Extended Heisenberg Models of Antiferromagnetism: Analogies to the Fractional Quantum Hall Effect

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The "valence-bond" ground states for extended Heisenberg models discussed by Affleck *et al.* are shown to be of a Jastrow form. We discuss a striking analogy between these models and the "truncated pseudopotential" approach to the fractional quantum Hall effect. The valence-bond states are in analogy to the Laughlin ground state, and the magnon spectrum is deduced by use of a single-mode approximation.

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Recently, Affleck, Kennedy, Lieb, and Tasaki (AKLT)[1] have discussed extended Heisenberg models whose exact "valence-bond" ground states can be readily determined. These models exist for lattices in any dimension, provided that the spin S is an integer multiple of half the lattice coordination number. The interactions are written in terms of projection operators for total bond spin, and are polynomial functions of $\mathbf{S}_i\cdot\mathbf{S}_j$. In this Letter we shall discuss a striking analogy between these antiferromagnetic spin models and the fractional quantum Hall effect (FQHE).

Laughlin's theory of the FQHE is based on a set of correlated wave functions of the Jastrow form, which are purported to be good *Ansatz* ground states for the interacting 2D electron gas in the lowest Landau level.[2] These trial states, which exist only when the filling fraction ν is an inverse odd integer, are exact when the interaction is sufficiently short ranged.[3,4] Thus, the coefficients in an expansion of the interaction $v(\mathbf{r})$ in terms of short-ranged "pseudopotentials" indicate roughly how far the true ground state is from the Laughlin *Ansatz*.[3] In spin-S Heisenberg systems, the interaction $\mathbf{S}_i\cdot\mathbf{S}_j$ can similarly be decomposed into total pair-spin projection operators, and for certain values of S a Jastrow (valence-bond) state exists which is exact if only certain projectors are kept. Furthermore, with a knowledge of the ground-state correlations, the magnon spectrum may be obtained in the "single-mode approximation."[5]

First, we briefly summarize the AKLT models, applying a more elegant formalism which permits us to write for the first time the general AKLT state. Consider a lattice of spin-S objects with rotationally invariant interactions. We start by writing $(\mathbf{S}_i\cdot\mathbf{S}_j)^m$ as a sum over projection operators $P_J^S(ij)$ for total bond spin J. One knows that there are $2S+1$ multiplets indexed by $J=0,1,\ldots,2S$. Using $\mathbf{S}_i\cdot\mathbf{S}_j=\frac{1}{2}(\mathbf{S}_i+\mathbf{S}_j)^2-S(S+1)$ and the completeness relation $1=\sum_{J=0}^{2S}P_J^S(ij)$, one finds

$$(\mathbf{S}_i\cdot\mathbf{S}_j)^m=\sum_{J=0}^{2S}[\tfrac{1}{2}J(J+1)-S(S+1)]^m P_J^S(ij). \quad (1)$$

This formula may be inverted, so that each projector may be represented by a polynomial of order $2S$ in $\mathbf{S}_i\cdot\mathbf{S}_j$. We shall make extensive use of the Schwinger boson representation of the spin algebra:

$$\begin{aligned} S_n^+&=a_n^\dagger b_n,\quad S_n^z=\tfrac{1}{2}(a_n^\dagger a_n-b_n^\dagger b_n),\\ S_n^-&=a_n b_n^\dagger,\quad \hat{S}_n=\tfrac{1}{2}(a_n^\dagger a_n+b_n^\dagger b_n),\end{aligned} \quad (2)$$

in which each spin is defined by two bosons, together with the constraint that the total Bose occupation n_a+n_b is constrained to be twice S. In the subspace defined by the constraint, one finds $\mathbf{S}_i\cdot\mathbf{S}_j=-\frac{1}{2}\mathcal{C}_{ij}^\dagger\mathcal{C}_{ij}+S^2$, with $\mathcal{C}_{ij}\equiv a_ib_j-b_ia_j$. The AKLT valence-bond states for an arbitrary lattice $\mathcal{L}$ of coordination number z may be compactly written as

