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1999 J. Phys.: Condens. Matter 11 L169

(http://iopscience.iop.org/0953-8984/11/16/001)

J. Phys.: Condens. Matter **11** (1999) L169–L174. Printed in the UK PII: S0953-8984(99)02724-1

LETTER TO THE EDITOR

On the behaviour of a two-dimensional Heisenberg antiferromagnet at very low temperatures

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Received 17 March 1999

Abstract. We present an analytical formula for the ratio of the physical spin correlation length of a two-dimensional Heisenberg antiferromagnet on a square lattice, and the one which is actually computed in numerical simulations. This latter correlation length is deduced from the second moment of the structure factor at the antiferromagnetic momentum Q. We show that the ratio is very close to one, in agreement with a previously obtained numerical result based on the $1/N$ expansion.

The two-dimensional Heisenberg antiferromagnet on a square lattice is one of the most extensively studied systems in condensed-matter physics. The interest in this model is twofold. On one hand, the Heisenberg antiferromagnet models a large number of real materials including parent compounds of high-T_c superconductors. On the other hand, its low-energy physics is adequately described by a field-theoretical σ-model thus allowing one to find similarities between condensed-matter physics and field theory.

The low-temperature behaviour of the Heisenberg antiferromagnet is understood in great detail [1–3]. For short-range interaction, the ground state is ordered unless one fine tunes the couplings between nearest and further neighbours. The ordered ground state is characterized by a sublattice order parameter, N_0, spin stiffness, ρ_s, and transverse susceptibility, $\chi_\perp = c^{-2}\rho_s$, where c is the spin-wave velocity. At any finite temperature, however, the system is disordered due to thermal fluctuations. The disordering means that the equal-time spin–spin correlation function decays exponentially with the distance, as $\mathrm{e}^{-r/\xi}$. The length scale ξ is the physical spin correlation length. Various approaches to 2D antiferromagnets all predict [1, 2, 4] that in the renormalized-classical region ($T \ll \rho_s$), which we consider here, ξ is exponentially large in T at low T and behaves as $\xi \sim \exp(2\pi\rho_s/T)$. Equal-time spin correlations at large distances can also be described by a static structure factor $S(k)$ for k near the antiferromagnetic momentum $Q = (\pi, \pi)$. At finite temperatures, $S(Q)$ scales as ξ^2 and is therefore also exponential in T.

The exponential temperature dependences of ξ and of $S(Q)$ have been verified in numerical simulations [5, 6], and by analysing the neutron scattering and NMR data for La_2CuO_4 and $Sr_2CuO_2Cl_2$ [2]. The accuracy of numerical simulations is however so high that one can not only check the temperature dependences but also compare the absolute value of the spin correlation length with the exact expression for ξ obtained some time ago by Hasenfratz and Niedermayer (see below). Recently, two groups [5, 6] performed such a detailed comparison and found a good agreement with the Hasenfratz and Niedermayer formula at very low T.

This comparison, however, requires care, as in numerical simulations one in fact measures not the physical spin correlation length ξ, but another length scale which differs from ξ by a constant factor which is not necessarily close to one. The point is that in numerical simulations one measures the spin structure factor $S(k)$ in the momentum space. Meanwhile, the physical spin correlation length is associated with the real-space behaviour of the structure factor: at large distances $S(r) \propto \mathrm{e}^{-r/\xi}$. To extract this ξ from $S(k)$, one has to move to the *imaginary* k-axis. Then ξ^{-1} is the scale at which $S(k)$ has a pole: $S^{-1}(k = \mathrm{i}\xi^{-1}) = 0$ [2]. In numerical simulations, however, the structure factor is evaluated only for *real* values of the momentum k. By agreement, the correlation length is identified as a second moment of $S(k)$ for $k = Q$, i.e., as $\tilde{\xi} = (-S^{-1}(Q)\, \mathrm{d}S(k)/\mathrm{d}k^2|_{k\to Q})^{1/2}$ [5, 6].

