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1999 J. Phys. A: Math. Gen. 32 867

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Finite-size scaling for the spin- $\frac{1}{2}$ Heisenberg antiferromagnetic chain

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Received 7 October 1998

Abstract. Corrections to the asymptotic correlation function in a Heisenberg spin- $\frac{1}{2}$ antiferromagnetic spin chain are known to vanish slowly (logarithmically) as a function of the distance r or the chain size L . This leads to significant differences with numerical results. We calculate the sub-leading logarithmic corrections to the finite-size correlation function, using renormalization group improved perturbation theory, and compare the result with numerical data.

The correlation function in the spin- $\frac{1}{2}$ Heisenberg antiferromagnetic chain is difficult to determine from the Bethe ansatz, so other methods are used for this purpose, such as bosonization and conformal field theory (CFT). These methods work very well as a tool to determine long-distance asymptotics. Numerical work [1–5], however, often questioned this approach. This has been explained by the fact that finite-size corrections vanish slowly at long distances, as $1/\ln L$, and $1/\ln(r)$, where L is the system size (periodic boundary conditions assumed) and r the separation of the two points, due to the presence of a marginally irrelevant operator [6, 7].

Following the methods and notation of [6, 8], the continuum limit of the Heisenberg model can be written in $SU(2)$ -symmetric form using non-Abelian bosonization [6]. The action for the $SU(2)$ -symmetric matrix field g_β^α includes the Wess–Zumino term with coefficient $k = 1$. This theory is equivalent to a free boson defined on a circle. The low-energy Hamiltonian in the continuum approximation is given by:

$$H = H_0 - 8\pi^2/\sqrt{3}\lambda \mathbf{J}_L \cdot \mathbf{J}_R \tag{1}$$

where H_0 is the Hamiltonian density for a free boson, $\mathbf{J}_{L,R}$ are left and right $SU(2)$ currents:

$$\mathbf{J}_L \equiv \frac{-i}{4\sqrt{\pi}} \text{tr}[g^\dagger \partial_- g \sigma] \quad \mathbf{J}_R \equiv \frac{i}{4\sqrt{\pi}} \text{tr}[\partial_+ g g^\dagger \sigma]. \tag{2}$$

(Here we use the notation λ for the marginal coupling constant rather than g as in [8].)

We now turn to the discussion of the asymptotic correlation function. The spin operators can be written in non-abelian bosonization notation as:

$$S_j = (\mathbf{J}_L + \mathbf{J}_R) + \text{const } i(-1)^j \text{tr}[g\sigma]. \tag{3}$$

Thus the correlation function has uniform and staggered terms,

$$G(r) = \langle S_0^z S_r^z \rangle \rightarrow G_u(r) + (-1)^r G_s(r). \tag{4}$$

Both terms vary slowly on the scale of the lattice spacing, and correspond to different Green functions in the continuum theory. In this paper we only consider the staggered term $G_s(r)$,

$$G_s(r) \propto \langle \text{tr}(\sigma^z \mathbf{g})(r) \text{tr}(\sigma^z \mathbf{g})(0) \rangle. \quad (5)$$

The staggered correlation function for a finite chain obeys the following renormalization group (RG) equations [6]:

$$[\partial/\partial \ln r + \beta(\lambda)\partial/\partial \lambda + 2\gamma(\lambda)]G_s(r, r/L, \lambda) = 0 \quad (6)$$

where $\beta(\lambda)$ is the beta function for the coupling constant λ in equation (1):

$$\frac{d\lambda}{d \ln r} = \beta(\lambda) \quad (7)$$

and $\gamma(\lambda)$ is the anomalous dimension. In equation (6) the r -derivative acts only on the first argument of G_s ; r/L is held fixed. Equation (6) expresses the fact that a rescaling of both lengths L and r by a common factor can be compensated for by a change in the effective coupling constant, $\lambda(r)$ and a rescaling of the correlation function. The solution of equation (6) has the form:

$$G_s(r, \lambda_0) = \exp\left(-2 \int_{r_0}^r d \ln r' \gamma[\lambda(r')]\right) F[r/L, \lambda(r)] \quad (8)$$

where $\lambda_0 \equiv \lambda(r_0)$ is the ‘bare’ coupling—a coupling at the ultraviolet cut-off scale r_0 , $F[r/L, \lambda(r)]$ is an arbitrary function of the effective coupling constant at scale r , $\lambda(r)$.

