"Spinon Gas" Description of the $S=\frac{1}{2}$ Heisenberg Chain with Inverse-Square Exchange: Exact Spectrum and Thermodynamics

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(Received 4 January 1991)

The exact spectrum and thermodynamics of the $S=\frac{1}{2}$ Heisenberg chain with inverse-square exchange are explicitly obtained in closed form, and a description in terms of semionic spin-$\frac{1}{2}$ "spinon" excitations is developed. The unexpected degeneracies of the spectrum lead to a new representation of the $k=1$ SU(2) Wess-Zumino-Witten conformal field theory that exposes an infinite set of SU(2) symmetries of that model.

PACS numbers: 75.10.Jm, 05.30.−d

A few years ago, a new solvable spin-$\frac{1}{2}$ Heisenberg chain—with exchange proportional to the inverse square of the distance between sites—was independently identified by myself[1] and Shastry.[2] The antiferromagnetic ground state has a Jastrow pair-product form,[1,2] and is equivalent to the one-dimensional (1D) versions of the Kalmeyer-Laughlin state,[3] the fully Gutzwiller-projected single-band spin-$\frac{1}{2}$ Fermi gas with one particle per site,[4] and Anderson's "resonating-valence-bond" state.[5] The ground-state correlations were explicitly found, and are related to a random-matrix problem solved by Dyson[6] (symplectic case, $\beta=4$). The full construction of the spectrum and of the thermodynamics was not accomplished in the original work.[1,2] In this Letter, I report the remarkably simple solution of this problem in terms of spin-$\frac{1}{2}$ "spinon" excitations, and from this obtain a new representation of the $k=1$ SU(2) Wess-Zumino-Witten (WZW) conformal field theory[7] (CFT), which exposes an infinite set of SU(2) symmetries of that model.

The model with periodic boundary conditions on a ring of N sites is

$$H=J\sum_{n<n'}[d(n-n')]^{-2}\mathbf{S}_n\cdot\mathbf{S}_{n'}, \tag{1}$$

where $d(n)=(N/\pi)\sin(\pi|n|/N)$ is the chord distance between spins n sites apart. In Ref. 1, a subset of the eigenstates was explicitly obtained using a relation between the model (1) and the continuum model (at coupling $\lambda=2$) of 1D nonrelativistic bosons with interaction potential $\lambda(\lambda-1)(\hbar^2/m)[d(x_i-x_j)]^{-2}$ solved by Sutherland.[8] Remarkably, numerical diagonalization[1] showed that because of unexpected degeneracies this incomplete set of states generates the *full* set of energy levels of (1). The explicitly found states are identified here as states where N_{sp} spin-$\frac{1}{2}$ spinon excitations of the spin-singlet antiferromagnetic ground state are present, and $S=S^z=N_{sp}/2$. I will refer to them as "fully (spin-)polarized spin gas" (FPSG) states. FPSG states have $M=(N-N_{sp})/2$ reversed spins; if $\{z_i\}=\{\exp(2\pi i n_i/N)\}$, where $\{n_i\}$ are the indices of sites with reversed spins, the wave functions are polynomials where $(z_i)^n$ occurs with powers in the range $0<n<N$, and have the form

$$\Psi=\phi(z_1,\ldots,z_M)\prod_{i<j}(z_i-z_j)^2\prod_i z_i, \tag{2}$$

where $\phi(\{z_i\})$ is a symmetric polynomial with degree $\leq N_{sp}$ in each variable z_i. The basis set of polynomials ϕ is spanned by "coherent states" $\phi=\prod_{ij}(z_i-Z_j)$ parametrized by N_{sp} complex "spinon coordinates" $\{Z_j\}$. Expansion in powers of $\{Z_j\}$ [which are *not* restricted to values where $(Z_j)^N=1$] gives a basis set of $g(N_{sp},M)=(N_{sp}+M)!/M!N_{sp}!$ independent symmetric polynomials. The polynomials corresponding to eigenstates of (1) are homogeneous solutions of the eigenvalue equation

$$\sum_i(z_i\partial_{z_i})^2\phi+\lambda\sum_{i<j}\frac{z_i+z_j}{z_i-z_j}(z_i\partial_{z_i}-z_j\partial_{z_j})\phi=\epsilon\phi, \tag{3}$$

with $\lambda=2$. Sutherland[8] has obtained the eigenvalues of (3) and an algorithm for generating the coefficients of the power-series expansion of the solutions ϕ.

