Role of domain walls in the ground-state properties of the spin-$\frac{1}{2}$ XXZ Hamiltonian in the linear chain

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(Received 10 August 1989)

The XXZ spin-$\frac{1}{2}$ Hamiltonian in the linear chain is exactly transformed into a model where the local degrees of freedom are domain walls between opposite antiferromagnetic domains. The ground state of the new Hamiltonian is studied with the Hartree-Fock approximation. This approximation is shown to become exact in the XY and extreme antiferromagnetic limits, with excellent results in between. Known results concerning the existence or nonexistence of long-range order and gap in the excitation spectrum are reproduced by our solution. Good quantitative agreement with representative properties of the exact solution is obtained. The domain-wall Hamiltonian is shown to be the natural framework for the understanding of the ground state and low-lying excited states of the XXZ system in the antiferromagnetic regime.

I. INTRODUCTION

In this paper we will be concerned with the zero-temperature properties of the antiferromagnetic (AF) spin-$\frac{1}{2}$ XXZ model in the linear chain:

$$\mathcal{H}=\sum_i (s_i^x s_{i+1}^x + s_i^y s_{i+1}^y) + \Delta \sum_i (s_i^z s_{i+1}^z) , \quad (1)$$

where $\Delta \geq 0$, and s_i^α represent the α component of the spin-$\frac{1}{2}$ operator of site i. This model plays a central role as one of the very few strongly interacting systems for which an exact solution can be obtained.[1-4] In spite of its apparent simplicity, the ground state (g.s.) is able to display ordered and disordered phases, with interesting critical behavior. Besides their intrinsic theoretical importance, quantum-spin Hamiltonians have been employed as starting models for realistic descriptions of quasi-one-dimensional magnetic materials[5] and, in recent times, we have witnessed a renewed interest in these models as part of the effort devoted to the understanding of high-T_c superconductors.

The fact that the model described by $\mathcal{H}$ is amenable to exact solution does not mean that the obtention of g.s. properties is an easy or closed task.[3] Since Bethe's original work,[1] the study of $\mathcal{H}$ (energy,[6,7] correlations,[8-12] long-range properties,[11] low-lying excitations,[13,11,14] etc.) has been a slow process where the connection with two-dimensional statistical models[15] has proved to be very useful. Even if one is able to obtain exact results with Bethe's ansatz, their interpretation is not always straightforward: The knowledge of the exact dispersion relation for low-lying excited states does not help in getting a physical picture of them, and controversies concerning the nature of these excitations have existed.[16,17]

Though approximate treatments of $\mathcal{H}$ cannot substitute the results obtained from the exact solution, they can shed light over our understanding of Bethe's solution and help gain a deeper insight into the problem. Many approximate schemes have been proposed (see Refs. 18–23, though the list is by no means exhaustive), and most of them have in common the reduction of the original $\mathcal{H}$ to an effective noninteracting Hamiltonian with local degrees of freedom given by the spin orientation (up-down). While the reduction to a noninteracting system is an almost unavoidable requisite for approximate theories, the choice of the spin orientation as the local degree of freedom is not. At least in the AF regime, there are strong indications[14,16,17,24] of domain walls (DW's) between opposite AF domains as the key elements in the properties of the g.s. of $\mathcal{H}$. This suggests the use of DW's rather than the spin orientation as the natural degree of freedom for the study of $\mathcal{H}$ in the specified regime.

In this paper we describe the form that $\mathcal{H}$ adopts when written in DW language. While the mapping to be described is exact and valid for the general XYZ Hamiltonian, we restrict its use to the XXZ Hamiltonian in the interval $0 \leq \Delta \leq \infty$. We will show that, upon choosing the proper DW version of the Hamiltonian, the simplest approximate variational treatment of it provides excellent results in the specified interval, becoming exact for $\Delta=0$ and $\Delta=\infty$. Exact results concerning the existence or nonexistence of long-range order and of gap in the spectrum of excitations are reproduced by our treatment. Good quantitative agreement is also found with the exact results for the g.s. energy and gap (when it exists). Our study allows us to support the interpretation[14,24] of low-lying excitations in the region $\Delta \geq 1$ as the creation of a pair of *free* DW's, each carrying a spin excess[16,17] of $\pm\frac{1}{2}$, being the destruction of long-range order at $\Delta=1$ signaled by the vanishing of the energy necessary for the creation of a DW. With this information, we believe that the present approach contributes to a deeper understanding of the physics involved in the exact solution of $\mathcal{H}$.