The coupling constant flows to zero as the distance r is increased, and one can use perturbative expressions for $\gamma(\lambda)$ and $\beta(\lambda)$ to determine long-distance properties. The universal terms in the perturbative expansion for the β -function [9] and the anomalous dimension [6, 7] are known,

$$\beta(\lambda) = -(4\pi/\sqrt{3})\lambda^2 - (\frac{1}{2})(4\pi/\sqrt{3})^2\lambda^3 \quad (9)$$

$$\gamma(\lambda) = \frac{1}{2} - (\pi/\sqrt{3})\lambda. \quad (10)$$

Thus the effective coupling is given by:

$$\frac{1}{\lambda(r)} - \frac{1}{\lambda_0} = (4\pi/\sqrt{3})\{\ln(r/r_0) + (\frac{1}{2})\ln[\ln(r/r_0)]\} + O(1). \quad (11)$$

Rewriting the integral in equation (8) using equation (9), one easily finds [8]:

$$\int_{\lambda_0}^{\lambda(r)} [\gamma(\lambda)/\beta(\lambda)] d\lambda = (\frac{1}{2})\ln(r/r_0) + (\frac{1}{4})\ln[\lambda(r)/\lambda_0] + \dots \quad (12)$$

Thus Green’s function has the expansion:

$$G_s(r, L, \lambda) = \frac{1}{r} \sqrt{\frac{\lambda_0}{\lambda(r)}} e^{\sum_{n=1}^{\infty} a_n [\lambda(r)^n - \lambda_0^n]} \sum_{m=0}^{\infty} F_m(r/L) \lambda(r)^m. \quad (13)$$

The coefficients, a_n and the functions $F_m(r/L)$ can be determined by doing perturbation theory in the bare coupling constant and then recasting the resulting expression in terms of the renormalized coupling constant in the form of equation (13). This automatically incorporates, at low orders, the leading log divergences to all orders in perturbation theory. This method is standard in quantum chromodynamics calculations and is known as ‘RG improved perturbation theory’.

The zeroth-order term of this sum, $F_0(r/L)$, is given by the free theory—the conformally invariant WZW model on a circle of length L , and can be obtained by conformal transformation. Since \mathbf{g} has scaling dimension $\frac{1}{2}$, for an infinite system:

$$\langle \text{tr}[\mathbf{g}(r)\sigma^z(r)] \text{tr}[\mathbf{g}(0)\sigma^z] \rangle = \frac{1}{r}. \quad (14)$$

(Here we have chosen a convenient normalization for the operator g .) For a finite system with periodic boundary conditions, we make a conformal transformation from the infinite plane to the cylinder, obtaining:

$$\langle \text{tr}[g(r)\sigma^z] \text{tr}[g(0)\sigma^z] \rangle = \frac{\pi}{L \sin(\pi r/L)}. \tag{15}$$

Thus we see that:

$$F_0(r/L) \propto \frac{(\pi r/L)}{\sin(\pi r/L)}. \tag{16}$$

Using equation (11), we thus obtain the asymptotic correlation function:

$$G_s(r, L) \rightarrow \frac{A}{(L/\pi) \sin(\pi r/L)} \{ \ln(r/r_0) + (\frac{1}{2}) \ln[\ln(r/r_0)] \}. \tag{17}$$

Essentially this result was obtained in [8]. For related work on the correlation function for the infinite length spin chain see [10].

