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Gap-behavior in the vicinity of a saturation transverse field

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Abstract. We have studied the behavior of the energy gap of the 1D AF spin-$\frac{1}{2}$ XXZ model in a transverse magnetic field (h) using the exact diagonalization technique. The ground state phase diagram consists of two spin-flop and paramagnetic phases. Using a modified finite-size scaling approach, we have computed the critical exponent of the energy gap in the vicinity of the critical transverse field $h_c(\Delta)$. Our numerical results confirm that the continuous phase transition from the spin-flop phase to the paramagnetic one is in the universality class of the Ising model in the transverse field (ITF). By applying conformal estimates of a small perturbation ($h \ll 1$), we have also justified our numerical results.

PACS. 75.10.Jm Quantized spin models – 75.10.Pq Spin chain models

1 Introduction

The 1D antiferromagnetic (AF) XXZ model in an external magnetic field has attracted much interest recently. The Hamiltonian of this model on a periodic chain of N sites, in a magnetic field is

$$H = \sum_{i=1}^{N} [J(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z) + hS_i^\delta], \quad (1)$$

where $J > 0$ is the exchange coupling, Δ is the anisotropy in the z direction and h is proportional to the longitudinal ($\delta = z$) or transverse ($\delta = x, y$) field. In the absence of an external magnetic field ($h = 0$), the exact solution is given by the Bethe ansatz [1]. In the regions $\Delta > 1$ and $\Delta \leq -1$, there is a gap in the excitation spectrum and the ground state is in the Néel and the ferromagnetic phase respectively. In the region $-1 < \Delta \leq 1$, the ground state is in the gapless spin-fluid phase with a power-low decay of correlations. The effect of a uniform longitudinal magnetic field is studied in great detail [1]. In this case, in the region $-1 < \Delta \leq 1$ the spectrum of the model remains gapless up to a saturation value of the longitudinal field $h = J(1 + \Delta)$.

Application of a transverse magnetic field on the 1D AF XXZ model is very interesting from the experimental [2,3] and theoretical [4–13] points of view. Adding a transverse field to the 1D AF 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 (the spin-flop phase). At a special field value $h_{cl} = \sqrt{2J(1+\Delta)}$ the ground state is known exactly to be of the classical Néel type [4,5]. The gap vanishes at the critical field $h_c(\Delta)$, where the transition to the paramagnetic phase (fully polarized phase in the field direction) occurs. Thus, in the case of the anisotropic AF XXZ chain ($-1 < \Delta < 1$), there are two phase transitions in the plane of the transverse magnetic field h vs. the anisotropic parameter Δ (see Fig. 1 of Ref. [7]). The first one (at $h_c = 0$) corresponds to the transition from the gapless spin-fluid phase to the gapped spin-flop phase. The second one (at $h_c(\Delta)$) represents the transition from the gapped spin-flop phase to the fully polarized phase.

Using quantum renormalization group (QRG) it is shown [6] that the anisotropy is not relevant and the universality class of the transition at $h_c(\Delta)$ is governed by the ITF model. Exact diagonalization data also supported the QRG results by calculating the spin structure factor and the magnetization of finite chain sizes. Using scaling estimations, the critical indices of the energy gap in the vicinity of the critical lines are obtained in reference [7]. It is shown that the critical exponent of the energy gap in the region $-1 < \Delta < 1$ at the phase transition between the spin-fluid phase and the spin-flop phase (at $h_c = 0$) is a function of the anisotropy parameter Δ

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

where θ is

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

A recent exact diagonalization approach [13,14] has shown very good agreement for the critical exponent of the energy gap in the vicinity of the critical field $h_c = 0$ and the whole range of the anisotropy parameter $-1 < \Delta < 1$. In this numerical work, the Δ-dependence of the critical

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exponent of the energy gap is computed using the relation between the divergence of the leading term in the perturbation expansion and the scaling behavior of the energy gap. Using a modified version of this approach we have also computed the critical exponent of the energy gap in the vicinity of the critical line $\Delta = -1$ in good agreement with the spin-wave approach [15].

