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Numerical Analysis of Spin-1/2 Alternating Heisenberg-XY Antiferromagnet in One Dimension

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The spin-1/2 alternating Heisenberg model with XY-like anisotropy is studied by numerical methods. This model exhibits critical behavior in the ground state as the bond-alternation parameter δ approaches 0. The critical exponents characterizing this ground-state critical point are estimated. The results agree well with those of the analytical calculation of Nakano and Fukuyama. A logarithmic correction of the type predicted by Black and Emery is found to be consistent with numerical data in the isotropic Heisenberg model but not in anisotropic models.

§1. Introduction

The spin degree of freedom of the organic compounds which fall into the spin-Peierls state at low temperatures is described by the one-dimensional alternating spin-1/2 Heisenberg model.[1] The ground state properties of this system attract strong attention[1] because a critical phenomenon is observed as the rate of bond alternation δ approaches 0. The quantities of current interest are the critical exponents a, b and ν which describe, respectively, the behavior of the ground-state energy, energy gap and correlation length near the critical point $\delta=0$. In the case of the isotropic Heisenberg model, analytical calculations[2-4] suggest $a=4/3$ and $b=\nu=2/3$ (possibly with logarithmic corrections[5]). Various numerical estimates fall close to these values.[6] If the interaction is of the form of the XY model, one can solve it exactly even in the presence of a finite bond alternation,[7] leading to the critical exponents $a=2$ (with logarithmic correction), $b=1$ and a power decay of the correlation function. When the exchange anisotropy lies between the XY and isotropic Heisenberg models, the method of phase Hamiltonian introduced by Nakano and Fukuyama (NF)[8] predicts a smooth interpolation of exponents between both limits (without logarithmic corrections). The Ising-like exchange anisotropy causes competition between the Néel state and the singlet-pair dominated state.[9]

In this situation we have investigated the systems with XY-like anisotropy by numerical methods to test the theoretical predictions of NF and others. The largest system size we have treated is $N=20$ and the data were analyzed by finite-size scaling and extrapolation techniques. A detailed description of our method of analysis is given in ref. 6 where the isotropic Heisenberg model is discussed. In the present work particular attention has been paid to the possible existence of logarithmic corrections to the critical exponents. We have found that the logarithmic corrections of the type of those predicted by Black and Emery[5] are limited, if any, to the isotropic Heisenberg model. The logarithmic corrections similar to that in the XY model are not likely to persist in the intermediate region between the XY and isotropic models. In this region only pure power singularities (no logarithmic corrections) exist in the relevant physical quantities, and the critical exponents assume very close values to those given by NF.

In the next section numerical data are presented and analyzed by finite-size scaling and extrapolation methods. In §3 the results are discussed and conclusions are given.

§2. Numerical Analysis

The Hamiltonian of our interest is

$$H=J\sum_j [1+(-1)^j\delta](S_j^xS_{j+1}^x+S_j^yS_{j+1}^y+\Delta S_j^zS_{j+1}^z). \quad (J>0,\ 0\leqslant\delta\leqslant 1,\ 0\leqslant\Delta\leqslant 1) \tag{1}$$

We have calculated numerically the ground-state energy $E_0(N, \delta)$ and the first excited state energy $E_1(N, \delta)$ using the computer program written by one of the authors (H. N.) and Taguchi.[10] The system size ranges from $N=8$ to $N=20$ (even numbers), and 23 values of δ were chosen ($\delta=0$, 0.001, $\cdots$, 0.8). The anisotropy parameter takes $\Delta=0.1$, 0.2, 0.3, $\cdots$, 1.0.

In the present model (1) the correlation function at $T=0$ has a power-low decay[11] if $\delta=0$, whereas an exponential decay is expected when $\delta>0$ because of formation of effective singlet pairs between pairs of sites with stronger interaction $J(1+\delta)$. Thus $\delta=0$ is regarded as a critical point. The critical exponents a, b and ν to be determined are defined as

$$\lim_{N\to\infty} G(N, \delta)\sim\delta^a, \tag{2}$$

$$\lim_{N\to\infty} \varepsilon_g(N, \delta)\sim\delta^b, \tag{3}$$

and

$$\xi\sim\delta^{-\nu},$$

where G denotes the energy gain per spin, ε_g is for the energy gap and ξ represents the correlation length:

$$G(N, \delta)=[E_0(N, 0)-E_0(N, \delta)]/N,$$

$$\varepsilon_g(N, \delta)=E_1(N, \delta)-E_0(N, \delta).$$

It is useful to employ the method of finite-size scaling to determine critical exponents from finite-size data.[12] As described in ref. 6 the hypothesis of finite-size scaling reads, in the present context, that G and ε_g have scaling forms as

