Finite Temperature Drude Weight of the One-Dimensional Spin-1/2 Heisenberg Model

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Using the Bethe ansatz method, the zero frequency contribution (Drude weight) to the spin current correlations is analyzed for the easy plane antiferromagnetic Heisenberg model. The Drude weight is a monotonically decreasing function of temperature for all $0 \leq \Delta \leq 1$; it approaches the zero temperature value with a power law and appears to vanish for all finite temperatures at the isotropic $\Delta = 1$ point. [S0031-9007(99)08507-5]

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The low frequency dynamics in one-dimensional spin chains is a long standing problem. It has recently attracted renewed interest, due partly to the fabrication of excellent quasi-one-dimensional, spin-1/2 magnetic materials as Sr_2CuO_3 and $CuGeO_3$. Detailed NMR experiments [1] revealed an unusually high value of the spin diffusion constant and nearly ballistic behavior.

The first issue on the question of spin diffusion is the zero frequency contribution (or Drude weight) to the dynamic spin current correlations at finite temperatures. If the Drude weight turns out to be finite, the current correlations do not decay to zero at long times, implying ideal conducting behavior. If they decay to zero, the question still remains open whether they decay fast enough so that transport coefficients can be defined. Several numerical studies have been devoted to the analysis of the diffusive behavior in the Heisenberg model [2–5] with suggestive, but not conclusive, results.

In relation to this problem, it has been proposed that the integrability of the spin-1/2 Heisenberg model implies pathological spin dynamics and presumably the absence of spin diffusion [2,6]. A straightforward demonstration on the way in which conservation laws, characterizing integrable systems, might affect the long time dynamics was pointed out in Ref. [7]. There it was shown that in several quantum integrable models the uniform current correlations do not decay to zero at long times due to the overlap of the currents to conserved quantities. Unfortunately, this simple idea turned out to be insufficient for deciding on the decay of spin currents in the spin-1/2 Heisenberg model at zero magnetic field.

On the other hand, a new method was proposed recently by Fujimoto and Kawakami [8] that allows the direct analytical evaluation of the Drude weight at finite temperatures. This procedure is based on the calculation of finite size corrections of the energy eigenvalues obtained by the Bethe ansatz method [9]. The analysis starts from a convenient expression for the finite temperature Drude weight as the thermal average of curvatures of energy levels in a Hamiltonian subject to a fictitious flux coupled to the hopping or spin-flipping term [10,11]. Note that the anisotropic Heisenberg model is equivalent to the model of spinless fermions interacting with nearest neighbor interaction using the Jordan-Wigner transformation [12]. The direct analogy between charge and spin current correlations also suggests the use of the name "Drude weight" in the context of spin correlations.

In this Letter, we calculate the Drude weight for the antiferromagnetic Heisenberg model using the procedure proposed in Refs. [8] and [9]. The formulation and notation of the thermodynamic Bethe ansatz equations by Takahashi and Suzuki [13] will be closely followed. This construction is based on the string assumption for the excitations, and it is particularly complex for arbitrary values of the anisotropy parameter Δ. The allowed type of strings are constrained by the normalizability of the wave functions [14]. Therefore, for simplicity and without loss of generality, the analysis will be limited at $\Delta = \cos(\pi/\nu)$, $\nu =$ integer, where only a finite number of string excitations is allowed.

The results presented here are in good agreement with numerical results obtained by exact diagonalization of the Hamiltonian matrix on finite size lattices [4]. They lend support to both the string construction and the novel procedure for calculating the Drude weight from finite size corrections to the Bethe ansatz eigenvalues.

