Prog. Theor. Phys. Vol. 73, No. 6, June 1985, Progress Letters

One-Dimensional Critical Exponent η as a Function of the Spin Quantum Number and Anisotropy

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(Received February 7, 1985)

The critical exponent η is calculated to order $1/S^2$ from the classical limit for the one-dimensional quantum anisotropic Heisenberg antiferromagnet at $T=0$. η of the transverse correlation function depends explicitly on S and anisotropy. Implications of the resulting values are discussed.

The correlation function of the spin-1/2 one-dimensional Heisenberg antiferromagnet

$$H=J\sum(S_j^xS_{j+1}^x+S_j^yS_{j+1}^y+\Delta S_j^zS_{j+1}^z)\qquad (J>0,\ 0\leq\Delta<1) \tag{1}$$

is known[1),2)] to decay by power laws at $T=0$:

$$\langle S_j^xS_{j+r}^x\rangle\sim(-1)^r r^{-\eta_x},\quad \eta_x=1-\mu/\pi \tag{2}$$

$$\langle S_j^zS_{j+r}^z\rangle\sim(-1)^r r^{-\eta_z},\quad \eta_z=(1-\mu/\pi)^{-1} \tag{3}$$

where $\cos\mu=\Delta$, $0<\mu\leq\pi/2$. On the other hand, in the classical limit $S\to\infty$, the same system (1) has a long-range order in the XY-plane; the transverse correlation (2) does not decay (which may be regarded as $\eta_x=0$) and the longitudinal correlation (3), normalized by S^2, identically vanishes. These two extreme cases, $S=1/2$ and ∞, suggest an explicit dependence of η on S. In fact, for $S\gg1$, Villain[3)] developed a spin wave theory to calculate η to order $1/S$ when $\Delta=0$. His result

$$\eta_x=-1/\sqrt{2}\pi S\,, \tag{4}$$

$$\eta_z=2 \tag{5}$$

is in good agreement with the exact values (2) and (3) if we set $S=1/2$ in (4). However he derived (4) and (5) with the aid of an uncontrolled decoupling approximation and did not estimate higher order corrections (order $1/S^2$ and higher) to (4) and (5). In the present paper we apply an enhanced version[4)] of his spin wave theory to obtain η_x to order $1/S^2$ for general Δ. η_z is found not to depend on $1/S$ or Δ and has the universal value of two as in (5). It should be mentioned that we have failed to prove exactness of our estimates of coefficients in the expansion of η_x by $1/S$. Nevertheless there are reasons to believe that our values are accurate (possibly exact) as will be noted. A major physical interest in the dependence of η_x on S and Δ comes from Haldane's predictions[5)~12)] on the ground-state properties of the present model (1). Among other assertions he maintains that, if S is an integer, the transverse correlation function at $T=0$ decays by power laws for $0\leq\Delta\leq\Delta_c$ with $\Delta_c<1$. Beyond Δ_c this correlation has an exponential decay, which continues to Δ larger than 1. At Δ_c, η_x takes the value 1/4. Our explicit expression of η_x as a function of S and Δ allows us to determine Δ_c by the criterion $\eta_x(\Delta_c)=1/4$.

In a previous paper[4)] we developed an enhanced version of Villain's spin wave theory.[3)] We calculated the ground-state energy of (1) (and of higher dimensional systems) to order $1/S^2$. To obtain the ground-state energy we had to derive an expression for the nearest neighbor correlation function. The same method applies to an arbitrary two-spin correlation function and we find

$$\langle S_j^xS_{j+r}^x\rangle=\langle S_j^yS_{j+r}^y\rangle=\frac{1}{2}\left(S+\frac{1}{2}\right)^2(-1)^r\Lambda_\perp[\Xi_r(\lambda_1,\lambda_2,1)]. \tag{6}$$

$\Lambda_\perp$ is an integral operator with the kernel of the Bessel function

$$\Lambda_\perp[f(\lambda_1,\lambda_2)]=\int_{-\infty}^{\infty}\frac{d\lambda_1}{2\lambda_1}J_1(\lambda_1)\int_{-\infty}^{\infty}\frac{d\lambda_2}{2\lambda_2}J_1(\lambda_1)f(\lambda_1,\lambda_2) \tag{7}$$

and

$$\Xi_r(\lambda_1,\lambda_2,1)=\exp\Big[-\frac{1}{2S+1}\frac{1}{N}\sum_k\{(1-\cos kr)/C_k+C_k(\lambda_1^2+\lambda_2^2-2\lambda_1\lambda_2\cos kr)/2\}\Big]. \tag{8}$$

