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Temperature-dependent logarithmic corrections in the spin-1/2 Heisenberg chain

Victor Barzykin

National High Magnetic Field Laboratory, Florida State University, 1800 E Paul Dirac Drive, Tallahassee, FL 32310, USA

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Abstract. We obtain the logarithmic corrections to the dynamic response function and nuclear magnetic resonance (NMR) T_1- and T_{2G}-rates in the spin-1/2 antiferromagnetic Heisenberg chain using the perturbative renormalization group for the leading irrelevant operator. The result is compared with NMR experiments on Sr_2CuO_3.

Quantum spin chains have attracted considerable interest for a long time, due to both the unconventional physics of the 1D materials and the sophisticated theoretical methods used in the analysis of the problem. In particular, it is well known [1] that the antiferromagnetic spin-1/2 XXZ-chain is critical for $J_x > J_z$ (the two exchange constants), and the spin correlators at $T = 0$ decay as a power law with distance. The critical theory can be mapped onto a theory of free bosons. For $J_x < J_z$ the system acquires a spin gap. At the quantum critical point, the Heisenberg XXX-chain, the spin-correlation function has logarithmic corrections to the free theory coming from the leading irrelevant operator, which becomes marginal. Thus, the asymptotic power-law behaviour of the correlator at long distances is modified [2, 3]. The staggered component of the spin–spin correlator has the following form:

$$\langle S^z(r)S^z(0)\rangle = (-1)^r D\frac{\sqrt{\ln(r/r_0)}}{r} \tag{1}$$

where the non-universal coefficient $D = 1/(2\pi)^{3/2}$ has been determined from the Bethe *ansatz* [4, 5].

Logarithmic corrections in the SU(2)-invariant models are very well known. For example, an RG calculation of the logarithmic corrections up to two loops was carried out for the fermion model with backward scattering [6], the sine–Gordon model [7], and the SU(2) Gross–Neveu model [8]. Logarithms appear in every physical property of the spin-1/2 Heisenberg chain as a result of the marginally irrelevant operator. They were first found in the seminal papers of Yang and Yang [9], who calculated $1/\ln(H)$ corrections to the magnetization using the Bethe *ansatz* (see also reference [10]). Higher-order two-loop calculations of the $\ln(\ln(H))/\ln^2(H)$ corrections to $\chi(H)$ were performed by Schlottmann [11, 12]. Also well known are the temperature-dependent $1/\ln(T)$ corrections to the bulk spin susceptibility [13], and $T/\ln^3(T)$ corrections to the specific heat [14].

The leading logarithmic behaviour of the staggered spin-correlation function has been known for a long time [2, 3]. However, numerical [15–20] and experimental [21, 22] tests of it

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have appeared only recently. To fit the numerical data, various phenomenological expressions were used [15, 18, 19, 23]. As was first pointed out by Nomura [24], using the RG scheme up to two loops greatly improves the asymptotic behaviour of the finite-size correction to the energy gap. For the equal-time correlator in a finite-size chain at $T = 0$, this fact has been recently proven in references [4, 25], where the two-loop expression was derived and compared with numerical DMRG results. In what follows we use a similar approach to obtain the staggered dynamic spin correlator, up to two-loop order in the perturbative renormalization group scheme. The imaginary part of the staggered dynamic spin susceptibility is observed in inelastic neutron scattering experiments, and determines the relaxation time T_1 in nuclear magnetic resonance (NMR) experiments. Another NMR relaxation time, T_{2G}, is found from the real part of the spin susceptibility.

