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Scaling behavior of the energy gap of the XXZ model in a transverse magnetic field

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Abstract

The energy gap of the one-dimensional (1D) spin- $\frac{1}{2}$ AF (antiferromagnetic) XXZ model in a transverse magnetic field (h) is studied by using the exact diagonalization technique. We have computed the energy gap in the region of anisotropy parameter $-1 < \Delta < 1$ and in the vicinity of the critical line $\Delta = -1$. By introducing a practical finite-size scaling approach, we have computed the correct critical exponent of the energy gap in good agreement with the field theoretical and spin-wave approaches. To check this approach, we have also studied the critical exponent of the energy gap of the 1D AF-Heisenberg chain in a staggered magnetic field (h_s).

1. Introduction

The effect induced by external magnetic fields in low-dimensional magnets has attracted much interest recently from the experimental and theoretical points of view. One of the most interesting examples is the effect of a transverse magnetic field on low-dimensional spin systems. The experimental observations [1, 2] on quasi-one-dimensional spin- $\frac{1}{2}$ antiferromagnetic Cs_2CoCl_4 are a realization of the effect of a noncommuting field on the low-energy behavior of a quantum model. A good candidate for explaining the low-temperature behavior of Cs_2CoCl_4 is the spin- $\frac{1}{2}$ XXZ model. The Hamiltonian of the XXZ model in a transverse field on a periodic chain of N sites is

$$H = J \sum_{i=1}^N (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z - h S_i^x), \quad (1)$$

where $J > 0$ is the exchange coupling in the xy easy plane, Δ is the anisotropy in the z direction, and h is proportional to the transverse field. However, since the integrability of the XXZ model will be lost in the presence of a transverse magnetic field, more intensive studies from the theoretical point of view are needed.

In the absence of a transverse magnetic field ($h = 0$), the exact solution is given by the Bethe ansatz [3]. The Ising regime is governed by $\Delta > 1$ and there is a gap in the excitation spectrum, while for $\Delta \leq -1$ the ground state is in the ferromagnetic phase and there is a gap

over the ferromagnetic state. In the region $-1 < \Delta \leq 1$, the ground state of the system is in the gapless spin-fluid phase with a power-low decay of correlations. The application of a transverse magnetic field breaks the rotational symmetry and destroys the integrability of the XXZ model except at special points $\Delta \rightarrow \pm\infty$ and $\Delta = 1$. In both limits, the system has the phase transition point $h_c = \frac{|\Delta|}{2}$, where the gap is closed and the long-range order in the z direction vanishes. Similar to these limiting cases, for any $|\Delta| > 1$ and $h < h_c(\Delta)$, the system has long-range order in the z direction.

In the isotropic antiferromagnetic case $\Delta = 1$, the model remains integrable. In this case, the direction of the magnetic field is not important and the ground state of the system remains a gapless spin-fluid state, up to the point $h = 2J$, where a Pokrovsky–Talapov-type phase transition occurs and the ground state becomes a completely ordered ferromagnetic state.

Adding a transverse field to the XXZ model in the region $-1 < \Delta < 1$ develops a gap. The ground state then has the long-range Néel order in the y direction (spin-flop phase). In fact, at a special field value $h_{cl} = \sqrt{2J(1+\Delta)}$, the ground state is known exactly to be of the classical Néel type [4–6]. The gap vanishes at the critical field h_c , where the transition to the paramagnetic phase occurs.

The implementation of the quantum renormalization group [7] shows that the transition at h_c is in the universality class of the Ising model in a transverse field (ITF). The scaling of the gap, the phase diagram, and some of the low excited states at h_{cl} of the XXZ model in the transverse field have been studied in [8]. In this approach, the scaling of the gap is given by the scaling of the operators S^x (in the region $-1 < \Delta < 1$) and S^z (on the line $\Delta = 1$). It is shown that the critical exponent of the energy gap in the region $-1 < \Delta < 1$ at the phase transition between spin-fluid phase and spin-flop phase is a function of the anisotropy parameter Δ as

