Variational Approach to the *XXZ* Spin-1 Linear Chain: Elementary Excitations and Haldane Conjecture

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The *XXZ* spin-1 chain is studied by means of a physically motivated variational approach. An effective Hamiltonian for the dynamics of spin-0 defects in antiferromagnetic environments (domain walls) is obtained, and its ground-state properties are analyzed. An order-disorder transition is found with critical behavior corresponding to the 2D Ising-model universality class, in complete agreement with Haldane's conjecture. The approximations involved in this variational scheme are carefully tested using known Monte Carlo results. In particular, excellent agreement with the recently calculated excited states at the Heisenberg (isotropic) point is found, clarifying the nature of these excitations.

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We are concerned with the ground-state (GS) properties of the following Hamiltonian:

$$\mathcal{H}=\mathcal{H}_{xy}+\mathcal{H}_z=\sum_{\langle i,j\rangle}(s_i^x s_j^x+s_i^y s_j^y)+\epsilon\sum_{\langle i,j\rangle}s_i^z s_j^z\,, \qquad (1)$$

where s_i^α represents the α component of the spin-1 operator of site i in an infinite (N) chain, and the sum is restricted to nearest neighbors. The GS of the spin-$\frac{1}{2}$ version of $\mathcal{H}$ is well understood.[1] On the antiferromagnetic side ($\epsilon>0$), in particular, it shows long-range order (LRO) for $\epsilon>1$ and a gapless, disordered, but critical phase with continuously varying exponents for $\epsilon\leq 1$. The transition between these two phases takes place when the symmetry of $\mathcal{H}$ changes ($\epsilon=1$), in accordance with simple universality ideas. Though no exact results exist for higher-spin chains, spin-wave analysis and the universality principle would suggest that the spin-$\frac{1}{2}$ phase diagram is valid for arbitrary spin. This was the prevailing opinion until recently, but Haldane's conjecture[2] of a fundamental difference between phase diagrams of integer and half-integer spins changed this situation drastically. Based on a mapping of $\mathcal{H}$ to the *nonlinear* σ model, Haldane proposed the following picture for integer-spin chains: The antiferromagnetically ordered phase ($\epsilon\gg 1$) would disappear at a point $\epsilon_c>1$, giving rise to a nondegenerate, disordered phase (Haldane phase), with a gap in the excitation spectrum and exponentially decaying correlations. (A further *XY*-like phase would eventually appear for smaller values of ϵ.) The critical point ϵ_c was predicted by Haldane to belong to the universality class of the 2D Ising model.

The controversy[3-6] that ensued this innovative proposal cannot be considered completely settled, but most theoretical[7] and even some experimental[8,9] results seem to support it. On the theoretical side, different approaches[10-12] have been employed to tackle this problem, but exact or Monte Carlo (MC) diagonalizations of finite spin-1 chains provide the best evidence.[13,14] These diagonalizations are the main source of information about this system, but because of its nature, it is not always easy to get a clear idea of the problem from them. This paper describes an alternative variational approach, simple enough to be fully analyzed, but with some features which, absent in most variational approaches, seem to be necessary to handle this problem. We study the transition from antiferromagnetic LRO to the Haldane phase by means of a variational Hamiltonian expected to be valid at least for $\epsilon\gtrsim 1$ (we quantify this validity at the end of the paper), and analyze its critical properties. This physically motivated approach allows us to verify the correctness of Haldane's predictions concerning the transition at ϵ_c, in addition to providing excellent quantitative agreement with known results, particularly the recently calculated excitation spectrum[15] at $\epsilon=1$.

The variational Hamiltonian for the spin-1 problem is constructed as follows. Keeping in mind our interest in the antiferromagnetically dominated regime ($\epsilon\geq 1$), we discard all the states with nearest-neighbor parallel rpins. Thus, the only sources of antiferromagnetic disorder are sites with $s_z=0$ (spin-0 defects, SZD). To specify completely the restricted basis set, it suffices to say that the two spins at the left and right of a single SZD (or of a sequence of contiguous SZD) should be antiparallel. This guarantees that an isolated SZD is an antiferromagnetic domain wall which can move freely along the chain (in the sense that its motion does not create additional disorder). A typical example of a state within this restricted set could have the following form:

$$\ldots\downarrow\uparrow\downarrow\circ\uparrow\circ\circ\downarrow\uparrow\ldots\,,$$

where arrows mean $s_z=\pm 1$ and circles mean $s_z=0$. Notice that, though the restricted states are locally antiferromagnetically ordered, this does not imply that we are dealing with long-range ordered states. In fact, we will see that both (long-range) ordered and disordered phases can be described with the same basis set.