Let us now show how the logarithms appear in the time-dependent staggered spin-correlation function. For this purpose it is more convenient to work in real space and imaginary time, so that one can easily apply bosonization and conformal invariance. One should then Fourier transform and analytically continue the result to real frequencies. At low temperatures and large distances we can use the continuum approximation. The theory can be written in terms of free bosons defined on a circle. In case of the SU(2)-symmetric Heisenberg model it is more convenient to use non-Abelian bosonization [2], which respects the symmetry. The action for the SU(2)-symmetric matrix field $\mathbf{g}^{\alpha}_{\beta}$ includes the Wess–Zumino term with coefficient $k = 1$. The Hamiltonian density takes the following form:

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

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

$$\boldsymbol{J}_L \equiv \frac{-\mathrm{i}}{4\sqrt{\pi}} \operatorname{tr}[\mathbf{g}^{\dagger}\, \partial_- \mathbf{g}\, \boldsymbol{\sigma}] \qquad \boldsymbol{J}_R \equiv \frac{\mathrm{i}}{4\sqrt{\pi}} \operatorname{tr}[\partial_+ \mathbf{g}\, \mathbf{g}^{\dagger} \boldsymbol{\sigma}]. \tag{3}$$

The spin operators can be written in non-Abelian bosonization notation as

$$\boldsymbol{S}_j = (\boldsymbol{J}_L + \boldsymbol{J}_R) + \text{constant} \times \mathrm{i}(-1)^j \operatorname{tr}[\mathbf{g}\boldsymbol{\sigma}] \tag{4}$$

so the correlation function has uniform and staggered terms:

$$\chi(r, \tau) = \langle S^z_0 S^z_r \rangle \to \chi_u(r, \tau) + (-1)^r \chi_s(r, \tau) \tag{5}$$

where τ is imaginary time. Both terms vary slowly on the scale of the lattice spacing, and correspond to different Green's functions in the continuum theory. The staggered susceptibility, which is enhanced near wave vector $q = \pi$, is observed by means of inelastic neutron scattering and NMR:

$$\chi_s(r, \tau) \propto \langle \operatorname{tr}(\boldsymbol{\sigma}^z \mathbf{g})(r, \tau) \operatorname{tr}(\boldsymbol{\sigma}^z \mathbf{g})(0) \rangle. \tag{6}$$

It is not difficult to determine the contribution of the free boson with radius $R = 1/\sqrt{2\pi}$ [26]—the conformally invariant WZW model on a circle of length $\beta = 1/T$ in the imaginary-time direction. Indeed, $\mathbf{g}$ has scaling dimension 1/2, so for an infinite system one writes

$$\langle \operatorname{tr}[\mathbf{g}(z, \bar{z})\boldsymbol{\sigma}^z] \operatorname{tr}[\mathbf{g}(0)\boldsymbol{\sigma}^z] \rangle = \frac{1}{\sqrt{z\bar{z}}} \tag{7}$$

where $z = \tau + \mathrm{i}x$, $\bar{z} = \tau - \mathrm{i}x$. Here we have chosen a convenient normalization for the operator $\mathbf{g}$. Here and below we use the units $c = k_B = \hbar = 1$. Making a conformal transformation from the infinite plane to the cylinder, one easily finds

$$\langle \operatorname{tr}[\mathbf{g}(z, \bar{z})\boldsymbol{\sigma}^z] \operatorname{tr}[\mathbf{g}(0)\boldsymbol{\sigma}^z] \rangle = \frac{\pi T}{\sqrt{\sin(\pi T z) \sin(\pi T \bar{z})}}. \tag{8}$$

The result for real time is given by a straightforward analytic continuation, $\tau = \mathrm{i}t$. To obtain $\chi''(q, \omega)$, one simply performs a Fourier transform. Integration over q in the limit $\omega \to 0$ gives the NMR T_1 [27]. These results are, of course, well known.