$$G(N, \delta)\sim N^{-a/\nu}g(N\delta^\nu), \tag{4}$$

$$\varepsilon_g(N, \delta)\sim N^{-b/\nu}f(N\delta^\nu), \tag{5}$$

where g and f are universal scaling functions. To use eq. (4) (or eq. (5)) we adjust the values of critical exponents so that the finite-size data fall in a single curve described by eq. (4) (or eq. (5)). Although there appear two exponents in both eqs. (4) and (5), it is possible to adjust parameters (exponents) one by one if we make use of data on $\varepsilon_g(N, 0)$ as well as the fact that $\varepsilon_g(N, 0)\sim N^{-1}$.[6] (Thus we do not have to adjust two parameters simultaneously.) In Figs. 1 and 2 we show the scaling plots of G and ε_g in the case of $\Delta=0.5$ as representative examples. The resulting values of critical exponents as functions of δ are displayed in Fig. 3 (exponent a) and Fig. 4 (ν). The exponent b agrees with ν within 3% errors as long as $\Delta\leq 0.9$. (Remember that one expects $b=\nu$ from the size dependence of gap ε_g at $\delta=0$.[6])

An alternative method of analysis of finite size data is a simple extrapolation to the limit $N\to\infty$ following the assumption

$$G(N, \delta)\sim G(\infty, \delta)+c_1/N+c_2/N^2. \tag{6}$$

We have analyzed only the energy gain by ex-

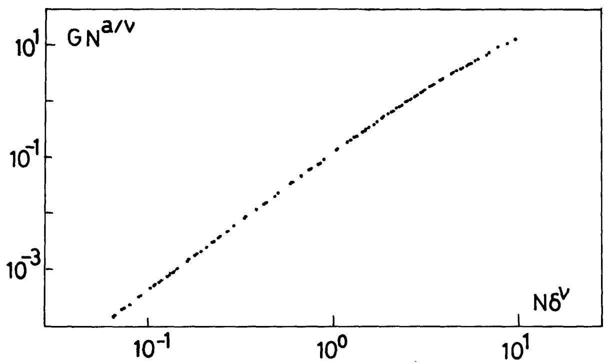

Fig. 1. The scaling plot of the energy gain $G(N, \delta)$ multiplied by $N^{a/\nu}$ as a function of $N\delta^\nu$. The anisotropy is $\Delta=0.5$. The exponents are $a=1.40$ and $\nu=0.81$.

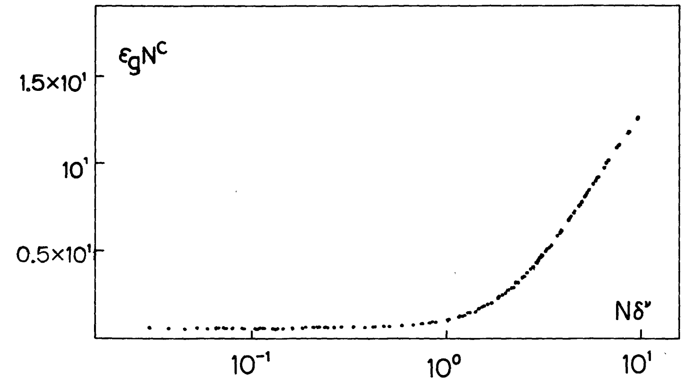

Fig. 2. The scaling plot of the energy gap $\varepsilon_g(N, \delta)$ multiplied by N^c $(=N^{b/\nu})$ as a function of $N\delta^\nu$. Here $\Delta=0.5$ and the exponents are $b=\nu=0.81$.

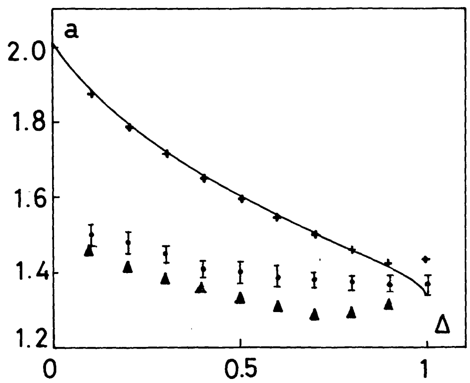

Fig. 3. The energy gain exponent a as a function of the anisotropy Δ. The finite-size scaling with the pure power assumption in eq. (4) yields the results written with error bars. The extrapolation method (6) gives the values denoted by solid triangles. The scaling hypothesis with lower order contribution numerically eliminated leads to the estimation represented by +. The solid curve is the prediction by NF.