II. DOMAIN-WALL HAMILTONIAN

In this section we describe the transformation of the original Hamiltonian into another completely equivalent

one, but with local degrees of freedom given by the bond status (ferro or antiferro) rather than the spin orientation (up-down). To each bond we associate a spin-$\frac{1}{2}$ z-component operator σ^z, with eigenvalues $+\frac{1}{2}$ if the bond is ferromagnetic ($\uparrow\uparrow$ or $\downarrow\downarrow$) and $-\frac{1}{2}$ if the bond is antiferromagnetic ($\uparrow\downarrow$ or $\downarrow\uparrow$). In terms of the original spin operators, the new bond operators have the expression $\sigma_i^z = 2s_i^z s_{i+1}^z$. To avoid ambiguities, we take an open linear chain and fix the orientation of the first spin to be always up $s_1^z = +\frac{1}{2}$. Thus, there is a one to one correspondence between the original s^z description and the σ^z description. For example, given a state with the following s^z form,

$$\uparrow\downarrow\uparrow\downarrow\downarrow\uparrow\downarrow\cdots$$

it would have the following representation in terms of the new σ^z variables:

$$\sigma_1^z = -\tfrac{1}{2},\quad \sigma_2^z = -\tfrac{1}{2},\quad \sigma_3^z = -\tfrac{1}{2},$$
$$\sigma_4^z = +\tfrac{1}{2},\quad \sigma_5^z = -\tfrac{1}{2},\quad \sigma_6^z = -\tfrac{1}{2},\ \cdots .$$

The state with perfect antiferromagnetic order in the original s^z representation corresponds to all bond operators σ^z having the value $\sigma^z = -\frac{1}{2}$. Therefore, every bond with value $\sigma^z = \frac{1}{2}$ represents a domain wall between two opposite antiferromagnetic domains.

Having described the new degrees of freedom, it is a trivial exercise to write the Hamiltonian in the new representation. After Wigner-Jordan fermionization[2] of bond operators, the domain-wall version of the Hamiltonian ($\mathcal{H}_{\rm DW}$) can be written as follows:

$$\mathcal{H}_{\rm DW} = \mathcal{H}_1 + \mathcal{H}_2 , \tag{2}$$

with

$$\mathcal{H}_1 = \frac{\Delta}{2}\sum_i (n_i - \tfrac{1}{2}) + \tfrac{1}{2}\sum_i (c_{i-1}^\dagger c_{i+1} + c_{i-1}^\dagger c_{i+1}^\dagger + \text{H.c.}) , \tag{2a}$$

$$\mathcal{H}_2 = -\tfrac{1}{2}\sum_i n_i (c_{i-1}^\dagger c_{i+1} + c_{i-1}^\dagger c_{i+1}^\dagger + \text{H.c.}) , \tag{2b}$$

where $c_i^\dagger (c_i)$ creates (annihilates) a domain wall at bond i and $n_i = c_i^\dagger c_i$, being the vacuum the state with perfect antiferromagnetic order in the s^z representation.

The one-body term $\mathcal{H}_1$ only couples second neighbor bonds and, as a consequence, DW's in the sublattices formed by even-numbered and odd-numbered bonds are not mixed by $\mathcal{H}_1$. It is only through the many-body term $\mathcal{H}_2$ that interaction between DW's in both sublattices takes place.

