Exact Jastrow-Gutzwiller Resonating-Valence-Bond Ground State of the Spin-$\frac{1}{2}$ Antiferromagnetic Heisenberg Chain with $1/r^2$ Exchange

F. D. M. Haldane
Department of Physics, University of California at San Diego, La Jolla, California 92093
(Received 15 December 1987)

A set of Jastrow wave functions comprises exact eigenstates of a family of $S=\frac{1}{2}$ antiferromagnetic chains with r^{-2} exchange. The ground state of the isotropic model is in this set, and is identical to the $U\to\infty$ limit of the Gutzwiller wave function, also identified as Anderson's "resonating-valence-bond" state. The full set of energy levels of this model is obtained; the spectrum exhibits remarkable "supermultiplet" degeneracies suggesting the existence of a hidden continuous symmetry.

PACS numbers: 75.10.Jm, 74.65.+n

In this Letter I construct the exact Jastrow-product ground-state wave function of the $S=\frac{1}{2}$ one-dimensional (1D) isotropic Heisenberg antiferromagnet with an exchange coupling falling off as the inverse square of the distance between sites. This state is found to be identical to the $U\to\infty$ limit of Gutzwiller's variational wave function[1-3] for the Hubbard chain, and to the 1D version of Anderson's "resonating-valence-bond" (RVB) state.[4,5] I also obtain the wave functions and correlation functions of a related set of exact eigenstates, give a construction for the full set of excitation energies, and discuss an anisotropic generalization of the model.

The model Hamiltonian is given by

$$H=\sum_{n<n'}J(n-n')(S_n^xS_{n'}^x+S_n^yS_{n'}^y+\Delta S_n^zS_{n'}^z), \qquad (1)$$

with $J(n-n')=d(n-n')^{-2}$, where d is the distance between sites. To impose periodic boundary conditions on a finite ring of N sites, I take d to be the chord distance $(N/\pi)\,|\sin[\pi(n-n')/N]\,|$.

The mathematical result underlying the solution of the model involves the sum

$$S_{pq}(J)=\sum_n{}' z^{nJ}(1-z^n)^{p-1}(1-z^{-n})^{q-1}, \qquad (2)$$

where p, q, and J are integers, $z=\exp(2\pi i/N)$, and the primed sum is from $n=1$ to $N-1$. J may be chosen in the range $1\le J\le N$. Then, for $0\le q\le J\le N-p\le N$, (a) $S_{pq}(J)=0$ for $p+q>2$, (b) $S_{pq}(J)=(-1)^p$ for $p+q=2$, (c) $S_{pq}(J)=-\frac{1}{2}-(p-q)(J-\frac{1}{2}N)$ for $p+q=1$, and (d) $S_{00}(J)=\frac{1}{12}(N^2-1)-\frac{1}{2}J(N-J)$. If p or q exceed the maximum values allowed by the inequality, $S_{pq}\neq 0$. This means that the set of values $\{S_{pq}(J),p+q=r\}$ are all zero only in the range $2<r\le\min(J,N-J)$.

It is convenient to choose the total azimuthal spin $S^z\ge 0$, and treat the system as a Bose lattice gas where $S_n^z=\sigma=+\frac{1}{2}$ represents an empty site, and $\sigma=-\frac{1}{2}$ an occupied site. There are $M=\frac{1}{2}N-S^z$ particles, with matrix elements $\frac{1}{2}d(n)^{-2}$ for a hop of n sites, and interaction energy $\Delta d(n)^{-2}$ between pairs n sites apart. The boson dispersion relation is given by $\epsilon(k)=\frac{1}{4}k(k-2\pi)$ for $0<k<2\pi$. In addition, there is an energy hift

$$E_0(M,\Delta)=\tfrac{1}{24}(2\pi/N)^2(N^2-1)[\tfrac{1}{4}N\Delta+M(1-\Delta)].$$

Motivated by Sutherland's solution[6] of the continuum limit of this problem, I consider the Jastrow wave functions

$$\psi(\{n_i\})=\prod_i\exp(2\pi iJn_i/N)\prod_{i<j}d(n_i-n_j)^m. \qquad (3)$$

J controls the particle current around the ring; the state is an eigenfunction of the translation operator with eigenvalue $T=\exp(iK)=\exp(2\pi iJM/N)$.

