Ground states of infinite-range spin-$\frac{1}{2}$ quantum Heisenberg antiferromagnets

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We study a class of infinite-range spin-$\frac{1}{2}$ quantum Heisenberg antiferromagnets. We show that, in addition to ground states with macroscopic net spin in one or several sublattices ("Néel states"), there are valence-bond (VB) states that are local spin singlets. We show that there is a class of perturbations that stabilizes the VB state. We characterize the excitation spectrum and find an order parameter for the VB states. Finally, we extend our method to find perturbations that stabilize microscopic as well as macroscopic chiral states.

I. INTRODUCTION

The subject of the possible ground states of quantum antiferromagnets has attracted considerable interest in the past year or so. Much of this effort is connected with the search of a possible magnetic mechanism for high-temperature superconductivity. However, this is a subject of considerable importance in its own right, in view of our poor understanding of what generically are called "Mott insulators."

Much of the recent effort has concentrated on classifying the possible ground states of these systems, particularly in two dimensions. In addition to various Néel states,[1] a host of new "phases" have been proposed: resonating valence bonds (RVB)[2] (both in its long-range[3] and short-range[4,5] forms), valence-bond (VB) crystals,[6,7] flux phases,[8,9] Laughlin states,[10] and parity-broken states.[11,12] Mean-field theories for Néel-type states are fairly standard and well understood. Usually they become exact in high dimensions, particularly in the infinite-range limit. This limit has been studied extensively in the framework of the theory of classical spin glasses.[13]

The present understanding of the "less conventional" phases is quite sketchy. In this paper, we study the infinite-range version of the Heisenberg model with an eye at developing a mean-field theory for "unconventional" ground states of the antiferromagnet using techniques which are well understood for Néel states. This may seem rather surprising at first sight. Indeed, common wisdom has it that the Néel state is stable at higher dimensions because the system effectively becomes classical. This, however, is not necessarily so. We show here that an infinite-range quantum Heisenberg antiferromagnet can have "unconventional" ground states just as easily. In fact, we have been able to generalize the infinite-range model so as to stabilize (i) Néel states (with two or more sublattices; this issue has been recently addressed by Ma[14]), (ii) valence-bond crystals, and (iii) chiral states. The RVB state does not have any simple representation in this model. Interestingly enough we find two types of chiral states. One type breaks parity at the microscopic level while the other does so at the macroscopic level.

The paper is organized as follows. In Sec. **II**, we discuss the infinite-range quantum Heisenberg antiferromagnet for spin $\frac{1}{2}$. In Sec. **III**, we introduce a hierarchy of interactions (an "architecture") which stabilizes either a Néel state or a VB crystal. We also discuss the low-energy spectrum associated with both regimes. In Sec. **IV**, we discuss microscopic and macroscopic chiral states. As a bonus multisublattice Néel states also are found. Section **V** is devoted to the conclusion.

II. INFINITE-RANGE QUANTUM HEISENBERG HAMILTONIAN

Let us consider the infinite-range quantum Heisenberg antiferromagnet for a system Ω of N (even) spins $\frac{1}{2}$. The Hamiltonian is

$$H_0=J\sum_{i<j}^{N}\mathbf{S}_i\cdot\mathbf{S}_j \ , \tag{2.1}$$

where the coupling constant J is positive. The operators $\mathbf{S}_i$, $i=1,\ldots,N$, represent spin-$\frac{1}{2}$ degrees of freedom and satisfy the algebra

$$[S_i^a,S_j^b]=\delta_{ij}(\epsilon^{abc}S_j^c),\quad i,j=1,..,N \ . \tag{2.2}$$

In this form, the infinite-range nature of the interaction is equivalent to the invariance of H_0 under any permutation of the N spins. To obtain the spectrum of H_0 and its eigenstates we make explicit the invariance of H_0 under global rotations of the system. If we denote with $\mathbf{S}$ the total spin of the system Ω, the Hamiltonian can be rewritten in the form

$$H_0=\frac{J}{2}(\mathbf{S}^2-\tfrac{3}{4}N) \ . \tag{2.3}$$

The eigenvalues of H_0 are labeled with the quantum number s of the total spin

$$E_0(s)=\frac{J}{2}[s(s+1)-\tfrac{3}{4}N],\quad s=0,1,\ldots,\frac{N}{2} \ . \tag{2.4}$$