The action of $\mathcal{H}_{\rm DW}$ can be understood as follows. The one-body term has a static contribution ($\sum_i n_i$) that merely counts the number of DW's (ferromagnetic bonds), and a dynamic part that creates (annihilates) and moves these DW's [$\sum_i (c_{i-1}^\dagger c_{i+1} + c_{i-1}^\dagger c_{i+1}^\dagger + \text{H.c.})$]. As mentioned, this one-body part separates even-numbered from odd-numbered bonds. The many-body term can be thought of as a modification of the dynamics of DW's in a given sublattice due to the presence of DW in the other sublattice: The expression $n_i(c_{i-1}^\dagger c_{i+1} + c_{i-1}^\dagger c_{i+1}^\dagger + \text{H.c.})$ allows creation (annihilation) and movement of DW's in bonds $i-1$ and $i+1$ if bond i (belonging to the other sublattice) is occupied ($n_i = 1$). The correspondence between terms in both $\mathcal{H}$ and $\mathcal{H}_{\rm DW}$ is as follows: The contribution $(\Delta/2)\sum_i (n_i - \frac{1}{2})$ in $\mathcal{H}_{\rm DW}$ comes from the Z part of $\mathcal{H}$ while the remaining terms in $\mathcal{H}_{\rm DW}$ come from the XY terms of $\mathcal{H}$.

It is important to stress the fact that no approximations are involved in obtaining the DW Hamiltonian from the original one. Fixing the orientation of the first spin and the need for an open chain can be thought of as peculiar boundary conditions, irrelevant in the macroscopic limit. In fact, we will ignore these boundary conditions and assume perfect translational invariance in our treatment of $\mathcal{H}_{\rm DW}$.

The XXZ Hamiltonian is invariant under rotations around the z axis, and eigenstates can be classified according to the value of the z component of the total spin S^z. It is illustrative to see the form that this conservation law adopts in the DW representation. Assuming, for simplicity, an even number of sites and DW's, then:

(i) States with $S^z = 0$ are those with DW configurations that can be reduced to the vacuum upon application of $\mathcal{H}_{\rm DW}$. This implies that there is, at least, one way of pairing DW's within each sublattice such that the number of DW's per sublattice in the interval between any pair is even.

(ii) States with $S^z = \pm 1$ are those with DW configurations that, upon application of $\mathcal{H}_{\rm DW}$, can be reduced to a state with only two nearest-neighbor (in different sublattices) DW's. The dynamics of DW's imposed by $\mathcal{H}_{\rm DW}$ is such that no further reduction is allowed.

(iii) States with $S^z = \pm 2$ are those with DW's configurations that, upon application of $\mathcal{H}_{\rm DW}$, can be reduced to a state with four nearest-neighbor DW's.

The rule for an arbitrary value of S^z is evident from the above examples. If we rewrite $\mathcal{H}_{\rm DW}$ in the following fashion,

$$\mathcal{H}_{\rm DW} = \frac{\Delta}{2}\sum_i (n_i - \tfrac{1}{2}) + \tfrac{1}{2}\sum_i (1-n_i)(c_{i-1}^\dagger c_{i+1} + c_{i-1}^\dagger c_{i+1}^\dagger + \text{H.c.}) , \tag{3}$$

we see that the above classification of eigenstates is a direct consequence of the dynamics of DW's: Creation (annihilation) and movement of DW's ($c_{i-1}^\dagger c_{i+1}^\dagger + c_{i-1}^\dagger c_{i+1} + \text{H.c}$) proceeds unperturbed within each sublattice unless the bond i of the other sublattice is occupied ($1-n_i$); in that case, the action between bonds $i-1$ and $i+1$ does not take place.

As indicated in the Introduction, the mapping described before can be applied to the general case of an XYZ Hamiltonian, giving the same structure for the resulting DW Hamiltonian. Even for a given XYZ Hamiltonian, different DW versions of it can be obtained

changing the quantization axis. Though all possible DW versions of the same Hamiltonian are equivalent, approximate solutions of them may not be. Therefore, it is important to evaluate which version is best suited for an approximate treatment. With this in mind, we write a complementary DW version of the XXZ Hamiltonian obtained when the quantization axis is chosen to lie in the XY plane ($\mathcal{H}'_{\rm DW}$):

$$\mathcal{H}'_{\rm DW}=\mathcal{H}'_1+\mathcal{H}'_2 , \tag{4}$$

with

$$\mathcal{H}'_1=\tfrac{1}{2}\sum_i (n_i-\tfrac{1}{2}) + \tfrac{1}{4}(1+\Delta)\sum_i (c^\dagger_{i-1}c_{i+1}+c^\dagger_{i-1}c^\dagger_{i+1}+\text{H.c.}) , \tag{4a}$$

$$\mathcal{H}'_2=-\frac{\Delta}{2}\sum_i n_i(c^\dagger_{i-1}c_{i+1}+c^\dagger_{i-1}c^\dagger_{i+1}+\text{H.c.}) . \tag{4b}$$

