Coherent states as solutions of the anisotropic Heisenberg antiferromagnetic chain

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We propose a *coherent*-state solution for the one-dimensional antiferromagnetic Heisenberg Hamiltonian in the quasi-Ising asymptotic regime. We discuss the nature of the spectrum and the eigenvectors as a function of the anisotropy parameter. Results for the energy of the ground state and the short-range-order correlation agree with exact numerical calculations in a wide range of variation of anisotropy. We also present a canonical formulation of the theory which interpolates continuously from the Ising limit to cases of lower anisotropies, thus yielding a novel view of antiferromagnetism. Finally we discuss possible connections with the theory of superconductivity of high-T_c ceramics.

I. INTRODUCTION

The interest in models that deal with many-body problems in low-dimensional systems has been recently revived due to the discovery of high-T_c superconductivity.[1] The anisotropic Heisenberg chain with antiferromagnetic coupling is one of them. By means of the Jordan-Wigner transformation, this model for spin $\frac{1}{2}$ can be mapped onto a fermion problem which is a lattice version of the massless Thirring model.[2] The latter has been recently used to formulate a theory of superconductivity which seems to apply to ceramic superconductors.[3]

In this contribution we want to concentrate on the study of the spin-$\frac{1}{2}$ Heisenberg antiferromagnetic chain. Preliminary results of this material have been published elsewhere.[4] Although the problem has been exactly solved in the past,[5] no light concerning the nature of the ground state (GS) has been shed. From the study of spin-wave excitations it is known that the GS is somewhat disordered and different from the standard Néel state.[6] It is surprising however that the spin-wave theory of antiferromagnets, as it is usually constructed, works properly and describes with success experimental data. Recently, Anderson and collaborators have put forward a trial solution based on the resonating-valence-bond concept,[7] obtaining a GS which is liquid-type disordered.

In this paper we want to present a solution which is exact in the high anisotropic limit (quasi-Ising regime), and is neither perturbative in relation to anisotropy nor variational. The wave function proposed corresponds to a *coherent state*,[8] different from the Néel state even for very high anisotropy. The apparent structure of this state is disorderedlike, similarly to the solution proposed by Anderson,[7] but on the average the antiferromagnetic ordering is preserved in the form

$$\langle S_z(m)\rangle \approx \begin{cases} \frac{1}{2} & \text{for } m \text{ even },\\ -\frac{1}{2} & \text{for } m \text{ odd },\end{cases} \tag{1}$$

where the angle brackets in (1) mean an average in relation to the GS and $S_z(m)$ is the z component of the spin at the mth site. This means that the usual picture of sublattices in antiferromagnets can be saved, in spite of the complications introduced by the GS structure. The GS energy obtained in our calculation is the same as the one provided by corrections from spin waves for high anisotropy, and compares very well with exact numerical results[5] for a wide range of variation of the anisotropy parameter α ($\alpha=0$ being the Ising limit and $\alpha=1$ the case of isotropic exchange).

Bose-type operators are constructed which coherently reverse pairs of neighboring spins. Disorder can be introduced into the Néel state by applying these operators, but since the final state is obtained as a coherent superposition, one can say that the final product is antiferromagnetically ordered in the sense given by (1). This consideration resolves the paradox concerning the formulation of the spin-wave theory in antiferromagnets: spin waves are actually constructed in relation to the true GS, as long as only relation (1) is used in the deduction. We will return to this point later on.

A broken symmetry is present in our formulation since one of the two possible Néel states is chosen as a reference state, and all operators are defined in relation to it. A similar construction can be done using the other Néel state; both are connected by the time-reversal operator and thus the GS is a doublet.[9] By flipping spin pairs in the Néel state we induce a number of different configurations within the manifold of total $S_z=0$: At a given site, the probability of finding the spin in either direction is finite. To illustrate the physical picture we quote Anderson:[6] "Therefore, while the spins of the two sublattices can certainly be said to be opposite in direction, in the ground state of the lattice, on an average basis, we cannot define the direction in space of the spin of either one."