In order to obtain the logarithm, one has to go further [2, 3] and carry out a perturbative expansion in the leading irrelevant operator in equation (2), and then collect the diverging terms in a renormalization group (RG) scheme [4, 25]. To the first order in the leading irrelevant operator the correction can easily be calculated. The details of a similar calculation for this diagram for a finite-size chain at $T = 0$ can be found in reference [25]. The first-order correction has the following form:

$$\delta\langle \mathrm{tr}[\mathbf{g}(z,\bar{z})\boldsymbol{\sigma}^z]\,\mathrm{tr}[\mathbf{g}(0)\boldsymbol{\sigma}^z]\rangle = \frac{\pi^2\lambda_0 T}{\sqrt{3\sin[\pi T z]\sin[\pi T \bar{z}]}} \times \left\{\ln\left[\frac{\sin[\pi T z]\sin[\pi T \bar{z}]}{(\pi T/T_0)^2}\right] + \text{constant}\right\}. \tag{9}$$

Here λ_0 is the 'bare' coupling constant for a theory defined with a cut-off at $T = T_0$.

We can now sum the leading logarithmic contributions using the standard Callan–Symanzik RG equations for the staggered spin-correlation function $\chi_s(r, \tau, T, \lambda)$:

$$[-\partial/\partial \ln T + \beta(\lambda)\,\partial/\partial\lambda + 2\gamma(\lambda)]\chi_s(r, rT, \tau T, \lambda) = 0 \tag{10}$$

where $\beta(\lambda)$ is the beta function for the coupling constant λ in equation (2):

$$\frac{\mathrm{d}\lambda}{\mathrm{d}\ln T} = -\beta(\lambda) \tag{11}$$

and $\gamma(\lambda)$ is the anomalous dimension. In equation (10) the T-derivative acts only on the first argument of χ_s; rT and τT are held fixed. The solution of equation (10) can be written as follows:

$$\chi_s(r, \tau, T, \lambda_0) = \exp\left(-2\int_{\lambda_0}^{\lambda(T)} \frac{\gamma[\lambda']}{\beta(\lambda')}\,\mathrm{d}\lambda'\right) F[\lambda(T), rT, \tau T] \tag{12}$$

where $\lambda_0 \equiv \lambda(T_0)$ is the 'bare' coupling—a coupling at the energy cut-off scale T_0; $F[\lambda(T), rT, \tau T]$ is an arbitrary function of the effective coupling constant at scale T, $\lambda(T)$.

Since the coupling constant flows to zero as T is decreased, one can use perturbative expressions for $\gamma(\lambda)$ and $\beta(\lambda)$ to determine the long-distance asymptotics for the staggered spin susceptibility. The universal terms in the perturbative expansion for the β-function [28] and the anomalous dimension [2, 3] are known:

$$\beta(\lambda) = -(4\pi/\sqrt{3})\lambda^2 - (1/2)(4\pi/\sqrt{3})^2\lambda^3 \tag{13}$$

$$\gamma(\lambda) = 1/2 - (\pi/\sqrt{3})\lambda. \tag{14}$$

Thus the effective coupling is given by

$$\frac{1}{\lambda(T)} = \frac{4\pi}{\sqrt{3}}\left\{\ln(\Lambda/T) + \frac{1}{2}\ln[\ln(\Lambda/T)]\right\} + \mathrm{O}(1) \tag{15}$$

where

$$\Lambda = \text{constant} \times \sqrt{\lambda_0}\mathrm{e}^{\sqrt{3}/(4\pi\lambda_0)}T_0. \tag{16}$$

Thus, we can rewrite the integral in equation (12):

$$\int_{\lambda_0}^{\lambda(T)} \frac{\gamma(\lambda)}{\beta(\lambda)}\,\mathrm{d}\lambda = \frac{1}{2}\ln\frac{T_0}{T} + \frac{1}{4}\ln\frac{\lambda(T)}{\lambda_0} + \cdots. \tag{17}$$

In general, one can expand the staggered spin-susceptibility expression, equation (12), in powers of $\lambda(T)$:

$$\chi_s(r,\tau,T,\lambda)=\frac{1}{r}\sqrt{\frac{\lambda_0}{\lambda(T)}}\exp\left(\sum_{n=1}^{\infty}a_n[\lambda(T)^n-\lambda_0^n]\right)\sum_{m=0}^{\infty}F_m(rT,\tau T)\lambda(T)^m. \tag{18}$$

The coefficients a_n and the functions $F_m(rT,\tau T)$ can be determined from the perturbative expansion in the leading irrelevant operator.