III. APPROXIMATE SOLUTION

In this section we solve the DW Hamiltonians ($\mathcal{H}_{\rm DW}$ and $\mathcal{H}'_{\rm DW}$) by means of a Hartree-Fock (HF) approximation. This approximation is the simplest variational approach dictated by the structure of these Hamiltonians, and reduces the many-body terms ($\mathcal{H}_2$ and $\mathcal{H}'_2$) to effective one-body Hamiltonians in which even and odd sublattices are decoupled. Before describing our approach, we study certain limits to clarify ideas about the region of validity of our treatment.

(i) When $\Delta\to\infty$, the system shows perfect antiferromagnetic order. The natural DW Hamiltonian to describe this limit corresponds to quantization along the z axis ($\mathcal{H}_{\rm DW}$). Perfect antiferromagnetic order means the vacuum state of our representation and, therefore, $n_i=0$. But if $n_i=0$, the many-body contributions vanish and our solution becomes exact. It is important to emphasize here that the fact that our approximation becomes exact in this limit applies not only to the g.s. (something trivial in this case of perfect AF order), but also to the first excited states. We will see how excited state properties like the gap approach the exact asymptotic limit rather quickly with increasing Δ. Our approach will allow us to give a clear physical picture of excited states in that limit.

(ii) When $\Delta\le 1$, one expects strong local antiferromagnetic correlations in the XY plane. Thus, the natural DW version of our Hamiltonian corresponds to quantization in the XY plane ($\mathcal{H}'_{\rm DW}$). For the particular case of the XY model[25] ($\Delta=0$), no coupling between even and odd sublattices takes place and, therefore, our treatment becomes exact. It is worth noticing that, in our DW representation, the XY model consists of two interpenetrating but noninteracting sublattices, the Hamiltonian for each sublattice being the fermionic version on the Ising plus transverse field[26] (ITF) model at its critical point. This new view of the XY model is at the basis of the characteristic alternating behavior of correlations in that model and, to our knowledge, has not been described previously.

We have shown two limits in which our HF approximation of the two DW Hamiltonians, $\mathcal{H}_{\rm DW}$ and $\mathcal{H}'_{\rm DW}$, becomes exact. We expect our HF treatment to be a good description of the model in between both limits. As mentioned in the preceding section, our approximate treatments of both $\mathcal{H}_{\rm DW}$ and $\mathcal{H}'_{\rm DW}$ are not equivalent. The HF approach being a variational approximation, the question of preference of one description over the other is decided on the basis of achieving the lowest value for the g.s. energy. Generally speaking, if we have two variational approaches for the same problem, the change from one approach to the other can take place at an arbitrary point, not necessarily related to the physics of the problem, but rather to the nature of the approximations. We will see that, in our case, the minimum value for the g.s. energy is obtained with the XY version ($\mathcal{H}'_{\rm DW}$) for $\Delta\le 1$, and with the Z version ($\mathcal{H}_{\rm DW}$) for $\Delta\ge 1$. Therefore, the change from one version to the other takes place at a point with physical content: The Heisenberg point ($\Delta=1$). This physical location of the transition point between the preferred variational solution is an additional indication of the validity of our treatment, and could have been anticipated noticing that the choice of quantization axis is irrelevant for any approximate solution at the isotropic point. Another way of looking at this is provided by the fact that both DW versions ($\mathcal{H}_{\rm DW}$ and $\mathcal{H}'_{\rm DW}$) are connected by a dual transformation.[27] The HF solutions of them are not linked by this duality relation except at the Heisenberg point, where both the Hamiltonian and its HF solution are self-dual.

