to M. This feature will be investigated in the next section.

IV. GROUND-STATE DEGENERACY AT THE POINTS WHERE THE PHASE BOUNDARIES MEET

According to (3.2) the phase boundary $\Delta_f(\alpha)$ of the ferromagnetic phase is defined by the degeneracy of two eigenstates with total spin $S_z=0$ and $S_z=N/2$, respectively. At the points $\Delta=-1,\alpha=0$ and $\Delta=-\frac{1}{2},\alpha=\frac{1}{2}$ where $\Delta_f(\alpha)=\Delta_a(\alpha)$, a much larger degeneracy of the ground state with respect to all values of $S_z=0,\ldots,N/2$ occurs. We are going to show now that the n-magnon states $S_+(p)^n|F-\rangle$—obtained by n-fold application of the rising operator

$$S_+(p)=\sum_l e^{ipl}S_l^+ \tag{4.1}$$

on the ferromagnetic state $|F-\rangle$—are eigenstates of the Hamiltonian

$$H(\alpha,\Delta,B)S_+(p)^n|F-\rangle=E_F S_+(p)^n|F-\rangle \tag{4.2}$$

for

$$\text{(a)}\quad \alpha=0,\quad \Delta=-1,\quad p=\pi, \tag{4.3}$$

$$\text{(b)}\quad -\infty<\alpha<\infty,\quad \Delta=-\frac{1}{2},\quad p=\frac{2\pi}{3},\quad p=\frac{4\pi}{3}. \tag{4.4}$$

Here

$$E_F=\frac{N}{4}(\Delta+\Delta\cdot\alpha) \tag{4.5}$$

is the energy of the ferromagnetic state. For the proof of (4.2) we start from the commutation relations:

$$[H(\alpha,\Delta,B),S_+(p)]=\sum_{j=1}^{2}\left(a_j\sum_l S_l^+S_{l+j}^z e^{ipl}+b_j\sum_l S_l^zS_{l+j}^+e^{ipl}\right), \tag{4.6}$$

where

$$a_1=-e^{ip}+\Delta,\quad b_1=-1+\Delta e^{ip},$$
$$a_2=\alpha(-e^{2ip}+\Delta),\quad b_2=\alpha(-1+\Delta e^{2ip}) \tag{4.7}$$

and

$$[[H(\alpha,\Delta),S_+(p)],S_+(p)]=\sum_{j=1}^{2}c_j\sum_l S_l^+S_{l+j}^+e^{2ipl}, \tag{4.8}$$

where

$$c_1=2e^{ip}(\Delta-\cos p),$$
$$c_2=2\alpha e^{2ip}(\Delta-\cos 2p). \tag{4.9}$$

All further commutators with $S_+(p)$ vanish identically. Application of (4.6) and (4.8) onto the ferromagnetic state $|F-\rangle$ yields

$$[H(\alpha,\Delta),S_+(p)]|F-\rangle=-2(\Delta-\cos p+\alpha(\Delta-\cos 2p))|p\rangle, \tag{4.10}$$

where $|p\rangle$ is the one-magnon state (3.6). Similarly one finds

$$[[H(\alpha,\Delta),S_+(p)],S_+(p)]|F-\rangle=2e^{ip}(\Delta-\cos p)|2p,1\rangle+2e^{2ip}\alpha(\Delta-\cos 2p)|2p,2\rangle, \tag{4.11}$$

where

$$|2p,j\rangle=\sum_l e^{2ipl}|l,l+j\rangle \tag{4.12}$$

are two magnon states with two spins up at sites l and $l+j$. Note that the right hand sides of (4.10) and (4.11) vanish for the two cases listed in (4.3) and (4.4), respectively. The first point (4.3) marks the transition from antiferromagnetism to ferromagnetism in the nearest neighbor XXZ model. Indeed, the rising operator $S_+(\pi)$ commutes with the Hamiltonian $H(\alpha=0,\Delta=-1)$.

Along the line (4.4), the endpoint of the dimerline ($\alpha=0.5,\Delta=-0.5$) is of special interest. Here the eigenvalues (1.5) of the dimer states (1.2), (1.3) are degenerate with the energy (4.5) of the ferromagnetic states. This also implies that the n-magnon states (4.2) are ground states for $\alpha=\frac{1}{2}$, which explains the degeneracy found in Fig. 4(a) for $\alpha=-0.5$.

