NMR relaxation in half-integer antiferromagnetic spin chains

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Nuclear relaxation in half-integer spin chains at low-temperatures ($T \ll J$, the antiferromagnetic exchange constant) is dominated by dissipation from a gas of thermally excited, overdamped, spinons. The universal low-temperature dependence of the relaxation rates $1/T_1$ and $1/T_{2G}$ is computed.

Nuclear magnetic resonance experiments have recently been shown to be a powerful tool in studying the electronic spin dynamics of the two-dimensional quantum antiferromagnets in the cuprate compounds.[1] The combined measurements of the longitudinal relaxation rate, $1/T_1$, and the spin-echo decay rate $1/T_{2G}$, over a wide temperature (T) range allow one to learn a great deal about the antiferromagnetic spin-fluctuation spectrum.[2-5]

Another class of Heisenberg antiferromagnets with novel properties are the one-dimensional spin chains with half-integer spins per site. Some nuclear relaxation measurements on such systems have been performed[6] and more detailed studies are under way.[7] Our theoretical understanding of the ground state properties of this system is in good shape,[8] and there has been limited discussion of the behavior at finite temperatures.[9-11] It is the purpose of this paper to use results on the T, wave vector, and frequency dependence of the uniform and staggered spin susceptibilities to obtain the NMR relaxation rates. There have been earlier discussions[6,12] of the T_1 relaxation rate in spin-1/2 chains and we will comment on their relationship to our results below.

An important difference between the two-dimensional antiferromagnets and the half-integer spin chains is that the latter are *generically* critical. This means that the zero-temperature spin correlators have power-law decays in both space and time, over a finite range of ratios of short-range exchange interactions—this happens because the critical fixed point has no relevant perturbations which respect the symmetry of the underlying Hamiltonian. However, for sufficiently large second-neighbor coupling (for example), there is a transition to a gapped, dimer phase which is not critical. We will restrict our attention here to the range of couplings where the ground state is critical. This immediately has important consequences for the finite temperature spin correlators: the entire low-temperature region ($T \ll J$) may be considered as the analog of the *quantum-critical region* of two-dimensional antiferromagnets.[13,14,3] There is now no requirement that the temperature be larger than some stiffness-associated energy scale, as there is no analog of the renormalized-classical[13] region. Of course, when the small interchain coupling is taken into account, three-dimensional long-range order, and the corresponding renormalized-classical region, can appear at very low temperatures.

The principles of conformal invariance allow one to obtain the exact scaling functions of the quantum-critical region of many one-dimensional quantum systems[15,9-11]. Half-integer spin chains however possess a complicating feature. There is a marginally irrelevant operator at the critical fixed point, which spoils conformal invariance by inducing logarithmic corrections to the leading scaling behavior.[16,17] There is no analog of this effect in the two-dimensional antiferromagnets. To keep the analysis simple, I will first discuss the computation in which this marginal operator is ignored. The logarithmic corrections induced by it will be discussed in the next section.

Let us first look at the staggered spin correlations of the half-integer spin chain. It is known[16,17] that the equal-time, ground state spin correlators have the staggered component

$$\langle S_i(0) S_j(R) \rangle_{T=0} = \delta_{ij}(-1)^R (\ln R)^{1/2} \frac{D}{R} \qquad (1)$$

at large spatial separation R. The constant D is nonuniversal and depends upon the choice of microscopic exchange couplings. In the absence of the $\ln R$ term, this result is sufficient to specify the staggered susceptibility at finite temperatures.[9-11] As noted above, we will proceed in the remainder of this section by ignoring the $\ln R$ term—we will put it back in the next section. Then, a simple application of the results of Refs. 11 gives us the following result for $\chi_s(k,\omega)$, the wave vector (k) and frequency dependent staggered susceptibility at finite T (for χ_s, k is the deviation of the wave vector from π/a, where a is the nearest-neighbor spacing):

$$\chi_s(k,\omega)$$

$$= \frac{D}{2k_B T} \frac{\Gamma\left(\frac{1}{4} - i\frac{\hbar(\omega + ck)}{4\pi k_B T}\right) \Gamma\left(\frac{1}{4} - i\frac{\hbar(\omega - ck)}{4\pi k_B T}\right)}{\Gamma\left(\frac{3}{4} - i\frac{\hbar(\omega + ck)}{4\pi k_B T}\right) \Gamma\left(\frac{3}{4} - i\frac{\hbar(\omega - ck)}{4\pi k_B T}\right)} \cdot$$

$$(2)$$

The quantity c is the $T = 0$ spinon velocity. Note that the only microscopic input into this result for the susceptibility are the values of c and D. A plot of the spectral function $\mathrm{Im}\chi_s(k,\omega)/\omega$ was presented in Ref. 11 for a different value of the critical exponents; here we present

the imaginary part of the result (2) in Fig. 1. For small wave vectors, with $\hbar ck$ smaller than or around $k_B T$, the peak in the spectral function is at $\omega = 0$, indicating the presence of overdamped excitations—spinon excitations interact strongly with other thermally excited spinons, acquiring a very short lifetime. We will see below that the NMR relaxation is dominated by the contribution of these spinons. At larger k, $\hbar ck \gg k_B T$, the peak in the spectral function moves to finite ω (see Fig. 1)—these are propagating spinons with a lifetime of order $\hbar/k_B T$.