The tensorial basis of the Hilbert space

$$\begin{aligned}\mathcal{H}(\Omega)&\equiv\mathcal{H}_{1/2}\otimes\cdots\otimes\mathcal{H}_{1/2}\\&\equiv a_0\mathcal{H}_0\oplus\cdots\oplus a_{N/2}\mathcal{H}_{N/2} \ ,\end{aligned} \tag{2.5}$$

diagonalizes H_0. $\mathcal{H}_j$, $j=0,\frac{1}{2},1,\ldots$, denotes the $j(j+1)$-dimensional Hilbert space associated with an irreducible representation of SU(2), and the a_j are integers. The degeneracy of the global singlet subspace is a_0. This degeneracy is a result of the discrete permutation symmetry. The states with the lowest energy $E_0(0)$ are global singlets. They span the subspace $\mathcal{H}_0(\Omega)\equiv a_0\mathcal{H}_0$ which is, for example, one dimensional for $N=2$ and two dimensional for $N=4$. In general, the dimensionality a_0 of $\mathcal{H}_0(\Omega)$ is[15]

$$\begin{bmatrix} N \\ N/2 \end{bmatrix} \frac{1}{N/2+1} .$$

Our goal is to construct for a large, even number of spins a class of perturbations of H_0 which lifts the degeneracy of the ground states. To this end, we need to understand the structure of $\mathcal{H}_0(\Omega)$. First, we choose a procedure for obtaining the total spin $\mathbf{S}$. There are $\frac{1}{2}N!$ systems of basis which diagonalize $\mathbf{S}$. Each system corresponds to the particular order chosen to add the spins. To motivate our choice consider four spins. Label them and add them according to the rule

$$\mathbf{S}=(\mathbf{S}_1+\mathbf{S}_2)+(\mathbf{S}_3+\mathbf{S}_4)\equiv\mathbf{S}_{11}+\mathbf{S}_{12} . \tag{2.6}$$

Now, $\mathbf{S}_{11}$ and $\mathbf{S}_{12}$ can be both in a singlet or in a triplet state while adding to a global singlet state. The global singlet subspace is thus two dimensional and a possible basis can be labeled, respectively, with the quantum number $(s,s_{11},s_{12})=(0;0,0)$ and $(s,s_{11},s_{12})=(0;1,1)$.

To extend this method to larger N, assume that

$$N=2^n, \quad n=1,2,3,4,\ldots .$$

Represent the basis elements of $\mathcal{H}_0(\Omega)$ with binary trees constructed in such a way that their vertices are associated with the total spin $\mathbf{S}_{ij}$ of a subset Ω_{ij} of spin $\frac{1}{2}$ belonging to the set Ω. More precisely,

$$\begin{aligned}
&\mathbf{S}_{ij}\equiv\mathbf{S}_{(i+1)(2j-1)}+\mathbf{S}_{(i+1)(2j)} ,\\
&i=1,\ldots,n \text{ and } j=1,\ldots,2^i ;\\
&\mathbf{S}_{nj}\equiv\mathbf{S}_j, \quad j=1,\ldots,N ;\\
&\Omega_{ij}\equiv\Omega_{(i+1)(2j-1)}\cup\Omega_{(i+1)(2j)} ,\\
&i=1,\ldots,n \text{ and } j=1,\ldots,2^i ;\\
&\Omega_{nj}\equiv\{j\}, \quad j=1,\ldots,N .
\end{aligned} \tag{2.7}$$

The first index i labels the ith generation of the tree. It runs from 1 to n. The second index j labels the branch of a given generation i. It runs from 1 to 2^i. A subset Ω_{ij} contains 2^{n-i} elements (spin $\frac{1}{2}$) and hence the conserved partial spin quantum numbers s_{ij} take the values

$$s_{ij}=0,1,\ldots,2^{n-i-1} . \tag{2.8}$$

We denote with $|s,m_z;\{s_{ij}\}\rangle$, $m_z=-s,\ldots,+s$, a state with total spin quantum number s and which can be viewed symbolically as a binary tree carrying the quantum numbers s_{ij} on its vertices. When $s=0$ the global singlet $|0;\{s_{ij}\}\rangle$ is uniquely defined up to a normalization constant. A necessary and sufficient condition for $|s,m_z;\{s_{ij}\}\rangle$ to be a global singlet is that there exists a generation i_s with

