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Scaling behaviour of the energy gap of spin-1/2 AF-Heisenberg chains in both uniform and staggered fields

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Abstract. The energy gap of the 1D AF-Heisenberg model in the presence of both uniform (H) and staggered (h) magnetic fields is investigated using the exact diagonalization technique. The opening of the gap in the presence of a staggered field is found to scale with h^{ν}, where $\nu = \nu(H)$ is the critical exponent, and depends on the uniform field. With respect to the range of the staggered magnetic field, two regimes are identified through which the dependence of the real critical exponent $\nu(H)$ on H can be calculated numerically. Our numerical results are in good agreement with the results obtained by other theoretical approaches.

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

1 Introduction

The effect of external magnetic fields on the quantum properties of low-dimensional magnets has been of much interest in recent years. Experimental and theoretical studies of these systems have revealed a plethora of quantum fluctuation phenomena, not usally observed in higher dimensions. The magnetization processes in antiferromagnetic (AF) spin chains and ladders have been under intensive investigation using novel numerical techniques. Crucial experimental insights into the subject have been provided by high-field neutron scattering measurements [1–3], and the synthesis of magnetic, quasi-one dimensional systems such as the spin-1/2 antiferromagnet Cu benzoate and Yb_4As_3 [4–6]. Consequently, it is now possible observe the effect of a staggered magnetic field (or even more complicated interactions) on the low energy behaviour of a one-dimentional quantum model in the laboratory.

There are several mechanisms for generating a staggered field in a real magnet [7–9]. In Cu benzoate the alternating crystal axes are the source of such a field. Dender et al. showed that an effective staggered field can be generated by an alternating g-tensor [1]. Afflec et al. have investigated theoretically how an effective staggered field is generated by Dzyaloshinskii-Moriya (DM) interactions when the crystal symmetry is sufficiently low [7]. They showed that in the presence of DM interactions along the AF chain, an applied uniform field $\overrightarrow{H}$ generates an effective staggered field $\overrightarrow{h}$. Ignoring small residual anisotropies, they obtained an effective Hamiltonian where a one-dimensional Heisenberg AF chain is placed in perpendicular, uniform (H), and staggered (h) fields:

$$\hat{H} = \sum_j \left[J \overrightarrow{S}_j . \overrightarrow{S}_{j+1} - H S_j^x + h\,(-1)^j\, S_j^z \right]. \qquad (1)$$

It is expected that a staggered field induces an excitation gap in the $S = 1/2$ Heisenberg antiferromagnetic (AF) chain, which should be otherwise gapless [7,10]. This excitation gap caused by the staggered field is indeed found in real magnets [1,6,11].

In the absence of the staggered magnetic field ($h = 0$) and the uniform magnetic field ($H = 0$), the spectrum is gapless. In the ground state, the system is in a spin-fluid phase, where the decay of correlations follow a power law. When a uniform magnetic field is applied, the spectrum of the system remains gapless until a critical field $H_c = 2J$ is reached. Here, a phase transition of the Pokrovsky-Talapov type [12] occurs and the ground state becomes a completely ordered ferromagnetic state [13]. Since the uniform magnetic field does not destroy the exact integrability of the Heisenberg model, the eigenspectrum is exactly solvable. The integrability is lost upon applying a staggered magnetic field. The application of a staggered magnetic field when $H = 0$, produces an antiferromagnetically ordered (Néel order) ground-state, and induces a gap in the spectrum of the model. The Heisenberg model in both staggered and uniform fields has recently been investigated using the density matrix renormalization group (DMRG) formalism [14]. It is shown that bound midgap states generally exist in open boundary

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AF-Heisenberg chains. The gap and midgap energies in the thermodynamic limit are obtained by extrapolating numerical results for small chain sizes up to 200 sites. It is revealed that some of the gap and midgap energies for the half-integer spin chains fit well to a scaling function derived from the quantum Sine-Gordon model, but other low energy excitations fit less well.

