Scaling behavior of the energy gap of spin-$\frac{1}{2}$ AF-Heisenberg chain in both uniform and staggered fields

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

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I. INTRODUCTION

The effect of external magnetic fields in 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 usually observed in higher dimensions. The magnetization processes in antiferromagnetic (AF) spin chains and ladders have been under intensive investigation using novel numerical techniques. The progress in the experimental front is achieved by introduction of high-field neutron scattering studies and synthesis of magnetic quasi-one dimensional systems such as the spin-$\frac{1}{2}$ antiferromagnet Cu benzoate and $YbAs$. Due to these developments we can now observe the effect of a staggered magnetic field (or even more complicated interactions) on the low energy behavior of a one-dimensional quantum model in the laboratory.

There exist different mechanisms for generating a staggered field in a real magnet. In Cu benzoate the alternating crystal axes is the source of such a field. Dender et al. showed that an effective staggered field can be generated by the alternating g-tensor. Theoretically, Affleck et al. have studied how an effective staggered field is generated by Dzyaloshinskii-Moriya (DM) interaction if the crystal symmetry is sufficiently low. They showed that in the presence of DM interaction along the AF chain, an applied uniform field $\overline{H}$ generates an effective staggered field $\overline{h}$. 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

$$\hat{H} = \sum_j [J \overline{S}_j \cdot \overline{S}_{j+1} - h S_j^z + h(-1)^j S_j^z] \quad (1)$$

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 the 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 occurs and the ground state becomes a completely ordered ferromagnetic state. Since the uniform magnetic field does not destroy the exact integrability of the Heisenberg model, the eigenspectra is exactly solvable. Applying a staggered magnetic field, the integrability is lost. The application of a staggered magnetic field when $H = 0$, produces an antiferromagnetically ordered (Neel order) ground-state and induces a gap in the spectrum of the model. Heisenberg model in both staggered and uniform fields has been recently studied using density matrix renormalization group (DMRG). It is shown that bound midgap states generally exist in open boundary AF-Heisenberg chains. The gap and midgap energies in the thermodynamic limit are obtained by extrapolating numerical results of 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 do not fit equally well.

In this paper, we present the numerical results obtained on the low-energy states of the 1D AF-Heisenberg model in both uniform and staggered fields using an exact diagonalization technique for finite systems. We calculate the spin gap as a function of applied staggered field in the presence of small uniform field ($0 \leq H < 0.1$). With respect to the range of the staggered magnetic field, we show that there are two regimes in which we can compute the real critical exponent of the energy gap and it is important to note to which one of these regimes the numerical data are related. In Sec. II we discuss the scaling behavior of the gap using the available limiting behaviors. The leading exponent of the staggered field $h$, depends on $H$ both in finite size and thermodynamic limit. In Sec. III, we explain how, in certain
limits the numerical calculations may produce incorrect result for the critical exponent. We apply a perturbative approach to find the correct critical exponent in the small-$x$ ($x = N h^{\nu(H)}$) regime. In Sec. IV, we increase the scaling parameter $x$ and find the correct critical exponent in the large-$x$ regime. Finally, the summary and discussion are presented in Sec. V.

II. THE SCALING BEHAVIOR OF THE GAP

In the high field neutron-scattering experiment on Cu benzoate, which is a quasi-one dimensional $S = \frac{1}{2}$ antiferromagnet, the magnetic field induces a gap in excitation spectrum of the magnet. The observed gap is proportional to $H_0^{0.65}$, where $H_0$ is the magnitude of the applied field. This exponent of about $\frac{1}{2}$ describing the field dependence of the gap obtained in different experiments identify the source of this gap as the staggered field.

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

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

where $\nu(H)$ is the critical exponent of the gap and when $H$ is strictly 0, $\nu(H = 0) = \frac{2}{3}$. The $H$-dependence of the exponent $\nu(H)$ is studied numerically in Ref. [15]. Their approach is based on the $\eta$-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 relation between the critical exponent of the gap and $\eta$-exponent. Then by computing the $\eta$-exponent of the structure factor of the model, they predict the $H$-dependence of $\nu(H)$. Similarly, in an interesting recent work, the effect of an external field on the gap of the 2D AF Heisenberg model with DM interaction has been studied. It is shown that the effect of the external field on the gap can be predicted by investigating the on-site magnetization of the model.