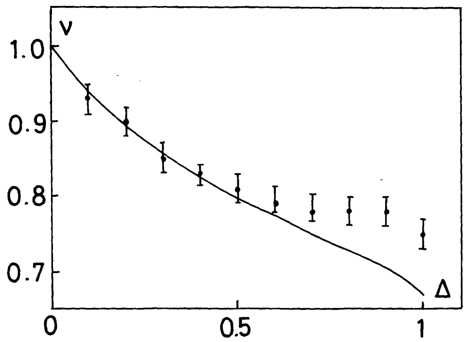

Fig. 4. The gap exponent ν given by the finite-size scaling analysis. The method of phase Hamiltonian[4,8] yields the solid curve.

trapolation (6) because the gap data for $N\leq 20$ do not have converged well enough to fit extrapolation formulas like eq. (6). In applying eq. (6) it is important to note the range of applicability of the extrapolation method. If we choose too small δ, finiteness of the system masks the infinite-size properties. A rough criterion for the validity of extrapolation is $N>\xi$ (the infinite-system correlation fits in the finite size system), or in other words $\delta^\nu > N^{-1}$. In Fig. 5 the extrapolated data $G(\infty, \delta)$ are shown as a function of δ in a log-log scale in the case of $\Delta=0.5$. It is apparent that we should accept $a=1.33$ instead of the small-δ result of $a=1.99$ $(=2.0)$. The latter value apparently reflects finite-size effects. (A simple perturbation with respect to δ is always valid if N is finite, leading to $G(N, \delta)$ proportional to δ^2 as will be discussed later.) The resulting value of a as a function of Δ is shown in Fig. 3 by ▲. The extrapolation and finite-size scaling methods yield very close values of the exponent a as seen in Fig. 3. An unexpected feature observed in Fig. 3 is a jump of a from $a=1.5$ at $\Delta=0.1$ to $a=2$ (with logarithmic correction) at $\Delta=0$, the latter being an exact result.[7] This point will be discussed later in relation to a logarithmic correction at $\Delta=0$.

It is interesting to check the existence of a logarithmic correction to critical properties at $\Delta=1$ as predicted by Black and Emery:[5]

$$G(\infty, \delta)\sim\delta^{4/3}/|\log\delta|, \tag{7}$$

$$\varepsilon_g(\infty, \delta)\sim G(\infty, \delta)^{1/2}. \tag{8}$$

Spronken, Fourcade and Lepiné[13] (SFL) used

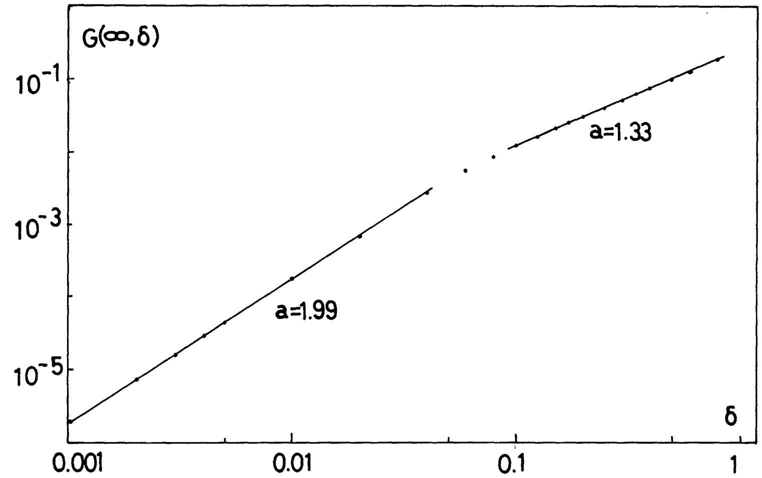

Fig. 5. The extrapolated energy gain $G(\infty, \delta)$ as a function of δ in a log-log scale. Two regions of $G(\infty, \delta)\sim\delta^{1.99}$ and $\sim\delta^{1.33}$ are clearly distinguished.