$$G(h) \sim \begin{cases} h^{\frac{1}{1-\theta/2}}, & -1 < \Delta < 0 \\ h^{\frac{2}{4-\theta-1/\theta}}, & 0 < \Delta < 1, \end{cases} \quad (2)$$

where θ is defined as

$$\theta = 1 - \frac{\arccos(\Delta)}{\pi}, \quad (3)$$

which shows theoretically that the critical exponent of the energy gap in the region $-1 < \Delta < 1$ is a function of the anisotropy parameter Δ . Also, the critical exponent of the energy gap in the phase transition between the spin-fluid phase (on the line $\Delta = 1$) and the Néel phase is a function of the transverse field. A very recent exact diagonalization approach [9] has given very good agreement on the critical exponent of the energy gap in the region $-1 < \Delta < 1$. In this numerical work, the Δ -dependence of the gap is computed with the relation between the divergence of the leading term in the perturbation expansion and the scaling behavior of the energy gap. Also, exact diagonalization [10] and density matrix renormalization group (DMRG) [11] results give us some knowledge on this model but not on the scaling of the gap. A bosonization approach to this model in certain limits leads to a nontrivial fixed point and a gapless line which separates two gapped phases [12]. Moreover, the connection to the axial next-nearest-neighbor Ising model has been addressed. The applicability of the mean-field approximation has been studied by comparing the DMRG results of magnetization and the structure factor [13]. Recently, the effect of a longitudinal magnetic field on both the Ising model in a transverse field [14] and the XXZ model in a transverse field has been discussed [15].

In this paper, we present our numerical results on the energy gap of the XXZ model in a transverse magnetic field. Our results are obtained using the exact diagonalization technique. In section 2, we discuss our practical finite-size scaling approach, and find the Δ -dependence of the correct critical exponent of the energy gap in the region $-1 < \Delta < 1$. In section 3, we calculate the critical exponent of the energy gap of the XXZ model close to the critical line

$\Delta = -1$. In section 4, we analyze the 1D AF-Heisenberg spin- $\frac{1}{2}$ model in a staggered magnetic field, using the method introduced in section 2. Finally, we conclude and summarize our results in section 5.

2. The finite-size scaling analysis

The finite-size scaling method is a way of extracting values for critical exponents by observing how measured quantities vary as the size $L = Na$ of the system being studied changes (where a is the lattice spacing and which we will consider to be 1). In fact, this method consists of comparing a sequence of finite lattices. The finite lattice systems are solved exactly, and various quantities can be calculated as a function of the lattice size L , for small L . Finally, these quantities are scaled up to $L \rightarrow \infty$ [16]. Two steps are needed before these ideas can be realized. First, one needs a procedure for solving the finite lattice system exactly. Second, one needs a procedure for extrapolating from finite to infinite L . In step one, we have used the modified Lanczos method [17] to obtain the excited-state energies at the same accuracy as the ground-state energy. The Lanczos method and the related recursion methods [18–21], possibly with appropriate implementations, have emerged as one of the most important computational procedures, mainly when a few extreme eigenvalues are desired. In the following, we present our practical finite-size scaling approach for the energy gap.

The energy gap as a function of the chain length (N) and the transverse field (h) is defined as

$$G(N, h) = E_m(N, h) - E_0(N, h), \quad (4)$$

where E_0 is the ground-state energy and E_m , in general, is the first or second excited-state energy. If the first excited state and ground state form a two-fold-degenerate ground state in the thermodynamic limit, then $E_1 - E_0$ vanishes [8] and the gap will be equal to $E_2 - E_0$.

In general, the critical point of an infinite system is defined, in the Hamiltonian formulation, as the value of the magnetic field h , at which the gap $G(h)$ vanishes as

$$G(h) \sim h^\varepsilon, \quad h \rightarrow h_c = 0, \quad (5)$$

where ε is the critical exponent of the energy gap. With our Lanczos scheme we can compute $G(N, h)$, which approaches $G(h)$ when N is large. We consider this, as a first condition. On the other hand, in the case of h equal to zero, the spectrum of the XXZ model is gapless. The gap vanishes in the thermodynamic limit proportional to the inverse of the chain length [22],