We can now improve using the RG the perturbative results equation (8) and equation (9). This can be done by expanding equation (18) to first order in the bare coupling constant, λ_0, and comparing it with the perturbative calculations. Indeed, if we substitute $\lambda(T)$ from equation (15) into equation (18), we easily find

$$\begin{aligned}&F_0(rT,\tau T)=1\\&F_1(rT,\tau T)=\tfrac{1}{4}\ln[\text{constant}\times\sin(\pi Tz)\sin(\pi T\bar{z})]\end{aligned} \tag{19}$$

where the constant is some non-universal constant. Also,

$$\begin{aligned}\chi_s(r,\tau,T,\lambda)=&\frac{1}{(2\pi)^{3/2}}\left[\pi T\sqrt{\ln\frac{\Lambda}{T}+\frac{1}{2}\ln\left(\ln\frac{\Lambda}{T}\right)}\Big/\sqrt{\sin(\pi Tz)\sin(\pi T\bar{z})}\right]\\&\times\left(1+\frac{1}{4\ln(\Lambda/T)}\ln[\sin(\pi Tz)\sin(\pi T\bar{z})]\right).\end{aligned} \tag{20}$$

This expression is our final perturbative result, which has to be Fourier transformed and continued analytically to real frequencies. For this purpose it is more convenient to work with the temperature-dependent anomalous dimension $\eta(T)$ instead of the form (20) with the logarithms. To the same order in λ we can write, using the identity

$$A^{1+x}\equiv\exp[(1+x)\ln A]\simeq A(1+x\ln A+\mathrm{o}(x^2))$$

valid at small x,

$$\chi_s(r,\tau,T,\lambda)=\frac{\pi T}{(2\pi)^{3/2}}\sqrt{\ln\frac{\Lambda}{T}+\frac{1}{2}\ln\left(\ln\frac{\Lambda}{T}\right)}(\sin(\pi Tz)\sin(\pi T\bar{z}))^{-\eta(T)/2} \tag{21}$$

where

$$\eta(T)=1-1\Big/\left(2\ln\frac{\Lambda}{T}\right). \tag{22}$$

The analytic continuation of equation (21) is then analogous to that in the case of a Luttinger liquid, which is well known [26, 29–31]. We therefore only discuss quantities which can be measured by means of inelastic neutron scattering and NMR. Continuing equation (21) to real frequencies, we get

$$\begin{aligned}\mathrm{Im}\,\chi(q,\omega)=&\frac{2^{\eta(T)-2}}{(2\pi)^{3/2}\pi T}\sin(\pi\eta(T)/2)\sqrt{\ln\frac{\Lambda}{T}+\frac{1}{2}\ln\left(\ln\frac{\Lambda}{T}\right)}\\&\times\mathrm{Im}\left\{B\left(\frac{\mathrm{i}(\omega-q)}{4\pi T}+\frac{\eta(T)}{4},1-\frac{\eta(T)}{2}\right)\right.\\&\left.\times B\left(\frac{\mathrm{i}(\omega+q)}{4\pi T}+\frac{\eta(T)}{4},1-\frac{\eta(T)}{2}\right)\right\}\end{aligned} \tag{23}$$

where $B(x,y)\equiv\Gamma(x)\Gamma(y)/\Gamma(x+y)$ is the beta function. An immediate consequence of the temperature-dependent anomalous dimension is that the correlation length acquires additional

logarithmic temperature dependence, which can be observed in inelastic neutron scattering experiments:

$$\xi^{-1} = \pi T\left(1 - \frac{1}{2\ln(T_0/T)}\right). \tag{24}$$

This also agrees with thermal Bethe *ansatz* calculations [32].