In this work we study the quantum phase transition between the spin-flop and fully polarized state at the finite critical field $h_c(\Delta)$. However, two problems arise if we are interested in using this numerical approach in the vicinity of the critical field $h_c(\Delta)$. First, the exact value of the critical field $h_c(\Delta)$ is not known. Second, the critical field in the finite size chains (the pseudocritical field) is a function of N and different from the exact value $h_c(\Delta)$. We should note that we face the same problem in most quantum phase transitions [16,17]. Thus, the main question is, "How can we find the critical exponent of the energy gap in this situation?" To answer this question, we have applied a modified finite-size scaling approach, which is applicable to more general cases.

In this paper, we present our numerical results obtained for the low-energy states of the 1D AF XXZ model in the vicinity of the critical field $h_c(\Delta)$. Using the exact diagonalization technique, we calculate the energy gap as a function of the applied transverse field. In Section 2, we define the pseudocritical field of a finite system. We describe two known methods for computing the critical field $h_c(\Delta)$ from finite systems, results. Using these methods we can solve the first problem. In Section 3, first, we show that the behavior of the energy gap in the vicinity of the pseudocritical field $h_c(N, \Delta)$ is perturbative. For this reason, we apply a perturbative approach [13] to study the scaling behavior of the gap in the vicinity of the critical transverse field $h_c(\Delta)$. Finally, the summary and discussion are presented in Section 4.

2 Pseudocritical field

In this section we consider the behavior of the model in the vicinity of the transition line $h_c(\Delta)$. Since, all types of long-range order except the long-range order along the transverse magnetic field must vanish at some value of the field, therefore the transition line $h_c(\Delta)$ must exist. In the region $h < h_c(\Delta)$, the ground state is in the spin-flop phase. To use conformal estimations for finding the critical exponent of the energy gap in the vicinity of the critical line $h_c(\Delta)$, it is convenient to rewrite the Hamiltonian (1) in the following form

$$\begin{aligned} H &= H_0 + V \\ H_0 &= \sum_{i=1}^{N} [J(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z) + h_c(\Delta) S_i^x] \\ V &= (h - h_c(\Delta)) \sum_{i=1}^{N} S_j^x, \end{aligned} \tag{4}$$

where $(h - h_c(\Delta))$ is very small. Therefore, for a small perturbation V, we can use conformal estimates. The long distance asymptote of the correlation function of the model on the critical line $h_c(\Delta)$ is obtained [7] as

$$\langle S_j^x S_{j+n}^x \rangle \propto \frac{1}{n^2}. \tag{5}$$

By investigating the perturbed action for the model and performing an infinitesimal renormalization group calculation with a scale λ ($x = \lambda x'$ and $t = \lambda t'$) and expressing $\lambda = \frac{\xi}{\xi'} = \frac{G'}{G}$, one can show that the energy gap scales as

$$G(h) \sim (h - h_c(\Delta))^{\varepsilon}, \qquad \varepsilon = 1, \tag{6}$$

which shows that the critical exponent of the energy gap ε in the vicinity of the critical line $h_c(\Delta)$ is independent of the anisotropy parameter Δ and equal to one. Since the transition to the paramagnetic phase occurs at the critical field $h_c(\Delta)$, we expect the critical exponent of the energy gap to be equal to one. This linear behavior is in good agreement with the exponent being equal to one, characteristic of the ITF universality class [18]. The above consideration is valid also for the case $h < h_c(\Delta)$ with the same critical exponent for the energy gap.

The critical exponent of the energy gap can also observed from the numerical calculations of finite size systems. We have used the modified Lanczos method [19] for solving the finite chains exactly. The modified Lanczos method is the best procedure to obtain the excited energies with the same accuracy as the ground state one. The Lanczos method and the related recursion method [20–23] have emerged as one of the most important computational procedures, mainly when a few extreme eigenvalues are desired. The energy gap as a function of the chain length N and the transverse field h is defined as

$$G(N, h) = E_m(N, h) - E_0(N, h), \tag{7}$$

where E_0 is the ground state energy and E_m is in general, the first or second excited state. Since the first excited state and the ground state form a twofold-degenerate ground state in the thermodynamic limit, then $E_1 - E_0$ vanishes [7] and the energy gap will be equal to $E_2 - E_0$.