Summarizing our analysis of the range of validity, the HF treatment of $\mathcal{H}_{\rm DW}$ becomes exact when $\Delta=\infty$, while that of $\mathcal{H}'_{\rm DW}$ is exact for $\Delta=0$. In between both limits, the HF solution of the XY version ($\mathcal{H}'_{\rm DW}$) is preferred in the range $0\le\Delta\le 1$, while the HF solution of the Z version ($\mathcal{H}_{\rm DW}$) has the lowest g.s. energy for $\Delta\ge 1$.

It is of interest to understand why our HF solutions are bound to fail when the system becomes increasingly ferromagnetic ($\Delta<0$). Let us consider, for example, the Heisenberg ferromagnet ($\Delta=-1$): The g.s. consists of all spins pointing along the same direction (Z axis, for instance). Our scheme is able to describe this trivial g.s.: It is simply the state in which all bonds have $\sigma^z=+\frac{1}{2}$. But our interest is not only the g.s. but rather low-lying excitations and the closely related long-range correlations. In this case the first excitations are spin waves formed by Bloch states with a single spin turned.[2] In our bond language, one spin turned amounts to a pair of nearest-neighbor antiferromagnetic bonds in a ferromagnetic background. This state demands a high degree of correlation between even and odd sublattices and, therefore, cannot be described by an approximation based on the decoupling between both sublattices.

Now we describe the technical details of the HF approach and present results for characteristic quantities. The many-body term is the same in both versions ($\mathcal{H}_{\rm DW}$ and $\mathcal{H}'_{\rm DW}$), and the HF decoupling is given by

$$n_i(c^\dagger_{i-1}c_{i+1}+c^\dagger_{i-1}c^\dagger_{i+1}+\text{H.c.})\approx\langle n_i\rangle(c^\dagger_{i-1}c_{i+1}+c^\dagger_{i-1}c^\dagger_{i+1}+\text{H.c.})$$
$$+n_i\langle(c^\dagger_{i-1}c_{i+1}+c^\dagger_{i-1}c^\dagger_{i+1}+\text{H.c.})\rangle-\langle n_i\rangle\langle(c^\dagger_{i-1}c_{i+1}+c^\dagger_{i-1}c^\dagger_{i+1}+\text{H.c.})\rangle\ , \quad (5)$$

where $\langle\ \rangle$ means g.s. average. There are more terms in a Wick factorization of the many-body contribution than those implied by the previous decoupling, but the self-consistent solution has always shown a null value for the other contributions. This means that, in our case, no additional restriction within the HF approximation is implied by the previous decoupling.

The structure of the effective one-body HF Hamiltonians is the same for both versions ($\mathcal{H}_{\rm DW}$ and $\mathcal{H}'_{\rm DW}$), and can be written in the following way:

$$\mathcal{H}_{\rm HF}=E_0\sum_i n_i+V\sum_i(c^\dagger_ic_{i+2}+c^\dagger_ic^\dagger_{i+2}+\text{H.c.})+\text{K}\ , \quad (6)$$

where the self-consistent parameters have the value

$$E_0=\begin{cases}\dfrac{\Delta}{2}-\dfrac{1}{2}\langle c^\dagger_ic^\dagger_{i+2}+c^\dagger_ic_{i+2}+\text{H.c.}\rangle, & \text{for } \mathcal{H}_{\rm DW}\ ,\\ \dfrac{1}{2}-\dfrac{\Delta}{2}\langle c^\dagger_ic^\dagger_{i+2}+c^\dagger_ic_{i+2}+\text{H.c.}\rangle, & \text{for } \mathcal{H}'_{\rm DW}\ ,\end{cases}$$
$$V=\tfrac{1}{2}(1-\langle n_i\rangle), \quad \text{for } \mathcal{H}_{\rm DW}\ ,$$
$$V=\tfrac{1}{4}(1+\Delta)-\frac{\Delta}{2}\langle n_i\rangle, \quad \text{for } \mathcal{H}'_{\rm DW}\ ,$$
$$K=\sum_i-\frac{\Delta}{4}+\frac{1}{2}\langle n_i\rangle\langle c^\dagger_{i-1}c_{i+1}+c^\dagger_{i-1}c^\dagger_{i+1}+\text{H.c.}\rangle, \quad \text{for } \mathcal{H}_{\rm DW}\ ,$$
$$K=\sum_i-\frac{1}{4}+\frac{\Delta}{2}\langle n_i\rangle\langle c^\dagger_{i-1}c_{i+1}+c^\dagger_{i-1}c^\dagger_{i+1}+\text{H.c.}\rangle, \quad \text{for } \mathcal{H}'_{\rm DW}\ . \quad (7)$$