The restriction of the original *XXZ* Hamiltonian to the described basis set is given, after Wigner-Jordan[1] fermionization, by

$$\mathcal{H}_{\rm eff}=\sum_i (c_i^\dagger c_{i+1}+c_i^\dagger c_{i+1}^\dagger+\text{H.c.}) +2\epsilon\sum_i (n_i-\tfrac{1}{2})-\epsilon\sum_i n_i n_{i+1}\,, \qquad (2)$$

where $c_i^\dagger$ (c_i) creates (annihilates) a SZD at site i, and $n_i \equiv c_i^\dagger c_i$. The last two terms of $\mathcal{H}_{\text{eff}}$ describe the energy of a static configuration of SZD's while the first term accounts for their creation (annihilation) and movement. This $\mathcal{H}_{\text{eff}}$ respects the rotational symmetry around the z axis of $\mathcal{H}$, and it is straightforward to show that the relevant long-range correlations are given in our restricted basis set by

$$|\langle s_i^z s_j^z\rangle| \propto \left\langle \exp\left[i\pi \sum_{i<l<j} n_l\right]\right\rangle ,$$
$$|\langle s_i^y s_j^y\rangle| = |\langle s_i^x s_j^x\rangle| \propto \left\langle \prod_{i<l<j} n_l\right\rangle , \tag{3}$$

where $\langle\,\rangle$ means GS average.

To study the GS of $\mathcal{H}_{\text{eff}}$ we note that the first two terms of $\mathcal{H}_{\text{eff}}$ are quadratic in fermion operators and thus, exactly solvable. They are, in fact, the fermionic version of the *Ising plus transverse field* (ITF) model,[16] whose critical properties are well known. We take this as the unperturbed Hamiltonian, and treat the many-body part ($n_i n_{i+1}$) in the Hartree-Fock (HF) approximation:

$$n_i n_{i+1} \approx (n_i + n_{i+1}) n_{\text{av}} - (c_i^\dagger c_{i+1} + \text{H.c.}) h + (c_i^\dagger c_{i+1}^\dagger + \text{H.c.}) s - (n_{\text{av}}^2 - h^2 + s^2) , \tag{4}$$

where $n_{\text{av}} \equiv \langle n\rangle$, $h \equiv \langle c_i^\dagger c_{i+1}\rangle$, and $s \equiv \langle c_i^\dagger c_{i+1}^\dagger\rangle$.

The resulting self-consistent Hamiltonian can be diagonalized with the usual Bogolubov-Fourier transformation[1] to new fermion operators $d_k^\dagger$ (d_k):

$$\mathcal{H}_{\text{eff, HF}} = \sum_k E(k) d_k^\dagger d_k + U , \tag{5}$$

with the excitation spectrum [$E(k)$] and the GS energy (U) given by

$$E(k)k = \{[2\epsilon_s + 2\nu\cos(k)]^2 + [2\nu'\sin(k)]^2\}^{1/2} ,$$
$$U = N(\epsilon_s - \epsilon) - \tfrac{1}{2}\sum_k E(k) + N\epsilon(n_{\text{av}}^2 - h^2 + s^2) , \tag{6}$$

where $\epsilon_s \equiv \epsilon(1 - n_{\text{av}})$, $\nu \equiv 1 + \epsilon h$, and $\nu' \equiv 1 - \epsilon s$.

Results for the gap[17] [$= E(k = \pi)$] are shown in Fig. 1. We see the existence of a critical value $\epsilon_c \cong 1.125$, at which the gap vanishes and the long-wavelength excitation spectrum develops Lorentz invariance. Borrowing results from the ITF model, critical properties are summarized as follows:

$$\xi^{-1} \sim \text{gap} \sim |\epsilon - \epsilon_c| ,$$
$$|\langle s_0^z s_\infty^z\rangle| \sim |\epsilon - \epsilon_c|^{1/4} \quad (\epsilon > \epsilon_c) ,$$
$$|\langle s_0^z s_l^z\rangle| \sim l^{-1/4} \quad (\epsilon = \epsilon_c) , \tag{7}$$
$$|\langle s_0^z s_\infty^z\rangle| = 0 \quad (\epsilon < \epsilon_c) ,$$
$$|\langle s_0^x s_l^x\rangle| \sim \exp[-l f(\epsilon)] ,$$

where ξ is the correlation length, and $f(\epsilon)$ is a continuous function at ϵ_c (note that $|\langle s_0^x s_l^x\rangle|$ is exponentially decaying even at the critical point).