The *XXZ* anisotropic Heisenberg Hamiltonian for a chain of N sites with periodic boundary conditions $S^a_{N+1} = S^a_1$ is given by

$$H = J \sum_{i=1}^{N} (S^x_i S^x_{i+1} + S^y_i S^y_{i+1} + \Delta S^z_i S^z_{i+1}), \qquad (1)$$

where $S^a_i = \frac{1}{2}\sigma^a_i$, σ^a_i are the Pauli spin operators with components $a = x, y, z$ at site i. The region $0 \leq \Delta \leq 1$ is parametrized by $\Delta = \cos\theta$, $\theta = \pi/\nu$, $\nu =$ integer. The pseudomomenta k_α and phase shifts $\phi_{\alpha\beta}$ characterizing the Bethe ansatz wave functions are expressed in terms of the rapidities x_α

$$\cot\left(\frac{k_\alpha}{2}\right) = \cot\left(\frac{\theta}{2}\right)\tanh\left(\frac{\theta x_\alpha}{2}\right),$$
$$\cot\left(\frac{\phi_{\alpha\beta}}{2}\right) = \cot\left(\frac{\theta}{2}\right)\tanh\left(\frac{\theta(x_\alpha - x_\beta)}{2}\right). \qquad (2)$$

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For M down spins and N-M up spins, the energy E and momentum K are given by

$$E = J \sum_{\alpha=1}^{M} (\cos k_\alpha - \Delta), \qquad K = \sum_{\alpha=1}^{M} k_\alpha . \quad (3)$$

Coupling the spin flipping term to a fictitious flux ϕ, the Hamiltonian becomes

$$H = J \sum_{i=1}^{N} \left(\frac{1}{2} e^{i\phi} \sigma_i^+ \sigma_{i+1}^- + \text{h.c.} \right) + \Delta S_i^z S_{i+1}^z . \quad (4)$$

The finite temperature Drude weight D can then be calculated by [11]

$$D = \frac{1}{N} \sum_n p_n \frac{1}{2} \frac{\partial^2 E_n(\phi)}{\partial \phi^2} \bigg|_{\phi \to 0} , \quad (5)$$

where E_n are the eigenvalues of the Hamiltonian and p_n are the corresponding Boltzmann weights. By imposing periodic boundary conditions on the Bethe ansatz wave functions, the following relations are obtained:

$$\left\{ \frac{\sinh \frac{1}{2}\theta(x_\alpha + i)}{\sinh \frac{1}{2}\theta(x_\alpha - i)} \right\}^N = -e^{i\phi N} \prod_{\beta=1}^{M} \left\{ \frac{\sinh \frac{1}{2}\theta(x_\alpha - x_\beta + 2i)}{\sinh \frac{1}{2}\theta(x_\alpha - x_\beta - 2i)} \right\}, \quad \alpha = 1,2,\ldots,M . \quad (6)$$

In the thermodynamic limit, the solutions of Eqs. (6) are grouped into strings of order n_j, $j = 1,\ldots,\nu$ and parity $v_j = +$ or $-$. For $\theta = \pi/\nu$ the allowed strings are of order $n_j = j$, $j = 1,\ldots,\nu - 1$ and parity $v_j = +$ of the form

$$x_{\alpha,+}^{n,k} = x_\alpha^n + (n + 1 - 2k)i + O(e^{-\delta N}), \quad k = 1,2,\ldots,n , \quad (7)$$

and strings of order $n_\nu = 1$ and parity $v_\nu = -$ of the form

$$x_{\alpha,-} = x_\alpha + i\nu + O(e^{-\delta N}), \qquad \delta > 0 . \quad (8)$$

By multiplying the terms in Eq. (6) corresponding to different members of a string and taking the logarithm, we obtain

$$N t_j(x_\alpha^j) = 2\pi I_\alpha^j + \sum_{k=1}^{\infty} \sum_{\beta=1}^{M_k} \Theta_{jk}(x_\alpha^j - x_\beta^k) + n_j \phi N, \quad \alpha = 1,2,\ldots,M_j . \quad (9)$$

I_α^j are integers (or half-integers) and M_k is the number of strings of type k,

$$t_j(x) = f(x; n_j, v_j) ,$$

$$\Theta_{jk}(x) = f(x; |n_j - n_k|, v_j v_k) + f(x; n_j + n_k, v_j v_k) + 2 \sum_{i=1}^{\min(n_j,n_k)-1} f(x; |n_j - n_k| + 2i, v_j v_k) ,$$

$$f(x; n, v) = 2v \tan^{-1}\{[\cot(n\pi/2\nu)]^v \tanh(\pi x/2\nu)\} .$$

Following Ref. [9], the finite size corrections to the energy eigenvalues for a system of size N are calculated by introducing the function g_{1j}, g_{2j}:

$$x_N^j = x_\infty^j + \frac{g_{1j}}{N} + \frac{g_{2j}}{N^2} , \quad (10)$$

where $x_N^j(x_\infty^j)$ are the rapidities for a system of size $N(\infty)$. Next, we expand Eq. (9) to orders of $1/N$ and, in the thermodynamic limit, introduce the densities of excitations ρ_j and hole densities ρ_j^h. The sums over the pseudomomenta are replaced by integrals over excitation densities plus boundary terms using the Euler-Maclaurin formula.