$$\lim_{N \rightarrow \infty} G(N, h = 0) \rightarrow \frac{A}{N}. \quad (6)$$

We consider this equation as the second condition for our procedure. The presence of the gap can be characterized by the following expression,

$$\frac{G(N, h)}{G(N, 0)} = 1 + f(x), \quad (7)$$

where $x = Nh^\varepsilon$ is a scaling parameter and $f(x)$ is the scaling function. If we consider the asymptotic behavior of $f(x)$ as

$$f(x) \sim x^\phi, \quad (8)$$

since we expect that equation (7) behaves in the combined limit

$$N \rightarrow \infty, \quad h \rightarrow 0 \quad (x \gg 1) \quad (9)$$

as equation (5), thus the ϕ -exponent in the large- x ($x \gg 1$) regime must be equal to one ($\phi = 1$). Then we get, in the large- x regime,

$$\lim_{N \rightarrow \infty (x \gg 1)} NG(N, h) \sim x. \quad (10)$$

This equation shows that the large- x behavior of $NG(N, h)$ is linear in x where the scaling exponent of the energy gap is ε .

We should note that, in using the Lanczos method, we are limited to considering the maximum value of $N = 24$. Moreover, to avoid the effect of level crossing, we should consider very small values of $h < 0.01$. Therefore, the value of x cannot be increased in this method. The same problem appears if the calculation is performed by DMRG. However, we are not allowed to read the scaling exponent of the gap which exists in the thermodynamic limit ($N \rightarrow \infty$ or $x \gg 1$). Thus, we have to find the scaling behavior from the small- x regime. In [9], we have introduced a perturbative approach to obtain the real critical exponent of the energy gap in the small- x regime. In this approach, we have shown that the coefficient of the leading term in the perturbation expansion diverges in the thermodynamic limit ($N \rightarrow \infty$). Then, using the relation between this divergence and the scaling behavior of the energy gap, we have calculated the Δ -dependence of the critical exponent of the energy gap. However, there is a restriction in this approach. When the first-order perturbation correction is not zero, the leading nonzero term in the perturbative approach is h , and therefore the coefficient of the first nonzero correction for the energy gap is not a well-defined function of N . Thus, the leading term in the perturbative expansion, of necessity, is not the size dependence. To avoid this restriction, we introduce a practical, more accurate procedure. We start from equation (7), since our numerical results are restricted to the small- x regime, the ϕ -exponent of the scaling function $f(x)$ is not exactly equal to one ($\phi \neq 1$). Now, let us consider the ratio of the gap in equation (7) as

$$K(N, h) = \frac{G(N, h)}{G(N, 0)} = 1 + N^\phi h^\alpha, \quad (11)$$

where the α -exponent is equal to $\varepsilon\phi$. If we can compute the exponents ϕ and α from the small- x regime, then the real critical exponent of the energy gap will be obtained as

$$\varepsilon = \frac{\alpha}{\phi}. \quad (12)$$

For this purpose, in the first step we have plotted, in figure 1(a), the ratio of the gap, $K(N, h)$ versus N for a fixed value of the transverse field $h = 0.002$ ($0.001 \leq h \leq 0.01$) which is very close to $h_c = 0$. The results have been plotted for different sizes, $N = 12, 14, \dots, 24$, to derive the ϕ -exponent at the small- x regime. In figure 1(a), we have considered the anisotropy parameter $\Delta = 0.5$ and found the best fit to our data for $\phi = 1.94 \pm 0.01$. In the second step, we have plotted, in the inset of figure 1(a), the scaling function $K(N, h)$ versus h for a fixed size N ($N = 24$) and anisotropy parameter $\Delta = 0.5$. The best fit to our data is obtained with $\alpha = 2.0005 \pm 0.0001$, which shows that the first nonzero correction in the perturbation expansion is second order [9]. In figure 1(b) we have shown the scaling function $K(N, h)$ versus $N^\phi h^\alpha$ for different chain sizes $N = 18, 20, 22, 24$ and different transverse fields $0.001 \leq h \leq 0.01$. It can be seen clearly that all the data with various N and h are on the universal scaling curve. This shows that the function $K(N, h)$ is universal for a wide range of $N^\phi h^\alpha$. If we choose the wrong values for the exponents ϕ and α , the universal curve splits into different curves for various N .

