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NMR relaxation rates in a spin-$\frac{1}{2}$ antiferromagnetic chain

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We consider the low-temperature behavior of NMR relaxation rates T_1 and T_{2G} in the spin-1/2 antiferromagnetic chain. We find that $T_1 \propto$ const and $T_{2G} \propto \sqrt{T}$, with logarithmic corrections. We determine both constants and logarithmic terms by matching perturbative renormalization-group with exact results, so that the final expressions for the relaxation rates do not contain any free parameters. Our theoretical results are in excellent agreement with NMR experiments in Sr_2CuO_3.

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There has been significant interest in the low-dimensional quantum spin systems and quantum critical phenomena in recent years due to the discovery of high-temperature superconductivity in layered cuprates. Nuclear magnetic resonance (NMR) has been a powerful tool in studying the spin dynamics of the cuprate compounds.[1] The measurements of the longitudinal relaxation rate $1/T_1$, the spin echo decay rate $1/T_{2G}$, and the Knight shift over a wide temperature range define the spectrum of antiferromagnetic fluctuations in the high-T_c cuprates.[2] These NMR experiments have been the basis of the phenomenological spin-fluctuation model,[3] which exhibits quantum critical behavior,[1] because the system always remains close to the antiferromagnetic instability.

A quantum spin-1/2 spin chain is another example of a quantum critical system with novel properties. The physical properties of this system are well understood theoretically. The XXZ spin-1/2 quantum spin chain is described by the Hamiltonian

$$H = J\sum_i \left[S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \gamma S_i^z S_{i+1}^z\right]. \tag{1}$$

This model exhibits quantum critical behavior for $-1 \leqslant \gamma \leqslant 1$, with asymptotic correlation functions vanishing with distance as a power law. Inverse temperature $1/T$ acts essentially as a finite system size, so that the power law for the correlation function crosses over to exponential decay at distances $r > \xi_T \simeq \hbar c/T$. For $|\gamma| > 1$ the spin-1/2 chain is equivalent to a model of massive free fermions, and the correlation functions decay exponentially with distance. Exactly at the Heisenberg point, $\gamma = 1$, logarithmic corrections to the correlation functions appear as a result of the presence of the leading marginally irrelevant operator.

Logarithmic corrections in the SU(2)-invariant models are well known. For example, a calculation of the logarithmic corrections up to two loops was done for the fermion model with backward scattering,[4] the sine-Gordon model,[5] and the SU(2) Gross-Neveu model.[6] Logarithms appear in every physical property of the spin-1/2 Heisenberg chain. For example, $1/\ln(H)$ dependence of magnetization on magnetic field was found in Ref. 7 and in Refs. 8 and 9. The temperature-dependent $1/\ln(T)$ corrections to the bulk spin susceptibility,[10] logarithmic behavior of the structure factor at low frequency, and logarithmic divergence of the spin autocorrelation function are other well-known consequences of the marginally irrelevant operator.[11] Finite-size scaling corrections to the staggered spin susceptibility were found in Ref. 12.

In what follows we determine the logarithmic behavior of the nuclear magnetic resonance (NMR) relaxation rates T_1 and T_{2G}. The measurement and interpretation of the NMR relaxation rates in spin-1/2 has a long history as well. First NMR experiments were performed more than 20 years ago[13–15] on $CuSeO_4 \cdot 5H_2O$ and $CuSO_4 \cdot 5H_2O$, where, surprisingly, it was found that T_1 was almost temperature independent. Later this fact was explained in a rather simple fashion by Sachdev,[16] who, however, did not find parameter-free expressions for T_1 and T_{2G}. Recent experiments by Takigawa *et al.*[23] have confirmed that both T_1 and $T_{2G}/\sqrt{T}$ are almost temperature independent in spin-1/2 chains.

Nuclear spins probe local spin environment. The Knight shift provides a measure of the uniform magnetic susceptibility at a particular nuclear site, while the experiments on the spin-lattice relaxation rate yield information on the imaginary and real parts of the dynamic spin susceptibility $\chi(\mathbf{q},\omega)$. The analysis of the NMR experiments begins with the magnetic hyperfine Hamiltonian, which couples nuclear spins and conduction electron spins:

$$H_{HF} = \sum_{\alpha,i,j} A_\alpha^{ij} I_{i\alpha} S_{j\alpha}, \tag{2}$$

where I is the nuclear spin, and S is the electron spin, and α enumerates spin projections for sites i and j. The following expressions can be obtained[17] for T_1 and T_{2G}:

$$\frac{1}{T_1} = \frac{2k_B T}{\hbar^2}\int \frac{dq}{2\pi} A_\perp^2(q)\frac{\mathrm{Im}\,\chi(q,\omega_0)}{\omega_0}, \tag{3}$$

$$\left(\frac{1}{T_{2G}}\right)^2 = \frac{0.68}{8\hbar^2}\left[\int \frac{dq}{2\pi} A_\parallel^4(q)\chi^2(q) - \left\{\int \frac{dq}{2\pi} A_\parallel^2(q)\chi(q)\right\}^2\right]. \tag{4}$$