Let us now compute the nuclear relaxation rates. Nuclear spins are coupled to electron degrees of freedom by the magnetic hyperfine Hamiltonian:

$$H_{HF} = \sum_{\alpha,i,j} A_\alpha^{ij} I_{i\alpha} S_{j\alpha}. \tag{25}$$

I is the nuclear spin, S is the electron spin, α enumerates spin projections for sites i and j. We will use the following expressions [33] for calculating T_1 and T_{2G}:

$$\frac{1}{T_1} = \frac{2k_B T}{\hbar^2}\int \frac{\mathrm{d}q}{2\pi}\, A_\perp^2(q)\frac{\operatorname{Im}\chi(q,\omega_0)}{\omega_0} \tag{26}$$

$$\left(\frac{1}{T_{2G}}\right)^2 = \frac{p}{8\hbar^2}\left[\int \frac{\mathrm{d}q}{2\pi}\, A_\parallel^4(q)\chi^2(q) - \left\{\int \frac{\mathrm{d}q}{2\pi}\, A_\parallel^2(q)\chi(q)\right\}^2\right]. \tag{27}$$

Here $A_\parallel(q)$ and $A_\perp(q)$ are the hyperfine couplings parallel and perpendicular to the easy axis of the crystal, and ω_0 is the nuclear resonance frequency, which is much smaller than any other electron energy scale. The magnetic field is directed along the c-axis. The q-dependence is smooth and arises from appropriate form factors. The susceptibility χ should, in principle, include contributions from both the uniform and staggered spin fluctuations. However, simple power counting [27] shows that the staggered component is dominant at small T. For the purpose of comparison of our theory with experiment, it is convenient to define normalized dimensionless NMR rates [34], which should be universal functions of T/J:

$$(1/T_1)_{norm} = \frac{\hbar J}{T_1 A_\perp^2(\pi)} \tag{28}$$

$$(\sqrt{T}/T_{2G})_{norm} = \left(\frac{k_B T}{pJ}\right)^{1/2}\frac{\hbar J}{A_\parallel^2(\pi)T_{2G}}. \tag{29}$$

A complete calculation of the NMR relaxation rates gives

$$(1/T_1)_{norm} = 2D\sqrt{\ln\frac{\Lambda}{T} + \frac{1}{2}\ln\left(\ln\frac{\Lambda}{T}\right)}\left(1 + \frac{\ln 2}{2\ln(\Lambda/T)} + \mathrm{O}\left[\frac{1}{\ln^2(\Lambda/T)}\right]\right) \tag{30}$$

$$(\sqrt{T}/T_{2G})_{norm} = \frac{\sqrt{I_0}D}{4\sqrt{\pi}}\sqrt{\ln\frac{\Lambda}{T} + \frac{1}{2}\ln\left(\ln\frac{\Lambda}{T}\right)} \times\left(1 - \frac{C + 3\ln 2 + I_1/(2I_0)}{2\ln(\Lambda/T)} + \mathrm{O}\left[\frac{1}{\ln^2(\Lambda/T)}\right]\right). \tag{31}$$

Here $D = 1/(2\pi)^{3/2}$ is the non-universal amplitude, $C \simeq 0.577\,2157$ is Euler's constant, while the integrals I_0 and I_1 are given by

$$\begin{aligned} I_0 &= \int_0^\infty \mathrm{d}x\, \left|\Gamma\left(\frac{1+\mathrm{i}x}{4}\right)\Big/\Gamma\left(\frac{3+\mathrm{i}x}{4}\right)\right|^4 \simeq 71.2766 \\ I_1 &= \int_0^\infty \mathrm{d}x\, \left|\Gamma\left(\frac{1+\mathrm{i}x}{4}\right)\Big/\Gamma\left(\frac{3+\mathrm{i}x}{4}\right)\right|^4 \operatorname{Re}\left[\Psi\left(\frac{1+\mathrm{i}x}{4}\right) + \Psi\left(\frac{3+\mathrm{i}x}{4}\right)\right] \simeq -259.94 \end{aligned} \tag{32}$$