$$s_{(i_s-1)j}=0, \quad j=1,\ldots,2^{i_s-1} . \tag{2.9}$$

For example, we can pair $\mathbf{S}_1$ and $\mathbf{S}_2$ into a singlet bond and repeat this for the remaining $N/2-1$ distinct pairs of spin $\frac{1}{2}$. The $N/2$ partial spins $\mathbf{S}_{(n-1)(j)}$ are by assumption singlets. Therefore, the associated global singlet is characterized uniquely by $i_s=n$. This state is called the valence-bond (VB) state and will be denoted with $|\psi_{\mathrm{VB}}\rangle$. In terms of the tree-like basis,

$$|\psi_{\mathrm{VB}}\rangle=|0;\{0,0\},\ldots,\{0,\ldots,0\},\{\tfrac{1}{2},\ldots,\tfrac{1}{2}\}\rangle .$$

Other global singlet states are generated by breaking two singlet bonds, say the singlet bonding between the pairs $(\mathbf{S}_{N-3},\mathbf{S}_{N-2})$ and $(\mathbf{S}_{N-1},\mathbf{S}_N)$, and by requiring that those triplet states combine into a singlet whenever they are added later on in the tree. The global singlets are not always uniquely characterized by i_s. The bipartite (semiclassical) Néel state [see (4.10c) and Ref. 16] corresponds, in this picture, to the global singlet state with $i_s=1$ and with the maximum, partial spin quantum number $s_{11}=N/4$. We will denote it with $|\psi_{\text{Néel}}\rangle_2^{\mathrm{cl}}$. In terms of the tree-like basis,

$$|\psi_{\text{Néel}}\rangle_2^{\mathrm{cl}}=|0;\{2^{n-i-1}\}\rangle .$$

More generally, we will call those global singlet states with one or several "sublattices" (Ω_{ij}) having a macroscopic net spin, Néel states. Whether we mean the bipartite Néel state or some less symmetric Néel state should be clear depending on the context.

III. NEEL STATE AND VALENCE-BOND STATE

A. Lifting of the degeneracy

We are now in position for constructing a class of perturbations which lifts the degeneracy of the subspace of global singlets $\mathcal{H}_0(\Omega)$. The idea is simply to introduce an operator which differentiates between basis states $|0;\{s_{ij}\}\rangle$ of $\mathcal{H}_0(\Omega)$. A possible choice is the class of operators

$$V(\{\lambda_{ij}\})\equiv\sum_{i=1}^{n}\sum_{j=1}^{2^i}\lambda_{ij}\mathbf{S}_{ij}^2 , \tag{3.1}$$

where $\{\lambda_{ij}\}$ is a set of real coupling constants. The effect of this perturbation is to merely change the couplings between pairs of spin $\frac{1}{2}$. Any operator of this form commutes with H_0 and, by construction, has only diagonal matrix elements in the basis $\{|0;\{s_{ij}\}\rangle\}$ of the global singlet subspace. Any element of this basis can have its unperturbed energy $E_0(0)$ lowered by the perturbation relative to all other basis states if the parameters λ_{ij} are chosen appropriately. For our purpose it is sufficient to consider the subclass of perturbations

$$V(\{\lambda_i\})\equiv\sum_{i=1}^{n}\lambda_i\sum_{j=1}^{2^i}\mathbf{S}_{ij}^2 , \tag{3.2}$$

where $\{\lambda_i\}$ is a set of real coupling constants. Although this class of operators has a degenerate spectrum in the subspace of global singlet states, the VB state as well as the bipartite Néel state are nondegenerate in $\mathcal{H}_0(\Omega)$ and have, respectively, the lowest and largest eigenvalues provided the λ_i, $i=1,\ldots,n$, are strictly positive:

$$V^{\mathrm{VB}}=\tfrac{3}{4}N\lambda_n \ , \tag{3.3a}$$

$$V^{\text{Néel}}=\sum_{i=1}^{n}\lambda_i 2^i\left[\frac{N}{2^{i+1}}\left[\frac{N}{2^{i+1}}+1\right]\right] . \tag{3.3b}$$

The perturbation $V(\{\lambda_i\})$ lifts the degeneracy of the subspace $\mathcal{H}_0(\Omega)$ by partially breaking the discrete permutation symmetry. This is clearly seen if we rewrite (3.2) in the form

$$V(\{\lambda_j\})=\sum_{i,j=1}^{N}J_{ij}^{(n)}(\{\lambda_i\})\mathbf{S}_i\cdot\mathbf{S}_j \ . \tag{3.4a}$$

