Exact Solution of an $S=\frac{1}{2}$ Heisenberg Antiferromagnetic Chain with Long-Ranged Interactions

B. Sriram Shastry[a]
Joseph Henry Laboratories of Physics, Princeton University, Princeton, New Jersey 08544
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The $S=\frac{1}{2}$ Heisenberg Hamiltonian

$$\mathcal{H}=\tfrac{1}{2}\sum_{n=1}^{N-1}\sum_{m=1}^{N} J_n \boldsymbol{\sigma}_m\cdot\boldsymbol{\sigma}_{m+n},$$

with $J_n=J_0/\sin^2(n\pi/N)$, is shown to have a simple singlet ground state in the form of a Jastrow function. The spectrum and correlations are explicitly known and the magnetic susceptibility is shown to be Pauli type at $T=0$. The model has a striking similarity to the nearest-neighbor isotropic Heisenberg model and may be viewed as a discretized version of the Sutherland-Calogero-Moser system.

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There has been a great interest recently in the properties of the Gutzwiller-projected Fermi wave function. The one-dimensional case corresponding to one electron per atom ($N_\uparrow=N_\downarrow=N/2$, N even) is a singlet wave function,

$$|\psi\rangle=P_G|\phi\rangle;\quad P_G=\prod_i(1-n_{i\uparrow}n_{i\downarrow}),$$
$$|\phi\rangle=\prod_{|k|<K_F}C^\dagger_{k\uparrow}C^\dagger_{k\downarrow}|0\rangle. \tag{1}$$

Elegant numerical work[1] has shown that $|\psi\rangle$ is an extremely good variational wave function for the nearest-neighbor isotropic Heisenberg (NNIH) model in that the energy is close to the Bethe *Ansatz* results, and also the spin correlations have a power-law behavior similar to the exact results. In fact, Gebhard and Vollhardt[2] have succeeded in computing the spin correlations analytically and find

$$\langle S_0^z S_n^z\rangle=\frac{\mathrm{Si}(\pi n)}{4\pi n}(-1)^n;$$
$$\mathrm{Si}(x)=\int_0^x\frac{\sin(\pi y)}{\pi y}\,dy. \tag{2}$$

I was motivated by the above to inquire further into the precise nature of the wave function $|\psi\rangle$ as a spin wave function. I show in this Letter that $|\psi\rangle$ is, in fact, an eigenfunction of a long-ranged Hamiltonian antiferromagnet described by the Hamiltonian (a periodic version of $1/r^2$ exchange)

$$\mathcal{H}'=\tfrac{1}{2}\sum_{m=1}^{N}\sum_{n=1}^{N-1}\frac{J_0}{\sin^2(n\pi/N)}\boldsymbol{\sigma}_m\cdot\boldsymbol{\sigma}_{m+n} \tag{3}$$

(N even and periodic boundary conditions).

As a prelude, let us examine the nature of the Gutzwiller projection in Eq. (1). It is convenient to work with the Klein operation $a_{n\uparrow}=c_{n\uparrow}$, $a_{n\downarrow}=c_{n\downarrow}\exp(i\pi\hat{N}_\uparrow)$, where $\hat{N}_\uparrow$ is the number operation for the up spins. (These operators have the property that $[a_{n\uparrow},a_{n\downarrow}]=0$.) A basis wave function for band electrons is written in the form

$$|\phi'\rangle=\prod_{k\in K}a^\dagger_{k\uparrow}\prod_{q\in Q}a^\dagger_{q\downarrow}|0\rangle, \tag{4}$$

where K is a set of $(N-M)$ momenta occupied by the up electrons and Q is the set of M wave vectors for the down electrons. We now perform a particle-hole transformation on the up-spin species generated by a unitary operator $U=(a^\dagger_{N\uparrow}+a_{N\uparrow})\cdots(a^\dagger_{1\uparrow}+a_{1\uparrow})$ and consider the state $|\bar\psi\rangle=UP_G|\phi'\rangle=\bar{P}_G U|\phi'\rangle$, where $\bar{P}_G=\prod_m(1-n_{m\downarrow}+n_{m\uparrow}n_{m\uparrow})$. The operator U can be commuted through the a's and we find

$$|\bar\psi\rangle=\bar{P}_G\prod_{k\in K}a_{-k\uparrow}\prod_{q\in Q}a^\dagger_{q\downarrow}\prod_{\forall l}a^\dagger_{l\uparrow}|0\rangle. \tag{5}$$