As indicated above, the self-consistent Hamiltonian for every sublattice is the fermionic version of the ITF (Ref. 26) model, whose well known properties will help us in understanding the nature of our solution. The $\mathcal{H}_{\rm HF}$ can be diagonalized by means of the usual Bogoliubov-Fourier transformation to new fermions operators[2] $d^\dagger_k(d_k)$, with the following result:

$$\mathcal{H}_{\rm HF}=\sum_k E_kd^\dagger_kd_k+U\ , \quad (8)$$

where U is the ground-state energy and $E_k=\{[E_0+2V\cos(k)]^2+[2V\sin(k)]^2\}^{1/2}$ is the dispersion relation for the excitations.

The self-consistent HF solution has the following properties.

(i) For $\Delta\geq 1$, the lowest g.s. energy is obtained using the Z-axis version ($\mathcal{H}_{\rm DW}$) as indicated previously. This g.s. shows long-range antiferromagnetic order and a gap in the excitation spectrum. Both gap and long-range order diminish with decreasing Δ, and vanish at the isotropic point $\Delta=1$, in agreement with the exact results.[11] For a quantitative evaluation of the approximation, in Figs. 1 and 2, we compare results for the g.s. energy and the gap in our approximation with those of the exact solution.[7,11] Concerning Fig. 2 we see that both the exact and approximate solutions tend to the asymptotic line[11,28] $gap=\Delta-2$. This limit is very revealing about the form of the excited states, and has a straightforward interpretation in our DW language: If we apply the operator $c^\dagger_{i-1}c^\dagger_{i+1}$ to the state with perfect AF order, we create two domain walls at bonds $i-1$ and $i+1$, with an increase in energy over the g.s. given by Δ. But this static configuration can reduce its energy by delocalizing DW's thanks to terms of the form $c^\dagger_jc_{j+2}+\text{H.c}$. According to $\mathcal{H}_{\rm DW}$, the dispersion relation associated with the motion

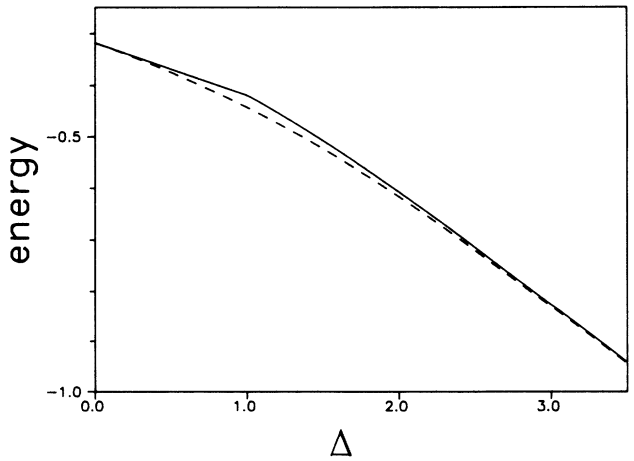

FIG. 1. Solid line: Hartree-Fock self-consistent results for the ground-state energy of $\mathcal{H}'_{\rm DW}$ ($\Delta\leq 1$) and $\mathcal{H}_{\rm DW}$ ($\Delta\geq 1$). Dashed line: Exact result.