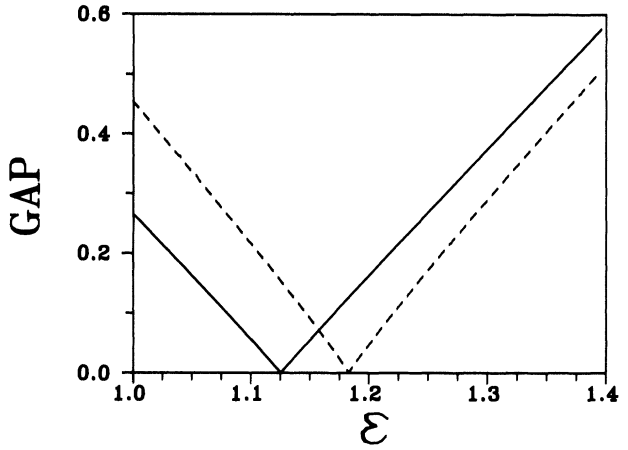

FIG. 1. Hartree-Fock self-consistent results for the excitation-spectrum gap of $\mathcal{H}_{\text{eff}}$ (continuous line) and $\mathcal{H}'_{\text{eff}}$ (dashed line).

Therefore, the antiferromagnetic phase gives rise to a disordered phase at a value $\epsilon_c > 1$, with critical behavior characterized by the 2D Ising-model (or ITF-model) universality class, *in complete agreement with Haldane's prediction.* It is interesting to note that the correlation $|\langle s_i^z s_j^z\rangle|$ depends on the parity of the number of SZD's between i and j: If the weights of even and odd configurations coincide, the correlation vanishes. In the ordered phase, even configurations dominate over long distances (bound SZD's). Below ϵ_c, SZD's behave independently and the difference between even and odd configurations vanishes exponentially with distance, in accordance with general statistical considerations. Thus, the transition at ϵ_c can be thought as a change from bound to free behavior of SZD's.

We now evaluate the validity of our treatment. Between the original XXZ Hamiltonian and our results, two independent approximate steps are involved: (i) restriction of $\mathcal{H}$ to $\mathcal{H}_{\text{eff}}$; (ii) HF treatment of the many-body part of $\mathcal{H}_{\text{eff}}$.

We begin by testing point (ii): correctness of our HF treatment of $\mathcal{H}_{\text{eff}}$. This is important because mean-field approximations are suspicious when critical behavior is involved in low-dimensional systems. To assert the validity of our results, we note that the one-body part of $\mathcal{H}_{\text{eff}}$ shows well defined critical properties and, thus, our problem reduces to studying the relevance or irrelevance of the many-body perturbation $n_i n_{i+1}$. The irrelevance of the many-body term can be shown, for instance, by means of a real-space renormalization-group calculation (details with be presented elsewhere for lack of space). This irrelevance implies that the critical behavior is that of the ITF model[16] and, therefore, no spurious effects are introduced by our HF approximation. Numerical diagonalizations of $\mathcal{H}_{\text{eff}}$ in finite chains of up to ten sites indicate that even the value of $\epsilon_c \cong 1.125$ is very accurate (to within 0.1%). This guarantees that our HF is not only

qualitatively valid (right critical behavior) but also quantitatively correct.

We now address point (i): the problem of the validity of $\mathcal{H}_{\text{eff}}$ as a faithful description of the original XXZ Hamiltonian. It was argued before that, since $\mathcal{H}_{\text{eff}}$ is dominated by $\mathcal{H}_z$, one can expect a range of validity given by $\epsilon \geq 1$. But since the physically interesting region ($\epsilon \cong \epsilon_c$) is so close to $\epsilon = 1$, it is important to make sure that the previous results are intrinsic features of the XXZ Hamiltonian, and not spurious results of its variational counterpart $\mathcal{H}_{\text{eff}}$. A first indication of the correctness of $\mathcal{H}_{\text{eff}}$ at the borderline value of $\epsilon = 1$ is given by its (variational) GS energy of -1.365, which compares very favorably to the MC value[14] of -1.401. In what follows we will show that an impressive agreement can be obtained between MC calculated properties of the XXZ Hamiltonian and those obtained from an improved (but essentially similar) version of $\mathcal{H}_{\text{eff}}$, in the vicinity of $\epsilon = 1$.