Here $A_\parallel(q)$ and $A_\perp(q)$ are the hyperfine couplings parallel and perpendicular to the easy axis of the crystal, 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[16] shows that the staggered component is dominant at small T. Indeed, the contribution of the uniform component scales as $1/T_1 \propto T$, $1/T_{2G} \propto T^0$, while for the staggered component $1/T_1 \propto T^0$, $1/T_{2G} \propto T^{-1/2}$.

For the purpose of comparison of theory with experiment, it is convenient to define normalized dimensionless NMR relaxation rates:

$$\left(\frac{1}{T_1}\right)_{norm} = \frac{\hbar J}{A_\perp^2 T_1}, \tag{5}$$

$$\left(\frac{\sqrt{2}}{T_{2G}}\right)_{norm} = \left(\frac{k_B T}{pJ}\right)^{1/2} \frac{\hbar J}{A_\parallel^2(\pi) T_{2G}}. \tag{6}$$

The calculation of the NMR relaxation rates are based on the continuum limit bosonized approximation to the Heisenberg model. The Hamiltonian density can be written as

$$H = H_0 - 2\pi g \vec{J}_L \vec{J}_R. \tag{7}$$

Here H_0 is the Hamiltonian density for a free boson of compactification radius $R = 1/\sqrt{2\pi}$, $\vec{J}_L$ and $\vec{J}_R$ are the left and right moving currents. The coupling constant obeys the renormalization-group equations known for the Kosterlitz-Thouless or the Kondo problem with ferromagnetic interactions:[18]

$$\beta \equiv dg/d\ln\Lambda = -g^2 - \frac{1}{2}g^3, \tag{8}$$

as the energy cutoff Λ varies.

The low-temperature asymptotics for NMR relaxation rates are determined by the staggered component of the dynamic spin correlator, which has the following general form:[19]

$$\chi_s(r,t,T,g_0) = DZ(g(T))F[g(T), rT/c, tT]. \tag{9}$$

Here $Z(g(T))$ is a cutoff-dependent renormalization factor, C is a nonuniversal constant. This scaling form can be easily obtained from the Callan-Symanzik renormalization group equations:

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

where $\beta(g)$ is the beta function for the coupling constant g in Eq. (7):

$$\frac{dg}{d\ln T} = -\beta(g) = g^2 - g^3/2 + O(g^4) \tag{11}$$

and $\gamma(g) \simeq 1/2 - g/4 + O(g^2)$ is the anomalous dimension. In Eq. (10) the T derivative acts only on the first argument of χ_s; rT and tT are held fixed. The solution of Eq. (10) can then be written in the form Eq. (9) with

$$D \propto \exp\left(2\int_0^{g_0} \frac{\gamma[g']}{\beta(g')} dg'\right), \tag{12}$$

$$Z(g) = \exp\left(-2\int_0^{g(T)} \frac{\gamma[g']}{\beta(g')} dg'\right), \tag{13}$$

where $g_0 \equiv g(\Lambda)$ is the ''bare'' coupling—the coupling at the energy cutoff scale Λ.

The leading behavior of $Z(g)$ is easily seen from perturbative expressions for $\beta(g)$ and $\gamma(g)$ given above,[20] $Z(g) \propto 1/\sqrt{g}$. Integrating Eq. (9) gives

$$\frac{1}{T_1} \propto Z(g(T))[1 + a_1 g(T) + a_2 g(T)^2 + \cdots],$$

$$\frac{1}{T_{2G}} \propto \frac{Z(g(T))}{\sqrt{T}}[1 + b_1 g(T) + b_2 g(T)^2 + \cdots]. \tag{14}$$

The nonuniversal constants a_i, b_i, the cutoff Λ, and common factor D in these expressions can be fixed using exact Bethe ansatz results on the correlation functions. The value of $D = 1/(2\pi)^{3/2}$ was determined in Refs. 21 and 22.