The new result which we derive here is the next order correction, $F_1(r/L)$, in equation (13). The first-order perturbation theory result, using the Hamiltonian of equation (1), gives:

$$\begin{aligned} \delta \langle \text{tr}[g(r)\sigma^z(r)] \text{tr}[g(0)\sigma^z] \rangle \\ = \frac{8\pi^2\lambda_0}{\sqrt{3}} \int d\tau dx \mathcal{T} \langle \text{tr}[g(r, 0)\sigma^z] \text{tr}[g(0, 0)\sigma^z] \mathbf{J}_L(x, \tau) \cdot \mathbf{J}_R(x, \tau) \rangle_L \end{aligned} \tag{18}$$

where \mathcal{T} denotes time-ordering. This correlation function can be evaluated using standard CFT techniques. We first obtain its value for an infinite system, then obtain the result for finite L by conformal transformation. Using the general result for three-point functions of primary operators we obtain:

$$\begin{aligned} \mathcal{T} \langle \text{tr}[g(r, 0)\sigma^z] \text{tr}[g(0, 0)\sigma^z] \mathbf{J}_L(x, \tau) \cdot \mathbf{J}_R(x, \tau) \rangle \\ \propto \frac{r}{(x + i\tau)(x - r + i\tau)(x - i\tau)(x - r - i\tau)}. \end{aligned} \tag{19}$$

The normalization constant can be fixed from the operator product expansion (OPE):

$$\mathbf{J}_L(x, \tau) \cdot \mathbf{J}_R(x, \tau) \text{tr}[g(0)\sigma^z] \rightarrow - \frac{\text{tr}[g(0)\sigma^z]}{16\pi^2(\tau^2 + x^2)} \tag{20}$$

and the normalization of the zeroth-order Green function in equation (14). This gives:

$$\begin{aligned} \mathcal{T} \langle \text{tr}[g(r, 0)\sigma^z] \text{tr}[g(0, 0)\sigma^z] \mathbf{J}_L(x, \tau) \cdot \mathbf{J}_R(x, \tau) \rangle \\ = - \frac{r}{16\pi^2(x + i\tau)(x - r + i\tau)(x - i\tau)(x - r - i\tau)}. \end{aligned} \tag{21}$$

The correlation function on the cylinder can be obtained by conformal transformation:

$$\begin{aligned} \mathcal{T} \langle \text{tr}[g(r, 0)\sigma^z] \text{tr}[g(0, 0)\sigma^z] \mathbf{J}_L(x, \tau) \cdot \mathbf{J}_R(x, \tau) \rangle_L \\ = - ((\pi/L)^3 \sin(\pi r/L)) (16\pi^2 \sin[\pi(x + i\tau)/L] \sin[\pi(x - r + i\tau)/L] \\ \times \sin[\pi(x - i\tau)/L] \sin[\pi(x - r - i\tau)/L])^{-1}. \end{aligned} \tag{22}$$

Thus the first-order correction is given by:

$$\begin{aligned} \delta \langle \text{tr}[g(r)\sigma^z(r)] \text{tr}[g(0)\sigma^z] \rangle_{>L} &= \left(\frac{-\lambda_0}{2\sqrt{3}} \right) \int_{-\infty}^{\infty} d\tau \int_0^L dx \\ &= ((\pi/L)^3 \sin(\pi r/L)) (16\pi^2 \sin[\pi(x + i\tau)/L] \sin[\pi(x - r + i\tau)/L] \\ &\quad \times \sin[\pi(x - i\tau)/L] \sin[\pi(x - r - i\tau)/L])^{-1}. \end{aligned} \tag{23}$$

This integral has a logarithmic ultraviolet divergence at $\tau \rightarrow 0$, and $x \rightarrow 0$ or r . This can be cut off by restricting the integral to $|x|^2 + \tau^2 > r_0^2$ and $|x - r|^2 + \tau^2 > r_0^2$. The resulting logarithmic dependence on r_0 is exactly what is needed in order for the resulting expression to have the form of equation (13), since:

$$\sqrt{\frac{\lambda_0}{\lambda(r)}} \approx 1 + \frac{2\pi\lambda_0}{\sqrt{3}} \ln(r/r_0). \quad (24)$$

