Spin Stiffness of Mesoscopic Quantum Antiferromagnets

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We study the spin stiffness of a one-dimensional quantum antiferromagnet in the whole range of system sizes L and temperatures T. We show that for integer and half-odd integer spin cases the stiffness differs fundamentally in its L and T dependences, and that in the latter case the stiffness exhibits a striking dependence on the parity of the number of sites. Integer spin chains are treated in terms of the nonlinear sigma model, while half-odd integer spin chains are discussed in a renormalization group approach leading to a Luttinger liquid with Aharonov-Bohm–type boundary conditions.

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Quantum one-dimensional antiferromagnets have been the subject of intensive studies since Haldane [1] conjectured that the spectrum of an integer spin S chain has a finite gap even in the absence of any anisotropy, while half-odd integer S chains are gapless. In both cases the Néel long-range order of the ground state is destroyed by quantum fluctuations. However, the "degree of destruction" is different: For integer S the correlation length is finite, which means that the elementary excitations have a gap, while for half-odd integer S the correlation length is infinite and excitations are gapless. By now, the presence of the Haldane gap for integer S chains is well understood theoretically [2] and has been confirmed in experimental [3] and numerical [4] studies. However, all these investigations were concentrated on the Haldane gap, i.e., on the energy spectrum itself. Thus a broader understanding of the Haldane conjecture is desirable, and the question naturally arises whether there are alternative manifestations of the fundamental difference between integer and half-odd integer spin chains. Indeed, it is the purpose of this work to provide an affirmative answer to this question and to discuss such a particular case in terms of the so-called spin stiffness.

Quite recently, there has been much interest in the spin stiffness (helicity modulus) ρ_s of *classical* Heisenberg ferromagnets [5–7]. ρ_s is defined as a change in the free energy F of the magnet when a twist is applied to the spins at the sample boundaries. When thermal fluctuations are taken into account, ρ_s is being renormalized with respect to its bare value and depends on the scale at which it is probed. Chakravarty [5] has recently shown that ρ_s exhibits features which are familiar from the behavior of the electrical conductance of a metal in the weak localization regime [8]. For instance, in 2D, the mean value of ρ_s depends logarithmically on the sample size L, while the rms value of its fluctuations is universal [9]. This similarity [10] makes the spin stiffness an equal member of the family of traditionally mesoscopic quantities such as a conductance or a persistent current. Also, the stiffness ρ_s serves as a useful (though not perfect) tool for characterizing magnetic long-range order; in particular, a vanishing value of ρ_s indicates absence of order [11].

Our goal here is to study ρ_s of a *quantum* one-dimensional antiferromagnet, where fluctuations are (i) quantum and (ii) topologically distinct for integer and half-odd integer S. We shall see that the behavior of ρ_s is, indeed, quite different for integer and half-odd integer S: ρ_s is renormalized with L in the former case (as it is for a classical 2D ferromagnet), whereas it is L independent (in leading order) in the latter. Moreover, for half-odd integer S, ρ_s is shown to exhibit a striking dependence on the parity of the total number N of spins. These results should be amenable to a direct check in numerical simulations (see, e.g., Refs. [7,12]) and, in particular, could be tested experimentally by measuring the stiffness of quasi-one-dimensional antiferromagnets of finite size using similar materials as in Ref. [3].

We start with the Heisenberg Hamiltonian for a spin chain with nearest-neighbor interactions

$$H = J_{\rm ex} \sum_{n=1}^{N} \mathbf{S}(n)\mathbf{S}(n+1), \tag{1}$$

where $J_{\rm ex} > 0$, and we consider the integer S case first. In this case, the long-wavelength limit of the partition function Z becomes the $(1+1)$D nonlinear σ model (NLσM) [13] with $Z = \int \mathcal{D}\mathbf{n}\, \delta(\mathbf{n}^2 - 1) \exp(-\mathcal{A})$, and the Euclidean action is given by

$$\mathcal{A} = \frac{1}{2g} \int_0^{L_T} \int_0^{L} dx_0\, dx (\partial_\mu \mathbf{n})^2, \qquad \mu = 0, 1, \tag{2}$$

where $g = 2/S$, $v_s = 2SJ_{\rm ex}a_0$ is the spin wave velocity (we set $k_B = \hbar = 1$), a_0 is the lattice constant, $L = a_0 N$, $L_T = \beta v_s$ is the wavelength of the thermal magnons, and $\mathbf{n}$ is the slow-varying component of the (staggered) magnetization satisfying the constraint $\mathbf{n}^2 = 1$. On the edges of the space-time domain $L \times L_T$ the boundary conditions are periodic in x_0, i.e., $\mathbf{n}(0,x) = \mathbf{n}(L_T, x)$, and correspond to a fixed twist of the $\mathbf{n}$ field applied in