If H^0 is the kinetic (hopping) term, and $H^0|\psi\rangle=|\chi\rangle$, then

$$\frac{\chi(\{n_i\})}{\psi(\{n_i\})}=\sum_n{}' f_n(J)\sum_i\prod_{j\neq i}[1-g_{ij}^{(n)}]^{m/2}, \qquad (4)$$

where $f_n(J)=\frac{1}{2}(2\pi/N)^2z^{nJ}(1-z^n)^{-1}(1-z^{-n})^{-1}$ and $g_{ij}^{(n)}=Z_{ij}^{-2}[(1-z^n)Z_i^2+(1-z^{-n})Z_j^2]$, where $Z_i\equiv z^{n_i}$ and $Z_{ij}=Z_i-Z_j$. If m is an *even integer*, the product in (4) can be expanded as a finite polynomial in $(1-z^n)^p(1-z^{-n})q$ with $p+q\le\frac{1}{2}m(M-1)$. *Provided* $\frac{1}{2}m(M-1)\le J\le N-\frac{1}{2}m(M-1)$, *terms with* $p+q>2$ *do not contribute to the right-hand side of (4).* This means that (4) only involves two-particle and three-particle terms; furthermore, the three-particle term may be eliminated with the identity $[\cot(\theta_1-\theta_2)\cot(\theta_2-\theta_3)+(\text{cyclic permutations of }1,2,3)\equiv 1]$. The right-hand side of (4) then is given by a constant minus $H^{\text{int}}(\{n_i\})$, the inverse-square interaction term with coupling $\Delta(m)=\frac{1}{2}m(m-1)$. Provided Δ takes a value corresponding to even-integral m, (3) is an eigenfunction of (1) with eigenvalue $E_0(M,\Delta)+\frac{1}{2}E_1$, where

$$E_1=(2\pi/N)^2[\tfrac{1}{24}m^2M(M^2-1)-\tfrac{1}{2}MJ(N-J)]. \qquad (5)$$

The lowest-energy eigenstate of the form (3) is obtained by our choosing M and J as close as possible to $\frac{1}{2}N$, while respecting the restrictions on M and J.

If (3) is multiplied by $\prod_{i<j}\mathrm{sgn}(n_i-n_j)$, it is found to be an exact eigenstate of the *spinless-fermion* version of the lattice-gas model provided $\Delta=\Delta(m)$ with *odd-integral m*. This variant model is not related to a simple Heisenberg chain with pairwise exchange. The cases $m=0$ and 1 correspond to free bosons and free spinless fermions.

The Bose lattice-gas pair correlation function is given by

$$M(M-1)C^{-1/2}\sum_{\{n_i,i>2\}}|\psi(\{n_i\})|^2, \quad (6)$$

where C is the normalization of ψ. To evaluate this, I note that $|\psi|^2$ is proportional to a power of a $M\times M$ Vandermonde determinant[2]:

$$[\det_{i,j}|\exp(ik_i'n_j)|]^{2m}, \quad (7)$$

where $k_{i+1}'=k_i'+(2\pi/N)$, and the set $\{k_i'\}$ is invariant under $k_i'\to -k_i'$, so that $|k_i'|\le\pi(M-1)/N$. The determinant can be expanded, and (6) reduces to a sum of terms made up of products of quantities $F(k_1,\ldots,k_{2m})$, where the k's are members of the set $\{k_i'\}$, and

$$F(\{k_j\})=\sum_n\prod_j e^{ik_jn}. \quad (8)$$

F vanishes unless the sum of the k's is a multiple of 2π, when it has the value N. Except for the limiting case $\frac{1}{2}m(M-1)=J=\frac{1}{2}N$ (which is excluded by the choice $S^z\ge 0$ for $m=2$) the restriction on M and J means that the sum of the k's cannot be equal to any multiple of 2π other than 0. The sum over the discrete integers $n=1,\ldots,N$ can then be simply replaced by an integral over continuous values of n from 0 to N, and *the real-space (N point) correlations of the lattice model are identical to those of the equivalent state of the continuum Bose gas model.* The same argument applies to the off-diagonal correlation functions.