Remarkably, the integrals can be done exactly. The x -integral can conveniently be done first using contour methods. This gives:

$$\begin{aligned} & \delta \langle \text{tr}[g(r)\sigma^z(r)] \text{tr}[g(0)\sigma^z] \rangle \\ &= \frac{i\pi^2\lambda_0}{2\sqrt{3}L} \int_{-\infty}^{\infty} du \left[\frac{1}{\sinh u \sinh(u + i\pi r/L)} - \text{complex conjugate} \right]. \end{aligned} \quad (25)$$

(Here $u \equiv 2\pi\tau/L$ and the integral is cut off at $|u| > r_0/L$.) This indefinite integral may be done exactly by changing variables to $\tanh u$, giving:

$$\begin{aligned} & \langle \text{tr}[g(r)\sigma^z(r)] \text{tr}[g(0)\sigma^z] \rangle \\ &= \frac{1}{(L/\pi) \sin[\pi r/L]} \left\{ 1 + \frac{2\pi\lambda_0}{\sqrt{3}} \{ \ln[(L/r_0) \sin(\pi r/L)] + \text{constant} \} \right\}. \end{aligned} \quad (26)$$

This is the result of perturbation theory to first order in the bare coupling constant λ_0 . The next step is to 'RG improve' this result by matching it to the expression in equation (13). Expanding this expression to first order in the bare coupling constant, using equation (11) gives:

$$G_s(r) \propto \frac{1}{(L/\pi) \sin[\pi r/L]} [1 + \lambda_0(2\pi/\sqrt{3}) \ln(r/r_0)] [1 + \lambda_0 F_1(r/L)/F_0(r/L)]. \quad (27)$$

Comparing equation (26) and (27) we see that:

$$F_1(r/L)/F_0(r/L) = \frac{2\pi}{\sqrt{3}} \ln \left[\frac{L}{r} \sin \left(\frac{\pi r}{L} \right) \right] + \text{constant}. \quad (28)$$

Thus our RG improved expression for the correlation function is:

$$G_s(r, L, \lambda_0) \propto \frac{1}{(L/\pi) \sin[\pi r/L]} \sqrt{\frac{\lambda_0}{\lambda(r)}} \left\{ 1 + \lambda(r) \left\{ \frac{2\pi}{\sqrt{3}} \ln \left[\frac{L}{r} \sin \left(\frac{\pi r}{L} \right) \right] + \text{constant} \right\} \right\}. \quad (29)$$

The advantage of this RG improved expression is that we may now go to arbitrarily large r , a limit in which the large logarithms, $\ln(r/r_0)$ invalidate finite-order perturbation theory and infinite resummations of most divergent diagrams are necessary. This is automatically taken care of by equation (29) together with the expression for $\lambda(r)$ in equation (11). In this asymptotic limit we may use:

$$\lambda(r) \approx \frac{\sqrt{3}}{4\pi \ln(r/r_0)} \quad (30)$$

for the factor of $\lambda(r)$ inside the curly brackets in equation (29). This gives:

$$\begin{aligned} G_s(r) &\rightarrow \frac{A}{(L/\pi) \sin[\pi r/L]} [\ln(Cr/r_0) + (\frac{1}{2}) \ln[\ln(r/r_0)]]^{1/2} \\ &\times \left\{ 1 + \frac{1}{2 \ln(r/r_0)} \left\{ \ln \left[\frac{L}{r} \sin \left(\frac{\pi r}{L} \right) \right] + \text{constant} \right\} \right\} \end{aligned} \quad (31)$$

where:

$$C \approx e^{\sqrt{3}/4\pi\lambda_0 + O(1)}. \quad (32)$$

We now see that the ‘constant’ term can be adsorbed, to lowest order in $1/\ln(r/r_0)$, into a rescaling of C (i.e. a shift of λ_0) so we henceforth drop it. This is all the information that can be extracted from the RG to this order. Two non-universal free parameters remain: the overall amplitude, A and the bare coupling λ_0 , appearing as the constant C in equation (31). The amplitude A was recently determined, from Bethe ansatz results [10] for the spin- $\frac{1}{2}$ Heisenberg model, to be [8] $A = (2\pi)^{-3/2}$. The bare coupling λ_0 (for some conveniently chosen value of r_0) is not known exactly for the spin- $\frac{1}{2}$ Heisenberg model. It can be determined by fitting numerical results. Since the same bare coupling constant also appears in various other finite size corrections, including the finite-size spectrum [6] various consistency checks could be made. However, this requires further calculations to ensure consistency of the cut-off schemes in various calculations and we do not attempt it here.