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

Let us rewrite the Hamiltonian (1) in the form

$$\hat{H} = \hat{H}_0 + V$$

$$\hat{H}_0 = \sum_j [J \hat{S}_j \hat{S}_{j+1} - H \hat{S}_j^z]$$

$$V = h \sum_j (-1)^j \hat{S}_j^z,$$

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 of the correlation function of the model in the absence of the staggered field ($h = 0$) is obtained as

$$\langle \hat{S}_j^z \hat{S}_{j+n}^z \rangle \sim (-1)^n n^{\alpha(H)},$$

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

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

which is also obtained with the bosonization technique in Ref. [7]. For example, in the absence of a uniform magnetic field, $\Delta \sim h^{\frac{2}{3}}$, in agreement with the bosonization and experimental results. Since, by increasing the uniform field, $\alpha(H)$ decreases, thus we can conclude that the gap scales as $H^\alpha$ by critical exponent

$$\nu(H) = \frac{2}{4 - \alpha(H)},$$

which is also obtained with the bosonization technique in Ref. [7].

To make a numerical check on effect of the uniform field the energy gap we have implemented the modified Lanczos algorithm on finite-size chains ($N = 12, 14, ..., 24$) using periodic boundary conditions to calculate the energy gap. We have computed the energy gap for different chain lengths in the cases of the uniform fields $0 \leq H < 0.1$. The energy gap as a function of the chain length $(N)$, uniform $(H)$ and staggered $(h)$ fields is defined as

$$\Delta(N, h, H) = E_1(N, h, H) - E_0(N, h, H),$$

where $E_0$ is the ground state energy and $E_1$ is the first excited state. In the absence of 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

$$\lim_{N \to \infty} \Delta(N, h = 0, H) \to \frac{A(H)}{N}.$$
as Eq. [2]. With our Lanczos scheme we can compute \( \Delta(N, h, H) \), which approaches \( \Delta(h, H) \) when \( N \) is large. The natural measure of the deviation of the finite system from the infinite one is \( \frac{L}{L_0} \), where \( L \) is the linear dimension of the finite system \( (L = Na, a \) is the lattice spacing) and \( L_0 \) is the correlation length of the infinite system \( (L_0 = \xi a) \). Thus, we assume that \( \Delta(N, h, H) \) depends on \( h \) through \( \frac{L}{L_0} \) as

\[
\Delta(N, h, H) \sim f\left(\frac{L}{L_0}\right) = f(x),
\]

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

\[
N \to \infty, \quad h \to 0 \quad (x \gg 1)
\]

as Eq. [2], thus we assume the asymptotic form of the scaling function \( f(x) \)

\[
f(x) \sim x^{\phi}.
\]

In addition, we need a factor to cancel the \( N \)-dependence of \( f(x) \) as \( N \to \infty \). This factor must be of the form \( N^{-1} \). Thus, we have

\[
\Delta(N, h, H) \sim N^{-1} f(x),
\]

If we multiply both sides of Eq. [12] by \( N \) we get

\[
\lim_{N \to \infty(x \gg 1)} N \Delta(N, h, H) \sim x.
\]

Eq. [13] shows that the large-\( x \) behavior of \( N \Delta(N, h, H) \) is linear in \( x \) where the scaling exponent of the energy gap is \( \nu(H) \).

III. SMALL-X REGIME

Since the scaling of the gap can only be observed in the thermodynamic limit and for very small value of \( h \), we compute the energy gap of the model for 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 \( 0 \leq H < 0.1 \). We have plotted the values of \( N \Delta(N, h, H) \) versus \( Nh^{\nu(H)} \) for \( H = 0, 0.03, 0.05, 0.07, 0.09 \). The results have been computed on a chain with the periodic boundary conditions. According to Eq. [13], we have found from our numerical results that the linear behavior is very well satisfied by \( \nu(H) \approx 2 \) independent of \( H \). This is very far from the correct value of critical exponent \( \nu(H) \leq \frac{4}{7} \) (Eq. [6]).

Note that the horizontal axes values in the small-\( x \) regime are limited to very small values of \( x = Nh^{\nu(H)} \leq 0.0024 \). Thus, we are not allowed to obtain the real scaling exponent of the gap which exists in the thermodynamic limit \( (N \to \infty \text{ or } x \gg 1) \).