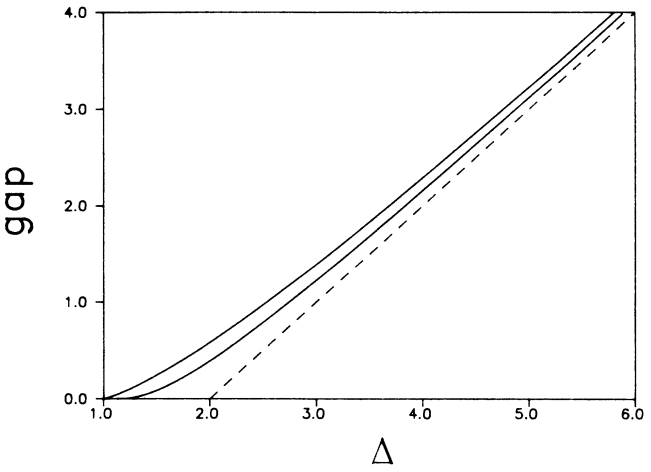

FIG. 2. Upper solid line: Hartree-Fock self-consistent results for the gap in the excitation spectrum of $\mathcal{H}_{\mathrm{DW}}$. Lower solid line: Exact result. Dashed line: Asymptotic limit ($\Delta \rightarrow \infty$) of both exact and approximate results.

of a single DW is given by $\cos(k)$, and the reduction in energy due to this motion is $\cos(k=\pi)=-1$ per DW. Therefore, the total increase in energy is given by $\Delta-2$, in agreement with the exact result. The described excited state has both DW's in the same sublattice and, therefore, has $S^z=0$, but the same energy would have the excited state with the pair of DW's in different sublattices ($S^z=\pm 1$). This degeneracy between excited states with $S^z=0$ and $S^z=\pm 1$ is also obtained from the exact Bethe ansatz solution.[29,30] At this point, it is important to notice that the real single particle excitation is an isolated free DW: the fact that we put two of them is merely to comply with the customary boundary conditions. It is easy to see that each isolated DW carries an excess spin of $\pm\frac{1}{2}$ and, therefore, the claim of Faddeev and Takhtajan[16,17] considering elementary excitations as kinks with spin $\frac{1}{2}$ is completely justified.

This pictorial image of excited states as the creation and posterior delocalization of a pair of DW's in a perfect AF background becomes quantitatively exact in the limit $\Delta=\infty$, but continuity arguments indicate that it should be qualitatively valid down to $\Delta=1$, where the gap vanishes. For $1\leq\Delta<\infty$, we can think of this pair of free DW's as moving in a background formed by the state of perfect AF order but with fluctuations due to virtual (not free) pairs of other DW's. The destruction of long-range order appears as a consequence of the fact that the gap for the creation of free DW's vanishes.

(ii) For $\Delta\leq 1$, the lowest g.s. energy is obtained with the XY-axis version ($\mathcal{H}'_{\mathrm{DW}}$), as indicated above. The HF Hamiltonian corresponds to the ITF model at its critical point. Consequently, there is no gap for the excitations, the g.s. lacks long-range order, and correlations decay algebraically, in agreement with the exact solution.[25,10] We can consider the behavior of DW's in the g.s. as that of a system at the (critical) boundary between free and virtual pairs of DW's. The comparison between exact[15] and approximate g.s. energy is shown in Fig. 1. In this interval of Δ, our approximation becomes quantitatively equivalent to that of Refs. 21 and 22, but the interpretation in terms of DW's is, to our knowledge, new.

Summarizing our results, we see that our approach reproduces exact results concerning the existence or nonexistence of long-range order and gap in the excitation spectrum. It gives a good quantitative approximation to the g.s. energy and the gap (when it exists), in addition to providing a physical description of the nature of excited states.

From Fig. 1 it is evident that the difference between the exact and approximate g.s. energy is largest at the isotropic point $\Delta=1$. To demonstrate that, even at that point, our approximation provides a fairly good description of the system, we show in Fig. 3 the des Cloizeaux–Pearson[13] (exact) dispersion relation for excited states together with our results for the continuum of pair excitations, whose lower edge corresponds to the des Cloizeaux–Pearson line.

Though our treatment has proved to be successful in describing long-range properties and the nature of low-lying excitations, shortcomings related to the mean-field nature of the HF approximation are bound to appear. The main limitations of our results are the following.