Note that if we chose $z \equiv (L/\pi) \sin(\pi r/L)$ instead of r as the length scale in equation (6), we would find, to this order, that the finite-size correlation function at distance r is given by an infinite-chain correlation function at z :

$$G_s(r, r/L) = G_s(z, 0) = \frac{1}{z(2\pi)^{3/2}} \{\ln(Cz/r_0) + (\frac{1}{2}) \ln[\ln(z/r_0)]\}^{1/2}. \quad (33)$$

However, this fact does not necessarily hold for higher-order RG. As follows from our result equation (31), the finite-size correction to the asymptotic correlation function vanishes as r^2/L^2 as one approaches the infinite-chain limit, $r/L \rightarrow 0$. The expansion in $1/\ln(r/r_0)$ remains, but the functions $F_m(r/L)$ (see equation (13)) approach constants in this limit. (We have only checked this for $F_0(r/L)$ and $F_1(r/L)$).

It is interesting to compare our result equation (31) with phenomenological expressions used to fit numerical data. Koma and Mizukoshi [5] used the scaling function of the form:

$$G_s(r, L) = \frac{A\{\ln[(L/\pi r_0) \sin(\pi r/L)]\}^{1/2}}{(L/\pi) \sin(\pi r/L)} \quad (34)$$

with $A = (2\pi)^{-3/2} \simeq 0.0635$, close to the exact answer. This form is equivalent to equation (33) with the slow log-log term replaced by a constant. The best fit was obtained for $A \simeq 0.065$, close to the exact answer. Kubo *et al* [1] and Hallberg *et al* [4] defined a scaling function $f(r/L)$,

$$G_s(r, L) = G_s(r, \infty) f(r/L) \quad (35)$$

and adopted a phenomenological expression,

$$f(x) \propto [1 + A \sinh^2(Bx)]^{2\eta}. \quad (36)$$

Note that equation (35) does not agree with our RG analysis. They found the best fit for $A = 0.288\ 22$, $B = 1.673$, $2\eta = 1.805$. As it has been noted by one of us, the form is remarkably (within 0.05%) close to the CFT prediction for the general xxz model, since

$$1 + 0.288\ 22 \sinh^2(1.673x) \simeq \left[\frac{\pi x}{\sin(\pi x)} \right]^{1/2}. \quad (37)$$

Further, for η close to 1 we can replace the phenomenological formula equation (36) by an equivalent,

$$[1 + 0.288\ 22 \sinh^2(1.673x)]^{2\eta} \simeq \left[\frac{\pi x}{\sin(\pi x)} \right] \left\{ 1 + (\eta - 1) \ln \left[\frac{\pi x}{\sin(\pi x)} \right] \right\}. \quad (38)$$

The scaling function $f(x)$ is similar to $F(\lambda(r), x)$ defined in equation (31). We find that η depends on r ,