For $m=2$, the continuum-model correlations have been obtained by Sutherland.[6] In the thermodynamic limit with $M/N\to\bar m$, $J/N\to\bar j$, $\bar m<\bar j<1-\bar m$, the longitudinal and transverse spin correlation functions on different sites are respectively given by $\langle S_n^zS_{n'}^z\rangle-\langle S_n^z\rangle\langle S_{n'}^z\rangle=C_\parallel(x)$ and $\langle S_n^xS_{n'}^x\rangle=\langle S_n^yS_{n'}^y\rangle=C_\perp(x)$, $x=2\pi(n-n')$:

$$C_\parallel=\bar m x^{-1}\mathrm{Si}(\bar m x)\cos\bar m x - x^{-2}[\mathrm{Si}(\bar m x)+\sin\bar m x]\sin\bar m x,$$
$$C_\perp=\tfrac{1}{2}x^{-1}\mathrm{Si}(\bar m x)\cos\bar j x, \quad (9)$$

where $\mathrm{Si}(x)$ is the sine integral. Note that the dominant asymptotic correlations are algebraic (times a periodic component) with exponent $\eta=\eta^{-1}=1$, *independent of* $\bar m$, and without logarithmic corrections. This is in contrast with calculated properties[7,8] of the chain with only nearest-neighbor exchange (where η is renormalized for $\bar m\ne\frac{1}{2}$), and indicates the absence of the "spin-umklapp"[7,9,10] (backscattering) processes that are present (with the marginally irrelevant sign of coupling) in the nearest-neighbor exchange model. With the other sign of coupling, these processes drive a transition to dimer order.[10,11]

Provided $\bar j$ is in the allowed range, it is found that the Fourier transform[6] of the transverse spin correlation function vanishes identically at $Q=0$. This shows that the states (3) are the top members of their multiplets with total spin quantum number $S=S^z$. For finite N, closer examination shows that states on the boundary of the allowed region $[J=\frac{1}{2}N\pm(M-1-\frac{1}{2}N)]$ have $S^z<S$ and are members of multiplets with top members in the interior region at $M-1$ and $J\pm1$. To keep only distinct states, the allowed range of J for $m=2$ can be reduced to $M\le J\le N-M$.

When $\bar m=\bar j-\frac{1}{2}$, the correlations are isotropic: $\langle S_n^\alpha S_0^\beta\rangle=\frac{1}{4}\delta^{\alpha\beta}(-1)^n\mathrm{Si}(\pi n)/(\pi n)$. *This is precisely the correlation function of the spin-singlet Gutzwiller-RVB wave function for the Heisenberg model recently obtained by Gebhard and Vollhardt.*[3]

It is straightforward to see that the wave functions (3) with $m=2$ are indeed Gutzwiller projections of free spin-$\frac{1}{2}$ lattice fermion wave functions into the subspace where every site is singly occupied. The wave functions can be rewritten as the amplitudes $\psi(\{\sigma_n\})$ for the system to be in the state $|\{\sigma_n\}\rangle$, where $\sigma_n=\pm\frac{1}{2}$ is the eigenvalue of S_n^z:

$$\psi\propto\prod_n\exp(2\pi iJn\sigma_n/N)\prod_{n<n'}d(n-n')^{\delta_{\sigma_n,\sigma_{n'}}}. \quad (10)$$

The Slater-determinant wave function where occupied states are Bloch states with consecutive crystal momenta k can be written as a Vandermonde determinant. The wave function (10) may be recognized as the product of two such Vandermonde determinants, one for the sites with $\sigma=+\frac{1}{2}$ and one for $\sigma=-\frac{1}{2}$ sites.

After obtaining the sign change when site-ordered products of fermion creation operators are factorized into separate products for each spin component, it is found that the states (3) are obtained from Gutzwiller projection on a free fermion state with $N-M$ consecutive occupied $\sigma=+\frac{1}{2}$ Bloch states and M consecutive occupied $\sigma=-\frac{1}{2}$ states. The centers of the two sets of occupied states are relatively displaced by $J-\frac{1}{2}N$ states; a uniform shift in k space of all the occupied states leaves the Gutzwiller-projection state unchanged. Except at the limiting values of J, the set of occupied $\sigma=-\frac{1}{2}$ states is contained entirely within the set of occupied $\sigma=+\frac{1}{2}$ states.

Sutherland[6] has constructed the set of excitation energies of the continuum model as the sum of kinetic energies $\epsilon(k_i)$, where $\{k_i\}$ are a set of M (real) distinct "pseudomomenta." For the discrete set of couplings $\Delta(m)$, m integral, Sutherland's equation fix the pseudomomenta to have values $k_i=2\pi m_i/N$, where m_i are *integers* satisfying the constraint $m_{i+1}\ge m_i+m$. Examination of the energies of states (3) shows that they are consistent with this construction, and have consecutive real pseudomomenta with $m_{i+1} = m_i + m$, where $\{m_i\}$ are restricted to the range $0 \le m_i \le N$. Comparison with the total number of states for a given M shows that the set of states with real pseudomomenta are incomplete for $m > 1$.