Finally, using equation (12), we obtained the critical exponent of the energy gap $\varepsilon = 1.03 \pm 0.01$, which shows very good agreement with the field theoretical results (equation (2)). We have also implemented our procedure for different values of the transverse magnetic field h

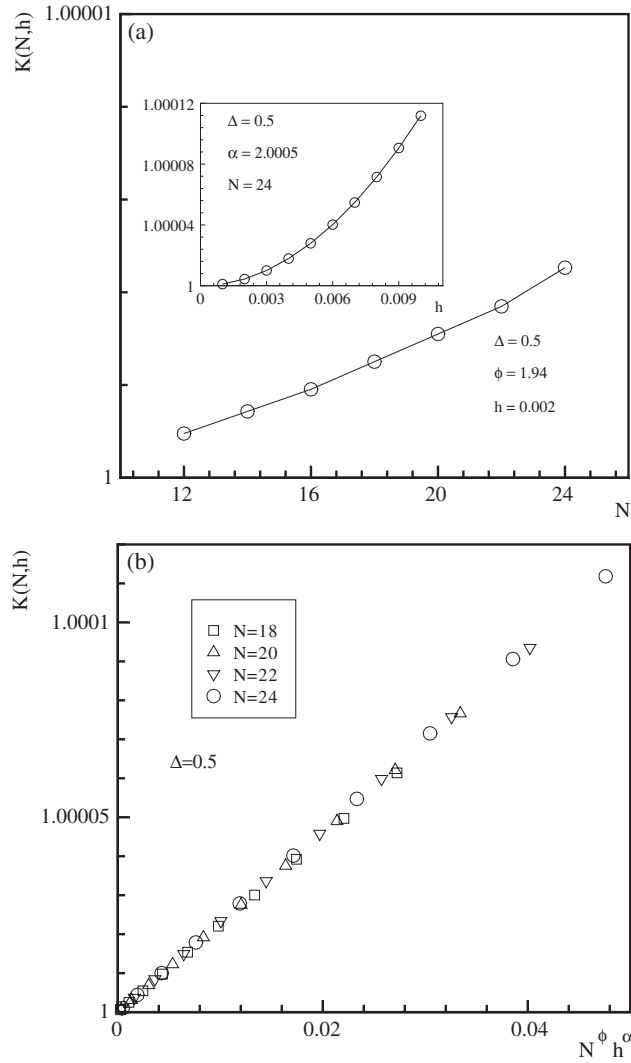


Figure 1. (a) The scaling function $K(N, h)$ versus N ($N = 12, 14, \dots, 24$) for the anisotropy parameter $\Delta = 0.5$ and transverse field $h = 0.002$. The best fit is obtained by $\phi = 1.94 \pm 0.01$. The inset shows the function $K(N, h)$ versus h for a fixed size $N = 24$. The best fit is obtained by using $\alpha = 2.0005 \pm 0.0001$. (b) The scaling function $K(N, h)$ versus $N^\phi h^\alpha$ for different chain sizes $N = 18, 20, 22, 24$ and different fields $0.001 \leq h \leq 0.01$.

($0.001 \leq h \leq 0.005$) very close to $h_c = 0$, and found the same results for the critical exponent of the energy gap, as we have expected.

We extended our numerical computations to consider other values of the anisotropy parameter Δ . The results have been presented in table 1. In this table, we have listed the ϕ -exponent of the scaling function $f(x)$ in the small- x regime, the α -exponent, the resulting critical exponent of the energy gap ε which is obtained from equation (12), and the corresponding value obtained by the theoretical approach ε_T for different values of the anisotropy parameter Δ . Our numerical results are in good agreement with the results of the field theoretical approach [8].

Table 1. The ϕ -exponent of the scaling function $f(x)$ in the small- x regime, the α -exponent, the resulting critical exponent of the energy gap ε which is obtained from equation (12), and the corresponding value obtained by the theoretical approach ε_T (equation (2)) for different values of anisotropy parameter $-1 < \Delta < 1$.