where $\Psi(x)$ is the digamma function. The $1/\ln(\Lambda/T)$ term could be incorporated to redefine the cut-off Λ as in reference [4]. Thus, up to terms $O(1/\ln^2(\Lambda/T))$ the temperature dependence for $1/T_1$ or $\sqrt{T}/T_{2G}$ is actually given by the square root of the log and log log terms in the numerator of equation (32). The ratio of the relaxation rates, however, is only weakly temperature dependent. We find

$$\left(\frac{T_{2G}}{T_1\sqrt{T}}\right)_{norm} \simeq 1.680\left(1+\frac{0.7632}{\ln(\Lambda/T)}\right). \tag{33}$$

To summarize, the new effects of the higher-order corrections in the leading irrelevant operator to the dynamic spin susceptibility are, apart from the log log term in the common factor $\sqrt{\ln(\Lambda/T)+0.5\ln[\ln(\Lambda/T)]}$, the temperature-dependent anomalous dimension, and logarithmic corrections to the correlation length. These only lead to an additional weak $O(1/\ln(\Lambda/T))$ temperature dependence for the relaxation rates $1/T_1$ and $1/T_{2G}$, which can be incorporated as a correction to the non-universal cut-off scale Λ. The relaxation rate ratio $(T_{2G}/(T_1\sqrt{T}))$, however, filters out the common factor, and therefore picks up a weak $1/\ln(\Lambda/T)$ temperature dependence, which we have calculated. We note that our result is similar to the phenomenological expression used by Starykh *et al* [23]. There are, however, important differences. Starykh *et al* [23] do not have the log log term, which turns out to be the most important correction in this approximation. The $1/\ln(T_0/T)$ weak temperature dependence for the ratio of the relaxation rates was also not explicitly obtained in reference [23]. Our theoretical results are in excellent agreement with experimental data of Takigawa *et al* [22, 34] on Sr_2CuO_3, as shown in figure 1.

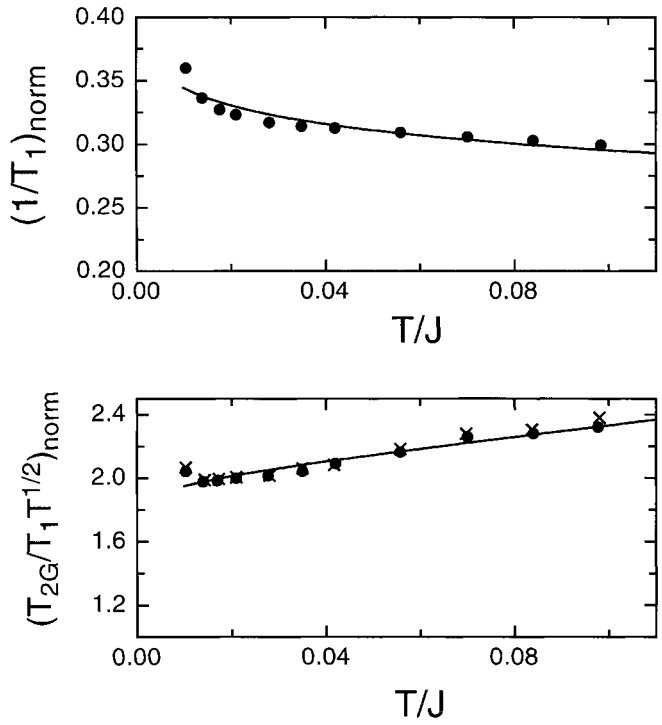

Figure 1. The NMR T_1 and $T_{2G}/(T_1T^{1/2})$ versus T/J from Takigawa *et al* [34] fitted to our expression, with $\Lambda = 5J$.

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