The eigenvalues of (1) can be described[1] in terms of M distinct "pseudomomenta" $\{k_i\}$, with $\exp(ik_iN)=1$, and $0<k_i<2\pi$, satisfying the Bethe-ansatz-like equation

$$k_iN=2\pi I_i+\pi\sum_{j=1}^{M}\mathrm{sgn}(k_i-k_j), \tag{4}$$

where the set of M distinct quantum numbers I_i can be chosen in ascending order, and take values in the range $I_0+1, I_0+2,\ldots,I_{M+1}-1$, where $I_0\equiv(M-1)/2$ and $I_{M+1}\equiv N-(M-1)/2$. There are $M+N_{sp}$ possible values in this range, M of which are "occupied" (i.e., contained in the set $\{I_i\}$) and N_{sp} of which are "empty" (not in that set). A configuration can be represented by a sequence such as 0100111011, where 1 represents a filled state and 0 an empty state. For a given N_{sp}, there are the same number $g(N_{sp},M)$ of possible configurations as independent symmetric polynomials in the basis set.

In terms of the $\{k_i\}$, the crystal momentum K is given by $\sum k_i (\text{mod} 2\pi)$, and the energy E/J is given by

$$\tfrac{1}{12}(\pi/N)^2 N(N^2-1)+\sum_i \bar{\epsilon}(k_i)\,, \tag{5}$$

where $\bar{\epsilon}(k)=\frac{1}{4}k(k-2\pi)$. Each FPSG state belongs to a multiplet with $S=N_{sp}/2$; in Ref. 1, it was noted that these states were in general degenerate with many other multiplets with $S<N_{sp}/2$, forming a "supermultiplet," but the precise nature of these degeneracies has not been identified until now.

Before describing these degeneracies, I present the full Schrödinger equation in Fourier space. In general, $M=(N-N_{sp})/2$ parametrizes the number of spinons, *not* the number M' of reversed spins, which is in the range $M\le M'\le N-M$. Let the symmetric function $\tilde{\Psi}^{FT}(q_1,\ldots,q_{M'})$ be the Fourier transform of the wave function $\Psi(\{n_i\})$; it is periodic in $q_i\to q_i+2\pi$. It is convenient to define a *nonperiodic* Fourier wave function $\tilde{\Psi}(\{q_i\})=\tilde{\Psi}^{FT}(\{q_i\})\prod_i v(q_i)$, where $v(q)=1$ if $0<q<2\pi$, $v(q)=\frac{1}{2}$ if $q=0$ or 2π, and $v(q)=0$ otherwise. $\tilde{\Psi}$ vanishes outside the M'-dimensional hypercube defined by $0\le q_i\le 2\pi$. For a given crystal momentum K in the range $|K|\le\pi$, the wave function $\tilde{\Psi}$ is confined to hyperplanes $\sum q_i=K+2\pi m$, with $0\le m\le M'$, and satisfies the boundary condition $\tilde{\Psi}(\ldots,0,\ldots)=\tilde{\Psi}(\ldots,2\pi,\ldots)$.

I define operators $\hat{t}_i^m(q)$ with the action

$$\hat{t}_i^m(q)\tilde{\Psi}(\ldots,q_i,\ldots)\equiv\tilde{\Psi}(\ldots,q_i+m\pi+q,\ldots)\,, \tag{6}$$

and introduce Lagrange multipliers η_{ij} that enforce the constraint $\Psi(\{n\})=0$ if $n_i=n_j$ for $i\ne j$. The Schrödinger equation for $\tilde{\Psi}(q_1,\ldots,q_{M'})$ has the form