The main limitation of the basis set of $\mathcal{H}_{\text{eff}}$ is that it does not include states with parallel nearest-neighbor spins. It turns out that one can include some of these states very easily, while preserving the basic structure of $\mathcal{H}_{\text{eff}}$. Consider one state $|\psi_1\rangle$ with a local configuration given by two contiguous SZD's in an antiferromagnetic environment:

$$|\psi_1\rangle = \ldots \uparrow\downarrow\uparrow\downarrow\circ\circ\uparrow\downarrow\uparrow\downarrow \ldots .$$

The XXZ Hamiltonian has a nonzero matrix element between $|\psi_1\rangle$ and the following $|\psi_2\rangle$, with two nearest-neighbor parallel spins:

$$|\psi_2\rangle = \ldots \uparrow\downarrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\uparrow\downarrow \ldots .$$

It is clear that we can include part of the effect of the forgotten states by considering a linear combination of the form

$$|\psi\rangle = \lambda_1 |\psi_1\rangle - \lambda_2 |\psi_2\rangle \quad (\lambda_1^2 + \lambda_2^2 = 1),$$

instead of restricting ourselves only to $|\psi_1\rangle$ (case of $\mathcal{H}_{\text{eff}}$). Using this improvement, we can cast the new Hamiltonian ($\mathcal{H}'_{\text{eff}}$) in a form very similar to that of $\mathcal{H}_{\text{eff}}$:

$$\mathcal{H}'_{\text{eff}} = \sum_i (c_i^\dagger c_{i+1} + \text{H.c.}) + \lambda_1 \sum_i (c_i^\dagger c_{i+1}^\dagger + \text{H.c.}) + 2\epsilon \sum_i (n_i - \tfrac{1}{2}) - \epsilon' \sum_i n_i n_{i+1}$$
$$+ (\lambda_1 - 1) \sum_i [n_{i-1}(c_i^\dagger c_{i+1} + \text{H.c.}) + (c_i^\dagger c_{i+1} + \text{H.c.}) n_{i+2}] , \tag{8}$$

where $\epsilon' = \epsilon\lambda_1^2 + 2\lambda_1\lambda_2$. This new $\mathcal{H}'_{\text{eff}}$ can be thought of as the renormalized version of $\mathcal{H}_{\text{eff}}$ when hopping to states like $|\psi_2\rangle$ is allowed (notice that for $\lambda_1 = 1$, $\mathcal{H}'_{\text{eff}}$ reduces to $\mathcal{H}_{\text{eff}}$). We could have dealt with $\mathcal{H}'_{\text{eff}}$ instead of $\mathcal{H}_{\text{eff}}$ from the beginning, but being basically equivalent, $\mathcal{H}_{\text{eff}}$ was chosen for the sake of simplicity.

Again, we treat many-body terms in $\mathcal{H}'_{\text{eff}}$ within the HF approximation, with λ_1 as an additional variational[18] parameter. The values of λ_1 obtained range from 1 ($\epsilon = \infty$) to 0.968 ($\epsilon = 1$). Therefore, though $\mathcal{H}'_{\text{eff}}$ remains very close to $\mathcal{H}_{\text{eff}}$, the improvement is enough to bring the results to very good agreement with known properties:

(i) The GS energy obtained from $\mathcal{H}'_{\text{eff}}$ at the "nominal" border of validity ($\epsilon = 1$) is -1.40 while the value quoted as the best MC results is -1.401.

(ii) The critical value of ϵ shifts from $\epsilon_c = 1.125$ in $\mathcal{H}_{\text{eff}}$ to $\epsilon_c = 1.184$ in $\mathcal{H}'_{\text{eff}}$ (see Fig. 1). The quoted[7] value for ϵ_c from MC calculations is 1.18–1.20. Thus, not only does the obtained (Haldane) transition not disappear when improving $\mathcal{H}_{\text{eff}}$, but it moves to the region of values obtained from MC calculations.

(iii) The XXZ Hamiltonian is isotropic at $\epsilon = 1$, but our variational approach does not respect the full global rotational symmetry at this point. Nevertheless, we can define the point of "local" isotropy as the value of ϵ at which the xx, yy, and zz nearest-neighbor correlations coincide. The GS of $\mathcal{H}'_{\text{eff}}$ exhibits this local isotropy at $\epsilon = 1.005$, extremely close to the true value of $\epsilon = 1$ for the XXZ Hamiltonian. Notice that nothing happens to the long-range-order properties at this point, showing an ability of our scheme to separate long-range from short-range behavior (something unusual in most variational-like approximations).