To $O(1)$ we recover the integral equations for the excitation densities in the thermodynamic limit [13]:

$$a_j = \lambda_j(\rho_j + \rho_j^h) + \sum_k T_{jk} \circ \rho_k . \quad (11)$$

$\circ$ denotes the convolution $a \circ b(x) = \int_{-\infty}^{+\infty} a(x - y)b(y)dy$, $T_{jk}(x) = (1/2\pi)d\Theta_{jk}(x)/dx$, and $a_j(x) = (1/2\pi)dt_j(x)/dx$. The sum over k is constrained to the allowed strings, given in our case by Eqs. (7) and (8) and $\lambda_j = 1$, $j = 1,\ldots,\nu - 1$, and $\lambda_\nu = -1$.

To $O(1/N)$,

$$\lambda_j g_{1j}(\rho_j + \rho_j^h) = -\sum_k T_{jk} \circ (g_{1k}\rho_k) + \frac{n_j \phi}{2\pi} . \quad (12)$$

To $O(1/N^2)$,

$$\lambda_j g_{2j}(\rho_j + \rho_j^h) + \sum_k T_{jk} \circ (g_{2k}\rho_k) = \frac{1}{2} \frac{d}{dx} \times \left\{ \lambda_j g_{1j}^2(\rho_j + \rho_j^h) + \sum_k T_{jk} \circ (g_{1k}^2 \rho_k) \right\} + \text{boundary terms} . \quad (13)$$

Minimizing the free energy we obtain the standard Bethe ansatz equations for the equilibrium densities $\eta_j = \rho_j^h/\rho_j$ at temperature $T(\beta = 1/\kappa_B T)$:

$$\ln \eta_j = -2\nu \sin(\pi/\nu) J a_j \beta + \sum_k \lambda_k T_{jk} \circ \ln(1 + \eta_k^{-1}) . \quad (14)$$

These relations define the temperature dependent effective dispersions $\epsilon_j = (1/\beta)\ln(\rho_j^h/\rho_j)$. In the string representation the energy is given by

$$E = N \sum_{j=1}^{\infty} \int_{-\infty}^{+\infty} dx \left[-2\nu \sin\left(\frac{\pi}{\nu}\right) J a_j(x) \right] \rho_j(x) . \quad (15)$$

Expanding this expression for the energy we find that the first order correction in $1/N$ vanishes. Therefore, the second derivative with respect to ϕ of the second order correction gives us the final expression for the Drude weight:

$$D = \frac{1}{2} \sum_j \int_{-\infty}^{+\infty} dx \left[(\rho_j + \rho_j^h) \frac{\partial g_{1j}}{\partial \phi} \right]^2 \frac{d}{dx} \left(\frac{-1}{1 + e^{\beta \epsilon_j}} \right) \times \left(\frac{1}{\rho_j + \rho_j^h} \frac{d\epsilon_j}{dx} \right) . \quad (16)$$

This expression is formally similar to the one obtained in Ref. [8] for the Drude weight in the Hubbard model. It has an elegant interpretation by comparing it to the analogous expression for independent fermions. Taking the second derivative of the free energy with respect to the flux ϕ, we find

$$\frac{\partial^2 F}{\partial \phi^2} = \sum_\mu \langle n_\mu \rangle \frac{\partial^2 \epsilon_\mu}{\partial \phi^2} - \beta \sum_\mu \langle n_\mu \rangle (1 - \langle n_\mu \rangle) \left(\frac{\partial \epsilon_\mu}{\partial \phi} \right)^2, \tag{17}$$

where $\langle n_\mu \rangle$ is the Fermi-Dirac distribution for particles with dispersion ϵ_μ. Considering that the left-hand side (the persistent current susceptibility) vanishes in the thermodynamic limit for any finite temperature and that the first term in the right-hand side is equal to $2ND$, we find that

$$D \simeq \frac{\beta}{2N} \sum_\mu \langle n_\mu \rangle (1 - \langle n_\mu \rangle) \left(\frac{\partial \epsilon_\mu}{\partial \phi} \right)^2 \bigg|_{\phi \to 0} . \tag{18}$$