For the Lorentzian form of $S(k)$, $S(k) \propto ((Q-k)^2 + m_0^2)^{-1}$, both ξ and $\tilde{\xi}$ are equal to the mean-field spin excitation gap m_0^{-1} and are therefore identical. However, the $1/N$ calculations for the $\mathrm{O}(N)$ σ-model rigorously demonstrated that $S(k)$ has a Lorentzian form only in the limit $N \to \infty$, while for arbitrary N, and, in particular, for physical $N = 3$, the momentum dependence of $S(k)$ is different from a simple Lorentzian [2]. In this situation, $\tilde{\xi}$ and the physical spin correlation length ξ differ by some constant factor.

To proceed further, we quote the exact theoretical result [2–4]

$$\xi^{-1}/m = \left(\frac{8}{\mathrm{e}}\right)^{1/(N-2)} \frac{1}{\Gamma(1 + 1/(N-2))} \tag{1}$$

where m is given by

$$m = \frac{T}{c}\left(2\pi\rho_s/((N-2)T)\right)^{1/(N-2)} \mathrm{e}^{-2\pi\rho_s/[(N-2)T]}. \tag{2}$$

This result is based on numerical results for $N = 3$ and $N = 4$ [4] and on $1/N$ expansion for the $\mathrm{O}(N)$ σ-model [2, 3]. For $N = 3$, this yields $\xi^{-1}/m = (8/\mathrm{e}) \approx 2.94$.

No exact expression, however, is known for $\tilde{\xi}$. The $1/N$ expansion for the $\mathrm{O}(N)$ σ-model yields [2]

$$\tilde{\xi}^{-1} = \xi^{-1}(1 + 0.003/(N-2)) \tag{3}$$

where the factor 0.003 arises from numerical evaluation of some complex integrals [7]. A formal application of this result to the physical case of $N = 3$ yields almost identical values for $\tilde{\xi}$ and ξ. This agreement was cited in [5, 6] as a justification for comparing $\tilde{\xi}$ extracted from the simulations with ξ.

A potential problem with this argument is that it in fact assumes that the result for any N can be obtained by just exponentiating the $1/(N-2)$ term (i.e. by replacing $1+(\log a)/(N-2)$ by $a^{1/(N-2)}$). This exponentiation rule works for temperature-dependent corrections due to the renormalizability of a classical σ-model in $2D$. For a quantum model, the renormalizability is however not guaranteed, and there is a concern that the smallness of the $1/N$ correction may be the result of a near cancellation between the two terms, only one of which survives for $N = 3$.

To illustrate that this concern is justified, we review the large-N expansion for ξ^{-1}/m [2,3]. To first order in $1/(N-2)$ this ratio behaves as

$$\xi^{-1}/m = \left(1 + \frac{1}{N-2}(\log(8/\mathrm{e}) + \gamma_E)\right) \tag{4}$$

where γ_E is the Euler constant. Comparing equation (4) with the exact result, equation (1), we see that the exponentiation rule works, but only provided that one *neglects* the Euler constant in (4). The latter in turn accounts for the appearance of the Γ function in (1) (recall that $\Gamma(1 + 1/(N-2)) = 1 - \gamma_E/(N-2) + \mathrm{O}(1/(N-2)^2)$. As $\Gamma(2) = \Gamma(1) = 1$, the term with the Euler constant actually does not contribute to ξ^{-1}/m for the physical case of $N = 3$. In other words, to obtain the exact result for ξ for $N = 3$, one first has to eliminate γ_E from the $1/N$ correction and only then exponentiate the rest.

The danger is that the same might also happen for the rescaling factor of ξ and $\tilde{\xi}$, i.e., that the ratio obtained numerically to first order in $1/N$ may in fact contain the Euler constant which would mask the actual value of the ratio.

In the present communication we address this issue. We compute explicitly the T-independent $1/N$ corrections to $\tilde{\xi}$ and show that the factor describing the rescaling between $\tilde{\xi}$ and ξ does not contain the Euler constant. This implies that the $1/N$ result for the ratio is very likely to be reliable, and the rescaling factor for the two correlation lengths is very close to one.