Expanding the plane-wave states in the Wannier basis and implementing $\bar{P}_G$ we find

$$|\bar\psi\rangle=\sum_{n_1,\ldots,n_M}\det(e^{iq_in_j})\det(e^{ip_in_j})b^\dagger_{n_L}\cdots b^\dagger_{n_M}|0\rangle, \tag{6}$$

where the p's are the set of wave vectors complementing the set $-K$ and $b^\dagger_n=a^\dagger_{n\uparrow}a^\dagger_{n\downarrow}$. The algebra of the operators b_n is identical to that of the Pauli spin operators and, in fact, this representation was first used by Anderson[3] in the context of the theory of superconductivity. To be precise, I write $S_n^+=b_n$, $S_n^z=\frac{1}{2}-b_n^\dagger b_n$. The state $|\bar\psi\rangle$ is thus isomorphic to the state

$$|\chi\rangle=\sum_{n_1,\ldots,n_M}\det(e^{iq_in_j})\det(e^{ip_in_j})S^-_{n_1}\cdots S^-_{n_M}|F\rangle, \tag{7}$$

where $|F\rangle$ is the ferromagnetic state. The totality of states $|\chi\rangle$ form an appropriate basis for the spin system since the determinant forces the vanishing of the wave function for coincident spin deviation (the kinematical constraint is fulfilled) and, moreover, the pair of determinants gives a Bose character to the wave function. In fact, if we chose p's such that $p_n+q_m\neq0$ (for any n,m), we have the result $S^+_{\rm tot}|\chi\rangle=\sum_n S_n^+|\chi\rangle=0$. Thus $|\chi\rangle$'s are a set of highest-weight states for the rotation group, and are also eigenfunctions of the translation operator. There is a redundancy though, since we can form ${}^NC_M\,{}^{N-M}C_M$ such states, whereas the number of independent states is only ${}^NC_M-{}^NC_{M-1}$, the overcount factor being ${}^{N-M+1}C_M$.

Let us now specialize to the case of a half-filled ($M=\frac{1}{2}$) linear chain and q's corresponding to the Fermi distribution, i.e., $q_n=k_1,k_1+\theta,k_1+2\theta,\ldots,k_1+(N-1)\theta$, where $\theta=2\pi/N$ and $k_1=2\pi N^{-1}(1-N/4)$ ($N/2$ even, $k_1=2\pi N^{-1}[(2-N)/4]$ ($N/2$ odd). Then the states $p_n=\pi-q_n$ and the two determinants become equal, apart from a phase, and we find the amplitude for spin deviation to be

$$\psi(n_1,\ldots,n_M)=e^{i\pi\sum n_i}|\det(e^{iq_in_j})|^2 \propto e^{i\pi\sum n_i}\prod_{i<j}\sin^2[\pi(n_j-n_i)/N]. \quad (8)$$

I have used the Vandermonde nature of the Fermi determinant in the above. The phase factor is precisely the "Marshall sign."[4,5] The above derivation in the form of the modulus square of the determinant is also true for the square and cubic lattices where π is replaced by a vector $\pi(1,1)$ or $\pi(1,1,1)$, but the Jastrow-type form is only true in 1D.

We now turn to the main result in this Letter; we inquire if the wave function ψ is the exact eigenfunction of any simple Hamiltonian. In this task we are guided by the remarkable results of Sutherland[6] for the continuum Bose gas in 1D; Sutherland showed that the many-body problem with a two-body potential $\sim 1/\sin^2(x_i-x_j)$ has a Jastrow wave function for its ground state. A simple calculation for $M=2$ shows that the Hamiltonian Eq. (3) does have the desired property, and I discuss below the proof of the result for $M\le N/2$. It is expedient to perform a unitary transformation on $\mathcal{H}$ generated by $\prod_{n\in\text{odd}}\sigma_n^Z$, which absorbs the phase in Eq. (8), and consider the Hamiltonian in the following form:

$$\mathcal{H}_r'=\tfrac{1}{2}\sum_{n=1}^{N-1}J_n^Z(N-4r)+2\mathcal{H}_r,\quad \mathcal{H}_r=-\tfrac{1}{2}\sum_n J_n^\perp(b_{m+n}^\dagger b_m+\text{H.c.})+\sum J_n^Z b_{m+n}^\dagger b_{m+n}b_m^\dagger b_m. \quad (9)$$