$$\frac{1}{N}\sum_{i<j}\sum_{|m|\le 1}\sum_{q'}V_{ij}^m(q_i,q_j,q')\hat{t}_i^m(q')\hat{t}_j^m(-q')\tilde{\Psi} = \left[\sum_{i=1}^{M}\bar{\epsilon}(k_i)-\sum_{i=1}^{M'}\bar{\epsilon}(q_i)\right]\tilde{\Psi}\,, \tag{7}$$

where

$$V_{ij}^m(q_1,q_2,q)=\pi v(q_1)v(q_2)[\eta_{ij}+V_m(q_1,q_2,q)]\,,$$

with $V_0(q_1,q_2,q)=-\pi-|q|$, and $V_{\pm1}(q_1,q_2,q)=(q_1+q_2)/2\pm\pi$.

For $M'=M$ (the FPSG case), if $\tilde{\Psi}$ vanishes except on the hyperplane $\sum q_i=\sum k_i$, and $v(q_i)=1$ at all points where $\tilde{\Psi}\ne0$, (7) reduces to the Schrödinger equation of the $\lambda=2$ Sutherland boson gas. Note that these Sutherland wave functions vanish if the set $\{q_i\}$ cannot be obtained from a permutation of $\{k_i\}$ by a succession of "squeezing operations" $\{q_i\}\to\{q_i'\}$, where, for some pair i,j, $q_k=q_k'$, $k\ne i,j$, $q_i+q_j=q_i'+q_j'$, and $|q_i'-q_j'|<|q_i-q_j|$ (this follows from a similar property of the polynomials ϕ established by Sutherland for arbitrary λ). *These Sutherland wave functions thus vanish outside a convex polygonal region of the hyperplane with vertices at the $M!$ permutations of $\{k_i\}$.* Provided $0<k_i<2\pi$, this region is in the interior of the hypercube where $v(q_i)=1$, and these wave functions also solve (7).

The general solution of (7) to obtain the wave functions of non-FPSG states is left as an open problem, but from further inspection of the results from numerical diagonalization of (1) for $N\le12$, I have identified the rule giving the full multiplicity and spin content of the spectrum. For a configuration characterized by a quantum number sequence such as 0100111011, every 0 corresponds to a spinon, and every sequence of n consecutive 0's represents a free spin with $S=n/2$. For example, the content of the supermultiplet with configuration 0100111011 is obtained by combining $S=\frac{1}{2}$ (twice) with $S=1$, which gives states with $S=2$, $S=1$ (twice), and $S=0$, and a total degeneracy of 12.

To interpret this, I note that the number $g(N_{sp},M)$ of FPSG states is the number of ways to put N_{sp} bosons into $M+1$ orbitals, and I assign Bose occupation numbers $\{n_k\}=\{I_i-I_{i-1}-1\}$, $i=1,\ldots,M+1$, where the boson orbitals are labeled by crystal momenta k in the range $-k_0,-k_0+2\pi/N,\ldots,k_0$, with $k_0=\pi M/N$. In this formulation, the total crystal momentum K is $\pi MN+\sum_k kn_k (\text{mod} 2\pi)$. *The full supermultiplet structure is recovered by taking the spinons to be spin-$\frac{1}{2}$ bosons, with $n_k=n_{k+}+n_{k-}$, so each orbital has a total spin $n_k/2$.* For a given N_{sp}, the total number of states is now the number of ways to place N_{sp} bosons in $2(M+1)$ orbitals, i.e., $g(N_{sp},2M+1)$; summing this over M leads to the full count of 2^N states. In this description E/J is given by $E_0(M)$ plus

$$\sum_{k\sigma}\epsilon_0(k)n_{k\sigma}+\frac{1}{2N}\sum_{k\sigma,k'\sigma'}V(k-k')n_{k\sigma}n_{k'\sigma'}\,, \tag{8}$$

where $\epsilon_0(k)=\frac{1}{2}(k_0^2-k^2)$, $V(k)=(\pi/2)(k_0-|k|)$, and $E_0(M)$ is $(\pi/N)^2$ times

$$\tfrac{1}{12}N(N^2-1)+\tfrac{1}{3}M(M^2+2)-\tfrac{1}{4}MN^2\,. \tag{9}$$

There is an independent SU(2) symmetry for *each* of the $M+1$ spinon orbitals.