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the x direction, i.e., $\mathbf{n}(x_0, 0) = (1,0,0)$ and $\mathbf{n}(x_0, L) = (\cos\theta, \sin\theta, 0)$, where θ is the twist angle. It is convenient to use the transformation [5,6,14] $\mathbf{n} = \mathcal{R}(\theta(x))\sigma$, where $\mathcal{R}$ is the rotation matrix about the z axis by the angle $\theta(x) = \theta x/L$, and σ satisfies the boundary conditions $\sigma_1 = 1$ and $\sigma_{2,3} = 0$, at $x = 0, L$. The action then takes the form

$$\mathcal{A} = \frac{1}{2g}\int d\mathbf{x}\left[(\partial_\mu \sigma)^2 + \frac{\theta^2}{L^2}(1 - \sigma_3^2) + 2\frac{\theta}{L}(\sigma_1\partial_x\sigma_2 - \sigma_2\partial_x\sigma_1)\right]. \quad (3)$$

We define the spin stiffness ρ_s in units of the velocity

$$\rho_s = \frac{1}{2}L\frac{\partial^2 F}{\partial\theta^2}\bigg|_{\theta=0}, \quad (4)$$

where $F = -T\ln Z$ [15]. With this definition, the bare value of ρ_s in the tree (classical) approximation is $\rho_s^0 = v_s/2g$. Corrections due to quantum and thermal fluctuations can be found in a loop expansion in g. In one-loop order, only quadratic terms in the action (3) are to be retained, and the third term in Eq. (3) reduces to a total derivative $\partial_x\sigma_2$, and, thus, vanishes as we shall restrict our consideration to the topological sector with zero winding number (Pontryagin index). Performing the functional integration, we get

$$\rho_s = \rho_s^0\left(1 - \frac{g}{LL_T}\sum_{\mathbf{q}}\frac{1}{\mathbf{q}^2}\right), \quad (5)$$

where $\mathbf{q} = (2\pi n/L_T, \pi m/L)$, $n = 0, \pm 1, \ldots$, $m = 1, 2, \ldots$. The sum in Eq. (5) can be evaluated in three limiting cases: (a) $L \ll L_T$ (quantum region), (b) $a_0 \ll L_T \ll L$ (classical renormalized region), and (c) $L_T \ll a_0$ (classical region). We have

$$\frac{\rho_s}{v_s} = \begin{cases} \ln(\xi_{\rm qm}/L)/4\pi, & \text{for (a)}, \\ [\xi(T) - L]/12L_T, & \text{for (b)}, \\ (\xi_{\rm cl} - L)/12L_T, & \text{for (c)}. \end{cases} \quad (6)$$

Here, $\xi_{\rm qm} = \alpha a_0 \exp(\pi S)$ is the correlation length in the quantum region. $\xi(T) = 3L_T\ln(\gamma\xi_{\rm qm}/L_T)/\pi$ is the classical correlation length $\xi_{\rm cl} = 6L_T/g$ renormalized by quantum fluctuations. α and γ are (cutoff dependent) nonuniversal constants of order one. We note that case (c) agrees with the 1D classical NLσM [5].

In all the regions, ρ_s goes to zero as the system size $L < \xi$ approaches the correlation length of the corresponding region [16]. This zero value of ρ_s is what a macroscopic system is expected to have in the absence of spontaneously broken symmetry [11] (the point $\rho_s = 0$ signals the breakdown of the one-loop order expansion).