Numerical study of small systems confirms that the energy levels predicted by the real pseudomomentum construction *are* found in the full spectrum, but that other energy levels also occur, which presumably involve complex k_i. Solution of the $M=2$ problem shows that in addition to the (real pseudomomenta) scattering states, there are $m-2$ bound-state bands *above* the top of the continuum of energies of asymptotically free two-particle states. (There is no such upper limit in Sutherland's continuous model.[6]) The top of the continuum consists of doubly degenerate states where one of the two m_i is either 0 or N. One linear combination of these is not a true scattering state, but is an incipient (algebraically decaying) bound state that evolves into a true bound state for $\Delta > \Delta(m)$. Further discussion of the $m > 2$ models is postponed to a separate publication.

For the *isotropic* model, the numerical study reveals a surprising fact: States are grouped into highly degenerate *supermultiplets*, and at every value of the crystal momentum and parity, *every energy level is contained in the set derived from states with real pseudomomenta, and the energies in units of* $\frac{1}{4}(\pi/N)^2$ *are all integers.* The $k=0$ boson creation operator is the lowering operator for total azimuthal spin; if $k_i = 0$ $(m_i = 0, N)$ is present in the set of pseudomomenta, it is found that the state is not the top member of its spin multiplet. If such states are excluded, the remaining states are all top members of their multiplets, and generate a complete set of energy levels. Sample spectra of small systems are given in Fig. 1. Spin multiplets are grouped into degenerate supermultiplets, and the state of maximum spin in each group is a real pseudomomentum state.

For even N, the ground state of the isotropic model is a nondegenerate spin singlet (the Gutzwiller-RVB state) with $\{m_i\} = \{1, 3, \ldots, N-1\}$, and $k = \frac{1}{2} N\pi$. The elementary excitation corresponds to a *hole* $(m_{j+1} = m_j + 2 + \delta_{j,i}$ for some $i)$ and is a spin-$\frac{1}{2}$ neutral fermion excitation that only occurs on its own in a system with odd N. Its allowed crystal momenta K span *half* the Brillouin zone, $|K - K_0| < \frac{1}{2}\pi$, $K_0 = \frac{1}{2}(N-1)\pi$, with the dispersion relation $E(K) = \frac{1}{2}[(\frac{1}{2}\pi)^2 - (K-K_0)^2]$. (It is the condition $m_i \ne 0, N$ that restricts the real pseudomomenta states with $S = \frac{1}{2}$ to half the Brillouin zone.) Note that because of the supermultiplet structure, the Gutzwiller-RVB ground state is the *only* nondegenerate state for even N, and the half-band of single elementary excitations for odd N are the *only* $S = \frac{1}{2}$ states without extra degeneracies.

The remarkable supermultiplet structure of the spectrum of the isotropic model suggests that hidden continuous symmetries in addition to those of the usual rotational SO(3) or SU(2) group are present. In the large-N limit, the low-energy states of the model are described[12] by the chiral-SU(2)–invariant $k=1$ Wess-Zumino-Witten model, which is a conformally invariant Gaussian field theory. The supermultiplets of states of the lattice model with the same crystal momentum K resemble those of the field theory (given by the Gaussian or "Luttinger liquid"[7] construction), although the grouping of states with different K into "conformal towers" only occurs in the field-theory limit. Clearly some subgroup of the large symmetry group of the field theory persists as a hidden continuous symmetry of this discrete-spin lattice model, and it will be interesting to elucidate this structure.

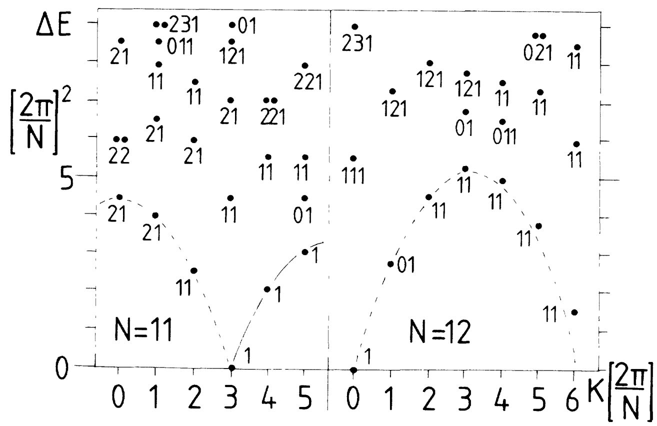

FIG. 1. Low-lying energy levels of the $N=11$ and $N=12$ models. Each real pseudomomentum state (with $m_i \ne 0, N$) is indicated by a filled circle (some degeneracies are present). Supermultiplet structure is also indicated; e.g., "231" indicates a group of states consisting of (for odd N) 2 $(S=\frac{1}{2})$, 3 $(S=\frac{3}{2})$, and 1 $(S=\frac{5}{2})$ multiplets. For even N, it means $(S=0)^2 \oplus (S=1)^3 \oplus (S=2)^1$. Broken lines are a guide to the eye indicating the bottom of the excitation continuum; the full line indicates the elementary $S=\frac{1}{2}$ fermion excitation.