$$\eta(r) \simeq 1 - \frac{1}{2 \ln(cr)}. \quad (39)$$

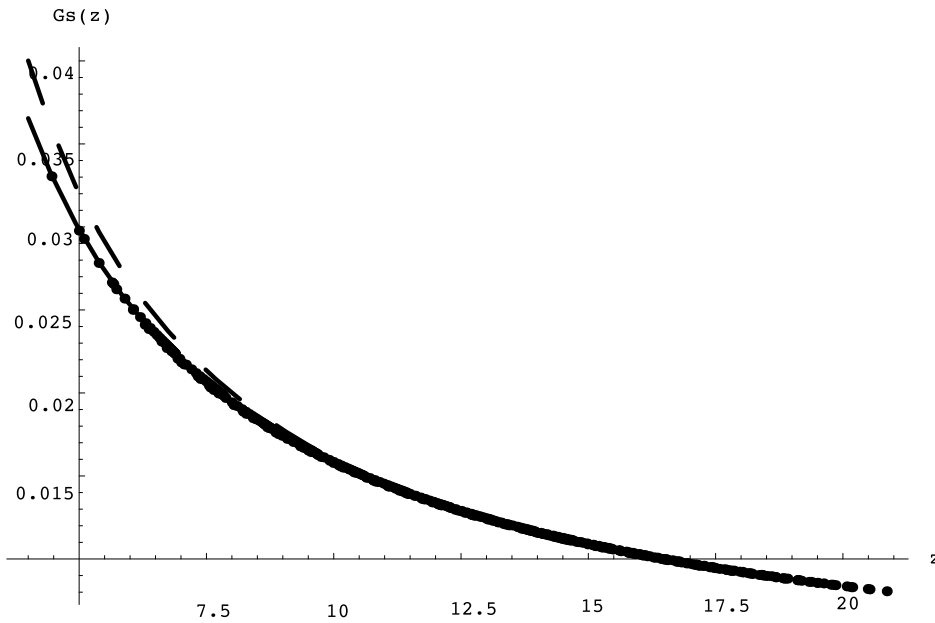


Figure 1. Scaled DMRG data for spin correlation function compared with one-loop theoretical expression (solid curve) and free boson result (dashed curve).

Finally, let us compare our theoretical expression equation (31) with DMRG data of [4]. We have found that the log–log term, which is higher order, is almost constant, and does not influence the comparison. Since adding a log–log term introduces one more free parameter, we decided to drop it. To obtain data collapse for $G_s(r, L)$ in a one-loop RG we use equation (33), with the log–log term dropped and use C as a free parameter. We compare this with a zero-order non-interacting result,

$$G_{\text{free}}(z) = \text{const} \frac{1}{z}. \quad (40)$$

The result is shown in figure 1. Both expressions use one free parameter. The better fit produced by our one-loop expression is obvious.

Alternatively, we can use the result equation (31), with $A = 1/(2\pi)^{3/2}$, the log–log term dropped, and C taken as a free parameter. (These two expressions are the same to the order that we have calculated in $1/\ln r$.) The comparison of this formula with numerical data is shown in figure 2. For comparison we also show the result without the correction that we have calculated,

$$G_s(r) = \frac{A[\ln(Cr/r_0)]^{1/2}}{(L/\pi) \sin[\pi r/L]}. \quad (41)$$

It is instructive to find the value of A from the numerical data to compare it with exact value. Using equation (31) with A and C as free parameters to fit the numerical data, we find $A = 0.063\,6427$, which differs only 0.2% from the exact answer. This is much better than what we would have found without the correction calculated in this paper, $A = 0.057\,8896$, which is off by some 9%.

Finally, we can extract from the data the behaviour of the correlation function at $L = \infty$,