Here I have specialized to the sector $M=r$ and the summations are in the region $1\le m\le N$, $1\le n\le N-1$. I define

$$J_n^Z=J_n=J_0/\sin^2(n\pi/N);\quad J_n^\perp=(-1)^{n+1}J_n. \quad (10)$$

Let us note that $\sum J_n^z\equiv x=J_0/3(N^2-1)$ and $\sum J_n^\perp\equiv y=J_0/3(N^2/2+1)$. Thus $\lambda_r=\frac{1}{2}x(N-4r)+2E_r$, where E_r is the eigenvalue of $\mathcal{H}_r$. Let us first note the case $r=1$, where $|\psi\rangle=\sum e^{ikn}S_n^-|F\rangle$. The eigenvalue $E_r(k)=-y+n_k$, where the single-particle energy is

$$n_k=\alpha k^2;\quad 0\le|k|\le\pi,\quad \alpha=J_0N^2/2\pi^2. \quad (11)$$

[This is to be contrasted to the usual spin-wave energy for the NNIH model $\sim(1-\cos k)$]. Consider the case $r=2$. We seek to satisfy the eigenvalue equation

$$E_2\psi(n,m)=2J_{n-m}^Z\psi(n,m)-\sum_r J_r^\perp[\psi(n+r,m)+\psi(n,m+r)] \quad (12)$$

with $\psi(n,m)=\sin^2[\pi(n-m)/N]$. The form of ψ essentially dictates that of J_n. To fulfill the recursion relation, we use the addition formula

$$\alpha(n+r)=\alpha(n)\gamma(r)+\alpha(r)+\beta(n)\beta(r), \quad (13)$$

where $\alpha(n)\equiv\sin^2(n\pi/N)$, $\gamma(n)=1-2\alpha(n)$, and $\beta(n)=(1/\sqrt{2})\sin(2\pi n/N)$. Substituting, we find the eigenvalue condition to be fulfilled with $E_2=4J_0-2y$, on using $\sum J_r^\perp\alpha(r)=J_0$. Next consider $r=3$. We look for the eigenvalue equation

$$E_3\psi(n_1,n_2,n_3)=2(J_{n_3-n_1}^Z+J_{n_3-n_2}^Z+J_{n_2-n_1}^Z)\psi(n_1,n_2,n_3) -\sum_r J_r^\perp[\psi(n_1+r,n_2,n_3)+\psi(n_1,n_2+r,n_3)+\psi(n_1,n_2,n_3+r)], \quad (14)$$

with $\psi(n_1,n_2,n_3)=\alpha(n_3-n_2)\alpha(n_3-n_1)\alpha(n_2-n_2)$. A typical term in the last sum looks like $\sum_r\alpha(n_3-n_2+r)\alpha(n_3-n_1+r)J_r^\perp$, which can be simplified with Eq. (13) and the result $\sum J_r^\perp f_r=0$, if $f_r=\alpha^2(r)$, $\beta(r)$, $\alpha(r)\beta(r)$, or $\beta(r)\gamma(r)$:

$$\sum_r J_r^\perp\psi(n_1,n_2,n_3+r)=\psi(n_1,n_2,n_3)\Big[\sum_r J_r^\perp\gamma^2(r)+\phi(n_3-n_1)\phi(n_3-n_2)\sum_r J_r^\perp\beta^2(r) +J_0\{\alpha^{-1}(n_3-n_1)+\alpha^{-1}(n_3-n_2)\}\Big], \quad (15)$$

where $\phi(r)=\beta(r)/\alpha(r)=\sqrt{2}\cot(\pi r/N)$. On adding the three terms from the right-hand side of Eq. (14), we find that the terms in Eq. (15) organize in the following way. The piece in the curly brackets cancels exactly the J^z terms in Eq.