Δ	ϕ	α	ε	ε_T
0.70	2.07	2.00	0.96	1.04
0.50	1.94	2.00	1.03	1.09
0.25	1.85	2.00	1.08	1.18
0.0	1.67	2.00	1.19	1.33
-0.25	1.56	2.00	1.28	1.26
-0.50	1.47	2.00	1.36	1.20
-0.70	1.50	2.00	1.33	1.14

This procedure is more accurate than the perturbative approach because, in general, in finite small systems the gap in the absence of the field [$G(N, 0)$] is not exactly proportional to the inverse of the chain length ($G(N, 0) \propto \frac{1}{N^\beta}$). Using the scaling function $K(N, h)$, we enter the deviation of the $\frac{1}{N}$ -behavior of the $G(N, 0)$ into our calculations, which causes our numerical results on the critical exponent of the energy gap to be more accurate. On the other hand, the second preference for this method is its ability to find the critical exponent of the energy gap when the first-order correction perturbation is nonzero. In this case, the coefficient of the first-order correction in the perturbation expansion for the energy gap is not a well-defined systematic function of N . But, by using the scaling function $K(N, h)$, the effect of the size dependence of $G(N, 0)$ on this coefficient shows the way to obtain the real critical exponent of the energy gap.

3. Vicinity of the line $\Delta = -1$

In this section, we consider our XXZ model in the vicinity of the critical line $\Delta = -1$. First, we rewrite the Hamiltonian (1) in the vicinity of this critical line as

$$H = J \sum_{i=1}^N (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y - S_i^z S_{i+1}^z - h S_i^x) + Jg \sum_{i=1}^N S_i^z S_{i+1}^z, \quad (13)$$

where $g = |1 + \Delta| \ll 1$ is a small parameter. By rotating the spins on each odd site by π around the z axis, the model becomes

$$H = -J \sum_{i=1}^N (\vec{S}_i \cdot \vec{S}_{i+1} - h(-1)^i S_i^x) + Jg \sum_{i=1}^N S_i^z S_{i+1}^z. \quad (14)$$

On the line $\Delta = -1$, this model reduces to the isotropic ferromagnet in a staggered magnetic field. The isotropic ferromagnetic chain in a staggered magnetic field is not exactly solvable. Reference [8] shows that the spectrum of low-lying excitations in the vicinity of the line $\Delta = -1$ can be described exactly by the spin-wave theory, which gives the energy gap as [23]

$$G = \sqrt{(\Delta + 1) \left(\Delta + 1 - \frac{h^2}{2} \right)}, \quad \Delta < -1. \quad (15)$$

We implemented our algorithm on sizes $N = 12, 14, \dots, 24$ in the vicinity of the line $\Delta = -1$ ($-1.01 \leq \Delta \leq -1.001$) and the transverse magnetic field $h = 0.05$. First, we checked the behavior of the gap, $G(N, g = 0)$, on the line $\Delta = -1$ as a function of $\frac{1}{N^\beta}$. We found that the best fit to our data yielded $\beta = 1.13 \pm 0.01$, which shows a small deviation

Table 2. The β -exponent of the function $G(N, g' = 0)$, ϕ , the α -exponent of the scaling function $K(N, g')$, and the resulting critical exponent of the energy gap ε , for different values of the transverse magnetic field h .

h	β	ϕ	α	ε
0.05	1.13	0.99	0.98	0.99
0.10	1.13	0.80	0.87	1.08

Table 3. The extrapolated energy gap and exact results obtained by spin-wave theory for a fixed transverse field $h = 0.1$ and different values of the parameter g .

g	G_{ext}	G_{sw}
0.001	0.002 5692	0.002 4495
0.002	0.003 6881	0.003 7417
0.003	0.004 8586	0.004 8990
0.004	0.005 9614	0.006 0000
0.005	0.007 0273	0.007 0711

from the $\frac{1}{N}$ -behavior. Then, we plotted the scaling function $K(N, g)$ versus N for a fixed value of the parameter $g = 0.002$ and found the best fit gave $\phi = 0.99 \pm 0.01$. By plotting the function $K(N, g)$ versus g for a fixed size $N = 24$ and $h = 0.05$, the best fit gave a value of $\alpha = 0.98 \pm 0.01$. Using equation (12), we obtained that the energy gap scales as g^ε with $\varepsilon = 0.99 \pm 0.01$. We also checked our numerical results for other values of the parameter g ($0.001 \leq g \leq 0.005$), and found the same results for the critical exponent of the energy gap.