Rewriting Eq. (16), we arrive at a similar expression:

$$D = \frac{1}{2} \beta \sum_j \int_{-\infty}^{+\infty} dx (\rho_j + \rho_j^h) \langle n_j \rangle (1 - \langle n_j \rangle) \times \left(\frac{\partial \epsilon_j}{\partial x} \frac{\partial g_{1j}}{\partial \phi} \right)^2 \tag{19}$$

with $\langle n_j \rangle = 1/(1 + e^{\beta \epsilon_j})$. Therefore, the Bethe ansatz expression for the Drude weight resembles that of independent fermionlike excitations.

To obtain the distributions ρ_j, ρ_j^h and $\frac{\partial g_{1j}}{\partial \phi}$, the coupled integral equations (11), (12), and (14) are numerically solved by iteration.

In Fig. 1, D is shown as a function of Δ for $2 \leq \nu \leq 16$ $(0 \leq \Delta < 0.98)$ and different characteristic temperatures. The main result is that the Drude weight D is a monotonically decreasing function of Δ and temperature. At $T = 0$, $D = \frac{\pi}{8} \frac{\sin(\pi/\nu)}{\frac{\pi}{\nu}(\pi - \frac{\pi}{\nu})}$ [15]. Most interestingly, D seems to vanish at all temperatures for $\Delta = 1$. This result excludes an ideal conducting behavior for the isotropic Heisenberg model. Still, an anomalously slow long time decay of the current correlation functions could lead to pathological low frequency dynamics and nondiffusive behavior. Furthermore, the vanishing of the Drude weight at the isotropic point suggests that it remains zero at all temperatures in the region $\Delta > 1$, the easy axis case (or insulating state in the fermionic model). This conclusion is in accord with the numerical results of Ref. [2]. We should note that numerical investigation close to the isotropic point is somewhat difficult since the number of equations to solve diverges.

In the high temperature limit ($\beta \to 0$), D is proportional to β. The constant of proportionality C_{jj}, equal to the long time asymptotic value of the current correlations [7], is compared with the results obtained in Ref. [4] by exact diagonalization of the Hamiltonian on finite size lattices extrapolated to the infinite size limit. The quantitative agreement obtained lends support to the assumptions

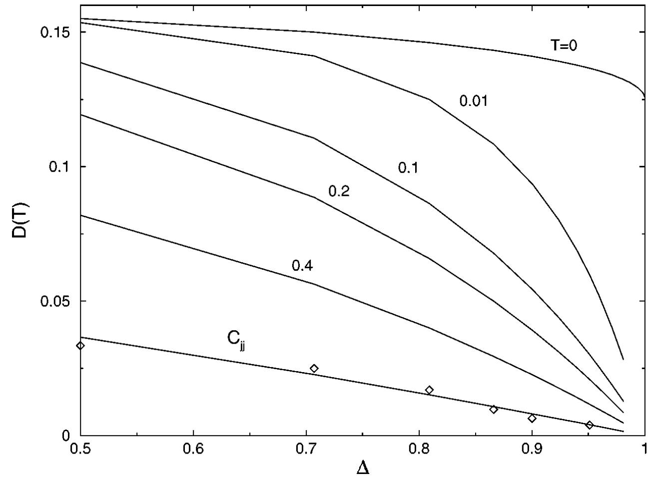

FIG. 1. $D(\Delta)$ evaluated at the points $\nu = 3, \ldots, 16$ and various temperatures. The continuous line is the high temperature proportionality constant $C_{jj} = D/\beta$. The diamonds (◇) indicate exact diagonalization results from Ref. [4].

involved in the whole Bethe ansatz procedure for calculating thermodynamic properties and finite size corrections.