In the Hamiltonian formulation, the critical point of an infinite system is defined as the value of the magnetic field h at which the gap $G(h)$ vanishes as in equation (6). Using the Lanczos method we can compute $G(N, h)$ which approaches $G(h)$ when N is large.

We have implemented the modified Lanczos algorithm on finite size chains ($N = 12, 14, ..., 24$) using periodic boundary conditions to calculate the energy gap as a function of the transverse magnetic field h. We have computed the energy gap for different values of the anisotropy parameter $-1 < \Delta < 1$ and the chain lengths. In Figure 1 we have plotted the h-dependence of the energy gap of the chain sizes $N = 12, 16, 20$ at the anisotropy parameter $\Delta = -0.25$. It can be seen that there are numerous level crossings between the states, which lead to incommensurate effects in the behavior of the spin structure factors. All crossings disappear at $h > h_c$. Because a finite system cannot have a phase transition, therefore $G(N, h)$ does not vanish at any finite value of the transverse field

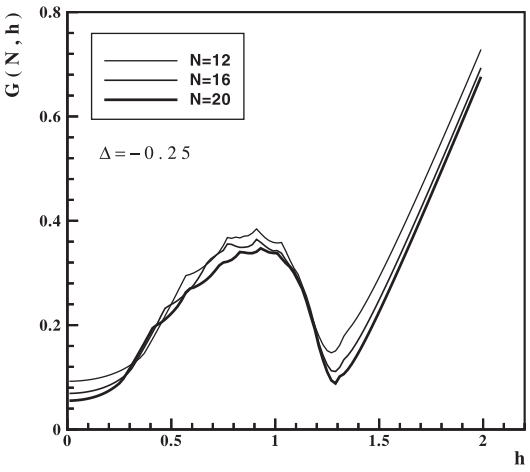

Fig. 1. The value of the energy gap $G(N,h)$ versus the transverse magnetic field for the anisotropy parameter $\Delta = -0.25$. The results reported are for different chain lengths $N = 12, 16, 20$.

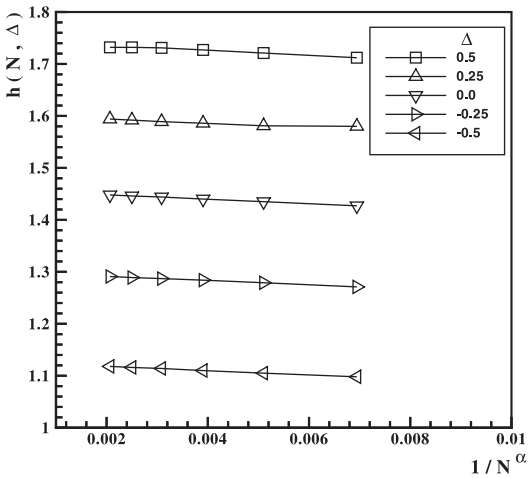

Fig. 2. The value of the Pseudocritical field $h_c(N,h)$ versus the parameter $1/N^{\alpha}$ for different values of the anisotropy parameter Δ. The best fit to our data is obtained using equation (8) with $\alpha = 2.0$.

h. We suggest, nevertheless, that one can extract $h_c(\Delta)$ from $G(N,h)$ by the following argument.

As it can be seen from Figure 1, the energy gap of a finite chain near h_{cl} decreases rapidly. Therefore we define the pseudocritical field of a finite system $h_c(N,\Delta)$ as the value of transverse field h at which the gap $G(N,h)$ is minimized and approaches $h_c(\Delta)$ as $N \longrightarrow \infty$. Using this procedure we have found the $h_c(N,\Delta)$ for different sizes $N = 12, 14, ..., 24$ and the anisotropy parameter $-1 < \Delta < 1$. We expect that the approach being characterized by the shift exponent α is defined by

$$\lim_{N\to\infty} h_c(N,\Delta) = h_c(\Delta) + \frac{B}{N^{\alpha}}. \qquad (8)$$

We have plotted in Figure 2, $h_c(N,\Delta)$ versus $1/N^{\alpha}$ for different values of the anisotropy parameter Δ. The results have been plotted for different sizes $N = 12, 14, ..., 22$ to derive $h_c(\Delta)$. The best fit to our data is obtained with $\alpha = 2.0$ for the anisotropy parameter $\Delta = 0$. Our numerical results show that the exponent α depends on Δ. But the deviation of $\alpha = 2.0$ is small. Since our numerical results are limited to small sizes up to $N_{max} = 24$, it becomes difficult to recognize the exact Δ-dependence of the exponent α.