In spite of those facts we will show here that a different spin representation can be chosen in such a way that the

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GS can be thought of as an "ordered" configuration. Local spin ladder operators are dressed with a boson field which delocalize their action along the chain. With such dressed operators all the formal developments of antiferromagnetism, including spin waves, can be maintained. In particular, the GS wave function can be obtained from the ferromagnetic aligned state by flipping the quasispin at even (odd) sites (we use the word "quasispin" to indicate that normal spins are dressed with a boson field). What our approach shows is the inadequacy of the basis of eigenvectors of the $[S_z(1)\otimes S_z(2)\otimes \cdots \otimes S_z(N)]$ operator. While they are eigenvectors of the Ising part of the Hamiltonian, they do not connect continuously with the eigenvectors of the total Hamiltonian when we adiabatically switch on the transverse part of it. In our formalism one interpolates continuously from the Ising limit of high anisotropy to lower anisotropies, yielding in this way a novel way to think of antiferromagnetic systems.

The GS doublet is separated by a gap from the excited states.[9] Unfortunately, in the highly anisotropic limit, excitation bands collapse into discrete boson levels. Excitations of arbitrary spin can be canonically constructed through application of the quasispin reversal operators. States of finite magnetization are of paramount importance in the construction of superconducting states,[3,10] since they represent non-half-filling cases in fermion language.

Our paper is organized as follows. In Sec. II we define our bosonlike operators and construct the GS as a coherent state. We also study the GS structure, its energy, and the short-range order correlation. In Sec. III we describe an equivalent canonical way of building the GS from the completely aligned ferromagnetic state. This procedure yields a clue for obtaining excitations of well defined spin. In the final section we discuss the connections with superconductivity and other implications of our solution.

II. CONSTRUCTION OF A COHERENT STATE

The anisotropic spin-$\frac{1}{2}$ Heisenberg Hamiltonian for antiferromagnetic coupling is written as

$$\hat{H}=J\sum_{m}^{N}\left[S_z(m+1)S_z(m)+\frac{\alpha}{2}\{S_+(m+1)S_-(m)+S_+(m)S_-(m+1)\}\right], \quad (2)$$

where $J>0$, $S_x(m)$, $S_y(m)$, and $S_z(m)$ are the spin components for the mth site of the chain, and α is the anisotropy parameter. In formula (2), $S_\pm$ are the spin ladder operators defined as

$$S_+(m)\equiv S_x(m)+iS_y(m)\,,\qquad S_-(m)\equiv S_x(m)-iS_y(m)\,. \quad (3)$$

Bosonlike operators which reverse spin pairs are defined through

$$\phi_e^\dagger\equiv\left[\frac{2}{N}\right]^{1/2}\left[\frac{1}{4}\alpha N+\sum_{m\ \mathrm{even}}S_+(m+1)S_-(m)\right],\qquad \phi_o^\dagger\equiv\left[\frac{2}{N}\right]^{1/2}\left[\frac{1}{4}\alpha N+\sum_{m\ \mathrm{odd}}S_+(m)S_-(m+1)\right], \quad (4)$$

where N is the total number of sites in the chain. For the large-N limit ($N\rightarrow\infty$), the formalism is symmetric in relation to both operators defined by (4). For finite chains there are boundary effects present which depend on the particular boundary condition chosen. For the free-end chain, boundary effects on the energy decay as $N^{-1/2}$, when N is large. We will not take the latter terms into account since we are mainly interested in the thermodynamic limit.

The commutator algebra for ϕ_e and ϕ_o can be straightforwardly calculated.[4] It yields rather complicated relations which can be simplified to a boson algebra if one assumes the quasi-Ising limit ($0\le\alpha\ll1$) and makes the replacement

$$S_z(m)\rightarrow\tfrac{1}{2}(-1)^m\,. \quad (5)$$

For this regime we obtain the following relations:

$$[\phi_e,\phi_e^\dagger]=[\phi_o,\phi_o^\dagger]=1\,,\qquad [\phi_e,\phi_o]=[\phi_e^\dagger,\phi_o]=0\,, \quad (6)$$

and also

$$[\hat{H}_o,\phi_e^\dagger]=J\left[\phi_e^\dagger-\frac{\alpha}{2}\left[\frac{N}{2}\right]^{1/2}\right],\qquad [\hat{H}_o,\phi_o^\dagger]=J\left[\phi_o^\dagger-\frac{\alpha}{2}\left[\frac{N}{2}\right]^{1/2}\right], \quad (7)$$

where $\hat{H}_o$ is the Ising part of the total Hamiltonian $\hat{H}$,

$$\hat{H}_o\equiv J\sum_m S_z(m+1)S_z(m)\,. \quad (8)$$

The transverse XY part of $\hat{H}$ can be written exactly in terms of the fields (ϕ_e,ϕ_o) in the following way:

$$\hat{H}_{XY}\equiv\hat{H}-\hat{H}_o=\frac{\alpha}{2}J\left[\frac{N}{2}\right]^{1/2}(\phi_e^\dagger+\phi_e+\phi_o^\dagger+\phi_o)-\tfrac{1}{2}\alpha^2NJ\,. \quad (9)$$