a finite-size scaling hypothesis consistent with the renormalization group equation of Black and Emery in order to analyze their numerical data up to $N=18$. They conclude that the logarithm-corrected forms (7) and (8) are more plausible than the simple power laws (2) to (5). We have used the same scaling hypothesis as SFL

$$G(N, \delta)\sim N^{-2}g(\delta^{\nu}N\sqrt{l_0/(l_0+\log N)}), \quad (9)$$

$$\varepsilon_g(N, \delta)\sim G(N, \delta)^{1/2}, \quad (10)$$

to see if our data of $N\leq 20$ satisfy these scaling forms in the range $0<\Delta\leq 1$ assuming that ν in eqs. (9) and (10) takes the value predicted by NF using the method of phase Hamiltonian[8] (*e.g.* $\nu=2/3$ for $\Delta=1$). When $\Delta=1$, we found a good fit of our data to eqs. (9) and (10) to the same degree of accuracy as in the case of the pure power scaling (4) and (5) with $a=1.37$ and $\nu=0.75$.[6] The parameter l_0 is found to assume 10 for the gain (9) and $l_0=0.5$ for the gap (10). The difference between $l_0=10$ for the gain and $l_0=0.5$ for the gap may be attributed to the fact that either the gain or gap data approach the critical scaling region faster as N is increased than the other data do. As soon as Δ is decreased from 1, the logarithm-corrected scaling (9) and (10) fails to explain the finite-size data if we use NF's ν.[8] More precisely, the gain data cannot be accomodated by eq. (9) for any value of l_0 if $\Delta\leq 0.9$ and the gap data are found to be consistent with eq. (10) with large l_0 (*e.g.* $l_0>10$ if $\Delta=0.6$). This inconsistency of the gain and gap results invalidates the assumption that both scaling forms (9) and (10) are simultaneously satisfied. Therefore, we believe, the logarithmic correction of the Black-Emery type (7) and (8) is not present when $\Delta<1$. We should remember here that SFL claim that their data for $\Delta=1$ did not satisfy the pure-power scaling, which they regard as evidence for the stronger plausibility of the Black-Emery logarithmic correction than the pure power law. But we did observe an excellent fit to the pure power law in the same situation, as explained in ref. 6. The origin of difference between us and SFL seems twofold. The first one is that we have treated N up to 20 in contrast to their 18. But this may not be essential because our analysis was not noticeably modified when we excluded the data of $N=20$. The second and more important difference is in the boundary condition. Our system has a periodic boundary in terms of spin variables while SFL used a slightly modified boundary condition in terms of a Fermion representation of the present system. They have shown that their boundary condition yields excellent results when $\Delta=0$ (*XY* model), but nothing is guaranteed in the case of $\Delta=1$. A possible origin of their failure to adjust their data to the pure power scaling (2) to (5) (while we succeeded in it) is that their boundary puts the finite size system farther away from the asymptotic scaling region than the simple periodic boundary condition does. It is thus impossible to rule out the pure power behavior when $\Delta=1$ as long as the degree of fit of finite size data to scaling is concerned. The only clear point is that the logarithmic correction of the type of eqs. (7) to (10) fails to explain the data for $\Delta<1$. We point out here the impossibility to detect the logarithmic corrections by the method of simple extrapolation such as eq. (6). It is necessary to use very small values of δ to verify the existence of a logarithmic term, which is beyond the capability of extrapolation method as explained before. In this regard we cannot accept the claim of Soos *et al.*[14] that they have confirmed the Black-Emery form (7). Further discussions on this point are given in ref. 6.

It is also impossible to detect the logarithmic correction of the type of the XY model[7]

$$G(\infty, \delta)\sim\delta^2|\log\delta|, \tag{11}$$

by extrapolation. For the XY model ($\Delta=0$) the exact solution is available even if the system size is finite.[13] From the exact solution of a finite system we have checked what size N is necessary to detect the logarithmic correction (11) by extrapolation. The result was of the order of 1000. Therefore one should not try to check the possible existence of the XY-type logarithmic corrections by extrapolation in the case of $\Delta>0$ from finite-size data as long as $N\ll 1000$.

An apparent and serious problem of our result in Fig. 3 is the discontinuity of a at $\Delta=0$ as noted before. A possible reason is the effect of logarithmic correction (11) in the XY model. This point can be clarified in the following example. The present model reduces to the massive Thirring model in certain approximation as pointed out by NF. The exact solution of the massive Thirring model by Bergknoff and Thacker reads (see ref. 8) in the limit of small Δ,

$$G(\infty, \delta)\sim\Delta^{-1}(\delta^{4\Delta/\pi}-1)\delta^2. \tag{12}$$

If one takes the limit $\Delta\to 0$ first, eq. (12) reproduces the logarithmic correction in the XY model ($\Delta=0$) as in eq. (11) while the change of the order of limits ($\delta\to 0$ and then $\Delta\to 0$) yields asymptotic pure power behavior