There is also another approach to find the critical field $h_c(\Delta)$ which is based on the static spin structure factor. The static spin structure factor at momentum q is defined as

$$S^{\delta\delta}(q) = \sum_r \langle S_0^{\delta} S_r^{\delta} \rangle, \qquad \delta = x, y, z. \qquad (9)$$

It is known that the spin structure factors give us a deeper insight into the characteristics of the ground state. We have plotted $S^{yy}(q=\pi)$ versus N for different transverse fields. We expect as long as $h > h_c(\Delta)$, $S^{yy}(q=\pi)$ grows slowly and shows saturation at a finite value when $N \longrightarrow \infty$. On the other hand, a superlinear behavior versus N shows divergence of the structure factor for $h < h_c(\Delta)$. This corresponds to the ordered spin-flop phase. Using this procedure we also computed the critical field $h_c'(\Delta)$. The results have been presented in Table 1. In this table, we have listed $h_{cl}(\Delta)$, the critical field $h_c(\Delta)$ which is obtained from equation (8), and the critical field $h_c'(\Delta)$ computed from the N-dependence of the spin structure factor $[S^{yy}(q=\pi)]$ for different values of the anisotropy parameter Δ. Our numerical results show that the value of the critical field $h_c(\Delta)$ is in good agreement with $h_c'(\Delta)$ and also is larger than $h_{cl}(\Delta)$, which is expected.

Table 1. The classical field $h_{cl}(\Delta)$, the critical field $h_c(\Delta)$ which is obtained from equation (8) and the critical field $h_c'(\Delta)$ which is obtained from the N-dependence of the spin structure factor $[S^{yy}(q=\pi)]$ for different values of anisotropy parameter $-1 < \Delta < 1$.

Δ	$h_{cl}(\Delta)$	$h_c(\Delta)$	$h_c'(\Delta)$
0.50	1.732	1.736	1.70
0.25	1.581	1.597	1.55
0.0	1.414	1.451	1.45
−0.25	1.224	1.294	1.25
−0.50	1.000	1.121	1.10

3 Finite-size scaling approach

Now, let us introduce a modified version of our previous finite-size scaling approach [13,14]. This modified version is also applicable in the cases where the critical field is not known exactly and is different from the finite size results. The presence of the gap can be characterized by the following expression,

$$G(N,h) \sim N^{-1} f(x), \qquad (10)$$

where $x = N(h - h_c(N,\Delta))^{\varepsilon}$ is the scaling variable and $f(x)$ is the scaling function. Multiplying both side of above

equation by N we get

$$\lim_{N\to\infty\ (x\gg 1)} NG(N,h) \sim N(h-h_c(\Delta))^{\varepsilon}, \qquad (11)$$

which shows that the large-x behavior of $NG(N,h)$ is linear in $N(h-h_c(\Delta))^{\varepsilon}$ where the scaling exponent of the energy gap is ε. On the other hand, since in using the Lanczos method we are limited to considering the maximum value of the spins, $N=24$, the value of x cannot be increased. Thus, we have to find the scaling behavior of the gap from the small-x regime. According to our computations for $N \leq 24$, the small-x regime is equivalent to very small values of the parameter $(h-h_c(N,\Delta))$. In this case the energy gap of the finite size system basically represents the perturbative behavior [13]

$$G(N,h) = A^{(0)}(N) + A^{(1)}(N)(h-h_c(N,\Delta)) + A^{(2)}(N)(h-h_c(N,\Delta))^2 + ... \qquad (12)$$