The $N\times N$ matrix $J_{ij}^{(n)}$ is obtained with the recursive formula

$$J_{ij}^{(n)}(\{\lambda_1,\ldots,\lambda_n\})=\begin{bmatrix}J_{ij}^{(n-1)}(\{\lambda_2,\ldots,\lambda_n\})+\lambda_1\mathbf{1}^{(n-1)} & \mathbf{0}\\ \mathbf{0} & J_{ij}^{(n-1)}(\{\lambda_2,\ldots,\lambda_n\})+\lambda_1\mathbf{1}^{(n-1)}\end{bmatrix}$$

where

$$\mathbf{1}^{(n-1)}\equiv\begin{bmatrix}\mathbf{1}^{(n-2)} & \cdots & \mathbf{1}^{(n-2)}\\ \mathbf{1}^{(n-2)} & \cdots & \mathbf{1}^{(n-2)}\end{bmatrix} ,$$

and initially,

$$J_{ij}^{(1)}\equiv\begin{bmatrix}\lambda_1 & 0\\ 0 & \lambda_1\end{bmatrix} \text{ and } \mathbf{1}^{(1)}\equiv\begin{bmatrix}1 & 1\\ 1 & 1\end{bmatrix} . \tag{3.4b}$$

One is easily convinced by explicitly constructing the effective interaction $J_{ij}^{(n)}(\lambda_1,\ldots,\lambda_n)$ between two spin-$\frac{1}{2}$ $\mathbf{S}_i$ and $\mathbf{S}_j$ for, say, $n=4$ or 8, that this effective interaction is determined solely by the position in the tree $\{\Omega_{ij}\}$ of their first common ancestor $\Omega_{k_i l_j}$. (In other words, $\Omega_{k_i l_j}$ is the smallest subset of Ω which contains the ith and jth spin $\frac{1}{2}$.) The class of perturbations (3.2) has induced an ultrametric topology in the space of coupling constants $\{J_{ij}^{(n)}|i,j=1,\ldots,N\}$.

The positive parameters λ_i, $i=1,\ldots,n$, are not arbitrary for the thermodynamic limit $N=2^n\to\infty$ to be well defined. Consider the ferromagnetic state

$$|\psi_F\rangle\equiv|N/2,m_z;\{2^{n-(i-1)}\}\rangle \ .$$

The sum of its unperturbed energy and perturbation energy is

$$\begin{aligned}E^F(N)&=\frac{J}{2}\left[\frac{N}{2}\left[\frac{N}{2}+1\right]-\tfrac{3}{4}N\right]\\&\quad+\sum_{i=1}^{n}\lambda_i 2^i\left[\frac{N}{2^{i+1}}\left[\frac{N}{2^{i+1}}+1\right]\right]\\&=\left[\frac{J}{8}+\tfrac{1}{4}\sum_{i=1}^{n}\frac{\lambda_i}{2^i}\right]N^2\\&\quad+\left[-\frac{J}{4}+\tfrac{1}{2}\sum_{i=1}^{n}\lambda_i\right]N \ .\end{aligned} \tag{3.5}$$

Since the ferromagnetic energy (3.5) is an upper bound to the spectrum of $H_0+V(\{\lambda_i\})$, the thermodynamic limit exists if and only if

$$J\propto\frac{1}{N} , \tag{3.6a}$$

$$\sum_{i=1}^{n}\frac{\lambda_i}{2^i}\propto\frac{1}{N} \ . \tag{3.6b}$$

Conditions (3.6a) and (3.6b) are met if we choose

$$\begin{aligned}J&=\frac{J_0}{N},\quad J_0>0 ,\\ \lambda_i&=\frac{\lambda_0}{N},\quad \lambda_0>0 \ .\end{aligned} \tag{3.7a}$$

With this choice, we get

$$\begin{aligned}\sum_{j=1}^{n}\frac{\lambda_i}{2^i}&=\frac{\lambda_0}{N}[1-(\tfrac{1}{2})^n] ,\\ \sum_{i=1}^{n}\lambda_i&=\frac{\lambda_0}{N}\frac{\ln N}{\ln 2} \ .\end{aligned} \tag{3.7b}$$