The rms fluctuation $\delta\rho_s^2 = (TL\partial/\partial\theta^2)^2\ln Z|_{\theta=0}$ is given by

$$\frac{\delta\rho_s^2}{v_s^2} = \frac{1}{2L^2L_T^2}\sum_{\mathbf{q}}\frac{1}{\mathbf{q}^4} = \begin{cases} \frac{\zeta(3)}{8\pi^3}\frac{L}{L_T}, & \text{for (a)}, \\ \frac{1}{180}\left(\frac{L}{L_T}\right)^2, & \text{for (b) and (c)}, \end{cases} \quad (7)$$

where $\zeta(x)$ is the Riemann ζ function. Contrary to the case of a classical ferromagnet [5], the fluctuations are *nonuniversal:* they depend on both L and T. Moreover, in the classical and classical renormalized regions, the fluctuations are abnormally large ($\delta\rho_s > \rho_s$), and, thus, the spin stiffness is not a self-averaging quantity. Finally, we note that the analogs of the regions we consider in the quantum NLσM can also be obtained in the classical 2D model, if one considers a rectangular instead of a square system.

We now turn to the half-odd integer spin case. The effective field-theoretical description of the long-wavelength excitations is not of much use here, since the partition function contains a Θ term and contributions from all topological sectors with different winding numbers [1,2,13], which makes the model hardly tractable. It is believed that the exactly solvable case of the spin 1/2 chain reproduces the generic features of all half-odd integer S chains [1,2,13], and we shall consider this case only. By using the Jordan-Wigner transformation [17]

$$\psi(n) = (-1)^n \exp\left(i\pi\sum_{j=1}^{n-1}[S_z(j) + \tfrac{1}{2}]\right)S_-(n), \quad (8)$$

where $S_\pm = S_x \pm iS_y$, the Hamiltonian (1) is mapped on to a system of spinless fermions on the lattice,

$$H = J_{\rm ex}\sum_{n=1}^{N}[-\tfrac{1}{2}\{\psi^\dagger(n)\psi(n+1) + \text{H.c.}\} + :\rho(n)::\rho(n+1):], \quad (9)$$

where $:\rho(n): = \psi^\dagger(n)\psi(n) - 1/2$ is the (Fermi-ordered) density operator. We now have to specify the boundary condition for the fermionic operators ψ. The quantum generalization of the classical boundary conditions for the spin field $\mathbf{n}$, used in the NLσM treatment of the integer S case, is $S_\pm(N+1) = e^{\pm i\theta}S_\pm(1)$ and $S_z(N+1) = S_z(1)$. The boundary condition for ψ then follows from Eq. (8),

$$\psi(N+1) = e^{i[\pi(N_F+N)-\theta]}\psi(1), \quad (10)$$

where the number of fermions is $N_F = N/2$, if N is even, and $N_F = (N+1)/2$, if N is odd. We have also used the fact that $\sum S_z(n) = 0\ (1/2)$ for even (odd) N. The problem defined by Eqs. (9) and (10) is similar to that of spinless electrons on a ring threaded by an Aharonov-Bohm flux θ, with the difference that here the boundary conditions depend on the parity of N. This parity dependence will result in a striking difference in the behavior of ρ_s for even and odd N.

Finite-size systems of interacting fermions with twisted boundary conditions have recently been studied in the framework of the Luttinger liquid approach [18]. The parity dependence of the boundary conditions, however, requires a reexamination of the bosonization scheme, which we now address. The left and right movers are introduced by $\psi(n) = e^{ink_F}\psi_+(n) + e^{-ink_F}\psi_-(n)$, where we choose $k_F = \pi/2$ for N even and odd. The boundary conditions for ψ_α, where $\alpha = \pm$, take the form

$$\psi_\alpha(N+1) = \begin{cases} e^{-i\theta}\psi_\alpha(1), & \text{for } N \text{ even}, \\ -\alpha i e^{-i\theta}\psi_\alpha(1), & \text{for } N \text{ odd}. \end{cases} \quad (11)$$