The next observation is that the Drude weight approaches the zero temperature value with a power law of the form

$$D(T) = D(T = 0) - \text{const} \times T^\alpha, \qquad \alpha = \frac{2}{\nu - 1} . \tag{20}$$

To indicate this point, in Fig. 2, $D(T = 0) - D(T)$ is shown for $\nu = 3, \ldots, 6$ in a logarithmic plot along with lines of slope α. Note that the exponent α is half that for the low temperature spin susceptibility as obtained by Abelian bosonization [16]. It is also consistent with the value $\alpha = 2$ for free fermions ($\nu = 2$).

The results presented above concern only the zero frequency contribution to the spin current correlations. A

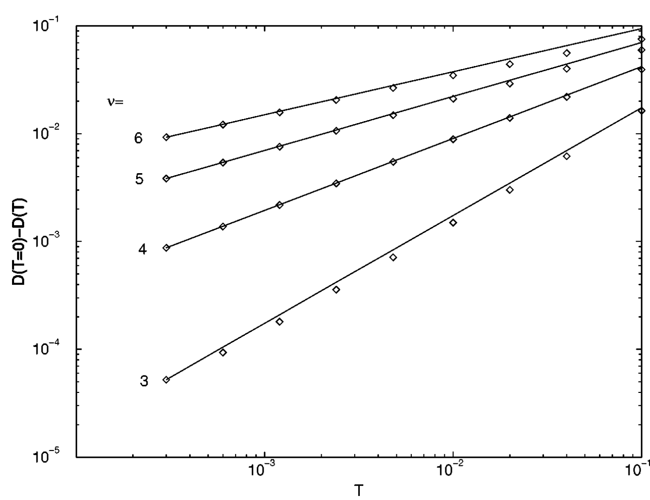

FIG. 2. $D(T = 0) - D(T)$ at different temperatures (◇'s) in a logarithmic scale. The lines indicate slopes $\alpha = 2/(\nu - 1)$.

reliable method for studying the *low frequency* behavior in integrable quantum many body systems (and the influence of nonintegrable perturbations) remains a challenging problem.

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[1] M. Takigawa, N. Motoyama, H. Eisaki, and S. Uchida, Phys. Rev. Lett. **76**, 4612 (1996).
[2] X. Zotos and P. Prelovšek, Phys. Rev. B **53**, 983 (1996).
[3] K. Fabricius and B. M. McCoy, Phys. Rev. B **57**, 8340 (1998) (this paper contains a critical discussion on the issue of spin diffusion and extensive references on previous works).
[4] F. Naef and X. Zotos, J. Phys. C **10**, L183 (1998).
[5] B. N. Narozhny, A. Millis, and N. Andrei, Phys. Rev. B **58**, R2921 (1998).
[6] B. M. McCoy, *Statistical Mechanics and Field Theory, Proceedings of the Seventh Summer Physics School* (World Scientific, Singapore, 1995).
[7] X. Zotos, F. Naef, and P. Prelovšek, Phys. Rev. B **55**, 11 029 (1997).
[8] S. Fujimoto and N. Kawakami, J. Phys. A **31**, 465 (1998).
[9] A. Berkovits and N. G. Murthy, J. Phys. A **21**, 3703 (1988).
[10] W. Kohn, Phys. Rev. **133**, 171 (1964).
[11] H. Castella, X. Zotos, and P. Prelovšek, Phys. Rev. Lett. **74**, 972 (1995).
[12] See, e.g., V. Emery, in *Highly Conducting One-Dimensional Solids*, edited by J. T. Devreese *et al.* (Plenum Press, New York, 1979), p. 247.
[13] M. Takahashi and M. Suzuki, Prog. Theor. Phys. **48**, 2187 (1972).
[14] M. Fowler and X. Zotos, Phys. Rev. B **24**, 2634 (1981); K. Hida, Phys. Lett. **84A**, 338 (1981).
[15] B. S. Shastry and B. Sutherland, Phys. Rev. Lett. **65**, 243 (1990).
[16] S. Eggert, I. Affleck, and M. Takahashi, Phys. Rev. Lett. **73**, 332 (1994).