$$|\psi(\mathcal{L},M)\rangle=\prod_{\langle ij\rangle}(a_i^\dagger b_j^\dagger-b_i^\dagger a_j^\dagger)^M|0\rangle, \quad (3)$$

where the product is over all bonds on $\mathcal{L}$. There are several important features associated with the state $|\psi(\mathcal{L},M)\rangle$. First, it is an eigenstate of $\hat{S}_n$ for all n with eigenvalue $S=\frac{1}{2}Mz$. Second, it is rotationally invariant, and hence has total spin zero. Third, and most to the point, $|\psi(\mathcal{L},M)\rangle$ has no projection onto the $J>2S-M$ subspace for any bond. ($J_{\max}^z=2S-M$ may be obtained by inspection, and $J_{\max}$ follows from rotational invariance.) Consequently, $|\psi(\mathcal{L},M)\rangle$ is an explicit zero-energy ground state for any Hamiltonian of the form

$$H=\sum_{\langle ij\rangle}\sum_{J=J_{\max}+1}^{2S}A_jP_J^S(ij).$$

Correlations within this formalism are easily evaluated

in a coherent-state Schrödinger representation. Within the spin-S sector of the Schwinger boson algebra, we can take $a^\dagger \to u$, $b^\dagger \to v$, $a \to \partial/\partial u$, $b \to \partial/\partial v$, with $u = \cos(\theta/2)e^{+i\phi/2}$, $v = \sin(\theta/2)e^{-i\phi/2}$. The inner product becomes $\langle f | g \rangle = \int d\Omega f^*(u,v)g(u,v)$, where the integration is with respect to solid angle. The operator $\hat{S}$ takes the form $\frac{1}{2}(u\,\partial_u + v\,\partial_v)$, and thus every spin-$S$ state is a homogeneous polynomial in u and v of order $2S$. In the calculation of matrix elements of operators $\hat{T}(\partial_u, \partial_v; u, v)$ which commute with $\hat{S}$, the following prescription is useful: First, write T in normal ordered form so that all derivative operators appear to the left. $\hat{T}$ therefore resembles $\hat{T} = \sum T_{klj}\,\partial_u^k \partial_v^l u^{k+j} v_{l-j}$. One then replaces $\partial_u^k \partial_v^l u^{k+j} v^{l-j}$ by

$$\prod_{m=2}^{k+l+1} (2S+m) u^{*k} v^{*l} u^{k+j} v^{l-j}.$$

The general state of Eq. (3) has the Schrödinger representation

$$\psi[u,v] = \prod_{\langle ij \rangle} (u_i v_j - v_i u_j)^M, \qquad |\psi|^2 = \prod_{\langle ij \rangle} \tfrac{1}{2}(1 - \hat{\Omega}_i \cdot \hat{\Omega}_j)^M, \tag{4}$$

where $\hat{\Omega}$ is a radius vector on the unit sphere. From Eq. (4), one can easily calculate the spin-spin correlation function $\langle \mathbf{S}_0 \cdot \mathbf{S}_n \rangle = (S+1)^2 \langle \hat{\Omega}_0 \cdot \hat{\Omega}_n \rangle$ of the spin-S chain via a transfer-matrix method ($n \neq 0$), yielding $\langle \mathbf{S}_0 \cdot \mathbf{S}_n \rangle = (-1)^n (S+1)^2 (1+2/S)^{-|n|}$, where we have taken the chain to have free ends. The correlation length is $\xi = 1/\ln(1+2/S)$ and the static structure factor is

$$s_{\alpha\beta}(k) = \frac{1}{N} \sum_{n,n'} e^{-ik(n-n')} \langle S_n^\alpha S_{n'}^\beta \rangle = \tfrac{1}{3} \delta_{\alpha\beta} (S+1) \left[\frac{1 - \cos k}{1 + \cos k + 2/S(S+2)} \right]. \tag{5}$$

Note that $s(k)$ is analytic in k^2 and vanishes as $k \to 0$, in accordance with the fact that $|\psi\rangle$ has zero total spin.