We have repeated our computations for the transverse magnetic field $h = 0.1$. The obtained results are presented in table 2. In this table, we list the β -exponent of $G(N, g = 0)$ in the small- x regime, the ϕ -exponent, the α -exponent and the resulting critical exponent of the energy gap ε . Our numerical results show a very good agreement with the results of the spin-wave theory (equation (15)).

In table 3, we also show the extrapolated values of the energy gap and the known exact analytical spin-wave results (equation (15)) for the transverse field $h = 0.1$ and different values of the parameter g . We have extrapolated our numerical results using the function $G(N, g) = a + \frac{b}{N^c}$. It can be seen that our extrapolated results are very close to the exact results. Close inspection of the data in table 3 shows that the difference between our numerical results and the analytical results is 0.0001.

4. The 1D AF-Heisenberg model in a staggered field

The general feature developed for the XXZ model in a transverse field can be applied to the 1D Heisenberg Hamiltonian with a staggered magnetic field h_s ,

$$H = J \sum_{i=1}^N [\vec{S}_i \cdot \vec{S}_{i+1} + h_s (-1)^i S_i^z]. \quad (16)$$

It is expected [24–27] that the staggered field induces an excitation gap in the $S = \frac{1}{2}$ AF-Heisenberg chain, which should otherwise be gapless. The excitation gap caused by the staggered field is indeed found in real magnets [28–30]. In the absence of the staggered field ($h_s = 0$), the eigenspectrum is exactly solvable. In the case of the staggered magnetic field ($h_s \neq 0$), the integrability is lost. The staggered magnetic field produces an antiferromagnetic