$$G(\infty, \delta)\sim\Delta^{-1}\delta^2. \tag{13}$$

In this argument it is important to treat the term of lower order in eq. (12) appropriately in the neighborhood of $\Delta\sim 0$ and $\delta\sim 0$. However numerical values of the leading term δ^2 and the next term $\delta^{2+4\Delta/\pi}$ are almost of the same order of magnitude for small (but not too small) δ and Δ, and it is difficult to extract only the leading order contribution from the numerical data. A result of simple analysis of raw data could thus be a wrong estimation of the exponent of the leading singularity. To avoid this sort of difficulties we used the following method so that only the leading order term is observed. If the system size is finite, it is possible to apply a simple perturbation theory with respect to δ to the ground state energy. Since the system is invariant by the change of sign of δ, we have even powers of δ:

$$G(N, \delta)\sim A(N)\delta^2+B(N)\delta^4+\cdots. \tag{14}$$

On the other hand the asymptotic scaling form is postulated as eq. (4). Agreement of eqs. (14) and (4) in the limit $\delta\to 0$ (N finite) is achieved if we assume that $g(N\delta^\nu)$ in eq. (4) behaves as $(N\delta^\nu)^{2/\nu}$ for small $N\delta^\nu$ because, then,

$$G(N, \delta)\sim N^{-a/\nu}(N\delta^\nu)^{2/\nu}=N^{(2-a)/\nu}\delta^2. \tag{15}$$

A comparison of eqs. (14) and (15) gives the asymptotic behavior of $A(N)$ as $N^{(2-a)/\nu}$ for large N. Taking account of the effects of finiteness of N, we may assume

$$A(N)\sim a_1N^{(2-a)/\nu}+a_2+a_3/N. \tag{16}$$

Hence, by extracting only the leading order term $a_1N^{(2-a)/\nu}$ in the coefficient $A(N)$, we can eliminate the effects of correction to the asymptotic scaling (4). This idea has been implemented by fitting the data of $N=14$, 16, 18 and 20 to eq. (16) to determine the parameters a_1, a_2, a_3 and $(2-a)/\nu$. We have used the value of ν derived by the method of phase Hamiltonian[4,8] to determine a from $(2-a)/\nu$. The result is shown in Fig. 3. Surprisingly excellent agreement with the prediction of NF on a is obtained. Almost the same result on a was derived when we used the value of ν from our finite size scaling estimation (Fig. 4). Therefore we conclude that the jump of a from 2 ($\Delta=0$) (exact) to 1.5 ($\Delta=0.1$) (numerical) is a consequence of non-negligible contribution of corrections of lower order to scaling. The assumption of pure power behavior with the NF values of the critical exponents explains the numerical data quite well in the range $0<\Delta<1$. Slight deviation of our predictions on exponents from the NF values near $\Delta=1$ may be attributed to the logarithmic correction of the type of Black and Emery.[5] At present we have no method to remove systematically lower order corrections to scaling in the neighborhood of the point where the Black-Emery logarithmic correction is present. The reason is that the energy gap has also a logarithmic correction in the Black-Emery case but our gap data are not accurate enough to allow an analysis as above.

§3. Summary

We have numerically calculated the ground state energy and the first excited state energy of the Hamiltonian (1). The finite-size scaling and extrapolation techniques were used to determine critical exponents from the obtained data. If we assume the simple power law behavior (2) and (3) both methods of analysis give consistent results as seen in Fig. 3. The assumption of the existence of logarithmic correction of the type of eqs. (7) to (10) is consistent with numerical data only when $\Delta=1$. The XY-type logarithmic correction (11) cannot be detected in straightforward analysis because of the smallness of N (≤ 20). In the neighborhood of $\Delta=0$, contribution from correction-to-scaling terms is significant, and we developed a method to extract only the leading order singularity from finite size data. The results indicate that the simple pure power behavior predicted by NF is consistent with numerical data if $0<\Delta<1$.

Thus a most plausible picture we have obtained in this work is as follows. The XY-type logarithmic correction (11) is restricted to the pure XY model. In the intermediate region $0<\Delta<1$ the system follows the pure power behavior with exponents quite close to those of NF. The logarithmic correction of the type of Black and Emery may be present only at $\Delta=1$. We cannot decisively rule out a pure power behavior at $\Delta=1$. If a pure power assumption at $\Delta=1$ is correct, the values of exponents are slightly deviated from those of NF in the neighborhood of $\Delta=1$.

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