The wave function in Eq. (4) bears a remarkable resemblance to the Laughlin state,[2]

$$\Psi = \prod_{j<k} (z_j - z_k)^m \exp\left(-\tfrac{1}{4} \sum_l |z_l|^2 \right),$$

which describes the fractional quantum Hall condensate at filling fraction $\nu = 1/m$ (m odd).[6] One can expand the (lowest Landau level restricted) interparticle interaction in terms of relative angular momentum projection operators: $v(\mathbf{r}_i - \mathbf{r}_j) = \sum_{k=0}^{\infty} V_k P_k(ij)$. For short-ranged potentials in which $V_k = 0$ when $k \geq m$, the Laughlin state is the exact ground state and there is a gap in the excitation spectrum. As Haldane has stressed,[3] the success of Laughlin's wave function for the Coulomb system is dependent on the difference between the $k = m-2$ and $k = m$ pseudopotential components V_k. This suggests that the Jastrow state of Eq. (3) is a good approximation to the true ground state for spin-spin interactions in which the coefficients of the projectors P_J^S for $J > J_{\max}$ are relatively large. Consider, for example, the $S = 1$ Heisenberg chain. From Eq. (1), we have $\mathbf{S}_i \cdot \mathbf{S}_j = -2 + P_1^1(ij) + 3P_2^1(ij)$. Recall that the state $|\psi(\text{chain}, M=1)\rangle$ of Eq. (3) is the exact ground state for a pure P_2^1 interaction (in this case it is also nondegenerate). The key point is that the coefficient of P_2^1 is greater than that of P_1^1, and we suggest that the difference is sufficiently large that the P_1^1 component can be treated perturbatively, without destroying the excitation gap. Since the largest $m = 1$ coefficients in Eq. (1) occur for the largest values of J, it is natural to ask how "close" the Heisenberg model is to the AKLT model; later we shall return to this point.

While the correlation functions for chains are simple to evaluate within the Schwinger boson formalism, the properties of the Jastrow state in more dimensions are not as clear. Much insight may be gained by an appeal to the Laughlin plasma analogy.[2] Interpreting the probability $|\psi|^2$ as a Boltzmann weight $e^{-\beta\Phi}$ of a classical system, we obtain $\beta = M/2$ and $\Phi = -\sum_{\langle ij \rangle} 2 \ln \sin^2 \frac{1}{2}\vartheta_{ij}$, with $\vartheta_{ij} = \cos^{-1} \hat{\Omega}_i \cdot \hat{\Omega}_j$. Thus, Φ is the energy of a classical assembly of spins (unit vectors) interacting via $v(\vartheta) = -2 \ln \sin^2 \frac{1}{2}\vartheta$; this potential strongly encourages spin antialignment on alternate sublattices.[7] We now see that these quantum mechanical systems are somewhat unusual in that their ground-state correlations are obtainable from classical models *in the same number of dimensions*. This feature explains the difference between the pure exponential behavior of the $d = 1$ correlations found above and the *two*-dimensional Ornstein-Zernike (OZ) form $(-1)^n |n|^{-1/2} \exp(-|n|/\xi)$ which is expected to describe the asymptotic correlations in the quantum $S = 1$ Heisenberg chain.[8] The correlations in the Jastrow state $|\psi(\mathcal{L}, M)\rangle$ are thus equivalent to those of a *classical* modified Heisenberg model on $\mathcal{L}$. The temperature $T = 2/M = z/S$ and dimensionality d should determine whether the spins are locked in a Néel phase (large S), or "disordered" (small S). A crude mean-field theory follows by our approximating $2 \ln \frac{1}{2}(1 - \hat{\Omega}_i \cdot \hat{\Omega}_j) \approx -(1 + \hat{\Omega}_i \cdot \hat{\Omega}_j)$ and taking $\langle \hat{\Omega} \rangle = \omega$, leading to the mean-field equation $\omega = \coth(S\omega) - (S\omega)^{-1}$, for which the "critical" spin is $S_c = 3$. This transition is valid only for $d > 2$. In dimensions $d \leq 2$, the ground state will be disordered for all S, the correlations will be of the OZ form $(-1)^n |n|^{(1-d)/2} \exp(-|n|/\xi)$, and the magnons discussed below will evidence a gap. Appealing to universality, we predict that the correlation length for the large-M Jastrow state should be identical to that for the classical Heisenberg model at $T = 2/M$, with $\xi(M) \sim M/2$ in $d = 1$ (as explicitly calculated above), and $\xi(M) \sim \exp(\pi M)$ in $d = 2$.[9]