We turn next to the uniform spin susceptibility, $\chi_u(k,\omega)$, where k is now the true wave vector, measured from the zone center. Unlike the staggered component, the overall normalization of the uniform spin susceptibility is not arbitrary, as the total spin is a conserved quantity. It is therefore useful to define a magnetization *density* $m_a(R)$ which is the spin per unit length. The $T = 0$ correlator of m is given by[8]

$$\langle m_a(R,\tau)m_b(0,0)\rangle_{T=0}$$

$$= -\frac{\delta_{ab}}{8\pi^2}\left(\frac{1}{(R+ic\tau)^2} + \frac{1}{(R-ic\tau)^2}\right) , \quad (3)$$

where τ is the Euclidean time. We can obtain the finite

FIG. 1. A plot of the universal spectral weight $[(k_B T)^2/D]\mathrm{Im}\chi_s(k,\omega)/\hbar\omega$ of the half-integer spin chain as a function of $\bar\omega = \hbar\omega/k_B T$ for various values of $\bar k = \hbar ck/k_B T$. The values for $\bar k = 1$ have been scaled down by a factor of $1/3$. Notice the overdamped peak at $\bar k = 1$ and the propagating peaks at $\bar k = 3, 5$.

T form of this correlator by conformally mapping onto a Matsubara strip, keeping in mind that the magnetization density is a component of a current and has nonzero conformal "spin." This procedure yields

$$\langle m_i(R,\tau)m_j(0,0)\rangle = -\frac{\delta_{ij}}{2}\left(\frac{k_B T}{\hbar c}\right)^2 \frac{\cosh(2\pi Rk_B T/\hbar c)\cos(2\pi\tau k_B T/\hbar) - 1}{[\cosh(2\pi Rk_B T/\hbar c) - \cos(2\pi\tau k_B T/\hbar)]^2} . \quad (4)$$

Performing a Fourier transform of this result to wave vectors k and Matsubara frequencies ω_n, we find the remarkably simple result

$$\chi_u(k,i\omega_n) = \frac{c}{2\pi\hbar}\frac{k^2}{c^2k^2 + \omega_n^2} . \quad (5)$$

Note that, unlike $\chi_s(k,\omega)$, all T dependence has disappeared. The T dependence in (4) is obtained while performing the discrete Fourier transform from frequency to time: the T dependence is contained entirely in the frequency spacing of the Matsubara sum. Analytically continuing to real frequencies we get

$$\chi_u(k,\omega) = \frac{c}{2\pi\hbar}\frac{k^2}{c^2k^2 - (\omega + i\epsilon)^2} , \quad (6)$$

where ϵ is a positive infinitesimal. A conspicuous property of this result is that there is no damping of the pole at $\omega = ck$, even at finite T. This is, of course, a property only of the scaling limit. Upon considering corrections to scaling, some damping should appear, but will be suppressed by powers of T/J. Related to the absence of damping is the fact that the spectrum of magnetization fluctuations is propagating and not diffusive. The spin diffusion constant is effectively infinite in the scaling limit.

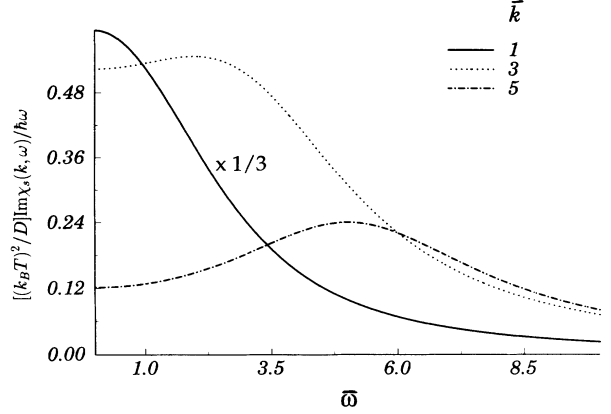One might, at this point, raise the issue of whether it is

legitimate to neglect the damping of the uniform magnetization modes: perhaps the damping coefficient will be dangerously irrelevant and will contribute a singular T dependence to the relaxation rates computed below. This possibility appears to me to be quite unlikely. The only role of temperature in all of the computations discussed here is to act as a finite-size cutoff in the imaginary-time direction to a critical theory: the $T = 0$ result should surely be obtained in the limit $T \to 0$.

