One-Dimensional Critical Exponent $\eta$
as a Function of the Spin Quantum Number and Anisotropy

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The critical exponent $\eta$ is calculated to order $1/S^2$ from the classical limit for the one-dimensional quantum anisotropic Heisenberg antiferromagnet at $T=0$. $\eta$ 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

$$H=J\Sigma(S_i \cdot S_{i+1} + S_i \cdot S_{i+2} + D S_i \cdot S_{i+1})$$

($J>0, 0<\Delta<1$) (1)

is known\textsuperscript{1-3} to decay by power laws at $T=0$:

$$\langle S_i \cdot S_{i+1} \rangle \sim (-1)^{r-r_i} , \quad \eta_x = 1 - \mu/\pi$$

(2)

$$\langle S_i \cdot S_{i+2} \rangle \sim (-1)^{r-r_i} , \quad \eta_z = (1 - \mu/\pi)^{-1}$$

(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 $\infty$, suggest an explicit dependence of $\eta$ on $S$.

In fact, for $S=1$, Villain\textsuperscript{10} developed a spin wave theory to calculate $\eta$ to order $1/S$ when $\Delta = 0$. His result

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

(4)

$$\eta_z = 2$$

(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\textsuperscript{9} of his spin wave theory to obtain $\eta_x$ to order $1/S^2$ for general $\Delta$. $\eta_z$ is found not to depend on $1/S$ or $\Delta$ 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 $\eta_x$ 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 $\eta_x$ on $S$ and $\Delta$ comes from Haldane's predictions\textsuperscript{9-12} 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 $0<\Delta<\Delta_c$ with $\Delta_c < 1$. Beyond $\Delta_c$, $\eta_x$ takes the value $1/4$. Our explicit expression of $\eta_x$ as a function of $S$ and $\Delta$ allows us to determine $\Delta_c$ by the criterion $\eta_x(\Delta_c) = 1/4$.

In a previous paper\textsuperscript{9} we developed an enhanced version of Villain's spin wave theory.\textsuperscript{9} 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

$$\langle S_i \cdot S_{i+1} \rangle = \langle S_i \cdot S_{i+1} \rangle$$

$$= \frac{1}{2} (S + 1)^2 (-1)^{r-r_i} \Lambda_x \Xi(\lambda_1, \lambda_2, 1).$$

(6)

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

$$\Lambda_x[f(\lambda_1, \lambda_2)] = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d\lambda_1}{2\lambda_1} \frac{d\lambda_2}{2\lambda_2} f(\lambda_1) f(\lambda_2)\phantom{1/s^2}$$

(7)

and

$$\Xi(\lambda_1, \lambda_2, 1) = \exp \left[ -\frac{1}{2S+1} \frac{1}{N} \sum_{k=1}^{N} \left( 1 - \cos k r \right) \right].$$

(8)

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

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

\[ J_3 = \frac{2}{\pi \sqrt{\Delta}} \left[ \sqrt{1 + a} - (1 + a) \log(1 + \sqrt{1 + a}) \right. \]

\[ + \left. \frac{1}{2} (1 + a) \log a \right], \tag{11} \]

where \( a = (1 - \Delta)/2\Delta \). To find 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 \( 1/S^2 \):

\[ A_\tau \sim \exp \left[ -\frac{1}{2} F_0(r) + \frac{1}{2} F_1(r)^2 \right] \]

\[ + 2 F_1(r) F_{-2} - 2 F_{-2} \]

\[ - \exp \left[ -\frac{1}{2} F_0(r) + \frac{1}{2} F_1(r)^2 + 2 F_1(r) F_{-2} \right] \]

\[ - \frac{1}{2} (F_0(r) + 2 F_{-2})^2 \] \tag{15}

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

\[ \langle S_x S_{y+x} \rangle \sim \left( S + \frac{1}{2} \right)^2 A_\tau \sim \left( S + \frac{1}{2} \right)^2 r^{-\eta_x} \]

with

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

When \( \Delta = 0 \), the first term on the right-hand side of (16) agrees with the corresponding result of Villain (4). The values of \( \eta_x \) for \( S = 1/2 \) and \( S = 1 \) are drawn in Figs. 1 and 2 as functions of \( \Delta \). 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, at the isotropic limit \( \Delta = 1 \).

It has been shown by Miyake (9) 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 for the constant \( F_1(r) \) and does not play a role in the following. As \( r \) tends to infinity, the function \( F_1(r) \) diverges logarithmically

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

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

Fig. 1. The anisotropy dependence of the critical exponent \( \eta_x \) 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 shown in the dashed line.
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 $\eta_\alpha$ 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\textsuperscript{19-23} has predicted that the spin wave picture (with gapless excitations) breaks down at $\Delta_c$ between 0 and 1 if $S$ is an integer. The exponent $\eta_\alpha$ is supposed to assume 1/4 at $\Delta_c$. Beyond $\Delta_c$ the correlation function decays exponentially. We apply our result (16) to the determination of $\Delta_c$ by the criterion $\eta_\alpha(\Delta_c) = 1/4$. (Remember that the spin wave results are valid in the interval $0 \leq \Delta \leq \Delta_c$ including $\Delta_c$.) We find $\Delta_c = 0.1528$ for $S = 1/2$, $\Delta_c = 0.9997$ for $S = 2$, and the critical $\Delta$ monotonically approaches 1 as $S$ increases. The asymptotic form for large $S$ is

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

It may seem strange for $\eta_\alpha$ 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 $\Delta \rightarrow 1$, which compensates for the smallness of $1/S^2$.

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

$$\langle S_i^z S_j^z \rangle \sim S r^{-2}$$

(17)

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

$$S^{-2} \langle S_i^z S_j^z \rangle \sim S^{-2} r^{-2} \rightarrow 0.$$

(We set $S \rightarrow \infty$ first and then $r \rightarrow \infty$.) The exact expression (3) for $S = 1/2$ shows $\eta_\alpha$ 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,\textsuperscript{6} breaks down near $\Delta = 1$. (In the case of $\eta_\alpha$, the exponent diverges at $\Delta = 1$.)

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