Excitations.—The Bijl-Feynman single-mode approximation (SMA), used with great success in deducing the phonon-roton curve in liquid ^{4}He, has also proved extremely accurate in its extension to the magnetophonon-

magnetoroton excitation spectrum in the FQHE.[5] In both instances the approximate ground state is of the Jastrow form. We now extend the theory to spins. Given a Hamiltonian $H=\sum_{\langle ij\rangle}Q(\mathbf{S}_i\cdot\mathbf{S}_j)$ where Q is an arbitrary polynomial function of its argument, and the *exact* ground state $|G\rangle$ (assumed to be normalized and of total spin zero), one constructs a candidate excited state at wave vector $\mathbf{k}$ by

$$|\mathbf{k}\rangle\equiv S^z_{\mathbf{k}}|G\rangle=N^{-1/2}\sum_i e^{i\mathbf{k}\cdot\mathbf{R}_i}S^z_i|G\rangle. \tag{6}$$

[The choice S^z in Eq. (6) is arbitrary; the magnon branch will be threefold degenerate.] The putative excitation energy is

$$\omega_{\mathbf{k}}=E_{\mathbf{k}}-E_0=\frac{1}{2}\frac{\langle G|[S^z_{-\mathbf{k}},[H,S^z_{\mathbf{k}}]]|G\rangle}{\langle G|S^z_{-\mathbf{k}}S^z_{\mathbf{k}}|G\rangle}, \tag{7}$$

and is a rigorous upper bound to the gap at wave vector $\mathbf{k}$. The gap is written as a ratio $\omega_{\mathbf{k}}=f(\mathbf{k})/s(\mathbf{k})$, where $s(\mathbf{k})=s_{zz}(\mathbf{k})=\frac{1}{3}s_{aa}(\mathbf{k})$ is the static structure factor, and $f(\mathbf{k})$ is the oscillator strength:

$$f(\mathbf{k})=\tfrac{1}{6}\langle G|[S^a_{-\mathbf{k}},[H,S^a_{\mathbf{k}}]]|G\rangle=\tfrac{1}{6}D\gamma_{\mathbf{k}},$$
$$D=\tfrac{1}{4}\langle G|[S^a_i-S^a_j,[Q(\mathbf{S}_i\cdot\mathbf{S}_j),S^a_i-S^a_j]]|G\rangle, \tag{8}$$

where (ij) is any nearest-neighbor pair and $\gamma_{\mathbf{k}}\equiv\sum_{\delta}(1-e^{-i\mathbf{k}\cdot\delta})$ is a sum over nearest-neighbor vectors. With the assumption of inversion symmetry, $f(\mathbf{k})$ vanishes as k^2 at long wavelengths. This proves gaplessness at the zone center if $s(\mathbf{k})$ vanishes more slowly than k^2, and at any point in the Brillouin zone where $s(\mathbf{k})$ diverges.