Since "spin-umklapp" processes[7,9,10] are (marginally) irrelevant and their coupling scales to zero in the gapless ground-state phase of the 1D spin-$\frac{1}{2}$ antiferromagnet,[10] the model solved here must represent the "fixed point" model Hamiltonian for this phase. The Gutzwiller-RVB wave function would thus seem to be the basic model for the gapless, nondimerized ground state; it seems likely that the hidden symmetries clearly present in this model are intimately related to the physics of the gapless phase. Since these symmetries of the fixed point are obscured by the irrelevant symmetry-breaking perturbations for other than inverse-square exchange, this model provides a valuable opportunity to clarify the nature of the RVB state and its neutral-fermion excitation spectrum.

In conclusion, I note that it is quite possible that Jastrow wave functions of the kind discussed here may have application in two or higher dimensions. Indeed, motivated by apparently very different arguments involving analogies to the fractional quantum Hall effect, Kalmeyer and Laughlin[13] have proposed that the RVB state of the triangular lattice antiferromagnet is related to just such a state. The condition $N \geq m(M-1)$ found here for the lattice-gas ground state to be a Jastrow state is also reminiscent of a similar condition[14] in the construction of the ground states of the "truncated pseudopotential" model for the fractional quantum Hall effect.

This work was initiated during and stimulated by the Summer Program of the Aspen Center for Physics. The author is an Alfred P. Sloan Foundation Fellow.

Note added.—Since submitting this Letter, I have received a preprint from Shastry, who independently reports that the Gutzwiller-RVB state is the ground state of (1) with $\Delta = 1$ and even N.[15]

[1]M. C. Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963).

[2]C. Gros, R. Joynt, and T. M. Rice, Phys. Rev. B **36**, 381 (1987).

[3]F. Gebhard and D. Vollhardt, Phys. Rev. Lett. **59**, 1472 (1987).

[4]P. W. Anderson, Mater. Res. Bull. **8**, 153 (1973); P. Fazekas and P. W. Anderson, Philos. Mag. **30**, 432 (1974); P. W. Anderson, G. Baskeran, Z. Zou, and T. Hsu, Phys. Rev. Lett. **58**, 2790 (1987).

[5]H. Yokoyama and H. Shiba, to be published.

[6]B. Sutherland, J. Math. Phys. **12**, 246,251 (1971), and Phys. Rev. A **4**, 2019 (1971), and **5**, 1372 (1972).

[7]F. D. M. Haldane, Phys. Rev. Lett. **45**, 1358 (1980).

[8]T. A. Kaplan, P. Horsch, and J. Borysowicz, Phys. Rev. B **35**, 1877 (1987).

[9]M. P. M. Den Nijs, Phys. Rev. B **23**, 61 (1981); J. Black and V. J. Emery, Phys. Rev. B **23**, 429 (1981).

[10]F. D. M. Haldane, Phys. Rev. B **25**, 4925 (1982), and **26**, 5257(E) (1982).

[11]Note that a previous study of the model with only first- and second-neighbor coupling found that the critical point where "spin-umklapp" terms vanished was at $J_2/J_1 \approx 0.24 \pm 0.005$, very close to the r^{-2} model. This calculation was based on the identification of *approximate* supermultiplet degeneracies at the critical point [R. Jullien and F. D. M. Haldane, Bull. Am. Phys. Soc. **28**, 344 (1983)].

[12]I. Affleck, Phys. Rev. Lett. **55**, 1355 (1985).

[13]V. Kalmeyer and R. B. Laughlin, Phys. Rev. Lett. **59**, 2095 (1987).

[14]F. D. M. Haldane, in *The Quantum Hall Effect,* edited by R. E. Prange and S. M. Girvin (Springer-Verlag, New York, 1987).

[15]B. Sriram Shastry, following Letter [Phys. Rev. Lett. **60**, 639 (1988)].