Using the commutation relations [(6) and (7)] and expression (9) (and neglecting boundary effects), one obtains

$$[\hat{H},\phi_e^\dagger]=J\phi_e^\dagger\,,\qquad [\hat{H},\phi_o^\dagger]=J\phi_o^\dagger\,, \quad (10)$$

meaning that the Hamiltonian can be diagonalized by the (ϕ_e,ϕ_o) operators within the manifold of total $S_z=0$. We then obtain

$$\hat{H}=J(\phi_e^\dagger\phi_e+\phi_o^\dagger\phi_o)+\hat{H}'(\alpha)+E_G(\alpha)\,, \quad (11)$$

where $E_G(\alpha)$ is the GS energy (absence of bosons described by the ϕ fields), and $\hat{H}'(\alpha)$ is a residual term such that

$$[\hat{H},\hat{H}'(\alpha)]=0 ,$$
$$[\hat{H}'(\alpha),\phi_e^\dagger]=[\hat{H}'(\alpha),\phi_o^\dagger]=0 . \quad (12)$$

The term $\hat{H}'(\alpha)$ represents all the elementary excitations which are additional to the bosonic degrees of freedom described by the fields (ϕ_e,ϕ_o). In particular, we might find there domain wall excitations and other excitations with $S_z \neq 0$ whose levels are remnants of spin-wave bands. We will disregard $H'(\alpha)$ for the time being, and will leave the formal demonstration that $H'(\alpha)=0$ in the $\alpha \to 0$ limit for the last part of this section.

The Néel state defined by relation (5) is trivially an eigenvector of operators (ϕ_e,ϕ_o):

$$\phi_e \,|\downarrow\uparrow\downarrow\uparrow \cdots\rangle = \frac{\alpha}{2}\left[\frac{N}{2}\right]^{1/2} |\downarrow\uparrow\downarrow\uparrow \cdots\rangle ,$$
$$\phi_o \,|\downarrow\uparrow\downarrow\uparrow \cdots\rangle = \frac{\alpha}{2}\left[\frac{N}{2}\right]^{1/2} |\downarrow\uparrow\downarrow\uparrow \cdots\rangle . \quad (13)$$

If we denote by $|N\rangle$ our choice for the Néel state, a standard coherent state can be constructed in the form[8]

$$|z\rangle = e^{z(\phi_e^\dagger-\phi_e)}e^{z(\phi_o^\dagger-\phi_o)}|N\rangle$$
$$= e^{-(z^2+2z\bar{z})}e^{z\phi_e^\dagger}e^{z\phi_o^\dagger}|N\rangle$$
$$= e^{-z(z+2\bar{z})}\sum_{\nu,\mu=0}^{\infty}\frac{z^{\nu+\mu}}{\nu!\mu!}(\phi_e^\dagger)^\nu(\phi_o^\dagger)^\mu|N\rangle , \quad (14)$$

where $\bar{z}\equiv\alpha/2(N/2)^{1/2}$.

As seen in relations (13), $|N\rangle$ is not the vacuum for the annihilation operator ϕ. From the basic Bose-type commutation relations (6), we obtain the identity

$$e^{-z\phi^\dagger}\phi e^{z\phi^\dagger}=\phi+z , \quad (15)$$

for any of the two operators ϕ. Applying ϕ_e over the $|z\rangle$ ket, and using relation (15) yields

$$\phi_e|z\rangle = e^{-z(z+2\bar{z})}\phi_e e^{z\phi_e^\dagger}e^{z\phi_o^\dagger}|N\rangle$$
$$= e^{-z(z+2\bar{z})}e^{z\phi_e^\dagger}(\phi_e+z)e^{z\phi_o^\dagger}|N\rangle$$
$$=(z+\bar{z})|z\rangle . \quad (16a)$$