In spin chains where S is half an odd integer, Haldane has predicted[8] that $\langle\mathbf{S}_0\cdot\mathbf{S}_n\rangle\sim(-1)^n|n|^{-1}+\mathcal{O}(n^{-2})$, in which case $s(k)$ vanishes linearly at the zone center and diverges logarithmically at the zone edge, in agreement with the commonly held belief that the spectrum is gapless at these points. The integer-S case is much different, and $s(k)$ is predicted to be analytic in k^2, giving a gap everywhere with a minimum at the zone edge. For the exactly solvable $H=\sum_n P^1_2(n,n+1)$ model, we find $f(k)=\frac{10}{27}(1-\cos k)$ and $s(k)=2(1-\cos k)/(5+3\cos k)$, yielding a magnon dispersion of $\omega_k=\frac{5}{27}(5+3\cos k)$ and an upper bound on the $k=\pi$ gap of $\Delta_{\mathrm{SMA}}=\frac{10}{27}\simeq 0.370$. Numerical work by one of us[10] on finite-sized (≤ 12 sites) chains yields a remarkably size-independent gap of $\Delta\simeq 0.350$ and furthermore verifies that the SMA dispersion is essentially exact throughout the region $\frac{1}{2}\pi\leq k\leq\pi$.[11]

Writing the dynamic structure factor as

$$\mathcal{S}_{\alpha\beta}(\mathbf{k},\omega)=\sum_j\langle G|S^{\alpha}_{-\mathbf{k}}|j\rangle\langle j|S^{\beta}_{\mathbf{k}}|G\rangle\delta(\omega-\omega_j), \tag{9}$$

with $\omega_j=E_j-E_0$, one sees that the oscillator strength $f(\mathbf{k})$ in Eq. (8) is the exact first moment of $\mathcal{S}(\mathbf{k},\omega)\equiv\frac{1}{3}\mathcal{S}_{aa}(\mathbf{k},\omega)$. It is easy to derive sum rules relating higher-order to ground-state correlations as well. The (normalized) second moment of $\mathcal{S}(\mathbf{k},\omega)$ is given by

$$\Gamma^2_{\mathbf{k}}\equiv\frac{1}{s(\mathbf{k})}\int_0^{\infty}d\omega\,\mathcal{S}(\mathbf{k},\omega)(\omega-\omega_{\mathbf{k}})^2$$
$$=\frac{\langle\mathbf{k}|H^2|\mathbf{k}\rangle}{\langle\mathbf{k}|\mathbf{k}\rangle}-\left[\frac{\langle\mathbf{k}|H|\mathbf{k}\rangle}{\langle\mathbf{k}|\mathbf{k}\rangle}\right]^2. \tag{10}$$

If, in the solvable $S=1$ chain, the *second* excited state at $k=\pi$ consists of three elementary $k=\pi$ magnons with no negative binding energy (this has been confirmed numerically), then a variational principle[12] gives that *if* $0\leq\Gamma^2_{\pi}\leq\frac{1}{3}\omega^2_{\pi}$ (where ω_k is the SMA energy), then the *exact* $k=\pi$ gap Δ satisfies

$$\textit{either } \tfrac{2}{3}\omega_{\pi}+\tfrac{1}{3}(\omega^2_{\pi}-3\Gamma^2_{\pi})^{1/2}\leq\Delta\leq\omega_{\pi},$$
$$\textit{or } 0\leq\Delta\leq\tfrac{2}{3}\omega_{\pi}-\tfrac{1}{3}(\omega^2_{\pi}-3\Gamma^2_{\pi})^{1/2}. \tag{11}$$

We find $\Gamma^2_k=\frac{10}{729}(5+3\cos k)$, giving either $0\leq\Delta\leq 0.169$ or $0.325\leq\Delta\leq 0.370$, which agrees nicely with numerical results. The SMA is so named because it amounts to our approximating $\mathcal{S}(\mathbf{k},\omega)\approx s(\mathbf{k})\delta(\omega-\omega_{\mathbf{k}})$. Within the SMA, the spin susceptibility is

$$\chi_{\alpha\beta}(\mathbf{k})=2\int_0^{\infty}\frac{d\omega}{\omega}\mathcal{S}_{\alpha\beta}(\mathbf{k},\omega)\approx 2\delta_{\alpha\beta}\frac{s(\mathbf{k})^2}{f(\mathbf{k})}. \tag{12}$$