(14), and the first term contributes to the eigenvalue. The dangerous unwanted term is

$$-\psi\sum J_r^{\perp}\beta^2(r)[\phi(n_3-n_1)\phi(n_3-n_2)+\phi(n_2-n_1)\phi(n_2-n_3)+\phi(n_1-n_2)\phi(n_1-n_3)]. \quad (16)$$

This term simplifies dramatically upon the use of the addition formula for ϕ's. Write $\pi/N(n_3-n_2)=x$, $\pi N^{-1}(n_2-n_1)=y$, $\pi N^{-1}(n_3-n_1)=x+y$; hence we find the term in square brackets in (16) to be $2[\cot(x+y)(\cot x+\cot y)-\cot x\cot y]$, which is equal to -2. Hence we find

$$E_3=-3\sum J_r^{\perp}r^2(r)+2\sum J_r\beta^2(r)=16J_0-3y. \quad (17)$$

We now turn to the general case of $r=M\leq N/2$ for which the eigenvalue problem reads

$$E_M\psi(n_1,\ldots,n_M)=2\sum_{i<j}J^Z_{n_j-n_i}\psi-\sum_{r,i}J_r^{\perp}\psi(n_1,\ldots,n_i+r,\ldots,n_M), \quad (18)$$

with $\psi=\prod_{i<j}\alpha(n_j-n_i)$. A typical term in Eq. (18) reads

$$\sum J_r^{\perp}\psi(n_1,\ldots,n_M+r)=\sum_r J_r^{\perp}[\alpha(n_M-n_1+r)\cdots\alpha(n_M-n_{M-1}+r)]. \quad (19)$$

On using Eq. (13), we find a total of 3^{M-1} terms; a generic term is

$$\Delta(M,v_1,v_2)\alpha(n_M-n_{i_1})\cdots\alpha(n_M-n_{i_{v_1}})\beta(n_M-n_{j_1})\cdots\beta(n_M-n_{j_{v_2}}), \quad (20)$$

$$\Delta(M,v_1,v_2)\equiv\sum_r J_r^{\perp}[\alpha(r)]^{v_1}[\beta(r)]^{v_2}[\gamma(r)]^{M-1-v_1-v_2};\ 0\leq v_i\leq M-1,\ 0\leq v_1+v_2\leq M-1. \quad (21)$$

Writing $\gamma(r)=1-2\alpha(r)$ and expanding, we find

$$\Delta(M,v_1,v_2)=\sum_{v_3=0}^{M-1-v_1v_2}(-2)^{v_3}\,{}^{M-1-v_1-v_2}C_{v_3}h(v_1+v_3,v_2), \quad (22)$$

$$h(v,v')\equiv\sum J_r^{\perp}[\alpha(r)]^{v}[\beta(r)]^{v'}. \quad (23)$$

I now crucially use the fact that the powers of $\alpha(r)$ and $\beta(r)$ are such that $v+v'\leq N/2$ and hence, in this region, assert that the only nonzero elements are $h(0,0)=y$, $h(0,2)=2J_0$, and $h(1,0)=J_0$. The details of the proof will be presented in a longer paper, but basically the vanishing of almost all the h's stems from the fact that $\alpha(r)J_r^{\perp}\sim(-1)^r$, i.e., possesses a "momentum" $\pi=(2\pi/N)\times(N/2)$, and the constraints on the values of v and v' force a multiplication of this function with *lower* momentum states. This implies the following nonvanishing Δ's: $\Delta(M,0,0)=y-2(M-1)J_0$, $\Delta(M,1,0)=J_0$, and $\Delta(M,0,2)=2J_0$; hence Eq. (19) reduces to

$$J_r^{\perp}\psi(n_1,\ldots,n_M+r)=\psi\left[y-2(M-1)J_0+J_0\sum_{j\neq m}\alpha^{-1}(n_M-n_j)+2\sum_{\substack{i,j\neq m\\ i<j}}\phi(n_M-n_i)\phi(n_M-n_j)\right]. \quad (24)$$

(This is the analog of the Liebnitz product rule for the difference operator $J^{\perp}$ acting on the test function ψ.) Substituting into Eq. (18) and using the addition theorem as in Eq. (16), we find that the eigenvalue problem is satisfied with

$$E_M=-My+2M(M-1)J_0+\tfrac{2}{3}J_0M(M-1)(M-2). \quad (25)$$

The last term arises from the ${}^MC_3$ triples each with a factor of -2, and the second term in (24) cancels exactly the first in Eq. (18). Combining, we find the eigenvalue of the Hamiltonian $\mathcal{H}$:

$$\lambda_M=\tfrac{1}{2}xN-2M(x+y)+4M(M-1)J_0+\tfrac{4}{3}J_0M(M-1)(M-2). \quad (26)$$

