Semiclassical Solitons and the $S=\frac{1}{2}$ Heisenberg Model

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We examine the statistical mechanics of the classically integrable Ishimori-Faddeev-Haldane lattice spin model. Thermodynamic properties can be exactly described in terms of an interacting soliton gas. Our semiclassical scheme can be used to calculate the low-temperature thermodynamics of the $S=\frac{1}{2}$ Heisenberg chain, in very good agreement with recent numerical calculations based on the quantum-mechanical Bethe ansatz.

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The $S=\frac{1}{2}$ ferromagnetic Heisenberg chain with nearest-neighbor interactions is one of the few nontrivial quantum-mechanical many-body problems amenable to an exact solution [1]. Nonetheless, a complete analytic description of its thermodynamic behavior in the vicinity of the ordered state ($T=0$) has proved elusive. Significant progress was achieved by recent independent numerical investigations [2,3] which suggest that the specific heat and the zero-field susceptibility are proportional to $T^{1/2}$ (spin-wave behavior) and T^{-2} (classical result [4]), respectively. There is yet no consensus regarding logarithmic corrections [2(b)] or exact analytic expressions for critical amplitudes.

In this paper we examine the thermodynamics of a related model, the Ishimori-Faddeev-Haldane [5-7] ferromagnetic chain, whose classical Hamiltonian is given by

$$H=-2JS^2\sum_n \ln(S^2+\mathbf{S}_n\cdot\mathbf{S}_{n+1}), \qquad (1)$$

where S is the value of the spin and $J>0$. At low temperatures neighboring spins are aligned and the physics of (1) reduces to that of the Heisenberg ferromagnet. Because of the complete integrability property of (1) [5-8], its thermodynamics can be exactly formulated [9] in terms of the phase shifts involved in the soliton interactions. Our statistical description is classical in the sense that it (i) assumes a continuum distribution of soliton action variables (magnetizations and momenta), and (ii) postulates that solitons would obey Boltzmann statistics if they were interaction free [9]. Assumption (i) is reasonable as long as the spectrum is gapless (our case [10]), or the temperature exceeds the value of the gap [11]. Assumption (ii) can be relaxed to allow for a different type of free-soliton statistics (e.g., fermions), resulting only in a 1% decrease in the critical amplitude of the specific heat. The fact that the value of S enters not only the energy scale [in the form JS^2, Eq. (1)], but also controls the phase-space measure determined by the rules of semiclassical quantization [10] [cf. Eq. (5) below], enables us to describe both classical *and* quantum regimes. Furthermore, the spin deviation due to solitons results in complete loss of long-range order for any $T>0$; this is an essential test of the validity of the thermodynamic soliton picture and contrasts favorably with the divergent spin deviation produced by a naive magnon gas description of the Heisenberg ferromagnet [12]. Our results, which describe the soliton statistical mechanics of (1), the only lattice spin model known to be classically integrable, thus provide a useful guide to the low-T behavior of the Heisenberg ferromagnet of *arbitrary* spin.

Soliton solutions of the Hamiltonian dynamics resulting from (1) are characterized [5,8] by two parameters w, k, with $0<w<\infty$ and $0<k<\pi$. It is possible to express the energy E, the magnetization M, and the canonical momentum P in terms of w and k; the exact expressions have been derived in the context of semiclassical quantization [10]. In the context of statistical mechanics we further need (i) the Jacobi determinant

$$\mathcal{J}(w,k)=\partial(P,M)/\partial(w,k)=32S^2w/(\cosh 2w-\cos 2k)^2$$

and, in order to describe the phase space of interacting solitons, (ii) the two-soliton phase shift

$$\Delta(w,k;w',k')=\frac{1}{2w}\ln\left[\frac{\cosh 2(w'+w)-\cos 2(k-k')}{\cosh 2(w'-w)-\cos 2(k-k')}\right], \qquad (2)$$

which can be derived by invoking the gauge equivalence of (1) with the discrete nonlinear Schrödinger model [5,13,14].