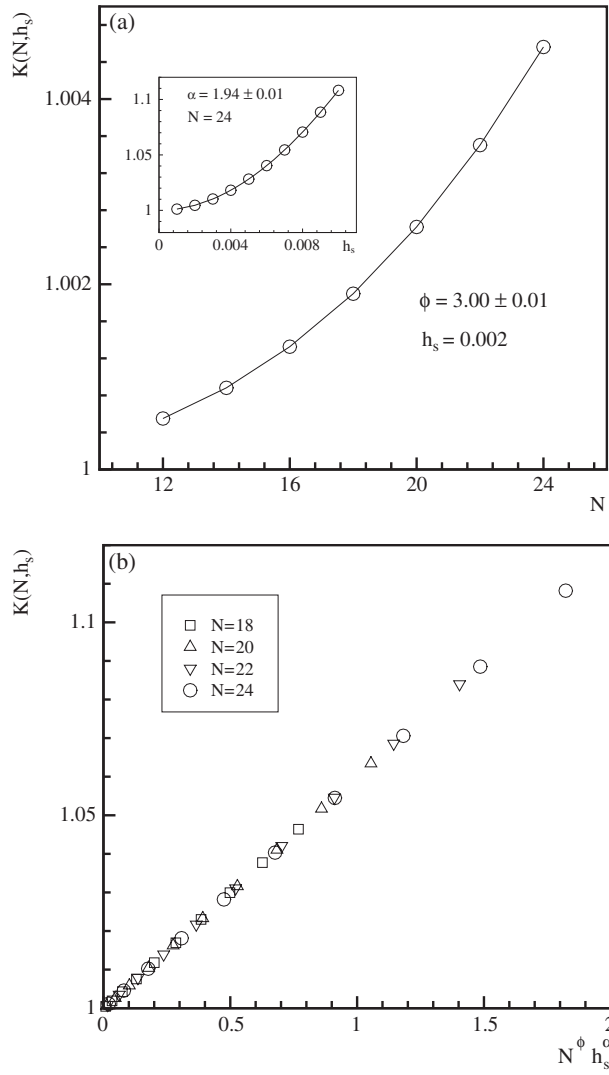


Figure 2. (a) The value of the scaling function $K(N, h_s)$ at the fixed staggered field $h_s = 0.002$ versus the chain length $N = 12, 14, \dots, 24$. The best fit is obtained by using $\phi = 3.00 \pm 0.01$. In the inset, the function $K(N, h_s)$ is plotted versus h_s ($0.001 \leq h_s \leq 0.01$) for the chain length $N = 24$. The best fit is obtained by $\alpha = 1.94 \pm 0.01$. (b) The scaling function $K(N, h_s)$ versus $N^\phi h_s^\alpha$ for different chain sizes $N = 18, 20, 22, 24$ and different staggered fields $0.001 \leq h_s \leq 0.01$.

ordered (Néel order) ground state. Affleck *et al*, using bosonization techniques, showed that the gap scales as [24],

$$G \sim h_s^{\frac{2}{3}}. \tag{17}$$

We have computed the scaling function $K(N, h_s)$ for different chain lengths ($N = 12, 14, \dots, 24$) in the cases of the staggered fields $0.001 \leq h_s \leq 0.01$. Our numerical data suggest that the function $G(N, h_s = 0)$ behaves as a function of $\frac{1}{N^\beta}$ with $\beta = 0.94 \pm 0.01$. In figure 2(a) we have plotted the scaling function $K(N, h_s)$ versus N for a fixed value of the

staggered magnetic field $h_s = 0.002$, and found the best fit for $\Phi = 3.00 \pm 0.01$. The inset of figure 2(a) shows the scaling function $K(N, h_s)$ versus h_s for a fixed size $N = 24$. In this case, the best fit yielded $\alpha = 1.94 \pm 0.01$. The value of the exponent $\alpha = 1.94 \pm 0.01$ shows that the second-order correction in the perturbation expansion is nonzero [31]. In figure 2(b) we have plotted the scaling function $K(N, h_s)$ versus $N^\phi h_s^\alpha$ for different chain sizes $N = 18, 20, 22, 24$ and different staggered fields $0.001 \leq h_s \leq 0.01$. It can be seen that all the data with various N and h_s are on the universal scaling curve.

Using equation (12), we found that the critical exponent of the energy gap is $\varepsilon = 0.65 \pm 0.01$, which is in good agreement with equation (17) and with the numerical results reported in [31].

5. Conclusions

In this paper, we have studied the energy gap of the 1D spin- $\frac{1}{2}$ AF XXZ model in a transverse magnetic field (h). We have implemented the modified Lanczos method to get the excited-state energies at the same accuracy as the ground-state energy. We have computed the energy gap in the region of anisotropy parameter $-1 < \Delta < 1$ and in the vicinity of the critical line $\Delta = -1$. We have shown that in the region $-1 < \Delta < 1$, the opening of the gap scales with h^ε , where ε is the critical exponent of the energy gap. On the other hand, the gap induced in the vicinity of the critical line $\Delta = -1$ scales with g^ε , where $g = |1 + \Delta| \ll 1$ is a parameter.

We have introduced a practical finite-size scaling approach for investigating the critical exponent of the energy gap ε . According to this approach, the presence of the gap can be characterized by the scaling function K . To find the correct critical exponent of the energy gap, we have plotted the best fit to the data of the scaling function K ($K(N, h) \propto N^\phi h^\alpha$ in the region $-1 < \Delta < 1$ and $K(N, g) \propto N^\phi g^\alpha$ in the vicinity of the critical line $\Delta = -1$). Using this procedure, we have computed the ϕ - and α -exponents of the scaling function K . We have shown that the critical exponent of the energy gap is related to the ϕ - and α -exponents by $\varepsilon = \frac{\alpha}{\phi}$. Finally we have computed the critical exponent of the energy gap of the 1D XXZ model in the region $-1 < \Delta < 1$ and in the vicinity of the critical line $\Delta = -1$. Our numerical results are in good agreement with the results obtained by the field theoretical and spin-wave approaches.

On the other hand, we have tested our procedure on the critical exponent of the energy gap of the 1D AF-Heisenberg chain in a staggered magnetic field (h_s), and showed that there is good agreement between results obtained by our practical approach and other numerical and theoretical approaches.

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