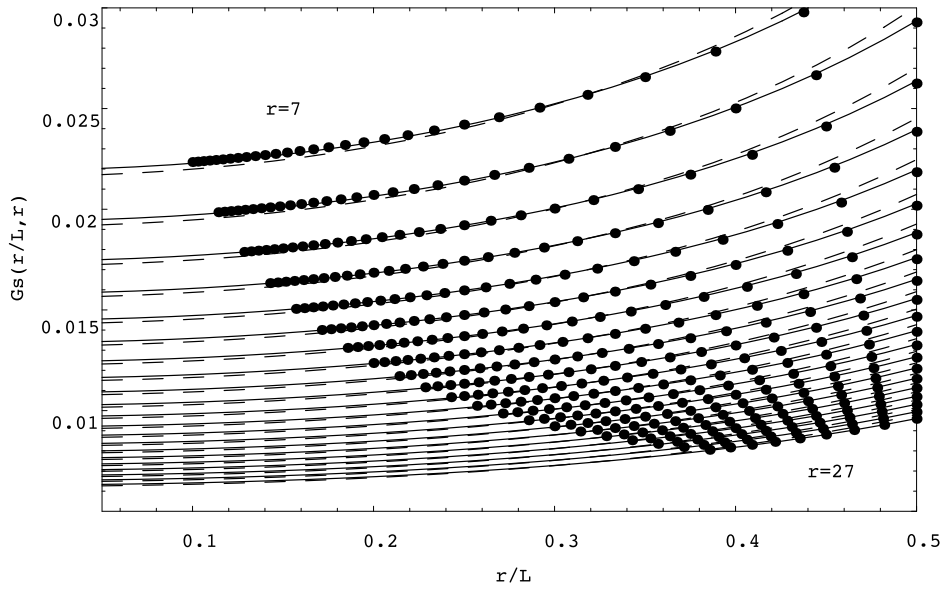


Figure 2. Numerical data for the spin-spin correlation function $G_s(r, L)$ from [4] versus r/L for $r = 7 - 27$. Solid curves—our one-loop result (with one parameter— c), dashed curve—the result without our correction (also with one parameter— c).

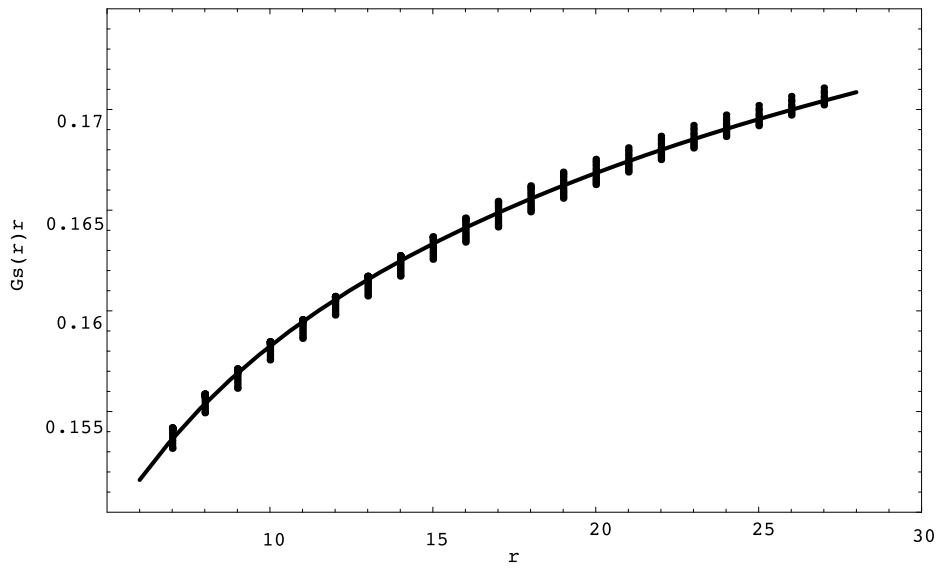


Figure 3. Spin-spin correlator multiplied by r , $rG_s(r, \infty)$, versus r extracted from the DMRG data of [4]. Solid curve—the one-loop result.

using equation (13) and dividing it by

$$F_0(r/L) + F_1(r/L)\lambda(r) = \left\{ 1 + \frac{1}{2 \ln(cr)} \ln \left[\frac{L}{\pi r} \sin \left(\frac{\pi r}{L} \right) \right] \right\} \frac{\pi r}{L \sin[\pi r/L]}. \quad (42)$$

The result is given by

$$G_s(r, \infty) = \frac{\sqrt{\ln(cr)}}{(2\pi)^{3/2}r} \quad (43)$$

with the same constant c . This way of extracting $L = \infty$ behaviour from finite-size data is different from the phenomenological scaling expression that Hallberg *et al* used in [4], $G_s(r, L) = G_s(r, \infty)f(r/L)$. The result is shown in figure 3.

In conclusion, we have shown that the bosonization approach provides an accurate description of the spin correlation function in a finite spin- $\frac{1}{2}$ Heisenberg spin chain. Our theoretical result equation (31) compares favourably with numerical data at long length scales.

Acknowledgments

We are grateful to K Hallberg for providing us numerical data from [4]. This work was supported by NSERC of Canada. VB acknowledges support by the NHMFL through NSF cooperative agreement no DMR-9527035 and the State of Florida.

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