Similarly one also gets the relation

$$\phi_o|z\rangle=(z+\bar{z})|z\rangle , \quad (16b)$$

illustrating the fact that coherent states are standardly constructed as eigenstates of the annihilation operators (ϕ_o,ϕ_e). What is different in our construction is that the Néel state is not the vacuum for the ϕ's and that the eigenvalue for $|z\rangle$ is $[z+\alpha/2(N/2)^{1/2}]$ and not simply z. Choosing $z=-\bar{z}=-(\alpha/2)(N/2)^{1/2}$ yields the ground state of our problem, which is the vacuum for the boson excitations described by the ϕ fields. The GS wave function is then given by

$$|G\rangle \equiv \left|z=-\frac{\alpha}{2}\left[\frac{N}{2}\right]^{1/2}\right\rangle , \quad (17)$$

and then we get from (14) and (16)

$$\phi_o|G\rangle=\phi_e|G\rangle=0 , \quad (18)$$

and

$$|G\rangle=\exp\left[-\frac{\alpha}{2}\left[\frac{N}{2}\right]^{1/2}(\phi_e^\dagger-\phi_e)\right]\exp\left[-\frac{\alpha}{2}\left[\frac{N}{2}\right]^{1/2}(\phi_o^\dagger-\phi_o)\right]|N\rangle ,$$
$$=\exp\left[\frac{\alpha^2N}{8}\right]\exp\left[-\frac{\alpha}{2}\left[\frac{N}{2}\right]^{1/2}\phi_e^\dagger\right]\exp\left[-\frac{\alpha}{2}\left[\frac{N}{2}\right]^{1/2}\phi_o^\dagger\right]|N\rangle ,$$
$$=\exp\left[\frac{\alpha^2N}{8}\right]\sum_{\nu,\mu=0}^{\infty}\frac{(-1)^{\nu+\mu}}{\nu!\mu!}\left[\frac{\alpha^2N}{8}\right]^{(\nu+\mu)/2}(\phi_e^\dagger)^\nu(\phi_o^\dagger)^\mu|N\rangle . \quad (19)$$

We see from the above formulas that $|G\rangle$ is not perturbative in relation to the anisotropy, since the α parameter always appears multiplied by $N^{1/2}$. We also get

$$\hat{H}|G\rangle=E_G(\alpha)|G\rangle . \quad (20)$$

For solving the GS energy $E_G(\alpha)$, the commutators given below are of value

$$[\hat{H}_o,e^{z\phi_e^\dagger}]=zJ\left[\phi_e^\dagger-\frac{\alpha}{2}\left[\frac{N}{2}\right]^{1/2}\right]e^{z\phi_e^\dagger} ,$$
$$[\hat{H}_o,e^{z\phi_o^\dagger}]=zJ\left[\phi_o^\dagger-\frac{\alpha}{2}\left[\frac{N}{2}\right]^{1/2}\right]e^{z\phi_o^\dagger} , \quad (21)$$

where $\hat{H}_o$ is the Ising part of the total Hamiltonian given by relation (8). A straightforward calculation yields,

$$\langle G|\hat{H}_o|G\rangle=-\frac{JN}{4}(1-\alpha^2) \quad (22)$$

which combined with expression (9) leads to the result

$$E_G(\alpha)=-\tfrac{1}{4}(1+\alpha^2)JN , \quad (23)$$

which is valid in the high anisotropy regime ($\alpha \ll 1$). It is worth mentioning that the energy given by relation (23) is the same energy that one obtains from spin-wave corrections to the energy of the Néel state in the high anisotropic limit (narrow spin-wave bands). The short-range-order parameter, which measures the quality of our solution, can be obtained immediately from relation (22). One finds the result

$$\langle S_z(m+1)S_z(m)\rangle = -\frac{1}{4}+\frac{\alpha^2}{4} , \tag{24}$$

which is independent of the site in the chain. In Fig. 1 we compare our results (23) and (24) with exact numerical calculations obtained by Orbach[5] as a function of the anisotropy parameter. Our results are exact in the asymptotic regime $\alpha \ll 1$, but even for lower anisotropies our wave function seems to describe with excellent accuracy the physical situation.

Defining the new operators

$$\tilde{\phi}_e^\dagger \equiv \phi_e^\dagger + \bar{z}, \quad \tilde{\phi}_o^\dagger \equiv \phi_o^\dagger + \bar{z} , \tag{25}$$

and substituting them in relation (7) yields:

$$\begin{aligned}[\hat{H}_o,\tilde{\phi}_e^\dagger] &= J\tilde{\phi}_e^\dagger , \\ [\hat{H}_o,\tilde{\phi}_0^\dagger] &= J\tilde{\phi}_o^\dagger ,\end{aligned} \tag{26}$$

which means that

$$\begin{aligned}\hat{H}_o &= J\sum_m S_z(m+1)S_z(m) \\ &= J(\tilde{\phi}_e^\dagger\tilde{\phi}_e + \tilde{\phi}_o^\dagger\tilde{\phi}_o) + E_N + H''(\alpha) ,\end{aligned} \tag{27}$$