Bosonic fields are introduced by $\psi_\alpha = (2\pi a_0)^{-1/2} e^{i\sqrt{\pi}\phi_\alpha}$, where $\phi_\alpha = \alpha\phi - \vartheta$, and $\partial_x \vartheta$ is the conjugate momentum of ϕ. The zero modes of ϕ and ϑ can be chosen in the form [18]

$$\begin{aligned} \phi_0 &= \phi_J/\sqrt{\pi} + \mathbf{M}\sqrt{\pi}x/L, \\ \vartheta_0 &= \vartheta_M/\sqrt{\pi} + (\mathbf{J} - \theta/\pi)\sqrt{\pi}(x + \tfrac{1}{2}L)/L, \end{aligned} \tag{12}$$

where $\mathbf{J}$ and $\mathbf{M}$ are the operators of the topological current and the number of particles above the ground state [19], respectively, which satisfy $[\phi_J, \mathbf{J}] = [\vartheta_M, \mathbf{M}] = i$. Next, using the Baker-Hausdorff formula, we write

$$e^{i\sqrt{\pi}\phi_\alpha} = \bar{\psi} e^{i(\pi/L)[\alpha x(M-1) - J(x+L/2)]}, \tag{13}$$

where $\bar{\psi}$ contains contributions from the nonzero modes and from ϕ_J and ϑ_M and is not parity dependent; $J(M)$ stands for the eigenvalue of $\mathbf{J}(\mathbf{M})$. It is convenient to introduce the topological indices κ_J and κ_M, such that $\kappa_J = 0$ (1), if J is even (odd); for even N, $\kappa_M = 0$ (1), if M is even (odd), and, for odd N, $\kappa_M = 0$ (1), if $M + 1/2$ is even (odd). By using Eqs. (11) and (13), we see that $\kappa_{J,M}$ must satisfy the following constraints: $\kappa_J = 1$, $\kappa_M = 0$ (and vice versa), if N is even, and $\kappa_J = \kappa_M$, if N is odd. By comparing these constraints with the analogous constraints of the fermionic problem [18], we can now say that the ground state of our spin system is *paramagnetic* for N even and *diamagnetic* for N odd.

The rest of the bosonization procedure is identical to that of Ref. [18], and the bosonized Euclidean action takes the sine-Gordon form

$$\mathcal{A}_b = \int_0^{\beta v_0}\int_0^L d^2x \{K_0(\partial_\mu\phi)^2 + (i/L)\sqrt{\pi}\theta_0\partial_0\phi - (g_0/a_0^2)\cos(4\sqrt{\pi}\phi)\}, \tag{14}$$

where $v_0 = v_s(1 + 4/\pi)^{1/2}$, $K_0 = v_0/2v_s$, $g_0 = 1/8\pi^2 K_0$, and $\theta_0 = \kappa_J - \theta/\pi$. The bosonic fields have been decompactified in the course of the functional integral derivation, and ϕ obeys now the boundary conditions $\phi(x_0 + k_0\beta v_0, x + k_1 L) = \phi(x_0, x) + k_0\sqrt{\pi}n + k_1\sqrt{\pi}(2m + \kappa_M)$, where n and m are the winding numbers in x_0 and x directions, respectively. The measure $\mathcal{D}\phi$ of the functional integral $Z = \int \mathcal{D}\phi \exp(-\mathcal{A}_b)$ includes the sums over the winding numbers n, m and over the topological indices $\kappa_{J,M}$. The last term in Eq. (14) corresponds to umklapp scattering processes between fermions. Since g_0/K_0 is small (≈ 0.02), this umklapp term can be treated perturbatively in a standard renormalization group (RG) approach leading to the following flow equations [20]:

$$\begin{aligned} \frac{dg}{dl} &= 2(K - 1)g, \qquad g(0) = g_0, \\ \frac{dK}{dl} &= 2\pi^2 g^2, \qquad K(0) = K_0, \end{aligned} \tag{15}$$

where $l = \ln(\mathcal{L}/a_0)$ with $\mathcal{L} = \min\{L, L_T\}$. Since we started with the isotropic Heisenberg model (1), the scaling dimension of the umklapp term is equal to the critical dimension of the model (= 2), i.e., this term is marginally relevant. In this case, the flow proceeds along the separatrix between massive and massless phase. On this line [21], the solutions to Eqs. (15) are with $\mathcal{L} \gg L_0$

$$K = K^* - \frac{1}{2\ln(\mathcal{L}/L_0)}, \qquad g = \frac{K^* - K}{\pi}, \tag{16}$$

where $K^* = K(\infty)$ is the fixed-point value, and the (nonuniversal) cutoff L_0 depends on (K_0, g_0) and is of the order a_0. At the fixed point ($\mathcal{L} \to \infty$), $g = 0$ and the action (14) renormalizes to that of a Luttinger liquid with a topological term ($\propto \partial_0\phi$), and with parameters renormalized through interactions: $(K_0, v_0) \to (K^*, v^*)$. By comparing with the exact Bethe-ansatz solution [22], one gets $K^* = 1$ and $v^* = \pi v_s/2$.