In order to get a sensible result in the thermodynamic limit, I chose $J_0=J/N^2$ so that the energy is extensive in N. Writing $M=N/2\bar{\mu}$ for $0\leq\bar{\mu}\leq1$, we obtain the energy

$$\lambda_M/NJ=[\tfrac{1}{6}-\tfrac{1}{2}\bar{\mu}+\tfrac{1}{6}\bar{\mu}^3]-(1+4\bar{\mu})/6N^2. \quad (27)$$

The minimum is achieved for $\bar{\mu}=1$ corresponding to a singlet state with $\lambda_{\min}=-1/6NJ+O(1/N)$. The magnetic susceptibility of the model follows from (27) and we find $\chi_{\text{spin}}=Ng^2\mu_B^2/4J$.

It is not *a priori* obvious that the wave function presented here is the ground-state wave function for the model. The phase factor in Eq. (8) is the correct phase factor for the nearest-neighbor model where the Frobenius-Perron-Marshall[4,5] criterion is applicable; however, this theorem does not apply in the present model since $J_n^{\perp}$ oscillates in sign. However, I find from small-cluster calculations ($N\leq6$) that the wave function is indeed the ground state and conjecture that it is so for the case of arbitrary (even) N. (The frustration in the model is weak, i.e., $|J_2|/|J_1|=\frac{1}{4}$, where J_1 and J_2 are first- and second-neighbor couplings, and hence the Frobenious-Perron-Marshall phase seems to survive.)

I have computed the excitation spectrum of the model following the strategy adopted by Sutherland for the Bose gas, and find near the ground state a spin-1 branch, analogous to the des Cloizeaux–Pearson branch for the NNIH model given by $\omega_q = 2J(|q|/\pi)(1-|q|/\pi)$, $0 \le |q| \le \pi$. This is renormalized with respect to the spin-wave theory by a factor of 2 (compared with $\pi/2$ for the nearest-neighbor model). Note that the product of χ_{spin} and the spin-wave velocity is $(Ng^2\mu_B^2) \times (1/2\pi)$ as in the NNIH model. This product is believed to be a universal number closely related to the "Wilson ratio." The present model is expected to be in the same universality class as the NNIH model, although the absence of logarithmic corrections in the correlations [Eq. (2)] suggests that this model has a vanishing coefficient of an appropriate marginal operator. I remark that the ground state in this model ($M = N/2$) possesses a momentum 0 if $N/2$ is even and π if $N/2$ is odd, just as in the case of the NNIH model. In fact, the wave function cannot be orthogonal to the NNIH ground state for finite-sized systems since both wave functions have $S=0$ and have an identical node structure. (For $N=4$, the wave functions are identical.) The overlap presumably vanishes for large N. A systematic exposition of the excited states and thermodynamics will be presented in a forthcoming paper.

The model presented and solved in this paper is seen to be closely connected to the continuum problem solved by Sutherland,[6] and corresponds to a particular way of discretizing the kinetic energy. This kind of discretization is, in fact, known in the high-energy physics literature as the SLAC derivative, and the model solved here was investigated approximately by Drell, Weinstein, and Yankielowicz.[7]

The wave function Eq. (8) also appears in the Dyson-Mehta-Gaudin[8] theory of random matrices if the location of n's are regarded as continuous variables. The present case corresponds to the circular ensembles with $\beta = 4$ (symplectic), for which the two-point correlation function [corresponding to Eq. (2)] is known exactly and agrees with Eq. (2). Also, the one-particle density matrix in this case is known from the work of Sutherland and it also agrees with Eq. (2). This perhaps unanticipated equality is, in fact, expected in the present model as a consequence of the singlet nature of the ground state (implying $\langle S_0^z S_n^z \rangle = \langle S_0^x S_n^x \rangle$). The discrete nature of the particle location thus seems unimportant to the correlation functions. If this is true generally, then we may infer *all* the n-point functions from the work of Dyson.[9]

Finally I note that the construction of the wave functions for the spin system in the present scheme utilizes a (many to one) correspondence between the states of a Fermi gas and the states of a spin system, and may be the natural setting to give a concrete form to the idea of a "pseudo Fermi surface" due to Anderson.[10]

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[a]On leave from Tata Institute of Fundamental Research, Bombay, India.

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