where E_N is the energy of the Néel state ($E_N = -JN/4$) and the term $H''(\alpha)$ is a residual part which commutes with the Ising term $\hat{H}_o$. But note that

$$\begin{aligned}J(\tilde{\phi}_e^\dagger\tilde{\phi}_e + \tilde{\phi}_o^\dagger\tilde{\phi}_0) = {} & J(\phi_e^\dagger\phi_e + \phi_o^\dagger\phi_o) \\ & + J\bar{z}(\phi_e^\dagger + \phi_e + \phi_o^\dagger + \phi_o) + 2\bar{z}^2 J .\end{aligned} \tag{28}$$

Comparing with expressions (9) and (11) we get

$$\hat{H}'(\alpha) \equiv \hat{H}''(\alpha) , \tag{29}$$

and so $\hat{H}'(\alpha)$ commutes with both, the total Hamiltonian and the Ising part of it (and hence it commutes with the transverse XY Hamiltonian). It follows that $H'(\alpha)$, in the extreme anisotropic limit, is a constant. But since E_G is the energy of the GS [see expression (11)] it follows that $H'(\alpha) \equiv 0$.

III. CANONICAL CONSTRUCTION OF THE GROUND STATE AND EXCITATIONS

Following the idea of des Cloizeaux and Gaudin,[5] one might think of generating the GS wave function from the ferromagnetic state $|F\rangle$ with saturated magnetization $M=\frac{1}{2}N$. In this state, all spins are pointing up and are parallel to each other. By means of spin flips one can generate any eigenstate of the total spin component S_z:

$$|\Omega\rangle = \sum_{\substack{n_1,\ldots,n_r \\ n_1<n_2\cdots<n_r}} a(n_1,n_2,\ldots,n_r)S_-(n_1)S_-(n_2)\cdots S_-(n_r)|F\rangle . \tag{30}$$

In particular our Néel state can be written as

$$|N\rangle = S_-(1)S_-(3)\cdots S_-(N-1)|F\rangle , \tag{31}$$

where we have assumed that the total number of sites N is an even number. If we write $|G\rangle$ in the following form:

$$|G\rangle = e^{-\alpha B}|N\rangle , \tag{32}$$

where the anti-Hermitian operator B is given by

$$B = \frac{1}{2}\left[\frac{N}{2}\right]^{1/2}(\phi_e^\dagger + \phi_o^\dagger - \phi_e - \phi_o) , \tag{33}$$

and use relation (31), one obtains

$$\begin{aligned}|G\rangle &= e^{-\alpha B}|N\rangle = e^{-\alpha B}S_-(1)S_-(3)\cdots S_-(N-1)|F\rangle \\ &= e^{-\alpha B}[S_-(1)S_-(3)\cdots S_-(N-1)]e^{\alpha B}|F\rangle ,\end{aligned} \tag{34}$$

where we have used the relation $e^{\pm\alpha B}|F\rangle = |F\rangle$, and, consequently, we get the result

$$|G\rangle = s_-(1)s_-(3)\cdots s_-(N-1)|F\rangle , \tag{35}$$

in complete analogy with the Néel wave function given by (31) but expressed now in terms of the operators

$$s_-(m) \equiv e^{-\alpha B}S_-(m)e^{\alpha B} . \tag{36}$$

These new operators correspond to spin lowering operators dressed by a boson field described by B. It can straightforwardly be shown that the action of $s_-(m)$ is delocalized around the mth site and can be described as a linear combination of lowering spin operators in all the chain. Since the transformation given by (36) is canonical, it preserves spin commutation relations, the ferromagnetic state is left invariant by it, and our GS is the transformed state which is in correspondence with the Néel state. The picture obtained is similar to the usual change of representation from Wannier to Bloch states in describing electronic properties of solids. Based on physical grounds one may write

$$s_-(m) = e^{-\alpha B}S_-(m)e^{\alpha B} = \sum_{n=-\infty}^{\infty} C_n(\alpha)S_-(m+n) , \tag{37}$$

where we have assumed an infinite chain with sites $-\infty < n < +\infty$. The amplitude $C_n(\alpha)$ is clearly a function of anisotropy and becomes more and more localized when $\alpha \to 0$. Precisely, for that limiting case one should obtain