Consequently with the choice (3.7a), as N goes to infinity the contribution to the energy (3.5) from $\sum_{i=1}^{n}\lambda_i/2^i$ is of order N while the contribution from $\sum_{i=1}^{n}\lambda_i$ is of order $\ln N$. This is important since it means that, on one hand, all those global singlets which are characterized by $\lim_{N\to\infty}i_s^{-1}=0$ [e.g., the VB state; see (2.9)] are again degenerate. Here, the largest subsets $\Omega_{i_s j}$ of those global singlets which carry nonvanishing partial spins $\mathbf{S}_{i_s j}$, only contain a finite number of spin $\frac{1}{2}$ in the thermodynamic limit. On the other hand, the perturbation still lifts partially the degeneracy of the global singlet states which have macroscopically large subsets of spin $\frac{1}{2}$ carrying nonvanishing, partial spin. The lifting is partial because two tree-like states are degenerate in the thermodynamic limit when they are characterized by $i_{s'}<i_{s''}<\infty$ and when they share the same quantum numbers s_{ij}, $i\geq i_{s''}$, while the $s_{i_{s'}j}, s_{(i_{s'}+1)j},\ldots,s_{(i_{s''}-1)j}$ are finite for the state with $i_{s'}$. But two tree-like states which differ only by having different macroscopic partial spins on the same generations of the tree, remain nondegenerate. Finally, we note that the preceding discussion is a simple consequence of the thermodynamic limit (3.6a) and (3.6b) and does not depend on the choice (3.7a) and (3.7b).

To recover the VB state as the nondegenerate ground state in the thermodynamic limit, we just modify a finite number of parameters $\{\lambda_i\}$ so as to penalize all other basis elements of $\mathcal{H}_0(\Omega)$. Define the class of Hamiltonian

$$H \equiv H_0 + V(\{\lambda_i\};\mu_1) \ , \tag{3.8}$$

where $\lambda_i > 0$, $i=1,\ldots,n$, $\mu_1>0$, and

$$V(\{\lambda_i\};\mu_1) \equiv \sum_{i=1}^{n} (\lambda_i + \delta_{n-1,i}\mu_1) \sum_{j=1}^{2^i} \mathbf{S}_{ij}^2 \ .$$

The parameters J and $\{\lambda_i\}$ are chosen so as to insure that the spectrum of H is extensive [condition (3.6)]. The indices of the positive parameter μ_1 stress the fact that a finite number of positive couplings can be introduced to stabilize other basis elements of $\mathcal{H}_0(\Omega)$. For example, in the context of a microscopic, chiral ground state, we will replace $\delta_{n-1,i}\mu_1$ with $\delta_{n-2,i}\mu_2$. In any case, the Hamiltonian (3.8) has the VB state for ground state or, if we were to reverse the sign of all $\{\lambda_i\}$ at once, the bipartite Néel state for ground state.

B. Excitation spectrum and order parameter for the Néel and VB state

The VB state,

$$|\psi_{\mathrm{VB}}\rangle \equiv |0;\{0,0\},\ldots,\{0,\ldots,0\},\{\tfrac{1}{2},\ldots,\tfrac{1}{2}\}\rangle \ ,$$

is the ground state of the class of Hamiltonians (3.8). There are $N/2$ pairs of spin-$\frac{1}{2}$ or valence bonds which are each forming a spin singlet. The energy of the VB state is

$$E^{\mathrm{VB}}(0) = E_0(0) + \tfrac{3}{4} N \lambda_n \ . \tag{3.9}$$

There are $N/2$ ways of breaking one singlet bond of the VB state. The resulting states, say

$$|1;\{1,0\},\ldots,\{1,0,\ldots,0\},\{\tfrac{1}{2},\ldots,\tfrac{1}{2}\}\rangle \ ,$$

have a global spin in the triplet state and the energy

$$E(1) = \frac{J}{2}[1(1+1)] + 1(1+1)\sum_{i=1}^{n-1}(\lambda_i + \delta_{n-1,i}\mu_1) + E^{\mathrm{VB}}(0) \ . \tag{3.10}$$

More generally, the breaking of m, $1 \le m \le N/2$, singlet bonds of the VB state costs at least an amount $1(1+1)m\mu_1$ in perturbation energy. The energy cost $1(1+1)\mu_1$ is a lower bound to the energy differences between the VB state and all the other states $|s,m_z;\{s_{ij}\}\rangle$ which can only become exact when $m=1$ and $N\to\infty$. As a result, in the thermodynamic limit, the lowest excitation states of (3.8) form an $(N/2)-$dimensional subspace of $\mathcal{H}_1$ [see (2.5)] and the energy gap between the VB state and those global spin-1 states is $2\mu_1$.