In this work, numerical results are presented for the low-energy states of the 1D AF-Heisenberg model in both uniform and staggered fields using an exact diagonalization technique for finite systems. The spin gap is calculated as a function of applied staggered field in the presence of a small uniform field ($0 \leq H < 0.1$). With respect to the magnitude of the staggered magnetic field, it is demonstrated that two regimes exist in which the real critical exponent of the energy gap can be calculated. It is important to note to which one of these regimes the numerical data are related. In Section 2, the scaling behaviour of the gap is considered, based upon available information about its limiting behaviour. The leading exponent of the staggered field h depends on H, both at finite sizes, and in the thermodynamic limit. In Section 3, an explanation is given for how, under certain conditions, the numerical calculations may produce incorrect results for the critical exponent. A perturbative approach[25] is applied to find the correct critical exponent in the small-x ($x = Nh^{\nu(H)}$) regime. In Section 4, the scaling parameter x is increased to investigate the critical exponent in the large-x regime. Finally, the summary and conclusions are presented in Section 5.

2 The scaling behaviour of the gap

In high field neutron-scattering experiments on Cu benzoate — which is a quasi-one dimensional $S = 1/2$ antiferromagnet — the magnetic field induces a gap in the excitation spectrum of the magnet [1]. The observed gap is proportional to $H_0^{0.65}$, where H_0 is the magnitude of the applied field. Other experiments (where the exponent is $\approx 2/3$) identify the cause of the gap as being due to the staggered field [6,11].

Using so-called bosonization techniques, Affleck et al. showed that, the gap scales as

$$\Delta(h, H) \sim h^{\nu(H)}, \tag{2}$$

where $\nu(H)$ is the critical exponent. When H is strictly 0, $\nu(H = 0) = 2/3$. The dependence of the exponent $\nu(H)$ on H is investigated numerically in reference [15]. Their approach is based on the η-exponent, defined through the static structure factor of the model in the absence of a staggered field ($h = 0$). They show that there is a relationship between the critical exponent of the gap and the η-exponent. Then, by computing the η-exponent of the structure factor of the model, they predict the H-dependence of $\nu(H)$. Similarly, the effect of an external field on the gap of the 2D AF Heisenberg model with DM interactions has been investigated [16]. It is shown that the effect of the external field on the gap can be predicted from the on-site magnetization of the model.

Here, the evolution of the gap is investigated using conformal estimates for a small perturbation $h \ll 1$, and finite-size scaling estimates of the energy eigenvalues of small chains in the presence of the staggered field ($h \neq 0$). We show that there are two regimes in which the real critical exponent can be calculated numerically, and it is important to note to which one of these regimes the numerical data are related.

The Hamiltonian (1) can be rewritten in the form

$$\begin{aligned} \hat{H} &= \hat{H}_0 + V \\ \hat{H}_0 &= \sum_j \left[J \overrightarrow{S}_j . \overrightarrow{S}_{j+1} - H S_j^x \right] \\ V &= h \sum_j (-1)^j S_j^z, \end{aligned} \tag{3}$$

where $\hat{H}_0$ is exactly solvable by the Bethe ansatz, and the staggered field $h \ll 1$ is very small. For a small perturbation V, we can use conformal estimates.

The large distance asymptotic behaviour of the correlation function of the model in the absence of the staggered field ($h = 0$) is given by [17]

$$\langle S_j^z S_{j+n}^z \rangle \sim \frac{(-1)^n}{n^{\alpha(H)}}, \tag{4}$$

where $\alpha(H)$ is a function of the uniform (H) field. This is found using the Bethe ansatz as

$$\alpha(H) \sim 1 - \frac{1}{2 \ln(1/H)}, \qquad H \to 0 \tag{5}$$

where $\alpha(0) = 1$ and $\alpha(2) = 1/2$.