We are now finally in a position to compute the nuclear relaxation rates. We will use the following expressions,[18] which are appropriate for the relaxation of a nucleus coupled to the electronic spins by a hyperfine term:

$$\frac{1}{T_1} = \lim_{\omega\to 0}\frac{2k_B T}{\hbar^2\omega}\int\frac{dk}{2\pi}A_\parallel^2(k)\mathrm{Im}\chi(k,\omega) ,$$

$$\left(\frac{\hbar}{T_{2G}}\right)^2 = \frac{1}{a}\int\frac{dk}{2\pi}A_\perp^4(k)\,[\chi(k,0)]^2$$

$$- \left[\int\frac{dk}{2\pi}A_\perp^2(k)\,\chi(k,0)\right]^2 , \quad (7)$$

where a is the lattice spacing, and $A_\parallel$ ($A_\perp$) are the hyperfine couplings parallel (perpendicular) to the field; their k dependence is expected to be smooth and arises from appropriate form factors. We have also neglected contributions from nucleus-nucleus dipolar couplings which could be important in some materials. The susceptibil-

ity χ should include contributions from both the uniform and staggered spin fluctuations. It is now a straightforward matter to insert (2) and (6) into (7) and obtain the T dependence of the rates. Simple power counting shows that the contribution of χ_s to the rates behaves as $1/T_1 \sim T^0$ and $1/T_{2G} \sim T^{-1/2}$, while the contribution of χ_u scales as $1/T_1 \sim T$ and $1/T_{2G} \sim T^0$. In both cases the contribution of the staggered component is dominant for small T. A complete calculation of this term yields finally the following leading low T result:

$$\frac{1}{T_1} = A_\parallel^2 (\pi/a) \frac{\pi D}{\hbar^2 c} \ ,$$

$$\frac{1}{T_{2G}} = A_\perp^2 (\pi/a) \frac{D}{2\hbar^2 c} \left(\frac{\hbar c}{k_B T a} \right)^{1/2} I \ , \tag{8}$$

where the numerical factor, I, is given by the integral

$$I^2 = \int_0^\infty dx \left| \frac{\Gamma[(1+ix)/4]}{\Gamma[(3+ix)/4]} \right|^4 = 71.276\,591\,604\ldots . \tag{9}$$

We emphasize that these results have neglected the logarithmic corrections to scaling which we will consider below. Note that the unknown prefactor D cancels out upon considering the ratio of the rates: this should be a convenient way of experimentally testing these results.

The T-independent behavior of $1/T_1$ (modulo logarithmic corrections discussed below) has already been noticed in previous analyses;[6,12] however a different T-independent value was obtained as these works did not account for the damping of the spinon states.

We now consider the consequence of the marginally irrelevant operator present in the field theory of half-integer spin chains.[8] The basic result is easy to state: both expressions for the relaxation rates in (8) acquire an identical, multiplicative prefactor of $\ln^{1/2}(J/T)$. Fur-

ther there are subdominant additive corrections which are suppressed by powers of $1/\ln(J/T)$: the form of these additive corrections will be different for the two relaxation rates. As these additive corrections are only logarithmically suppressed, it may be necessary to have T significantly smaller than J before the leading results (8) with their $\ln^{1/2}(J/T)$ are accurate.

The arguments for the logarithmic corrections are simple and closely parallel those presented in Refs. 16 and 17. One begins by writing down the Callan-Symanzik equation for $1/T_1(T, \Lambda)$, where $\Lambda \sim J$ is an ultraviolet cutoff. It is known that this quantity is finite in the limit $\Lambda \to \infty$ after multiplication by a Λ-dependent renormalization factor Z_Λ. This fact can be used to derive a Callan-Symanzik equation for $1/T_1$ in which the temperature T scales under its canonical dimension as it is nothing but an inverse length in Matsubara time direction. Integrating the Callan-Symanzik equation[16,17] to a scale where $T \sim \Lambda$, expresses $1/T_1$ as $\ln^{1/2}(\Lambda/T)$ times the value of $1/T_1$ in a system in which the coefficient of the marginally irrelevant coupling $\sim 1/\ln(\Lambda/T)$. To leading order, we can neglect this coupling and carry out the latter calculation in the critical theory with no marginal coupling, which is exactly what was done above. A similar argument can be made for $1/T_{2G}$: the $\ln^{1/2}(\Lambda/T)$ factor will be the same because the rescaling factor Z_Λ is identical to that for $1/T_1$. However, the perturbative corrections in powers of the coupling constant $\sim 1/\ln(\Lambda/T)$ should be different in the two rates.[19]

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