The variational parameter C_k should be expanded to order $1/S$ to obtain the correlation (6) to order $1/S^2$:

$$C_k=\left(\frac{1-\cos k}{1+\Delta\cos k}\right)^{1/2}\times\left\{1-\frac{2J_1-\Delta J_3}{4S}+\frac{(\Delta+\cos k)J_3}{4S(1+\Delta\cos k)}\right\},\tag{9}$$

where the lattice sums

$$J_1=\frac{1}{N}\sum_k\sqrt{(1-\cos k)(1+\Delta\cos k)}\ ,$$

$$J_3=\frac{1}{N}\sum_k\cos k\sqrt{(1-\cos k)/(1+\Delta\cos k)}\tag{10}$$

should not be confused with the Bessel functions. In one-dimension J_1 and J_3 can be evaluated explicitly:

$$J_1=\frac{2\sqrt{\Delta}}{\pi}\left\{\sqrt{1+a}+a\log(1+\sqrt{1+a})-\frac{1}{2}a\log a\right\},$$

$$J_3=\frac{2}{\pi\sqrt{\Delta}}\left\{\sqrt{1+a}-(1+a)\log(1+\sqrt{1+a})+\frac{1}{2}(1+a)\log a\right\},\tag{11}$$

where $a=(1-\Delta)/2\Delta$. To find out the asymptotic form of the correlation function (6) as $r\to\infty$ for large S, we first keep r finite and expand (6) in powers of $1/S$ to order $1/S^2$:

$$A_r\equiv\Lambda_\perp[\Xi_r(\lambda_1,\lambda_2,1)]=1-F_1(r)-2F_2+\frac{1}{2}F_1(r)^2+2F_1(r)F_2-2F_2{}^2+\frac{1}{2}F_3(r)^2\ ,\tag{12}$$

where

$$F_1(r)=\frac{1}{2S+1}\frac{1}{\pi}\times\int_0^\pi dk(1-\cos kr)\left(\frac{1+\Delta\cos k}{1-\cos k}\right)^{1/2}\times\left\{1+\frac{2J_1-\Delta J_3}{4S}-\frac{(\Delta+\cos k)J_3}{4S(1+\Delta\cos k)}\right\},$$

$$F_3(r)=\frac{1}{2S+1}\frac{1}{\pi}\int_0^\pi dk\cos kr\left(\frac{1-\cos k}{1+\Delta\cos k}\right)^{1/2}\times\left\{1-\frac{2J_1-\Delta J_3}{4S}+\frac{(\Delta+\cos k)J_3}{4S(1+\Delta\cos k)}\right\}.\tag{13}$$

F_2 is a constant (independent of r) and does not play a role in the following. As r tends to infinity, the function $F_1(r)$ diverges logarithmically

$$F_1(r)\sim\frac{\sqrt{1+\Delta}}{\sqrt{2}\pi S}\left\{1-\frac{1-J_1}{2S}-\frac{(1+\Delta)J_3}{4S}\right\}\log r\ ,\tag{14}$$

while $F_3(r)$ approaches a finite value. Hence, collecting the divergent terms in (12), we obtain

$$A_r\sim\exp\log\left\{1-F_1(r)+\frac{1}{2}F_1(r)^2+2F_1(r)F_2-2F_2\right\}\sim\exp\left\{-F_1(r)+\frac{1}{2}F_1(r)^2+2F_1(r)F_2-\frac{1}{2}(F_1(r)+2F_2)^2\right\}\sim\exp\{-F_1(r)\}.\tag{15}$$

We are now ready to derive the exponent η_x from (6), (12), (14) and (15):

$$\langle S_j^xS_{j+1}^x\rangle\sim\left(S+\frac{1}{2}\right)^2A_r\sim\left(S+\frac{1}{2}\right)^2r^{-\eta_x}$$

with

$$\eta_x=\frac{\sqrt{1+\Delta}}{\sqrt{2}\pi S}-\frac{\sqrt{1+\Delta}}{2\sqrt{2}\pi S^2}\left\{1-J_1+\frac{1}{2}(1+\Delta)J_3\right\}.\tag{16}$$

When $\Delta=0$, the first term on the right-hand side of (16) agrees with the corresponding result of Villain (4). The values of η_x for $S=1/2$ and $S=1$ are drawn in Figs. 1 and 2 as functions of Δ. The second order estimate (16) for $S=1/2$ is seen to agree well with the exact value (2). We notice the logarithmic divergence of the second order estimate at $\Delta=1$. This divergence may be attributed to the breakdown of the XY-like picture, from which we developed the enhanced spin wave theory,[4] at the isotropic limit $\Delta=1$.