In Fig. 5 we have plotted the ground-state energies $\epsilon(M,\alpha,\Delta=-0.5)$ on a ring with 18 sites along the line (4.4), where the degeneracy of the n-magnon states (4.2) has been proven. For $\alpha<0.5$ the ground-state energies $\epsilon(M,\alpha,\Delta=-0.5)$ are monotonically increasing with M; i.e., the corresponding ground states cannot be identified with the degenerate n-magnon states (4.2). The ground-state energies $\epsilon(M,\alpha,\Delta=-0.5)$ meet each other for all M at $\alpha=0.5$ and stay very close together in the interval $0.5<\alpha<0.6$. This leads to the narrow width of the metamagnetic phase in Fig. 3 for $0.5<\alpha<0.6$. For $\alpha>0.6$ the quasidegeneracy with respect to M is lifted again.

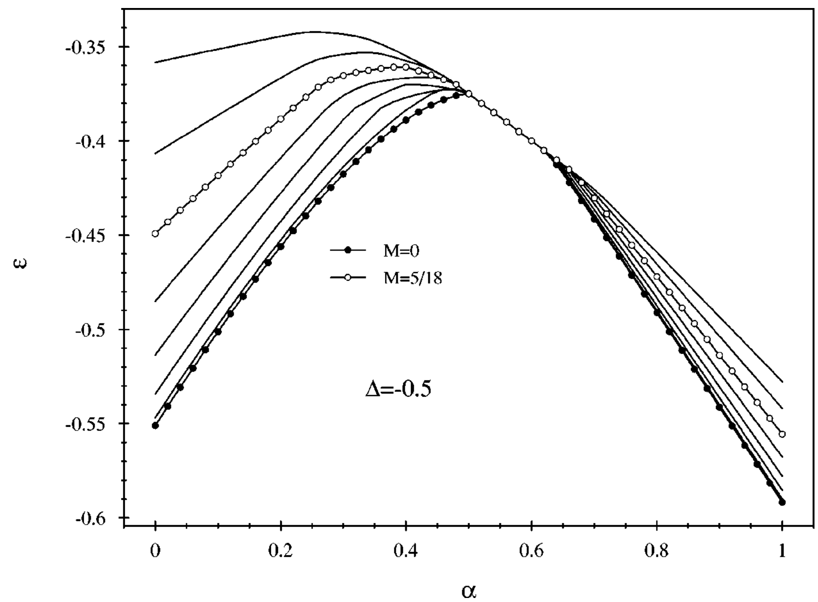

FIG. 5. α and M dependence of the ground-state energies $\epsilon(M,\Delta,N=18)$ along the line $\Delta=-0.5$.

V. DISCUSSION AND CONCLUSION

Metamagnetism denotes a mixed phase between ferromagnetism and antiferromagnetism, which has been observed in various substances such as, e.g., $Fe_xMn_{1-x}TiO_3$. The characteristic signal is a rapid increase (or discontinuity) in the magnetization curve, if the external field exceeds a critical value B_c. For $B>B_c$ the substance is almost fully magnetized. In this paper we have shown that the phenomenon of metamagnetism can be observed in the one dimensional spin-1/2 *XXZ* model with next-to-nearest-neighbor coupling α and anisotropy Δ. The phase diagram in the $\alpha-\Delta$ plane (Fig. 3) contains three regimes: the antiferromagnetic one with $\Delta>\Delta_a(\alpha)$, the ferromagnetic one with $\Delta<\Delta_f(\alpha)$ and the metamagnetic one in between $\Delta_a(\alpha)\geqslant\Delta\geqslant\Delta_f(\alpha)$. The metamagnetic phase shrinks to zero at $\alpha=0$ and $\alpha=0.5$, where $\Delta_a(\alpha)=\Delta_f(\alpha)$. At these points there is a direct transition from antiferromagnetism to ferromagnetism and the ground state turns out to be highly degenerate — namely with respect to $S_z=0,1,2,\ldots,N/2$. These states can be identified with n-magnon states.

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