By examining the response of the model to a perturbation, and performing an infinitesimal renormalization group with a scale λ, one can show that the staggered magnetic field scales as $h' = h\lambda^{2-\alpha(H)/2}$. Hence, the energy gap scales according to equation (2), where the critical exponent is

$$\nu(H) = \frac{2}{4 - \alpha(H)}. \tag{6}$$

This result is also obtained using the bosonization technique in reference [7]. For example, in the absence of a uniform magnetic field, $\Delta \sim h^{2/3}$, in agreement with the bosonization and experimental results. Increasing the uniform field H, makes $\alpha(H)$ smaller, which implies that the critical gap exponent $\nu(H)$ decreases with increasing uniform field H.

To examine the effect of the uniform field on the energy gap, we have implemented the modified Lanczos algorithm [18] for finite-size chains ($N = 12, 14, \ldots, 24$) using periodic boundary conditions. The energy gap is calculated for different chain lengths and uniform fields in the interval $0 \leq H < 0.1$. The energy gap as a function of the chain length (N), uniform (H) and staggered (h) fields is defined as

$$\Delta(N, h, H) = E_1(N, h, H) - E_0(N, h, H), \tag{7}$$

where E_0 is the ground state energy and E_1 is the first excited state. In the absence of a staggered field ($h = 0$), the spectrum of the AF Heisenberg model is gapless up to $H = 2J$. The gap vanishes in the thermodynamic limit, proportional to the inverse of the chain length [19]

$$\lim_{N\to\infty} \Delta\left(N, h = 0, H\right) \longrightarrow \frac{A(H)}{N}. \tag{8}$$

The coefficient A is known exactly from the solution to the Bethe ansatz [20]. In principle, it also can be computed by methods based on conformal invariance and finite-size scaling [21–23].

When the staggered field is applied, a non zero gap develops. Thus, the staggered field $h_c = 0$ is a critical point for the model. In general, the critical point h_c of an infinite system in the Hamiltonian formulation, is defined as the value of h at which the mass gap $\Delta(h, H)$ vanishes as equation (2). Using the Lanczos scheme $\Delta(N, h, H)$ can be calculated. This approaches $\Delta(h, H)$ when N is large. The natural measure of the deviation of the finite system from the infinite one is L/L_0, where L is the linear dimension of the finite system ($L = Na$, and a is the lattice spacing) and L_0 is the correlation length of the infinite system ($L_0 = \xi a$). Thus, it can be assumed that $\Delta(N, h, H)$ depends on h through L/L_0 as

$$\Delta\left(N, h, H\right) \sim f\left(\frac{L}{L_0}\right) = f\left(x\right), \tag{9}$$

where $x = Nh^{\nu(H)}$ is a scaling parameter, and $f(x)$ is the scaling function. As expected, the behaviour of this equation in the combined limit,

$$N \longrightarrow \infty, \qquad h \longrightarrow 0 \qquad (x \gg 1), \tag{10}$$

is consistent with equation (2). Thus, it can be assumed that the asymptotic form of the scaling function $f(x)$ is

$$f\left(x\right) \sim x^{\phi}. \tag{11}$$

In addition, we need a factor to cancel the dependence of $f(x)$ on N when $N \longrightarrow \infty$. This factor must be of the form N^{-1}; therefore,

$$\Delta\left(N, h, H\right) \sim N^{-1} f\left(x\right). \tag{12}$$

Multiplying both sides of equation (12) by N gives

$$\lim_{N\to\infty (x\gg 1)} N\Delta\left(N, h, H\right) \sim x. \tag{13}$$

Equation (13) shows that the large-x behaviour of $N\Delta(N, h, H)$ is linear in x where the scaling exponent of the energy gap is $\nu(H)$.

3 The small-x regime

Since the scaling of the gap can only be observed in the thermodynamic limit, and for very small values of h, the energy gap of the model is calculated using several values of staggered field $0.001 \leq h \leq 0.01$, and different chain lengths $N = 12, 14, \ldots, 24$, for fixed uniform fields $0 \leq H < 0.1$. When $N\Delta(N, h, H)$ versus $Nh^{\nu(H)}$ is plotted for $H = 0, 0.03, 0.05, 0.07, 0.09$, using periodic boundary conditions, then the linear behaviour of equation (13) is described well by $\nu(H) \cong 2.0$, independent of H. This is very far from the correct value of critical exponent $\nu(H) \leq 2/3$ (Eq. (6)).