The occupation probability $\bar{n}\equiv\exp[-\beta\varepsilon(\Gamma)]$ of a point $\Gamma\equiv(w,k)$ in phase space is then determined by the quasienergy $\varepsilon(\Gamma)$, given by the integral equation [9]

$$\varepsilon(\Gamma)=E(\Gamma)+(1/2\pi\beta)\int d\Gamma'\Delta(\Gamma',\Gamma)\exp[-\beta\varepsilon(\Gamma')], \qquad (3)$$

where $\beta=1/T$, $E(\Gamma)=8JS^2w$ is the bare soliton energy, and $d\Gamma'=J(w',k')dw'dk'$. Equation (3) forms [15] the basis of statistical mechanics for particles interacting via phase shifts only. In the form given, Eq. (3) neglects the presence of extended vibrational modes (magnons), an approximation which seems justified by the form of the semiclassical spectrum [10]. At low temperatures ($\beta JS^2 \gg 1$) we expect that only modes with $w \ll 1$ can contribute. It is then possible to simplify the two-dimensional integral equation (3) by using the approximate form

$$\Delta(w,k;w',k') = \frac{2\pi}{w}\min(w,w')\delta(k-k'). \tag{4}$$

The approximation (4) satisfies the exact sum rule $\int_0^\pi dk\,\Delta(w,k;w',k') = 2\pi\min(1,w'/w)$ and is similar in spirit to the one successfully employed [11] in the classical limit of sine-Gordon statistical mechanics. Using (4) it becomes possible to reduce (3) to the one-dimensional integral equation

$$\beta\varepsilon(w,k) = 8\beta JS^2 w + 8S^2\int_0^\infty dw' \frac{\min(w,w')}{(w'^2+\sin^2 k)^2} e^{-\beta\varepsilon(w',k)}. \tag{5}$$

It turns out [14] that the basic thermodynamic quantities, as defined in, e.g., Ref. [9], demand only some global features of the solution of the integral equation (3) or its simplified form (5). These are

$$V_0(k,\beta) = \lim_{w\to 0} \partial[\beta\varepsilon(w,k)]/\partial w$$

and

$$C_\infty(k,\beta) = \lim_{w\to\infty} [\beta\varepsilon(w,k) - V_\infty w],$$

where

$$V_\infty = \lim_{w\to\infty} \partial[\beta\varepsilon(w,k)]/\partial w = 8\beta JS^2.$$

As a function of V_0 and C_∞, the total density of solitons is [14]

$$n_s = \frac{1}{\pi}\int_0^{\pi/2} dk \left\{1 - \left(\frac{\partial V_0}{\partial V_\infty}\right)_k\right\}, \tag{6}$$

the energy per site

$$u = -\frac{T}{\pi}\int_0^{\pi/2} dk \left(\frac{\partial C_\infty}{\partial \ln\beta}\right)_k, \tag{7}$$

and the magnetization per site (for $T \neq 0$)

$$m = \lim_{k\to 0}\left(\frac{\partial V_0}{\partial V_\infty}\right)_k; \tag{8}$$

the expressions (6)-(8) can be derived from the full two-dimensional integral equation (3), using the symmetries of the phase shifts (2). The one-dimensional version (5) yields the same expressions, provided that the reasoning which leads to (4) is applied consistently. The integral equation (5) is equivalent to the ordinary differential equation

$$\frac{d^2x}{dt^2} = -\frac{8}{(1+at^2)^2}e^{-x}, \tag{9}$$

where $x \leftrightarrow \beta\varepsilon$, $t \leftrightarrow Sw/\sin^2 k$, and $a \leftrightarrow \sin^2 k/S^2$, subject to the *initial* condition $x(0)=0$ and the *final* condition

$$v_\infty = \lim_{t\to\infty}(dx/dt) = 8\beta JS\sin^2 k \equiv V_\infty \sin^2 k/S.$$

Equation (9) can be thought of as describing a nonautonomous mechanical system. The problem then is to determine the initial velocity $v_0 = (dx/dt)_{t=0} = V_0 \sin^2 k/S$ and the asymptotic spatial shift $C_\infty = \lim_{t\to\infty}\{x(t) - v_\infty t\}$ as a function of the parameters β, k, and S (which define a and the final velocity v_∞).