The effect of higher-order terms can be neglected for $(h-h_c(N,\Delta)) \leq 0.01$ to a very good approximation. We have checked the first coefficient in the perturbation expansion $(A^{(0)}(N))$ as a function of N. Our numerical results show that, this coefficient behaves as $A^{(0)}(N) \sim \frac{1}{N}$, which is expected. Now let us rewrite equation (10) as [24]

$$G(N,h) \sim N^{-1} f[(N)^{1/\varepsilon}(h-h_c(N,\Delta))]. \qquad (13)$$

This implies

$$\frac{\partial^m G}{\partial h^m}\,|_{h=h_c(N,\Delta)} = N^{-1+\frac{m}{\varepsilon}} \times \text{const.}, \qquad (14)$$

where m is the order of the leading term in the perturbation expansion. Using equation (12) we obtain

$$A^{(m)}(N) \propto N^{-1+\frac{m}{\varepsilon}}. \qquad (15)$$

Now, if we consider the large-N behavior of $A^{(m)}(N)$ as

$$\lim_{N\to\infty} A^{(m)}(N) \simeq a_1 N^{\beta}, \qquad (16)$$

we find that the real critical exponent of the energy gap is related to the β-exponent as,

$$\varepsilon = \frac{m}{1+\beta}. \qquad (17)$$

The above arguments suggested that we look for the large-N behavior of $A^{(m)}(N)$. To do this, in the first step we plotted in Figure 3 the energy gap $G(N,h_c(N,\Delta))$ versus h $[0.001 \leq (h-h_c(N,\Delta)) \leq 0.01]$ for a fixed size $N=24$ and the anisotropy parameter $\Delta=0$. The best fit to our data is obtained with $\gamma = 2.2$ $(G(N,h_c(N,\Delta)) \propto (h-h_c(N,\Delta))^{\gamma})$, which shows that the first nonzero correction in the perturbation expansion is second-order $(m=2)$. We have also implemented our procedure for different values of the sizes $N=12,16,20$ and found the same results for m as we expected. In the second step, we fitted the results of the energy gap $G(N,h_c(N,\Delta))$ to the

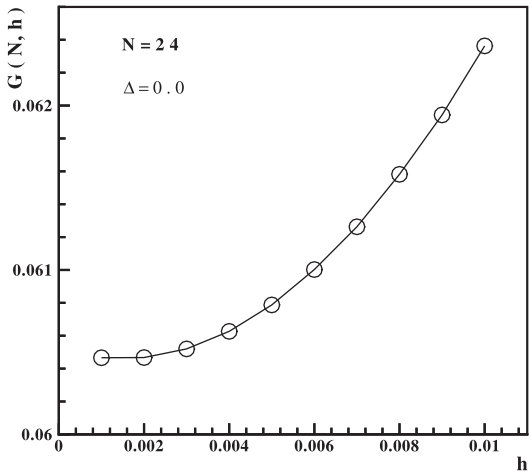

Fig. 3. The value of the energy gap $G(N,h)$ versus the transverse magnetic field close to critical field $h_c(N,\Delta)$ for the anisotropy parameter $\Delta=0$. The results reported are for a chain length $N=24$.

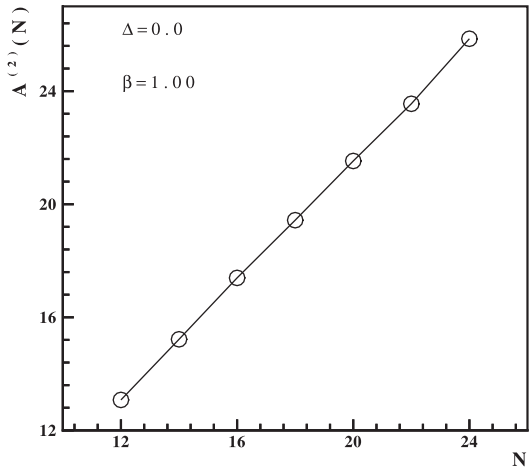

Fig. 4. The value of the scaling function $A^{(2)}(N)$ versus the chain length $N=12,14,...,24$ for the anisotropy parameter $\Delta=0$. The best fit is obtained by using equation (16) with $\beta = 1.00 \pm 0.07$.