Note that the horizontal axes values in the small-x regime are limited to very small values of $x = Nh^{\nu(H)} < 0.0024$. Thus, it is not possible to obtain the real scaling exponent of the gap in the thermodynamic limit when $N \longrightarrow \infty$ or $x \gg 1$.

When x is small, meaning h is very small, this may be too far from the thermodynamic behaviour that is needed to observe the correct scaling. For very small h in the finite size systems ($N \sim 24$) the value of x will be small ($x \ll 1$), which prevents information on the large-x behaviour of the scaling function $f(x)$ from being obtained. In effect here, the values of the energy gap coming from a finite system represent perturbative behaviour [25]. This is reproduced here for convenience, as follows.

Starting from the Hamiltonian equation (3), the energy eigenstates of $\hat{H}_0$ carry momentum $p = 0$ or $p = \pi$.

$$T\ |\psi_n(h = 0, H)\rangle = \pm\ |\psi_n(h = 0, H)\rangle, \tag{14}$$

where, T is translation operator, and $\{|\psi_n(h = 0, H)\rangle\}$ are eigenstates of the unperturbed Hamiltonian $\hat{H}_0$. The operator $\sum_j (-1)^j S_j^z$ changes the momentum of the state by π; therefore,

$$\langle\psi_n(0, H)\ |\ V\ |\psi_n(0, H)\rangle = 0. \tag{15}$$

Thus, the gap can be rewritten in the following form.

$$\Delta\left(N, h, H\right) = \Delta\left(N, 0, H\right) + g_1\left(N, H\right) h^2 + \cdots + g_n\left(N, H\right) h^{2n}, \tag{16}$$

where n is an integer. Higher order terms can be neglected for $h \leq 0.01$. The second-order perturbation correction is not zero in the staggered field: the leading nonzero term is h^2. If the small-x behaviour of the scaling function is defined as $f(x) \sim x^{\phi_s}$, then

$$\nu(H)\phi_s = 2. \tag{17}$$

This shows that in the small-x regime, $N\Delta(N, h, H)$ is a linear function of $x^{2/(\nu(H))}$. This is in agreement with the data in the small-x regime, where $\phi_s = 1$, and according to equation (17), the value of $\nu(H)$ is found to be $\nu(H) = 2.0$.

The large-N behaviour of $g_1(N, H)$ at fixed H is given by

$$\lim_{N\to\infty} g_1(N, H) \simeq a_1\left(H\right) N^{\mu(H)}. \tag{18}$$

This leads to

$$\Delta\left(N, h, H\right) \simeq \frac{A\left(H\right)}{N}\left(1 + b_1\left(H\right) N^{\mu(H)+1} h^2\right), \tag{19}$$

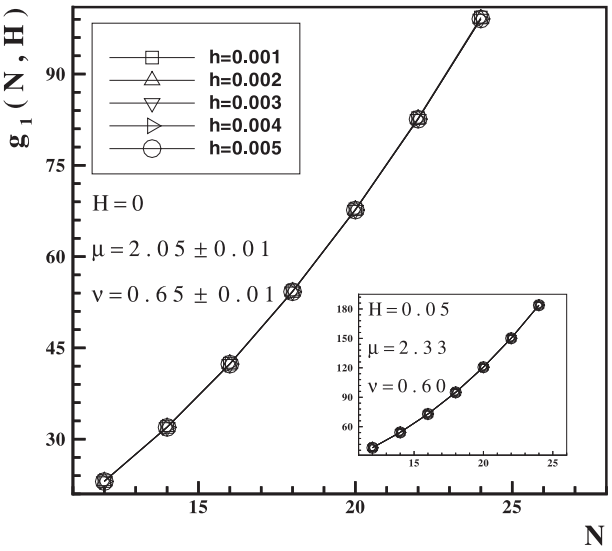

Fig. 1. The value of scaling function $g_1(N, H)$ at the fixed uniform field $H = 0$, versus the chain length $N = 12, 14, \ldots, 24$. The best fit is obtained by $\nu(H = 0) = 2.05 \pm 0.01$. In the inset, the function $g_1(N, H)$ is plotted versus N at the uniform field $H = 0.05$. The best fit is obtained using $\nu(H = 0.05) = 2.33 \pm 0.01$. Data for different staggered fields $0.001 \leq h \leq 0.005$ coincide exactly.