(iv) The most clear evidence for the validity of our approach is provided by the spectrum of elementary excitations at the borderline value $\epsilon = 1$. Very recently, Takahashi[15] has succeeded with a new MC technique in obtaining the lower edge of the spectrum of excited states as a function of wave vector k, for the spin-1 Heisenberg antiferromagnetic chain. He has also made a conjecture about the nature of these excitations: single-particle-like in the vicinity of $k = \pi$ and two-particle-like near $k = 0$. In Fig. 2 we show his MC results together with the single-particle spectrum and the lower edge of the continuum of two-particle excitations obtained from our HF solution of $\mathcal{H}'_{\text{eff}}$. We see that the agreement is very impressive, substantiating his conjecture about the nature of elementary excitations.

In judging the quality of the numbers presented, it should be remembered that no arbitrary parameter enters in the calculations: Once $\mathcal{H}'_{\text{eff}}$ is written, everything follows from minimization of the energy. Therefore, I believe that the numerical evidence presented shows unambiguously that $\mathcal{H}_{\text{eff}}$ and, more precisely, its improved version $\mathcal{H}'_{\text{eff}}$ are very faithful descriptions of the original XXZ Hamiltonian in the region $\epsilon \geq 1$.

In conclusion, a simple but physically sound model has been presented to study the behavior of the XXZ spin-1

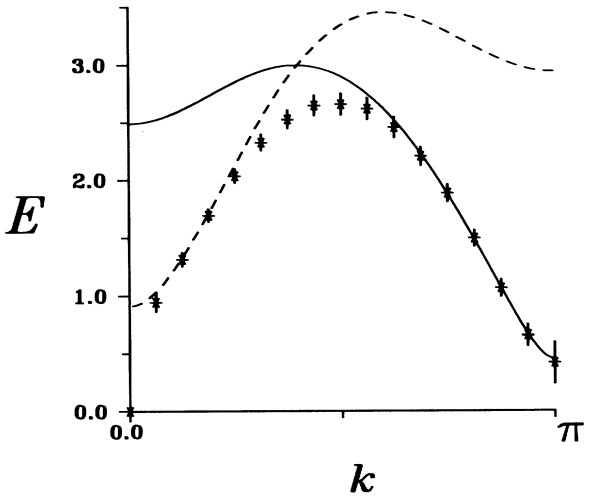

FIG. 2. Asterisks: MC results (Ref. 15) for the excitation spectrum of the Hamiltonian at $\epsilon=1$, as a function of wave vector k. Continuous line: single-particle excitation spectrum from $\mathcal{H}'_{\text{eff}}$. Dashed line: lower edge of continuum of two-particle excitation spectrum from $\mathcal{H}'_{\text{eff}}$.

chain in the antiferromagnetic regime. We have identified domain walls (SZD's) as the relevant excitations, and written a variational Hamiltonian for them. This Hamiltonian has been approximately solved, the validity of its solution asserted, and its critical properties fully analyzed, obtaining complete agreement with Haldane's proposal. The basic validity of our restricted $\mathcal{H}_{\text{eff}}$ as a faithful description of the original XXZ $\mathcal{H}$ has been proved by showing that an improved (but essentially similar) version of $\mathcal{H}_{\text{eff}}$ ($\mathcal{H}'_{\text{eff}}$) gives excellent agreement with all MC-calculated properties of the XXZ Hamiltonian, even at the nominal limit of validity $\epsilon=1$. In particular, the recently obtained excited states[15] at $\epsilon=1$ are very well reproduced by our calculation, providing support for a conjecture[15] concerning the nature of these states.

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[17]Because of our way of constructing $\mathcal{H}_{\text{eff}}$, we restrict ourselves to either open chains with an arbitrary number of sites, or closed rings with an odd number of sites. Boundary conditions are not expected to be relevant in the macroscopic limit.

[18]If we restricted ourselves to considering groups of contiguous SZD's of, at most, two sites, then $\mathcal{H}'_{\text{eff}}$ would be variational again. We do not enforce such a restriction and, therefore, $\mathcal{H}'_{\text{eff}}$ should be considered as an "almost" variational Hamiltonian. In principle, there is no difficulty in treating variationally groups of 3,4,5,... contiguous SZD's sites, but the number of variational parameters and of HF terms from decoupling of many-body operators grows rapidly. A proper variational treatment of groups of three contiguous SZD's indicates that the correction to our GS energy is of the order of 0.0003, for $\epsilon=1$. This justifies our treatment of $\mathcal{H}'_{\text{eff}}$ as an almost variational Hamiltonian.