Except in the case $a=0$ (autonomous limit), it is not possible to integrate (9) analytically. However, the analytical solution [11,14] [cf. (ii) below] can serve as a useful guide in two physically significant limiting cases. First, one can obtain the classical limit [4], corresponding to $J\to 0$, $S\to\infty$ with $JS^2 \to j$. In this limit, it can be shown that for large but finite values of S there will be a temperature range $j/S \ll T \ll j$ in which the system can be described as a *dense* soliton gas ($n_s \to \frac{1}{2}$), which exhausts all degrees of freedom, and exhibits low-temperature *classical* behavior [4], i.e., a constant specific heat. The other limiting case, as will become clear below [(i)-(iii)], is the approach to zero tempera-

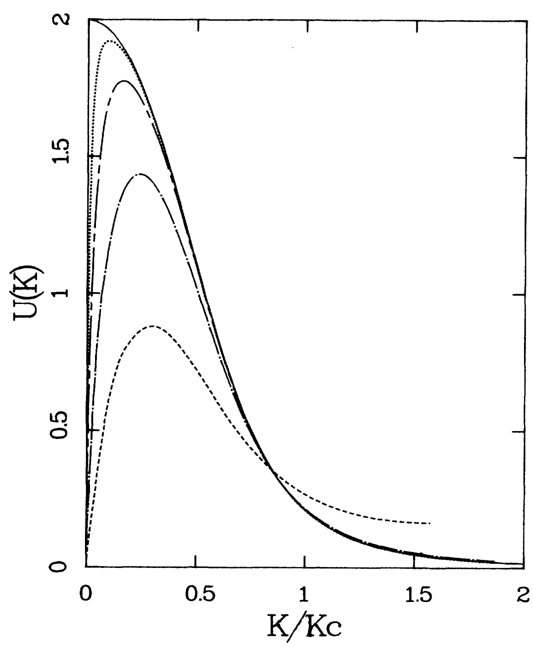

FIG. 1. The energy density in k space $U(k) = -(\partial C_\infty/\partial\ln\beta)_k$ as a function of k/k_c, where $k_c = \beta^{-1/2}$, for various values of β. The solid line corresponds to the limit $\beta\to\infty$. The four other curves correspond, from top to bottom, to $\beta = 10^6$, 10^4, 10^2, and 1, respectively.

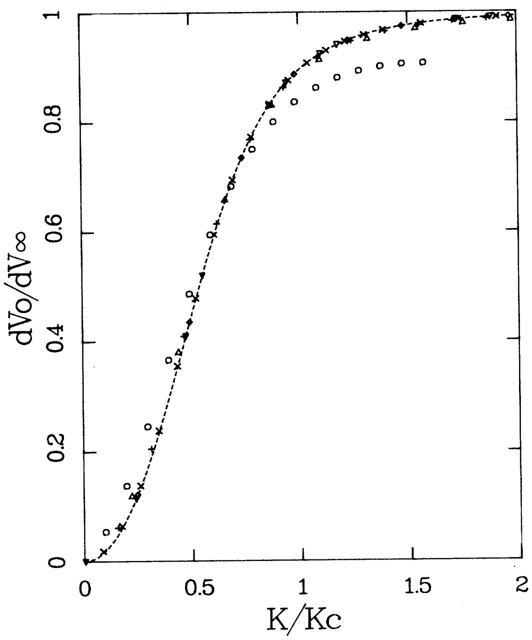

FIG. 2. The quantity $(\partial V_0/\partial V_\infty)_k = (\partial v_0/\partial v_\infty)_k$ as a function of k/k_c where $k_c = \beta^{-1/2}$, for various values of β. ○, $\beta=1$; △, $\beta=5$; +, $\beta=10$; ×, $\beta=50$; ♦, $\beta=100$; ▽, $\beta=500$. For large values of β the results are indistinguishable from the predictions of the autonomous (scaling) limit $a=0$ [cf. Eq. (9), dashed curve].