It is now straightforward to obtain the equilibrium thermodynamics: If the limit as $N\to\infty$ of the ensemble average $\langle n_{k\sigma}\rangle$ is the function $\bar{n}_\sigma(k)$, then the limit of $\langle n_{k\sigma}n_{k'\sigma'}\rangle$ is $\bar{n}_\sigma(k)\bar{n}_{\sigma'}(k')$ if $k\sigma\ne k'\sigma'$ (each occupation number is coupled to infinitely many others in this limit, and a "mean-field theory" in occupation number space becomes exact). Then $\delta E/\delta n_{k\sigma}=J\epsilon(k)$, where

$$\epsilon(k)=\epsilon_0(k)+\sum_\sigma\int_{-k_0}^{k_0}\frac{dk'}{2\pi}V(k-k')\bar{n}_\sigma(k')\,, \tag{10}$$

which satisfies the differential equation

$$\epsilon''(k)=-\left[1+\frac{1}{2}\sum_\sigma\bar{n}_\sigma(k)\right], \tag{11}$$

with boundary conditions $\epsilon'(\pm k_0)=\mp\pi/2$. The entropy density $\bar{s}=S/Nk_B$ has the usual Bose form

$$\sum_\sigma\int_{-k_0}^{k_0}\frac{dk}{2\pi}(\bar{n}_\sigma+1)\ln(\bar{n}_\sigma+1)-\bar{n}_\sigma\ln\bar{n}_\sigma\,. \tag{12}$$

Minimizing $\bar{e}-h\bar{\sigma}-\beta^{-1}\bar{s}$, where $\bar{e}=\langle H\rangle/N$ and $\bar{\sigma}=\langle S^z\rangle/N$, by varying $\bar{n}_\sigma(k)$ and k_0 subject to the constraint $N_{\rm sp}/N=1-2k_0/\pi$, leads to the Bose distribution

$$\bar{n}_\pm(k)=\{[1+\exp(\mp\beta h)]\exp[\beta J\epsilon(k)]-1\}^{-1}, \quad (13)$$

where $\epsilon(k)$ and $\bar{n}_\sigma(k)$ are even functions, $\epsilon(k_0)=0$, and $\bar{n}_\pm(k_0)=\exp(\pm\beta h)$.

The differential equation (11) can now be solved in terms of the velocity variable $v=d\epsilon/dk$; $v\,dv/d\epsilon=dv/dk$ is given by the right-hand side of (11), expressed as a function of ϵ using Eq. (13). In terms of $f(v)\equiv[v^2-(\pi/2)^2]/4$,

$$\bar{n}_\pm=\exp(2\beta Jf\pm\tfrac{1}{2}\beta h)[(1+\gamma^2)^{1/2}\pm\gamma], \quad (14)$$

where $\gamma=\exp(2\beta Jf)\sinh(\beta h/2)$. Substitution of the expressions for $\bar{n}_\pm(v)$ and dv/dk into (12) gives the entropy density $\bar{s}(\beta J,\beta h)$; given the limits $\bar{e}\to 0$ as $\beta J\to 0$, and $\bar{\sigma}\to 0$ as $\beta h\to 0$, this fully defines the thermodynamics.

For $h=0$, the entropy density $\bar{s}$ is

$$\frac{2}{\pi}\int_0^{\pi/2}dv\,\{\ln[2\cosh(\beta Jf)]-\beta Jf\tanh(\beta Jf)\}. \quad (15)$$

This has the unexpected symmetry $\bar{s}(\beta J)=\bar{s}(-\beta J)$. Similarly, the energy density $\bar{e}$ is an even function of J, despite the fact that for finite N, the energy-level structures of H and $-H$ are quite different. Also, $k_0(\beta J)$ decreases monotonically from $\pi/2$ to 0 as βJ decreases from ∞ to $-\infty$, with the property $k_0(\beta J)+k_0(-\beta J)=\pi/2$. The $h=0$ magnetic susceptibility $\chi=\partial\bar{\sigma}/\partial h$ has no such symmetry, and is given by

$$\chi=\frac{\beta}{3N}\sum_{n,n'}\langle\mathbf{S}_n\cdot\mathbf{S}_{n'}\rangle=\frac{\beta}{2\pi}\int_0^{\pi/2}dv\exp(2\beta Jf). \quad (16)$$