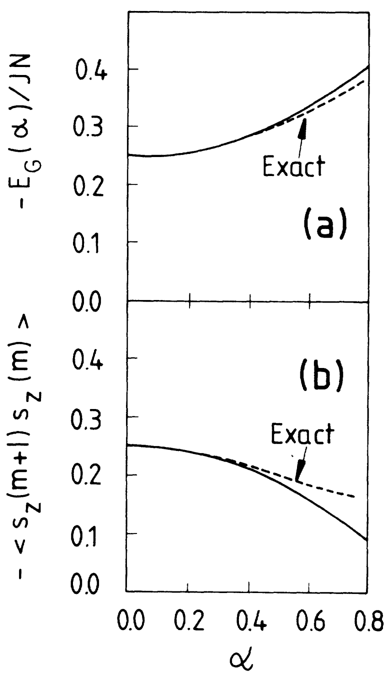

FIG. 1. The ground-state energy (a) and the short-range order parameter (b) as functions of the anisotropy α. Continuous lines represent the results obtained with our asymptotic ($\alpha \approx 0$) theory. They are compared with exact results from Orbach's calculation (Ref. 5) (dashed lines). Values at $\alpha=0$ (Ising case) yield the energy and correlation of the Néel state. Our theory has no adjustable parameter.

$$\lim_{\alpha \to 0} C_n(\alpha) = \delta_{n,0} \; , \tag{38}$$

where $\delta_{n,0}$ is the Krönecker symbol. Therefore, it can be seen that the α parameter plays the role of the electronic hopping when one does the analogy with the electronic systems. A cumbersome but straightforward calculation of commutators in the quasi-Ising regime leads to

$$\begin{aligned} s_{\pm}(m) &= e^{-\alpha B} S_{\pm}(m) e^{\alpha B} \\ &= \sum_{-\infty < n < \infty} \epsilon_n J_n(\alpha) S_{\pm}(m-n) \; , \end{aligned} \tag{39}$$

where $J_n(\alpha)$ is the Bessel function of nth order and ϵ_n is a sign given by

$$\epsilon_n = \frac{1+(-1)^n}{2}(-1)^{n/2} + \frac{1-(-1)^n}{2}(-1)^{(n-1)/2} \; . \tag{40}$$

Using the relations

$$S_-(m)S_+(m) = \tfrac{1}{2} - S_z(m) \; ,$$

$$S_+(m)S_-(m) = \tfrac{1}{2} + S_z(m) \; ,$$

one can immediately obtain the averages over the GS of the local z component of the spin, namely

$$\begin{aligned} \langle S_z(m) \rangle_{m \text{ odd}} &= -\tfrac{1}{2} + \sum_{n \text{ odd}} [J_n(\alpha)]^2 \\ &\approx -\tfrac{1}{2} + \frac{\alpha^2}{2} + o(\alpha^4) \; , \\ \langle S_z(m) \rangle_{m \text{ even}} &= \tfrac{1}{2} - \sum_{n \text{ odd}} [J_n(\alpha)]^2 \\ &\approx \tfrac{1}{2} - \frac{\alpha^2}{2} + o(\alpha^4) \; , \end{aligned} \tag{41}$$

which tell us that the deviation is second order in the anisotropy parameter α.

Excited states within the manifold of total $S_z=0$ can be obtained through application of the bosonic operator $\phi_e^\dagger$ and $\phi_o^\dagger$:

$$| \nu_e \nu_o \rangle \equiv \frac{(\phi_e^\dagger)^{\nu_e} (\phi_o^\dagger)^{\nu_o}}{\sqrt{\nu_e!}\sqrt{\nu_o!}} | G \rangle \; , \tag{42}$$

and the energy for each excitation is J. In the case of excitations of finite magnetization one should proceed differently. The canonical way of obtaining the GS through formula (35) can be used as an heuristic starting point for generating states which are approximate eigenvectors of the total Hamiltonian and have finite magnetization. For example, one can write a completely symmetrized state with $S_z=1$ in the following form:

$$\begin{aligned} | E \rangle &\equiv \left[\frac{2}{N} \right]^{1/2} \sum_{j=0}^{N/2-1} s_+(2j+1) | G \rangle \; , \\ &= \left[\frac{2}{N} \right]^{1/2} \sum_{j=0}^{N/2-1} \sum_{n=-N}^{N} \epsilon_n J_n(\alpha) S_+(2j+1-n) | G \rangle . \end{aligned} \tag{43}$$

This state can be thought to originate from the ferromagnetic $| F \rangle$ state by omitting one of $N/2$ lowering operators in (35), i.e.,

$$| E \rangle = \left[\frac{2}{N} \right]^{1/2} \sum_{j=0}^{N/2-1} s_-(1) s_-(3) \cdots \hat{s}_-(2j+1) \cdots s_-(N-3) s_-(N-1) | F \rangle \; , \tag{44}$$

where the caret here means omission of the corresponding operator.