When \( x \) is small, or in other words \( h \) is very small, we might be away from the thermodynamic behavior 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 avoid us to get the information on the large-\( x \) behavior of the scaling function \( f(x) \). In this case, the values of the energy gap coming from a finite system are basically representing the perturbative behavior, which we reproduce for the convenience .

We start from the Hamiltonian Eq. [3]. The energy eigenstates of the \( \hat{H}_0 \) carry momentum \( p = 0 \) or \( p = \pi \)

\[
T \mid \psi_n(h = 0, H) \rangle = \pm \mid \psi_n(h = 0, H) \rangle,
\]

where, \( T \) is translation operator and \( \{ \mid \psi_n(h = 0, H) \rangle \} \) are eigenstates of unperturbed Hamiltonian \( \hat{H}_0 \). Since the operator \( \sum_j (-1)^j S_j^z \) changes the momentum of the state by \( \pi \), we obtain that

\[
\langle \psi_n(0, H) \mid V \mid \psi_n(0, H) \rangle = 0
\]

Thus, the gap can be rewritten in the following form

\[
\Delta(N, h, H) = \Delta(N, 0, H) + g_1(N, H)h^2 + \cdots + g_n(N, H)h^{2n},
\]

where \( n \) is an integer. It is a good approximate to neglect the effect of higher order terms for \( h \leq 0.01 \). Because the second-order perturbation correction is not zero in the staggered field, the leading nonzero term is \( h^2 \). If the small-\( x \) behavior of the scaling function is defined as \( f(x) \sim x^{\phi_x} \), we find that

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

Let us consider the large-$N$ behavior of $g_1(N, H)$ at fixed $H$ as

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

This leads to

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

where $b_1(H)$ is a constant (at fixed $H$). We can write Eq. (19) in terms of the scaling variable $x$

$$N\Delta(N, h, H) \simeq A(H)(1 + N^{\nu(H)+1}x^{-\nu_h}) \quad (20)$$

For large-$N$ limit this equation should be independent of $N$, leading to the relation between $\mu(H)$ and $\nu(H)$ as

$$\nu(H) = \frac{2}{\mu(H) + 1} \quad (21)$$

The above arguments propose to look for the large-$N$ behavior of $g_1(N, H)$. To determine the $\mu(H)$ exponent, we have plotted in Fig.1 the following expression versus $N$

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

for fixed values of staggered field $h$ ($0.001 \leq h \leq 0.005$), and different sizes, $N = 12, 14, ..., 24$ at the uniform field $H = 0$. We found the best fit to our data for $\mu(H = 0) = 2.04 \pm 0.01$. The inset in Fig.1 shows the $g_1(N, H)$ versus $N$ at fixed $H = 0.05$. In this case, the best fit, found for $\mu(H = 0.5) = 2.33 \pm 0.01$. Our data for different $h$ values, fall perfectly on each other, which shows that our results for $g_1(N, H)$ in fixed uniform field $H$, are independent of the staggered field $h$ as expected. By using Eq. (21) we have found, $\nu(H = 0) = 0.66 \pm 0.01$ and $\nu(H = 0.05) = 0.60 \pm 0.01$. We have also implemented our numerical tool to calculate the critical exponent $\nu(H)$ at $H = 0.03, 0.07, 0.09$. The results have been presented in Table I.

IV. LARGE-X REGIME

In our numerical calculations because of memory issues, we were limited to consider the maximum chain length $N = 24$. Therefore the value of $x$ cannot be increased by increasing the size of chain. The problem appears if the calculation is done by density matrix renormalization group (DMRG) method. In that case, we may extend the calculation to larger sizes, $N \sim 200$, which cannot increase $x$ much larger than one (for $0.001 < h < 0.01$). On the other hand we may increase the staggered field for increasing $x$. But we should note that, in general there is usually level crossing between the energy levels in finite size systems. Which can change the behavior of the gap and lead to incommensurate effects. As an example, the dependences on the excitation energies of the three lowest levels on the
should be mentioned that if we choose another value for $\nu$ the plot will not be linear in $x$. Also, our data for different size chains fall perfectly on each other, which is expected from the scaling behavior.