A complete calculation of the NMR relaxation rates gives

$$(1/T_1)_{norm} = 2D\sqrt{\ln\frac{\Lambda}{T} + \frac{1}{2}\ln\left(\ln\frac{\Lambda}{T}\right)}\left(1 + O\left[\frac{1}{\ln^2\frac{\Lambda}{T}}\right]\right), \tag{15}$$

$$(\sqrt{T}/T_{2G})_{norm} = \frac{\sqrt{I_0}D}{4\sqrt{\pi}}\sqrt{\ln\frac{\Lambda_1}{T} + \frac{1}{2}\ln\left(\ln\frac{\Lambda_1}{T}\right)} \times \left(1 + O\left[\frac{1}{\ln^2\frac{\Lambda_1}{T}}\right]\right). \tag{16}$$

Here $D = 1/(2\pi)^{3/2}$ is the nonuniversal amplitude, $C \simeq 0.577\,215\,7$ is Euler's constant, while the integrals I_0 and I_1 are given by

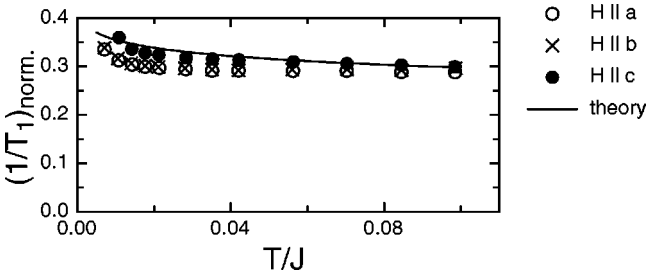

FIG. 1. NMR $1/T_1$ for magnetic fields along different crystal axes in Sr_2CuO_3 from Takigawa *et al.* (Ref. 23) compared to our theoretical expression with no adjustable parameters.

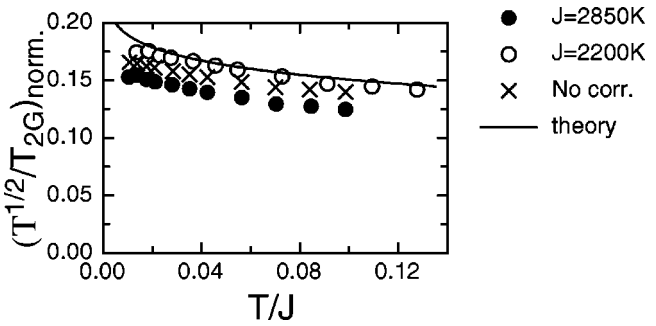

FIG. 2. NMR $T^{1/2}/T_{2G}$ from Takigawa *et al.* (Ref. 23) vs our low-temperature result. The data show different assumptions for the value of J (fitted from the spin susceptibility data). The crosses are the data for $J=2850$ K not corrected for the I_z fluctuations.

$$I_0=\int_0^\infty dx \left| \frac{\Gamma\left(\frac{1+ix}{4}\right)}{\Gamma\left(\frac{3+ix}{4}\right)} \right|^4 \simeq 71.2766,$$

$$I_1=\int_0^\infty dx \left| \frac{\Gamma\left(\frac{1+ix}{4}\right)}{\Gamma\left(\frac{3+ix}{4}\right)} \right|^4 \mathrm{Re}\left[\Psi\left(\frac{1+ix}{4}\right)+\Psi\left(\frac{3+ix}{4}\right) \right]$$

$$\simeq -259.94, \tag{17}$$

where $\Psi(x)$ is digamma function. The $1/\ln(\Lambda/T)$ term is incorporated in the cutoff as in Ref. 19. 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 loglog terms in the numerator of Eq. (17). The cutoff parameters Λ can be determined using exact methods:

$$\Lambda = 2\sqrt{2\pi}e^{C+1}J \simeq 24.27J, \tag{18}$$

$$\Lambda_1 = \frac{\sqrt{2\pi}e}{8} e^{-I_1/2I_0} J \simeq 5.27J. \tag{19}$$

The ratio of the relaxation rates, however, is only weakly temperature dependent,

$$\left(\frac{T_{2G}}{T_1\sqrt{T}}\right)_{norm} \simeq 1.680\left(1+\frac{0.7632}{\ln(\Lambda/T)}\right). \tag{20}$$

In summary, I have presented theoretical low-temperature results for NMR rates T_1 and T_{2G}. The temperature dependence of $1/T_1$ is logarithmic, which is expected in the presence of the leading irrelevant operator. The main improvement over past theories is that the amplitude and the cutoffs were also calculated, so our expressions do not contain any free parameters. This has been a matter of confusion in the past.[23] In particular, cutoffs have been fitted and used together with 1/log terms which redefine them. Presumably, this explains the difference of our cutoff Λ with a fitted value of $4.5J$ used in Ref. 23. Our theoretical results agree reasonably well with experimental data of Takigawa *et al.*[23] on Sr_2CuO_3, as shown in Figs. 1 and 2.

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