As an input for our calculations, we use the results of the $1/N$ expansion for O(N) σ-model [2, 3]. At $N = \infty$, the mean-field consideration is exact, and the static structure factor is given by [2]

$$S(k) = \sum_{i=1}^{N} S_{ii}(k) = \frac{T N_0^2 N}{\rho_s} \frac{1}{m_0^2 + (Q-k)^2} \tag{5}$$

where

$$m_0 = (T/c)\mathrm{e}^{-2\pi\rho_s/(NT)}.$$

At finite N, this simple expression is modified due to interaction between low-energy transverse spin fluctuations. It has been shown in [2, 3] that there exist two different types of $1/(N-2)$ corrections: singular ones which contain $\log(T/m_0)$ and $\log(\log(T/m_0))$, and T-independent, non-singular corrections which account for the renormalizations of the overall factors in $S(k)$ and m. The renormalizability of the classical 2D σ-model implies that logarithmical and double-logarithmical perturbation series are geometrical and therefore can be simply exponentiated. The non-singular $1/(N-2)$ corrections however require special care, as was demonstrated above. Collecting both singular and non-singular $1/N$ corrections and exponentiating the singular ones, one obtains [2]

$$S(k) = 2\pi N_0^2 \frac{N}{N-2} \left(\frac{(N-2)T}{2\pi\rho_s} \right)^{(N-1)/(N-2)} P(k) \tag{6}$$

where for k comparable to the inverse correlation length

$$P(k) = \frac{1}{Zm^2 + (Q-k)^2 + \Sigma(k)}. \tag{7}$$

Here m is given by (2), and Z and $\Sigma(k) \propto (Q-k)^2$ account for the temperature-independent $1/(N-2)$ corrections.

The expressions for Z and $\Sigma(k)$ have been obtained in [2] but not explicitly presented in that paper. Here we list the catalogue of the results which we will need:

$$\begin{aligned} Z &= 1 + \frac{2}{N}\left(2\log 2 - 1 - 3\int_0^\infty \mathrm{d}x\ \log\log\frac{x+\sqrt{x^2+4}}{2}\frac{x}{(x^2+1)^2}\right) \\ \Sigma(k \to Q) &= -\frac{4(Q-k)^2}{N}\int_0^\infty \mathrm{d}x\ \log\log\frac{x+\sqrt{x^2+4}}{2}\frac{x(7x^2-2)}{(x^2+1)^4} \\ \Sigma(k = \mathrm{i}m) &= -\frac{m^2}{N}\int_0^\infty \mathrm{d}x\ \log\log\frac{x+\sqrt{x^2+4}}{2}\left(\frac{(x-\sqrt{x^2+4})^2}{\sqrt{x^2+4}} - 6\frac{x}{(x^2+1)^2}\right). \end{aligned} \tag{8}$$

For the two correlation lengths we then obtain

$$\xi^{-2} = m^2 Z\left(1 + \frac{\Sigma(k=\mathrm{i}m)}{m^2}\right) \qquad \tilde{\xi}^{-2} = m^2 Z\left(1 - \frac{\Sigma(k)}{(Q-k)^2}\right)\Bigg|_{k\to Q}. \tag{9}$$

Performing simple manipulations, we find that

$$\xi^{-1} = m\left(1 + \frac{1}{N}(2\log 2 - 1 - A)\right) \tag{10}$$

where

$$A = \int_0^\infty \mathrm{d}x\ \log\log\frac{x + \sqrt{x^2+4}}{2}\left(\frac{(x - \sqrt{x^2+4})^2}{2\sqrt{x^2+4}}\right). \tag{11}$$

Introducing

$$t = \log\frac{x + \sqrt{x^2+4}}{2}$$

and integrating by parts, we immediately obtain $A = -(\gamma_E + \log 2)$. A substitution of this result into (10) yields equation (4).