polynomials for h close to $h_c(N,\Delta)$ up to $m=2$. Using this procedure we found the coefficient of the second-order correction perturbation, $A^{(2)}(N)$, as a function of N. Finally we plotted in Figure 4 the function $A^{(2)}(N)$ versus N for the value of the anisotropy parameter $\Delta=0$. The results have been plotted for different sizes $N=12,14,...,24$ to derive the β-exponent defined in equation (16). We found the best data fit for $\beta = 1.00 \pm 0.07$. Therefore, $\varepsilon = 1.00 \pm 0.07$ which shows very good agreement with equation (6). Moreover, our data for $h < h_c(N,\Delta)$, lead to $\varepsilon = 1.0 \pm 0.1$, as we expected. We have extended our numerical computations to consider other values of the anisotropy parameter Δ. The results have been presented in Table 2. We have listed the resulting ε which is obtained from equation (17), and the result of the theoretical approach ε_{th} for different values of the anisotropy parameter Δ. Our numerical results show very good agreement with

Table 2. The critical gap exponent ε which is obtained from equation (17) and theoretical gap exponent ε_{th} for different values of the anisotropy parameter $-1 < \Delta < 1$.

Δ	ϵ	ε_{th}
0.50	1.13	1.00
0.25	1.15	1.00
0.0	1.00	1.00
−0.25	0.99	1.00
−0.50	0.99	1.00

the exponent derived from the theoretical point of view, equation (6). The slight deviation in the region $\Delta > 0$ is the result of numerical computations and also limitation on the size of the system.

4 Conclusions

To summarize, we have studied the behavior of the energy gap of the 1D AF spin-$\frac{1}{2}$ XXZ model in a transverse magnetic field h. We have implemented the modified Lanczos method to obtain the excited state energies with the same accuracy as the ground state one. Adding a transverse field to the 1D AF XXZ model in the region $-1 < \Delta < 1$, develops a gap. There are two phase transitions in the plane of the transverse magnetic field h vs. the anisotropic parameter Δ (in the region $-1 < \Delta < 1$). The first one (at $h_c = 0$) corresponds to the transition from the gapless spin-fluid phase to the gapped spin-flop phase. The second one (at $h_c(\Delta)$) represents the transition from the gapped spin-flop phase to the fully polarized phase. In our previous work [13], we introduced an approach to obtain the real critical exponent of the energy gap from the finite size results in the vicinity of the critical field $h_c = 0$. However, two problems arise if we are interested in using this numerical approach in the vicinity of the critical field $h_c(\Delta)$. First, the exact value of the critical field $h_c(\Delta)$ is not known. Second, the critical field in the finite size chains is a function of N and different from the exact value $h_c(\Delta)$.

In this paper, we have shown that the modified approach is applicable to more general cases where the critical point is not exactly known and is different from the finite size results. First, we have defined the pseudocritical field of a finite system as $h_c(N, \Delta)$. To find the true critical field ($h_c(\Delta)$), we have plotted the best fit to the data of the function $h_c(N, \Delta)$ by using equation (8).

Then, we have shown that the behavior of the energy gap of the finite size chains ($G(N, h)$) in the vicinity of the pseudocritical field $h_c(N, \Delta)$ is perturbative. For this reason, we have applied a modified version of our previous perturbative approach [13] to study the scaling behavior of the gap in the vicinity of $h_c(\Delta)$. According to this approach, the scaling variable is defined as $x = N(h - h_c(N, \Delta))$. The small-$x$ regime is equivalent to very small values of the parameter $(h - h_c(N, \Delta))$. In this case we have written a perturbative expansion for the energy gap in the vicinity of the pseudocritical field $h_c(N, \Delta)$. To find the correct exponent of the energy gap in the small-x regime, one should plot the best fit to the data of the scaling function $A^{(m)}(N)$, which is the coefficient of the m-order perturbation expansion. Finally, we have found a relation between the divergence of the leading term $A^{(m)}(N)$ in the perturbative expansion and the scaling behavior of the energy gap as equation (17). Using this approach we have found that the critical exponent of the energy gap in the vicinity of the critical line $h_c(\Delta)$ is independent of the anisotropy parameter Δ and equal to one. This linear behavior shows that the continuous phase transition from the spin-flop phase to a paramagnetic one is in the universality class of the ITF model. By applying the conformal estimates of the small perturbation ($h \ll 1$), we have also justified our results theoretically (Eq. (6)).

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