This state is clearly orthogonal to $| G \rangle$ and its energy exceeds in J the energy of the GS (energy necessary to flip a spin in the Néel state). The calculation of the energy proceeds in the following way:

$$\langle E \mid \hat{H} \mid E \rangle = \frac{2}{N} \sum_{j,j'=0}^{N/2-1} \langle G \mid s_-(2j'+1)\hat{H} s_+(2j+1) \mid G \rangle$$
$$= \frac{2}{N} \sum_{j,j'=0}^{N/2-1} \langle N \mid S_-(2j'+1) e^{\alpha B} \hat{H} e^{-\alpha B} S_+(2j+1) \mid N \rangle \ . \tag{45}$$

We use the identity

$$e^{\alpha B}\hat{H}e^{-\alpha B} = \hat{H} + \alpha[B,\hat{H}] + \frac{\alpha^2}{2!}[B,[B,\hat{H}]] + \cdots \ , \tag{46}$$

which yields the result

$$e^{\alpha B}\hat{H}e^{-\alpha B} = \frac{JN\alpha^2}{4} + \hat{H} - J\alpha\tilde{B} \ , \tag{47}$$

where the Hermitian operator $\tilde{B}$ is given by

$$\tilde{B} \equiv \left[\frac{N}{2} \right]^{1/2} [\tfrac{1}{2}(\phi_e^\dagger + \phi_e) + \tfrac{1}{2}(\phi_o^\dagger + \phi_o)] \ . \tag{48}$$

A lengthy but straightforward calculation leads to

$$\langle E \mid \hat{H} \mid E \rangle = \frac{JN\alpha^2}{4} + E_N + J - \frac{JN\alpha^2}{2}$$
$$= E_G(\alpha) + J \ , \tag{49}$$

where E_N is the energy of the Néel state and $E_G(\alpha)$ the energy of the GS. In the limit of complete anisotropy one gets

$$\mid E \rangle \xrightarrow[\alpha \to 0]{} \left[\frac{2}{N} \right]^{1/2} \sum_{j=0}^{N/2-1} S_+(2j+1) \mid N \rangle \ , \tag{50}$$

with energy

$$\langle E \mid \hat{H} \mid E \rangle \xrightarrow[\alpha \to 0]{} E_N + J \ . \tag{51}$$

We have then obtained an approximate eigenstate of $\hat{H}$ (it is exact in the limit $\alpha \to 0$), with $S_z = 1$, and J being the energy of excitations. This state is a remnant of a spin-wave band which narrows as long as the anisotropy is increased. In fact, a wave-vector dependent state can be defined as

$$\mid E;k \rangle \equiv \left[\frac{2}{N} \right]^{1/2} \sum_{j=0}^{N/2-1} e^{ik(2j+1)} s_+(2j+1) \mid G \rangle \ , \tag{52}$$

where k is a wave number in the Brillouin zone corresponding to a sublattice (odd sites). A calculation similar to the one described above for $\mid E \rangle$, shows that states $\mid E;k \rangle$ are degenerate with $\mid E \rangle$, and that they represent possible excitations with energy J. In particular

$$\mid E \rangle = \mid E;k=0 \rangle \ , \tag{53}$$

and they are orthogonal,

$$\langle E;k' \mid E;k \rangle = \delta_{kk'} \ . \tag{54}$$

In the limit of high anisotropy all these states are piled up into a single degenerate level which is also superposed with the one-boson excitations described by $\phi_e^\dagger$ and $\phi_o^\dagger$.

Other excited states with arbitrary total z component of the spin can similarly be constructed. These states are of concern when treating the corresponding fermion models to describe high-T_c superconductivity.[10] A thorough study of the excitation spectrum is currently under way and will be published elsewhere.[10]

IV. FINAL COMMENTS

We have succeeded in obtaining for the Heisenberg antiferromagnetic chain a solution which is asymptotically exact in the limit of high anisotropy. Since our solution is in closed analytical form we gain a deep insight concerning the structure of the GS and its excitations. We also obtain a systematic way of improving our approximation for finite anisotropy by means of relations (41), which measure the deviation from the antiferromagnetic ordering, i.e., all the theory can be reformulated including corrections to the quasi-Ising regime. One hopes that this latter calculation should lead to spin-wave bands of finite width. Numerical calculations for the high anisotropic limit should be of value in order to test our predictions, but apart from obtaining the energy spectrum one should numerically study the nature of eigenvectors. This fact seriously limits the size of systems under study.[9]