where $b_1(H)$ is a constant (at fixed H). equation (19) can be written in terms of the scaling variable x:

$$N\Delta\left(N,h,H\right) \simeq A\left(H\right)\left(1+N^{\mu(H)+1-2/(\nu(H))}x^{2/(\nu(H))}\right). \tag{20}$$

For large-N limit this equation should be independent of N; hence, the relation between $\mu(H)$ and $\nu(H)$ is

$$\nu\left(H\right) = \frac{2}{\mu\left(H\right)+1}. \tag{21}$$

Therefore, an examination of the large-N behaviour of $g_1(N, H)$ is warranted. To determine the exponent $\mu(H)$, the expression

$$g_1\left(N,H\right) \simeq \frac{\Delta\left(N,h,H\right)-\Delta\left(N,0,H\right)}{h^2} \tag{22}$$

versus N is plotted in Figure 1 for fixed values of staggered field h ($0.001 \leq h \leq 0.005$), and different sizes, $N = 12, 14, \ldots, 24$, at the uniform field $H = 0$. The best fit to the data has $\mu(H = 0) = 2.04 \pm 0.01$. The inset in Figure 1 shows $g_1(N, H)$ versus N at fixed $H = 0.05$. Here, the best fit has $\mu(H = 0.5) = 2.33 \pm 0.01$. The data for different h values, fall exactly on each other, which shows that the results for $g_1(N, H)$ in fixed uniform field H, are independent of the staggered field h, as expected. Using equation (21) it is found that, $\nu(H = 0) = 0.66 \pm 0.01$ and $\nu(H = 0.05) = 0.60 \pm 0.01$. The numerical tool is also used to calculate the critical exponent $\nu(H)$ at $H = 0.03, 0.07, 0.09$. The results are given in Table 1.

Table 1. The exponent of $g_1(N, H)$ and gap exponent versus different values of the uniform field H in small-x and large-x regimes.

H	μ	ν_S	ν_L
0.0	2.05	0.65	0.66
0.03	2.20	0.63	0.64
0.05	2.33	0.60	0.63
0.07	2.58	0.56	0.62
0.09	2.80	0.53	0.60

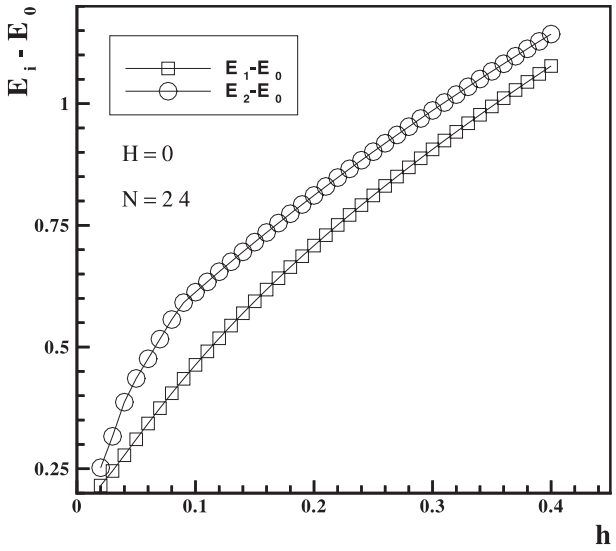

Fig. 2. Difference between the two lowest energy levels and the ground state energy as a function of the staggered magnetic field h, for finite chain length $N = 24$, and $H = 0$, over the interval $0.01 \leq h \leq 0.4$.