(i) The solution for $\Delta\leq 1$ is basically that of an XY model and,therefore, the power of the algebraically decaying correlations does not change with Δ.

(ii) Although the value $\Delta=1$ is a critical point for the approximate solution of $\mathcal{H}_{\mathrm{DW}}$ ($\Delta\geq 1$), the universality class is that of the ITF model and not that corresponding to the exact solution. For example, the correlation length in the vicinity of $\Delta=1$ diverges with a power law and not with the correct exponential behavior of the exact ground state.[11]

IV. SUMMARY

We have presented a new version of the spin-$\frac{1}{2}$ XXZ Hamiltonian in the linear chain with local degrees of free-

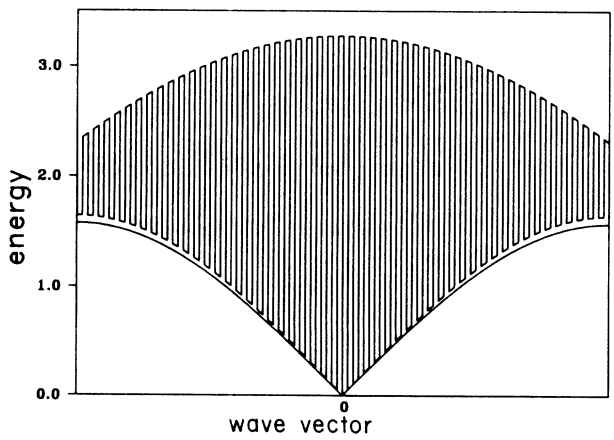

FIG. 3. Excitation spectrum at the Heisenberg point ($\Delta=1$) vs wave vector in the first Brillouin zone. Solid line: Des Cloizeaux–Pearson exact result. Shaded region: Continuum of pair excitations from the Hartree-Fock solution of $\mathcal{H}_{\mathrm{DW}}$.

dom characterized by the bond status (ferro or antiferro) rather than the spin orientation (up-down), with (fermionic) DW's between AF domains as the relevant dynamical variables. The mapping presented is exact and gives the same structure for the general XYZ Hamiltonian, though we have made use of it only in its XXZ version.

We have considered two equivalent versions of the DW Hamiltonian, obtained by choosing the quantization axis either along the Z ($\mathcal{H}_{\rm DW}$) direction or in the XY plane ($\mathcal{H}'_{\rm DW}$). The DW Hamiltonians have a one-body part characterized by independence between the sublattices formed by even-numbered and odd-numbered bonds, plus a many-body contribution where interaction between DW's in both sublattices takes place. This form of the DW Hamiltonians suggests an HF approximation based on a decoupling of the many-body term dictated by the two-sublattice structure.

Choosing the appropriate DW version, we have shown that our HF treatment provides very good results in the AF interval $0 \leq \Delta \leq \infty$, becoming exact in the limits $\Delta = \infty$ and $\Delta = 0$. In particular, we have shown that, for $\Delta \geq 1$, our solution has long-range AF order and a gap in the spectrum of excitations. Both gap and long-range order vanish at $\Delta = 1$, in agreement with the exact solution. Our treatment has allowed us to interpret the nature of the lowest excited states as the creation and delocalization of a pair of domain walls, giving an explanation for the exact asymptotic behavior of the gap in the limit $\Delta \to \infty$. In the region $0 \leq \Delta \leq 1$, our HF solution describes a critical system with no gap in the excitation spectrum and algebraically decaying correlations, also in agreement with exact results.

The difficulties associated with the mean-field nature of our approach are rather mild, and show up as an incorrect universality class for the critical behavior at $\Delta \gtrsim 1$, and an inability to change from its XY value the power of algebraically decaying correlations in the interval $0 \leq \Delta \leq 1$.

In conclusion, I have presented a mapping of the XXZ Hamiltonian whose approximate solution provides a simple, useful, and physically sound description of the ground state and low-lying excited states of that system in the AF regime.

Note added in proof. A partial account of this work has been presented at the 34th Conference on Magnetism and Magnetic Materials, Boston 1989 (Proceedings to appear in J. Appl. Phys.).

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