In the antiferromagnetic case ($J>0$), the ground state of the system (with even N) has $S=0$, and the elementary excitation (created only in pairs) is the $S=\frac{1}{2}$ spinon, with dispersion

$$\epsilon^{\rm spinon}(k)=\tfrac{1}{2}J(k_0^2-k^2),\quad |k|\le k_0=\pi/2. \quad (17)$$

At low energies ($|k|\to\pi/2$) the velocity v_0 is $(\pi/2)J$.

In conformal field theory, the low-temperature, zero-field behavior of the antiferromagnet is classified[7] as that of the $k=1$ SU(2) WZW model, a model with conformal anomaly $c=1$. The solution of the present model allows a new representation of the spectrum of this CFT, which exposes an infinite set of SU(2) symmetries. In the conformal limit, the energy spectrum of right-moving spinons is given by

$$\frac{2\pi v_0}{N}\left[\left(\frac{N_{\rm sp}}{2}\right)^2+\sum_{m=0}^{\infty}m(n_{m+}+n_{m-})\right], \quad (18)$$

where $N_{\rm sp}=N_++N_-$, $S^z=(N_+-N_-)/2$, and $N_\sigma=\sum n_{m\sigma}$, where $\{n_{m\sigma}\}$, $m=0,\ldots,\infty$, are a set of non-Abelian SU(2) boson (spinon) occupations. This separates kinematic degeneracies only present in the conformal limit from those resulting from the independent SU(2) symmetries of *each spinon orbital,* which form a much larger symmetry group than the standard product of separate global SU(2) symmetries of right and left movers in CFT. Related symmetries occur in the free spin-$\frac{1}{2}$ Fermi gas, which in the conformal limit is the sum of two independent $k=1$ SU(2) WZW CFT's, one for spin and one for charge degrees of freedom. The generators of the symmetries of (18) must correspond to configuration-dependent combinations of those of the Fermi gas.

The antiferromagnetic ground state in a finite magnetic field h has the magnetization $\bar{\sigma}=[\mathrm{sgn}(h)/2][1-(1-|h|/h_c)^{1/2}]$ for $0\le|h|\le h_c=(\pi/2)^2J$. This corresponds to Bose condensation of equal numbers of fully spin-polarized spinons into the orbitals with $k=\pm k_0$, $k_0=(\pi/2)(1-2|\bar{\sigma}|)$. In the low-energy limit, the spinon velocity $v(\bar{\sigma})$ is given by $(\pi/2)J(1-2|\bar{\sigma}|)$; the nonanalyticity of $v(\bar{\sigma})$ as $\bar{\sigma}\to 0$ appears to be a consequence of the long-range exchange, and would not be expected in a finite-range model.

For $|h|<h_c$, the low-temperature entropy per site is $\pi k_B^2T/3v(\bar{\sigma})$, as predicted from Abelian bosonization.[9,10] The $T=0$ susceptibility χ is $1/2\pi v(\bar{\sigma})$, consistent with the absence of a magnetization-dependent renormalization of the longitudinal and transverse spin-correlation exponents $\eta_\parallel=\eta_\perp=1$ seen in the explicit calculation of ground-state correlations at finite magnetization.[1] The relation $2\pi v\chi=\eta_\parallel=\eta_\perp^{-1}$ is predicted by the "Luttinger liquid" theory,[10,11] which today can be recognized as the $c=1$, U(1) case of the subsequently developed conformal field theory.