The anisotropic Heisenberg chain for $S=\frac{1}{2}$ can be mapped into a fermion model by means of the Jordan-Wigner transformation.[2] If we write that transformation as

$$S_-(n) = \exp\left[-\pi i \sum_{m=1}^{n-1} C_m^+ C_m \right] C_n \ , \tag{55}$$

where the $(C_i^\dagger, C_i)$ are fermion operators, one finds that Hamiltonian (2) transforms into

$$H = \tfrac{1}{2}\alpha J \sum_m (C_{m+1}^+ C_m + C_m^+ C_{m+1})$$
$$+ J \sum_m (n_{m+1} - \tfrac{1}{2})(n_m - \tfrac{1}{2}) \ , \tag{56}$$

where $n_m \equiv C_m^\dagger C_m$ is the fermion number operator which is related to $S_z(m)$ by

$$n_m = C_m^\dagger C_m = S_z(m) + \tfrac{1}{2} \ . \tag{57}$$

There is then a relation between the total number of fermions and the total magnetization as follows:

$$N_f \equiv \sum_m C_m^+ C_m = \sum_m [S_z(m) + \tfrac{1}{2}] \ . \tag{58}$$

The fermion Hamiltonian given by (56) includes a hopping part which is proportional to αJ, and a Coulomb repulsion between nearest neighbors which is proportional to J. For states with zero total magnetization one gets the result

$$\langle N_f \rangle = \left\langle \sum_m C_m C_m \right\rangle = \frac{N}{2} , \tag{59}$$

i.e., we are dealing with half-filling cases. It is known[11] that those states are insulators; there is a gap separating the GS from the excited levels, and there is long-range order in the sense that $\langle n_i \rangle \approx 1$ for even sites while $\langle n_i \rangle \approx 0$ for odd sites, which is the fermion similar of relation (1). Our solution (19) applies here for the case of strong Coulomb repulsion between nearest neighbors.

The physical situation changes dramatically[3,10] if one allows for states of finite magnetization, where the fermion occupation number is smaller than $N/2$. For these latter cases, the GS is a superposition of many configurations that *coherently* tunnel among them, yielding a paramount mobility along the chain. Indeed, it has been shown in Ref. 3 that those states are superconductors. For this picture, the mechanism that produces superconductivity is the Coulomb repulsion in a system with low density of carriers. As long as the repulsion is increased, the band moves further away from the GS and the electrons become more localized, but the GS wave function still maintains its properties which are fully many-body effects. Further work in this direction is in progress.

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[1] J. G. Bednorz and K. A. Muller, Z. Phys. B **64**, 188 (1986).

[2] E. Lieb, T. Schulz, and D. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961); W. E. Thirring, *ibid.* **3**, 91 (1958).

[3] M. Lagos, M. Kiwi, and R. Ramirez (unpublished).

[4] M. Lagos and G. G. Cabrera, Solid State Commun. (to be published).

[5] H. Bethe, Z. Phys. **71**, 205 (1935); L. Hulthén, Ark. Mat. Astron. Fys. **26A**, 1 (1938); R. Orbach, Phys. Rev. **112**, 309 (1958); J. Bonner and M. E. Fisher, *ibid.* **135**, A640 (1964); J. des Cloizeaux and M. Gaudin, J. Math. Phys. **7**, 1384 (1966).

[6] P. W. Anderson, Phys. Rev. **86**, 694 (1952).

[7] G. Baskaran, Z. Zou, and P. W. Anderson, Solid State Commun. **63**, 973 (1987); P. W. Anderson, Mater. Res. Bull. **8**, 153 (1973).

[8] J. R. Klauder and B. Skagerstam, *Coherent States: Applications in Physics and Mathematical Physics* (World-Scientific, Singapore, 1985).

[9] Appart from exact calculations this result has also been obtained numerically using finite-size scaling techniques [M. Kolb, R. Botet, and R. Jullien, J. Phys. A **16**, L673 (1983)].

[10] M. Lagos and G. G. Cabrera (unpublished).

[11] G. Spronken, R. Jullien, and M. Avignon, Phys. Rev. B **24**, 5356 (1981); E. R. Gagliano, E. Dagotto, A. Moreo, and F. C. Alcaraz, *ibid.* **34**, 1677 (1986).