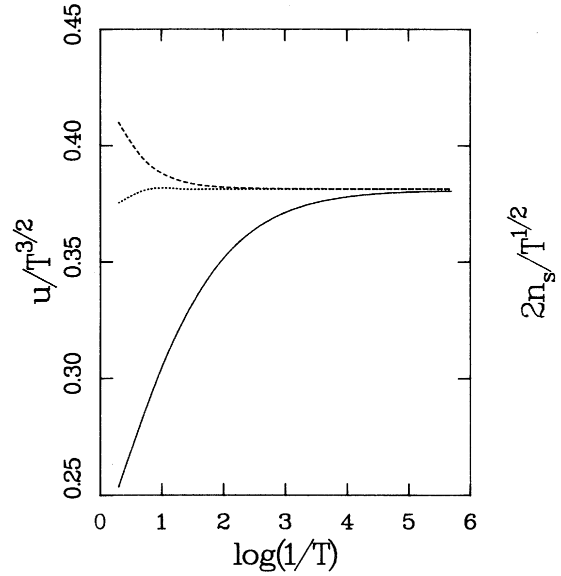

FIG. 3. Solid line: the quotient $u/T^{3/2}$, where u is the energy per site [Eq. (7)], as a function of $\log(1/T)$. Dotted line: the quotient $2n_s/T^{1/2}$, where n_s is the soliton density calculated from (6) and (9). Dashed line: the two quantities are identical in the autonomous (scaling) limit $a=0$ [cf. Eq. (9)].

ture (regardless of the value of S) and corresponds to explicitly quantum behavior, i.e., $0 < T \lesssim JS$.

It should be noted that in the autonomous limit the parameters β and k enter the solution in the combination $\beta\sin^2 k$, i.e., this limiting case is characterized by a scaling property.

We have performed the numerical integration of (9) using the Bulirsch-Stoer method [16] for a variety of β and k values, and $J=1$, $S=1$. The choice of a particular value of $S \sim O(1)$ does not affect the *leading asymptotic* behavior as $T \to 0$ except for a rescaling of constants. Our results can be summarized as follows:

(i) As the value of β increases, the integrand of (7), which represents the soliton energy density in k space, approaches a limiting function determined by the autonomous limit of Eq. (9) (Fig. 1).

(ii) The quantity $(\partial v_0/\partial v_\infty)_k$ tends to zero as $k \to 0$, in accordance with the requirement of vanishing long-range order, *for all finite temperatures* (Fig. 2); the same quantity appears in the integrand of (6), which determines the soliton density. Note that the approach to the asymptotic limit (determined by the relationship $v_0^2 = 16 + v_\infty^2$) is now much more rapid.

(iii) A detailed study of asymptotic behavior reveals that the energy per site and the soliton density approach the values $2AT^{3/2}$ and $AT^{1/2}$, respectively (Fig. 3), where $A = (2\pi)^{1/2}/[\Gamma(\frac{1}{4})]^2 = 0.1907$. The fact that $n_s \to 0$ explicitly confirms the presence of a dilute soliton gas. The ratio $2T$ is consistent with the principle of energy equipartition implicit in our "classical logic." Since the asymptotic limit depends on the combination βJS (cf. the expression for v_∞ above), our result translates to a free energy per site $f = -4AT(T/JS)^{1/2} = -1.0787T^{3/2}$ in the case of $S=\frac{1}{2}$. Our value of the critical amplitude lies within the estimated accuracy of the best numerical estimates based on the full quantum-mechanical Bethe ansatz (BA) [2,3], obtained using several hundreds of coupled integral equations. It deviates very slightly from the value 1.042 predicted within the free-magnon-gas framework [3]. Whether it represents a better approximation to the *exact* BA value is clearly a matter that can only be settled in the context of the BA formalism (in this framework Schlottmann [2(b)] gives an estimate of 1.1).

In summary, we have formulated and derived the equilibrium statistical mechanics of the only available discrete spin model which has the property of classical integrability. The soliton gas has been shown to be dilute at low temperature, and the nontrivial dependence of thermodynamic quantities on S allows us to describe the quantum-mechanical regime. The leading-order asymptotic behavior can be described analytically, and the computational effort involved in extending results to higher temperatures (while still satisfying $\beta JS^2 \gg 1$) can be kept at a minimum. Since the model by construction reduces to the Heisenberg model at very low temperatures, the results derived here reflect the asymptotic behavior of the latter.

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