A magnetization-dependent renormalization of the correlation exponent would usually be expected as a consequence of low-energy "spin backscattering" or "umklapp" processes.[10,12] A vanishing coupling for these processes at low energies places a model precisely at the critical point for the dimerization instability.[12] As identical particles in 1D, spinons can be considered to undergo only forward-scattering collisions; with this convention, these processes can be described as *spin exchange between spinons* during collisions. The special feature of this model is evidently that spin exchange between spinons is *entirely absent* at *all energies,* which also explains the remarkable level degeneracies.

Long-range ferromagnetic order appears as $\beta J\to-\infty$, where χ (and the correlation length) diverges exponentially:

$$\chi\sim\tfrac{1}{4}\beta(|\beta J|\pi/2)^{-1/2}\exp(|\beta J|\pi^2/8). \quad (19)$$

The ferromagnetic ($J<0$) ground state is ordered with $S=N/2$. This corresponds to Bose condensation of spinons into the zero-velocity orbital. The single magnon excitation ($\Delta S=-1$) has a dispersion

$$\epsilon^{\text{magnon}}(k)=\tfrac{1}{4}|J|(2\pi|k|-k^2),\quad |k|\le\pi. \tag{20}$$

At low energies ($|k|\to 0$) this has the same limiting velocity as the antiferromagnetic spinon (17). This ferromagnet has a linear magnon dispersion because of the long range of the exchange: For a ferromagnetic chain with exchange $J(n)\sim|n|^{-\alpha}$, $1<\alpha<3$, the long-wavelength magnon dispersion vanishes as $|k|^{\alpha-1}$.

A CFT-like description of the low-energy excitation spectrum can be developed: right- and left-moving parts each have the form

$$\frac{2\pi v_0}{N}\left[M^2+\sum_{m=1}^{M}m(n_{m+}+n_{m-})\right], \tag{21}$$

where $M=M^R$ or M^L is the number of right- or left-moving pseudomomenta $\{k_i\}$ (magnons) in (5); this fixes the *finite* number of spinon orbitals, which have occupations $\{n_{m\sigma}\}$, $m=1,\dots,M$. The Bose-condensed zero-velocity state has macroscopic occupancy $n_{0+}+n_{0-}=N-2(M^R+M^L)-(N_{\text{sp}}^R+N_{\text{sp}}^L)$: This degree of freedom is the ferromagnetic order parameter.

At *fixed* N_{sp} a bosonic description (8) of the spinon spectrum has proved useful. However, the behavior of the spinon gas as N_{sp} varies has a clearly "semionic" (half-fractional statistics) character (as in the 2D case[3]), intermediate between fermions and bosons. This is seen in the counting of the FPSG states: Addition of $2n$ spinons reduces the number of orbitals into which the next spin-polarized spinon can be placed by n as compared to $2n$ or 0 in the cases of spin-polarized free fermions or bosons. This definition of statistics as the rate at which a band (or Landau level) fills as particles are added coincides with the usual Berry's phase definition in the case of the fractional quantum Hall effect: The number of states in a Landau level is proportional to the total flux times the particle charge, and this changes as particles carrying flux are added.

In conclusion, the model (1) has proved explicitly solvable to a remarkable extent, and it seems appropriate to consider it in some sense as an "ideal spinon gas." Various unsolved problems remain: The general solution of (7) for the non-FPSG wave functions is needed, and the generators of the hidden SU(2) symmetries of (1) and the $k=1$ SU(2) WZW CFT must be found; an obvious question is whether they are special to this case or also occur in other CFT's. Another issue is the identification of the operator algebra underlying the evident integrability of the system, and its relation to that of the nearest-neighbor exchange model solved by Bethe.[13] In this context, Inozemtsev[14] has recently given persuasive arguments for the integrability of the family of $S=\frac{1}{2}$ Heisenberg chains with exchange

$$J(n)=J\sum_{m=-\infty}^{\infty}\left[\frac{\sinh\kappa}{\sinh[\kappa(n+mN)]}\right]^2, \tag{22}$$

which interpolates between the two models. Further evidence that (22) is integrable comes from a numerical-diagonalization study[15] of the relation of the spinon quantum numbers of the $\kappa=0$ model (1) to the complex rapidities of Bethe's $\kappa=\infty$ model.

This work was supported in part by NSF Grant No. DMR-8901985.

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