It has been shown by Miyake[13] that the expansion coefficients to order $1/S^2$ of the ground-state energy by the present method are exact if the dimensionality exceeds one (except

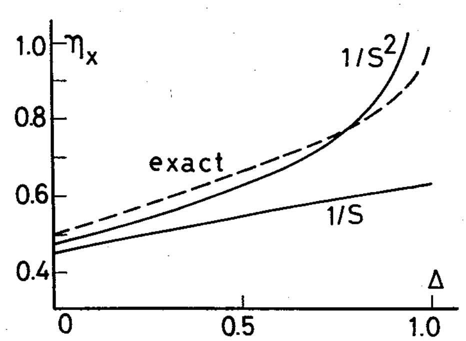

Fig. 1. The anisotropy dependence of the critical exponent η_x for $S=1/2$. If we truncate the formula (16) at the first order term, we obtain the line denoted as $1/S$. The full expression (16) yields the curve marked $1/S^2$. The exact value is drawn in a dashed line.

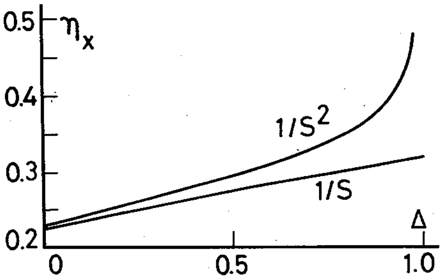

Fig. 2. The same exponent η_x as in Fig. 1 is plotted for $S=1$. The symbols $1/S$ and $1/S^2$ imply the order of expansion as in Fig. 1.

for non-bipartite lattices). Although a proof is lacking, it is reasonable to expect the same conclusion for a linear chain as well as for the expansion coefficients of an arbitrary correlation function (16). In addition, if $S\geq 1$, the good agreement of our result with the exact value for $S=1/2$ as in Fig. 1 supports the reliability of the value of η_x estimated from (16) (the expansion by $1/S$ would give better values for larger S).

Let us turn to an interesting consequence of the expansion (16). Haldane[5)~12)] has predicted that the spin wave picture (with gapless excitations) breaks down at Δ_c between 0 and 1 if S is an integer. The exponent η_x is supposed to assume $1/4$ at Δ_c. Beyond Δ_c the correlation function decays exponentially. We apply our result (16) to the determination of Δ_c by the criterion $\eta_x(\Delta_c)=1/4$. (Remember that the spin wave results are valid in the interval $0\leq\Delta\leq\Delta_c$ *including* Δ_c.) We find $\Delta_c=0.1528$ for $S=1/2$, $\Delta_c=0.9997$ for $S=2$, and the critical Δ monotonically approaches 1 as S increases. The asymptotic form for large S is

$$\Delta_c=1-\exp(-\pi^2S^2/2).$$

It may seem strange for η_x to assume $1/4$ when S is large: $1/S$ and $1/S^2$ in (16) are small numbers if S is large enough. However, J_3 in the coefficient of $1/S^2$ diverges as $\Delta\to 1$, which compensates for the smallness of $1/S^2$.

It is straightforward to apply the present method to the longitudinal correlation function to prove

$$\langle S_j^z S_{j+1}^z\rangle\sim Sr^{-2} \tag{17}$$

to the same accuracy as (16). The exponent does not depend on S or Δ. The classical limit is achieved by dividing (17) by S^2:

$$S^{-2}\langle S_j^z S_{j+1}^z\rangle\sim S^{-1}r^{-2}\to 0\,.$$

(We set $S\to\infty$ first and then $r\to\infty$.) The exact expression (3) for $S=1/2$ shows η_z varies from 2 ($\Delta=0$) to 1 ($\Delta=1$). Although our result (17) gives the constant value two, this fact should not be regarded as a fatal deficiency of the present method: Our XY-like picture, from which we developed a spin wave theory,[4)] breaks down near $\Delta=1$. (In the case of η_x, the exponent diverges at $\Delta=1$!)

Critical reading of the manuscript by Professor S. J. Miyake is gratefully acknowledged.

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