The operator

$$M^{\mathrm{VB}} \equiv -\frac{\partial}{\partial \mu_1} H = -\sum_{j=1}^{2^{n-1}} \mathbf{S}_{n-1,j}^2 \ , \tag{3.11a}$$

has the eigenvalues

$$\{0,-1\times 2,-2\times 2,\ldots,-m\times 2,\ldots,-(N/2)\times 2\} \tag{3.11b}$$

for our tree-like basis. The VB state is a nondegenerate eigenstate of M^{VB} with the largest eigenvalue. The states obtained by breaking one, two, ..., all the bonds of the VB state have decreasing eigenvalues. The bipartite Néel state and, in this respect, the ferromagnetic state belong to the same eigenspace of M^{VB} (namely, the one with the lowest possible eigenvalue). For this reason we interpret the operator M^{VB} as the order operator for the VB state.

If we reverse the sign of all parameters $\{\lambda_i\}$, the bipartite Néel state becomes the ground state of (3.8). For example, the global singlet state

$$|0;\{N/4-1,N/4-1\},\{N/8,\ldots,N/8\},\ldots,\{1/2,..,1/2\}\rangle$$

has the excitation energy $|\lambda_1|N = |\lambda_0|$, while the global triplet state $|1,m_z;\{2^{n-(i+1)}\}\rangle$ has the excitation energy $(J_0/2N)1(1+1)$. We see that in the thermodynamic limit, all the states with $s_{11}=s_{12}=N/4$ and s finite are degenerate in energy with the bipartite Néel state.

The order operator for the bipartite Néel state is the staggered magnetization

$$M_2^{\text{Néel}} \equiv S_{11}^z - S_{12}^z \ , \tag{3.12a}$$

with the eigenvalues

$$\{0,\pm 1,\ldots,\pm N/2\} \ . \tag{3.12b}$$

Here, the bipartite Néel state is the nondegenerate eigenstate with the eigenvalue of magnitude $N/2$ while the VB state as well as the ferromagnetic state are eigenstates with the eigenvalue 0. The bipartite Néel state order operator is not invariant under a uniform rotation of all spin $\frac{1}{2}$ in the system. This behavior is crucially different from that of the VB order operator (3.11a) which is left unchanged under the local transformation

$$\exp\left[i\sum_{j=1}^{2^{n-2}} \alpha_{(n-1)j}\cdot \mathbf{S}_{(n-1)j} \right] \ ,$$

where the $\alpha_{(n-1)j}$, $j=1,\ldots,2^{n-2}$, are local angles of rotation. In other words, the Néel state breaks spontaneously the rotational symmetry of the Hamiltonian (3.8) in sharp contrast to the VB state. It would seem that, in accordance to Goldstone theorem, it is precisely the spontaneous symmetry breaking of the rotational symmetry for the Néel case which causes the energy spectrum to become gapless in the thermodynamic limit. Conversely, the absence of spontaneous symmetry breaking of a continuous symmetry in the VB case explains why the energy spectrum has a gap in the thermodynamic limit. In the present context, however, the former result cannot be obtained from Goldstone theorem since the theorem only applies to spontaneously broken theories with sufficiently local (i.e., short range) interactions.[17] For example, the infinite-range ferromagnetic Heisenberg model (2.1) with

$J<0$ has an energy gap between the ground-state energy and the first excited energy level which survives the thermodynamic limit, namely

$$\lim_{N\to\infty}[E_0(s)-E_0(s-1)]|_{s=N/2}=|J_0| \ .$$

Hence, the prediction of the Goldstone theorem is not fulfilled in the ferromagnetic case since no new degenerate states are added to the ground-state subspace $\mathcal{H}_{N/2}$ [see (2.5)] in the thermodynamic limit.