We can now calculate the fixed-point value of the spin stiffness, ρ_s^*, and its finite size and finite temperature corrections. Upon integrating out the zero modes, the twist-dependent part of Z becomes

$$Z_\theta = \sum_{\kappa_J, \kappa_M} e^{-\kappa_M b}\theta_3(z_J, e^{-a})\theta_3(z_M, e^{-4b}), \tag{17}$$

where $\theta_3(z, q) = \sum q^{n^2} e^{2inz}$ is the Jacobi θ function, $z_J = \pi\theta_0/2$, $a = \pi K^* L/L_T^*$, $b = \pi K^* L_T^*/L$, $z_M = 2i\kappa_M b$, and $L_T^* = \beta v^*$. The results for the spin stiffness take simple forms in the limiting cases of low and high temperatures. For $L \ll L_T^*$, we obtain from (4) and (17)

$$\rho_s^* = \begin{cases} -(v^*/8K^{*2})L_T^*/L, & \text{for } N \text{ even}, \\ v^*/4\pi K^*, & \text{for } N \text{ odd}, \end{cases} \tag{18}$$

while for $L \gg L_T^*$ we get

$$\rho_s^* = (-1)^{N+1} 2(L/L_T^*) e^{-\pi\chi L/L_T^*}, \tag{19}$$

where $\chi = K^* + 1/4K^*$. To obtain the value of ρ_s away from the fixed point, we go back to the full action (14) and replace (K_0, g_0) by (K, g) from Eq. (16), treating the deviations from the fixed-point values as perturbations [21,23,24]. In first order, the umklapp term gives no contribution, while the perturbation in $K - K^*$ leads to

$$\rho_s = \rho_s^* \times \begin{cases} 1 + 1/\alpha_N \ln(L/L_0), & \text{for } L \ll L_T^*, \\ \exp[3L\pi/8L_T^* \ln(T_0/T)], & \text{for } L \gg L_T^*, \end{cases} \tag{20}$$

where $\alpha_N = 1$ for even N, and $\alpha_N = 2$ for odd N; the cutoff T_0 is of the order of v^*/L_0. The last equation is valid for $T \leq T^* < T_0$, where $L_T(T^*) = a_0$. The L- and T-dependent corrections to ρ_s^* resulting from the perturbation of the fixed-point action by the marginally irrelevant operator are larger than those coming from the expansion of Eq. (17) in $(L/L_T^*)^{\pm 1}$ at the fixed point. In particular, the exponential dependence of ρ_s^* on K^* in the high-temperature regime results in a significant T-dependent renormalization. This renormalization may be conjectured to remain significant in the intermediate regime $L \simeq L_T^*$ as well. We also note that the umklapp processes lead to the breakdown of the single-parameter scaling of ρ_s: The latter scales with L/L_T^* at the fixed point but acquires additional L/L_0 and T/T_0 scalings away from the fixed point (for a rough estimate, $L_0 \simeq a_0$, and $T_0 \simeq J_{ex}$). This breakdown can be detected in numerical and real experiments. The fluctuations in ρ_s can be calculated along the same lines as for ρ_s itself, and, in marked contrast to the integer S case, turn out to be exponentially small for all L/L_T.

The negative value of ρ_s for even N simply reflects the fact that in this case the free energy has a maximum at $\theta = 0$, and an arbitrarily small twist drives the system out of this state. Analyzing ρ_s at finite θ (and low temperatures) we can see that ρ_s vanishes at some $\theta^* \simeq L/L_T^* \ll 1$ and then remains positive for all θ, thus exhibiting a crossover from the paramagnetic to the diamagnetic regime. The parity effects in the spin stiffness are quite similar to that in persistent currents of electronic systems [18,25,26]; in particular, the result obtained above can be checked without approximations for the special case of the XY model by mapping it on to the exactly solvable problem of free fermions [27].

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