For the ratio of ξ and $\tilde{\xi}$, the same manipulations yield a more complex expression:

$$\tilde{\xi} = \xi\left(1 + \frac{1}{N}(\gamma_E + I)\right) \tag{12}$$

where $I = 3I_2 - 14I_3 + 18I_4$, and

$$I_n = \int_0^\infty \mathrm{d}t\ \frac{\sinh t \log t}{(2\cosh t - 1)^n}. \tag{13}$$

Notice that the integrals I_n are all convergent and hence are determined by energy scales which are much smaller than the upper cut-off. At this scale, the system behaviour is universal, and therefore the overall factor in $\tilde{\xi}$ is the universal number. Note in passing that similar integrals appear in the calculations of the d.c. Hall conductivity near the fractional quantum Hall critical point [8].

To evaluate the integrals (13), we introduce the auxiliary function

$$\Phi_n(t) = \sinh t \log^2(-t)/(2\cosh t - 1)^n$$

and integrate Φ_n over a contour which consists of a circle of infinite radius and a cut along the positive real t-axis. The contour integral yields $-4\pi \mathrm{i} I_n$ and simultaneously it is equal to the sum of the residues (modulo $2\pi\mathrm{i}$) of the poles along the imaginary t-axis. Performing calculations and making use of the summation formula

$$\sum_{n=0}^{\infty}\frac{\log(2\pi n + \pi(1-a))}{2n + (1-a)} - \frac{\log(2\pi n + \pi(1+a))}{2n + (1+a)} = \frac{\pi}{2}(\log\pi - \gamma_E)\tan\frac{\pi a}{2} - \int_0^\infty \mathrm{d}u\ \frac{\sinh ua}{\sinh u}\log u \tag{14}$$

we can explicitly pull out the Euler constant from the integrals

$$\begin{aligned} I_2 &= -\frac{\gamma_E}{2} - \frac{\tilde{I}_2}{2} \\ I_3 &= -\frac{\gamma_E}{4} - \frac{\tilde{I}_2}{12} + \frac{\tilde{I}_3}{12} \\ I_4 &= -\frac{\gamma_E}{6} - \frac{\tilde{I}_2}{18} + \frac{\tilde{I}_3}{36} - \frac{\tilde{I}_4}{36} \end{aligned} \tag{15}$$

where

$$\tilde{I}_2 = \int_0^\infty \mathrm{d}x \; \frac{\log x}{\sinh \pi x} \frac{\sinh 2\pi x/3}{\sin 2\pi/3}$$
$$\tilde{I}_3 = \int_0^\infty \mathrm{d}x \; \frac{x \log x}{\sinh \pi x} \frac{\cosh 2\pi x/3}{\cos 2\pi/3} \tag{16}$$
$$\tilde{I}_4 = \int_0^\infty \mathrm{d}x \; \frac{x^2 \log x}{\sinh \pi x} \frac{\sinh 2\pi x/3}{\sin 2\pi/3}.$$

The analytical expression for $\tilde{I}_2$ has been known for some time [10], whereas the ones for $\tilde{I}_{3,4}$ have been obtained very recently [9], It turns out that these integrals can be expressed in terms of the derivatives of the Hurvitz zeta function $\mathrm{d}\zeta(x,\alpha)/\mathrm{d}x$ at $x = 0, -1, -2$ and $\alpha = 1/6, 1/3, 1/2, 2/3, 5/6, 1$. Explicitly, we obtained [11]

$$\tilde{I}_2 = -\log R_0$$
$$\tilde{I}_3 = 6 \log R_{-1} - 3 \log 6 \tag{17}$$
$$\tilde{I}_4 = 36 \log R_{-2} + 3 \log 6$$

where

$$R_{-s} = \frac{\Gamma_{-s}(1/3)\Gamma_{-s}(1/2)}{\Gamma_{-s}(5/6)\Gamma_{-s}(1)} \left(\frac{\Gamma_{-s}(7/6)\Gamma_{-s}(1)}{\Gamma_{-s}(2/3)\Gamma_{-s}(1/2)} \right)^{(-1)^s} \tag{18}$$

and the Γ_s are the generalized Gamma functions introduced via

$$\mathrm{d}\zeta(x,\alpha)/\mathrm{d}x|_{x=-n} = \log(\Gamma_{-n}(\alpha)/\sqrt{2\pi})$$

(Γ_0 is a conventional Γ function)

Assembling now all contributions to I and substituting the result into (12), we find that the Euler constant is cancelled out. The rest is combined into

$$\tilde{\xi} = \xi \left(1 + \frac{1}{2(N-2)} \log[6 R_0^{8/3} R_{-1}^{-8} R_{-2}^{-36}] + \mathrm{O}\left(\frac{1}{(N-2)^2} \right) \right). \tag{19}$$

This expression is the central result of the paper.