4 The large-x regime

Due to computer memory constraints, the maximum chain length considered in the numerical calculations is $N = 24$. Therefore, the value of x cannot be increased by increasing the size of chain. The problem appears when the calculation employs the density matrix renormalization group (DMRG) method. When this occurs, the calculation may be extended to larger sizes, $N \sim 200$, subject to the restriction that this does not allow x to be much larger than one (for $0.001 < h < 0.01$). Instead, the staggered field may be increased to reach larger x. Note here that, in general, level crossing usually occurs between the energy levels in finite size systems. This can change the behaviour of the gap and lead to incommensurate effects [24]. When, for example, the excitation energies of the three lowest levels as a function of h ($0.01 \leq h \leq 0.4$) are calculated for $N = 24$ and $H = 0$, it turns out that the two lowest excited states do *not* cross each other (see Fig. 2). This means that x can be made larger by increasing h up to $h = 0.4$. Since the regime where the correct scaling of the gap can be observed is only when h is small, $h = 0.4$ is made the upper limit used in the calculations. Figure 3 shows the results of calculations for large-x, made using the Hamiltonian equation (1), and taking into account

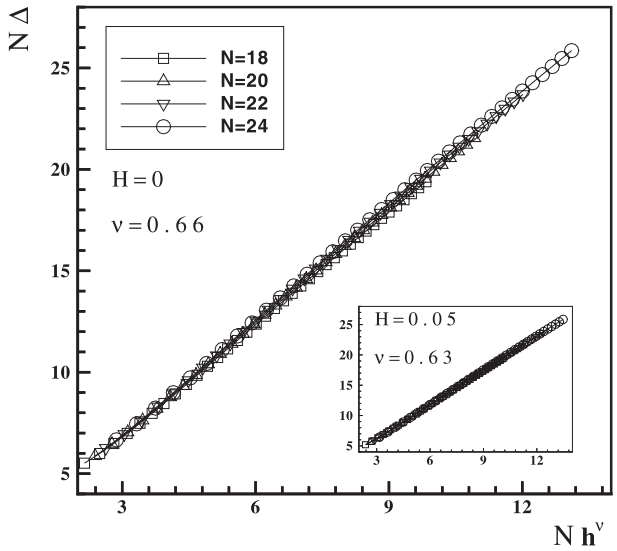

Fig. 3. The product of energy gap and chain length ($N\Delta$) versus $Nh^{\nu(H)}$ at the uniform field $H = 0$. Over the interval $0.04 \leq h \leq 0.4$, linear behaviour is obtained by choosing $\nu(H = 0) = 0.66$ for all chain lengths, $N = 18, 20, 22, 24$. In the inset, $N\Delta$ is plotted for uniform field $H = 0.05$. The linear behaviour is obtained with $\nu(H = 0.05) = 0.63$. Data for different chain lengths coincide.

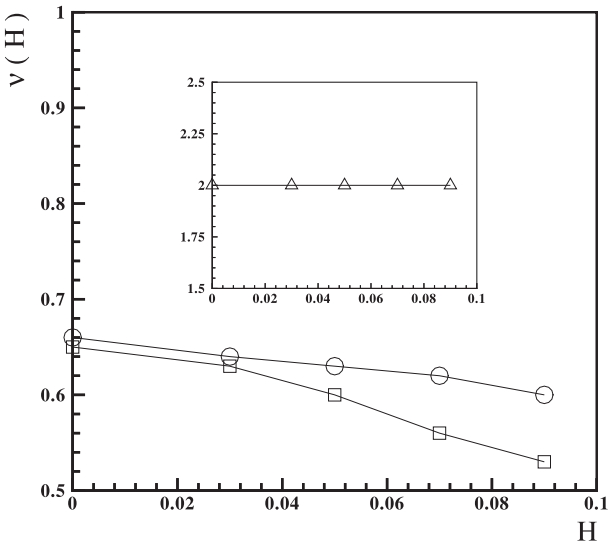

Fig. 4. Graph of the critical exponent ν versus uniform field H. Both critical exponents ν_s (squares) and ν_l (circles) start at the known value 2/3 and then decrease with the increasing uniform field H. In the inset, the critical exponent ν is plotted. This is obtained directly by extrapolating the numerical results for the energy gap over the interval $0.001 \leq h \leq 0.01$.