We have extended our numerical computations to consider values of the uniform field in the small region $0 \leq H < 0.1$. The results have been presented in Table I. We have listed $\mu$, the resulting $\nu$, that is obtained from perturbative approach, and result of the large-$x$ regime $\nu_l$ for different values of the uniform field $H$. In Fig.4 we have plotted the critical exponent $\nu(H)$ versus the uniform field $H$. As it is clearly seen from this figure, $\nu_s$ and $\nu_l$ start at the known value $\frac{2}{5}$ and then drop with the increasing uniform field $H$. The exponent are in good agreement with each other and show good agreement with the exponent derived in the field theoretical approach (Eq.(6)). The inset in Fig.4 shows the H-dependence of the critical exponent $\nu$ which is obtained directly by extrapolating the numerical results of the energy gap in the range of the staggered field $0.001 \leq h \leq 0.01$.

On the other hand, Fouet et.al studied the gap induced by the staggered field $H_c$ at the saturation uniform field $H_c = 2J$. Using field theoretical arguments, they found that the gap scales as $\Delta(h, H_c) \sim h^\nu$. By applying the DMRG method for system sizes up to $N = 100$, they have also computed the exponent of the energy gap $\nu(H_c) = 0.81$. We have extended our numerical computations to consider the uniform field at the saturation value $H_c$. In this case, we have obtained, $\nu_s(H_c) = 0.78$ and $\nu_l(H_c) = 0.82$ in good agreement with the Poet results.

### V. CONCLUSIONS

In this paper, we have studied the energy gap of the 1D AF-Heisenberg model in the presence of both uniform ($H$) and staggered ($h$) magnetic fields using the exact diagonalization technique. We have implemented the modified Lanczos method to obtain the excited state energies with the same accuracy as the ground state one. We have been limited to a maximum of $N = 24$, because of memory considerations. We have shown, if the energy gap in the thermodynamic limit had been obtained by extrapolating the numerical results for finite systems, then the behavior of the gap may deviate from the predicted scaling behavior. This deviation depends on the range of the staggered magnetic field ($h$). We have found in the range of very small values of the staggered magnetic field ($0.001 \leq h \leq 0.01$), the values of the energy gap coming from a finite system basically represent the perturbative behavior. We have shown that in this range of the staggered magnetic field, we are not allowed to read the scaling exponent of the energy gap directly from the

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**TABLE I:** The exponent of $\nu_s(N,H)$ and gap exponent versus different values of the uniform field $H$ in small-$x$ and large-$x$ regimes.

| $H$   | $\mu$ | $\nu_s$ | $\nu_l$ |
|-------|-------|---------|---------|
| 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    |

staggered field $h$ ($0.01 \leq h \leq 0.4$) are shown in Fig.2 for $N = 24$ and $H = 0$. From this figure, it can be seen that the two lowest excited states do not cross each other in this case. This means that we can increase the value of $x$ by increasing $h$ up to $h = 0.4$. Since that the regime where we can observe the right scaling of the gap is in very small value of $h$, we have restricted our numerical computations to upper limit of staggered field $h = 0.4$. In this respect, we have performed some numerical computations on the Hamiltonian Eq.(1) for large-$x$ values, and the results are plotted in Fig.3. In this figure the range of the staggered field is $0.04 \leq h \leq 0.4$, which causes that we get large-$x$ values for the considered chain lengths $N = 18, 20, 22, 24$ and $H = 0$. The inset in Fig.3 shows $N\Delta(N,h,H)$ versus $x = Nh^{\nu(H)}$ at fixed uniform field $H = 0.05$. In this case, we have obtained, $\nu(H = 0) = 0.66$ and $\nu(H = 0.05) = 0.63$. It should be mentioned that if we choose another value for $\nu$.
extrapolated numerical results.

We have applied a general finite size scaling procedure for investigating the $H$-dependence of the critical exponent of the gap. We have identified two regimes through which the real critical exponent $\nu(H)$ can be numerically calculated. To find the correct exponent of the gap in small-$x$ regime ($x = Nh^{\nu(H)} \ll 1$), we have used the scaling behavior of the coefficient of the leading term in the perturbation expansion, which is introduced by authors in Ref.[25]. In the large-$x$ regime using the standard finite size scaling Eq.(13), we have computed the correct critical exponent. On the other hand, using the conformal estimates of the small perturbation ($h \ll 1$), we have found the $H$-dependence of the critical exponent (Eq.(6)) from the theoretical point of view. Our numerical results in both regimes are in well agreement with the results obtained by the theoretical and numerical approaches.

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