The next issue is how to account for the higher-order terms in $1/(N-2)$. Here we use the same assumption as was proven to work for ξ, namely that after the Euler constant is subtracted, the rest of the $\mathrm{O}(1/(N-2))$ correction can be exponentiated. Using this assumption, we finally obtain

$$\tilde{\xi}^2 = \xi^2 (6 R_0^{8/3} R_{-1}^{-8} R_{-2}^{-36})^{1/(N-2)}. \tag{20}$$

For $N = 3$ this yields $\tilde{\xi}^2/\xi^2 = 0.993$; i.e. the ratio is indeed very close to one. This result may sound intuitively obvious, but we emphasize again that it is not based on any physical reasoning and therefore had to be verified by explicit calculations. This is what we did.

The extreme closeness of the ratio $\tilde{\xi}/\xi$ to 1 is consistent with recent claims that at $T \to 0$, the numerically computed spin correlation length [5, 6] approaches the Hasenfratz–Niedermayer result, equation (1).

Using our expressions for Z and ξ, we can also compute the overall factor for the structure factor $S(Q)$. This quantity was also targeted in numerical simulations. The numerical evaluation of the first $1/(N-2)$ correction yields

$$P(Q) \equiv 1/(Zm^2) = \xi^2(1 + 0.188/(N-2))$$

(see equation (6)). Exponentiating this result, one obtains $P(Q)/\xi^2 \approx 1.2$. Numerical simulations [6], on the other hand, reported that the actual rescaling factor is more than three times larger than this number. We performed analytical calculations along the same lines as the above and obtained

$$P(Q) = \xi^2\left[1 + \frac{1}{N-2}\,(2\gamma_E - \log 2 + 6I_2)\right] \tag{21}$$

where I_2 is given by (15). Substituting the result for I_2 into this expression, we obtain

$$P(Q) = \xi^2\left[1 + \frac{1}{N-2}\,(-\gamma_E + 3\log(R_0) - \log 2)\right]. \tag{22}$$

This result coincides with the one obtained earlier by Campostrini and Rossi [3], and cited previously in [12]. We see now that the Euler constant is present in the perturbation series, i.e. one cannot simply exponentiate the lowest-order result. Using the same procedure as before, i.e., treating γ_E as coming from the expansion of $\Gamma(1+1/(N-2))$, and exponentiating the rest of (22), we obtain

$$P(Q) = 2^{1/(2-N)}\Gamma\left(\frac{N-1}{N-2}\right)\left(\frac{\Gamma(1/3)\Gamma(7/6)}{\Gamma(5/6)\Gamma(2/3)}\right)^{3/(N-2)}\xi^2. \tag{23}$$

For $N = 3$, this yields $P(Q)\xi^{-2} = 2.149$ which is about double the value obtained by formally exponentiating the whole $1/(N-2)$ correction. Still, however, this result does not fully agree with quantum Monte Carlo simulations at low T which reported $P(Q)\xi^{-2} \approx 4$ for both $S = 1/2$ [6] and $S = 1$ [13]. The series expansion results [14] reported a somewhat smaller $P(Q)\xi^{-2} \approx 3.2$ for $S = 1/2$. The reason for the discrepancy is not clear to us. Possibly, the numerical simulations for $S(Q)$ were not performed deep enough inside the asymptotic scaling regime at $T \to 0$. Another possibility is that something may be wrong with the exponentiation of the first $1/N$ correction to $S(Q)$, though this is unlikely in view of the fact that this procedure definitely works for the correlation length ξ.

We would like to thank V Adamchik, S Sachdev, M Troyer, R Wickham and M Zhitomirsky for fruitful discussions.

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