the limitations previously described. Therefore, these results are over the interval $0.04 \leq h \leq 0.4$, which provides large-x using chain lengths $N = 18, 20, 22, 24$, and $H = 0$. The inset in Figure 3 shows $N\Delta(N, h, H)$ versus $x = Nh^{\nu(H)}$ at fixed uniform field $H = 0.05$. This yields $\nu(H = 0) = 0.66$, and $\nu(H = 0.05) = 0.63$. These represent the unique values for ν which give linear behaviour. Moreover, the results for different size chains coincide exactly, which is expected from the scaling properties.

The results of further calculations covering the low uniform field region over the interval $0 \leq H < 0.1$ are given in Table 1. The quantities μ, the resulting ν_s that is obtained from perturbative approach, and the corresponding result for the large-x regime ν_l, for different values of the uniform field H are included.

Figure 4 shows the critical exponent $\nu(H)$ versus the uniform field H. The quantities ν_s and ν_l start at the known value 2/3, and then decrease with the increasing uniform field H. The exponents are in good agreement with each other, and are in accord with the exponents derived using the field formalism (Eq. (6)). The inset in Figure 4 shows the dependence on H of the critical exponent ν. This is obtained directly by extrapolating the numerical results for the energy gap using a staggered field over the interval $0.001 \leq h \leq 0.01$. Clearly, the behaviour of the gap in finite systems is different from its behaviour at the thermodynamic limit. Furthermore, the behaviour of the gap also deviates from the predicted scaling behaviour with respect to the magnitude of the staggered magnetic field.

Fouet et al. investigated the gap-induced by the staggered field h at the saturation uniform field $H_c = 2J$ [26]. Using field theoretical arguments, they find that the gap scales as $\Delta(h, H_c) \sim h^{4/5}$. By applying the DMRG method to systems with sizes up to $N = 100$, they also estimate that the exponent of the energy gap is 0.81. The results of calculations extended to H_c in the present work yield similar values: $\nu_s(H_c) = 0.78$ and $\nu_l(H_c) = 0.82$.

5 Conclusions

The 1D AF-Heisenberg model in the presence of both uniform (H) and staggered (h) magnetic fields is investigated using the exact diagonalization technique in this work. The modified Lanczos method is implemented to obtain the excited state energies to the same accuracy as in the ground state. This formalism is applied to model chains up to $N = 24$ in length (limited by presently available computer resources). When the energy gap in the thermodynamic limit is obtained by extrapolating the numerical results for finite systems, it is found that the behaviour of the gap apparently deviates from the predicted scaling properties. This deviation depends on the magnitude of the staggered magnetic field (h). For small values of the staggered magnetic field ($0.001 \leq h \leq 0.01$), the energy gap of a finite system behaves essentially in a perturbative manner. Thus, the scaling exponent of the energy gap cannot be extrapolated from numerical results in this regime.

Results, based on a general finite size scaling procedure, are presented for the H-dependence of the critical exponent of the gap. Two regimes are identified where the real critical exponent $\nu(H)$ can be calculated numerically. To find the correct exponent of the gap in small-x regime ($x = Nh^{\nu(H)} \ll 1$), the scaling behaviour of the

coefficient of the leading term in the perturbation expansion is used, as described previously in reference [25]. In the large-x regime, the correct critical exponent is calculated using standard finite size scaling via equation (13). In addition, conformal estimates of the small perturbation ($h \ll 1$) are used to provide the dependence of the critical exponent on H (Eq. (6)). The numerical results for both regimes in this work are in good agreement with others obtained by theoretical and numerical approaches.

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