Because of the large susceptibility at the zone edge, spin chains have a tendency to dimerize in the presence of a staggered interaction such as

$$H_d=\sum_n\{1+(-1)^n\lambda\}\mathbf{S}_n\cdot\mathbf{S}_{n+1}.$$

For this Hamiltonian, we construct the dimerized trial ground state

$$|\psi\rangle=\prod_n(\mathcal{O}^{\dagger}_{2n-1,2n})^{S+p}(\mathcal{O}^{\dagger}_{2n,2n+1})^{S-p}|0\rangle, \tag{13}$$

where $p=-S,-S+1,\ldots,S$, and where S is an integer *or* half an odd integer. $|\psi\rangle$ describes a spin-S chain, and the variational parameter p is determined by our minimizing the energy per spin,

$$\frac{\langle H_d\rangle}{N}=-(S+1)^2+2(S+1)^2\left[\frac{S+2-\lambda p}{(S+2)^2-p^2}\right], \tag{14}$$

yielding $p^*=(S+2)[1-(1-\lambda^2)^{1/2}]/\lambda$, where p^* must of course be rounded off to the nearest allowed value. The correlations decay exponentially with $\xi=2/\ln\{[(S+2)^2-p^2]/(S^2-p^2)\}$.[13]

How well do the AKLT models approximate more realistic (e.g., pure Heisenberg) models? As mentioned by Affleck *et al.*, employment of the $(d=1,S=1)$ AKLT state as a trial Heisenberg-chain ground state gives an energy within 5% of the numerical value. One might further suspect that the SMA formula of Eq. (7) would yield an acceptable approximation to the gap, even though the AKLT state is not the exact ground state.[5] However, one finds that the SMA expression yields a

value about twice too large. In two dimensions, it has been proven[1,14] that for $S \geq \frac{3}{2}$ on a honeycomb lattice and for $S \geq 1$ on a square lattice, Néel order exists in the Heisenberg ground state. Yet we have shown above that the AKLT-state correlations are short ranged for $d \leq 2$! In this regard, it is worth emphasizing that the peculiar "reduced dimensionality" OZ correlations mentioned above arise because of the special form of the interaction. As one moves away from the AKLT points in the space of models by turning on the "disallowed" pseudopotential components A_J where $J \leq 2S - M$, a crossover to the expected $(d+1)$-dimensional OZ form will occur. If one strays far enough, a phase transition may occur, as happens in the case of the $d=2$ Heisenberg models discussed above. In one dimension, there also exist extended Heisenberg models with broken-symmetry ground states, but it appears that for the pure Heisenberg model, the AKLT states may be a good starting point for perturbation theory in the range of the interaction. Recently, one of us has shown explicitly how this dimensional crossover occurs in the vicinity of the $(d=1, S=1)$ AKLT point by expressing the difference $H - H_{\mathrm{AKLT}}$ in terms of SMA magnon operators.[10]

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[6]The wave functions appear almost identical if the Laughlin state is written in a spherical geometry (Ref. 3): $\Psi = \prod_{i<j}(u_i v_j - v_i u_j)^m$. The difference is that the Laughlin state is a product over *all* $N(N-1)/2$ pairs of electrons, while the AKLT state is a product over the $zN/2$ nearest-neighbor bonds.

[7]We assume $\mathcal{L}$ to be bipartite.

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[11]At $k=0$, e.g., the lowest-lying excitation is a *pair* of elementary $k=\pi$ magnons. The numerical value of half the $k=0$ gap is $\Delta(0)/2 \simeq 0.36$.

[12]Let $e^{\frac{1}{2}}$ and $E_2^{\frac{1}{2}}$ be the lowest two eigenvalues with crystal momentum $\mathbf{k}$. Then $\langle \mathbf{k} | (H - E^{\frac{1}{2}})(H - E_2^{\frac{1}{2}}) | \mathbf{k} \rangle \geq 0$, from which Eq. (11) follows.

[13]When S is half an odd integer, Eq. (13) yields a dimer state for all p (e.g., for $S = p = \frac{1}{2}$, $|\psi\rangle$ corresponds to an alternating chain of singlet pairs), and hence $|\psi\rangle$ is not a good trial ground state for λ sufficiently close to zero.

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