Finally, we note that the perturbation (3.1) could be used to stabilize any global singlet state. In particular, it can stabilize extensions of the bipartite Néel state to 2^i-partite Néel state (i finite). First, define for $i=1,\dots,n$, the operator

$$M_{2^i}\equiv\sum_{j=1}^{2^i}(-1)^j S_{ij}^z \ . \tag{3.13}$$

Note that the VB state is an eigenstate with eigenvalue 0 for M_{2^i}, $i=1,\dots,n-1$, while it is projected onto its orthogonal space when $i=n$. Consequently, the expectation value of (3.13) for the VB state vanishes for all generations i. Now, the 2^i-partite Néel state is the global singlet state which is the nondegenerate eigenstate of (3.13) with the eigenvalue of magnitude $N/2$ and for which the S_{ij}^z give extensive eigenvalues of magnitude $N/2^{i+1}$, $i=i_s$ being independent of N when the thermodynamic limit is taken [i.e., $i=i_s$ is finite and according to the discussion following (2.9), there are macroscopically large subsets of spin-$\frac{1}{2}$ carrying a macroscopic partial spin].

IV. MICROSCOPIC AND MACROSCOPIC CHIRAL STATES

A. Microscopic chiral state and excitation spectrum

Besides the VB state or the bipartite Néel state, other types of ground states can be stabilized starting from the class of infinite-range Hamiltonian (3.8). For example, the analog of the chiral state introduced on a square lattice[12] can be obtained as follows. Consider the class of Hamiltonian (3.8) with μ_1 replaced by μ_2. In other words, the ground-state subspace is now $2^{N/4}$ dimensional. It is spanned by all those tree-like states with singlet, partial spin on all the disjoint subsets $\Omega_{(n-1)j}$, $j=1,\dots,N/4$, consisting of four spin $\frac{1}{2}$. Define the operators

$$\chi_{123}^{(j)}\equiv\frac{4}{\sqrt{3}}\mathbf{S}_{4j-3}\cdot(\mathbf{S}_{4j-2}\times\mathbf{S}_{4j-1}) \ , \quad j=1,\dots,2^{n-2} \ , \tag{4.1a}$$

which all commute with $\mathbf{S}_{123}^{(j)}\equiv\mathbf{S}_{4j-3}+\mathbf{S}_{4j-2}+\mathbf{S}_{4j-1}$, $j=1,\dots,2^{n-2}$ [although not with the spins on the nth and on the $(n-1)$th branches of the binary tree] and moreover have the eigenvalues $c_j=-1,0,+1$ with the corresponding eigenstates

$$|s_{123}^{(j)},m_{s_{123}^{(j)}};c_j\rangle\in\{|\tfrac{1}{2},m_{1/2};-1\rangle,|\tfrac{3}{2},m_{3/2};0\rangle,|\tfrac{1}{2},m_{1/2};1\rangle\}, \quad m_{s_{123}^{(j)}}=-s_{123}^{(j)},\dots,+s_{123}^{(j)} \ . \tag{4.1b}$$

Any arbitrary $\chi_{123}^{(j)}$ breaks parity (P) and time-reversal (T) symmetry. Indeed under a time-reversal transformation the spin operators change signs. The $\chi_{123}^{(j)}$ also changes sign under an odd permutation of the three spin operators. Geometrically, an odd permutation of (123) amounts to reversing the direction of circulation around a triangle with vertices labeled 1,2,3. In this sense, the nonvanishing expectation value of $\chi_{123}^{(j)}$ is interpreted as the breaking of parity. Consequently, the chiral state

$$|\{c_j\}\rangle\equiv\prod_{j=1}^{2^{n-2}}\left[\frac{1}{\sqrt{2}}\left|\frac{1}{2},+\frac{1}{2};c_j\right\rangle\otimes\left|-\frac{1}{2}\right\rangle-\frac{1}{\sqrt{2}}\left|\frac{1}{2},-\frac{1}{2};c_j\right\rangle\otimes\left|+\frac{1}{2}\right\rangle\right] \tag{4.2}$$

is one such that the expectation value $\langle\{c_j\}|\chi_{123}^{(j)}|\{c_j\}\rangle$ is nonvanishing for any $j\in\{1,\dots,2^{n-1}\}$.

We use (3.8) with μ_1 replaced by μ_2 to define

$$H_{mc}\equiv H+H_I \ , \tag{4.3a}$$

where $H_I\equiv-\sum_{j=1}^{2^{n-2}}h(j)\chi_{123}^{(j)}$ and $h(j)\neq 0$, $j=1,\dots,N/4$. The ground state of this class of Hamiltonian is unique and has the form (4.2) in the thermodynamic limit (for which the $\lambda_{n,n-1}$ vanish). If the "magnetic" field $h(j)$ is chosen to be uniform, then the quantum numbers of the ground state are $c_j=\mathrm{sgn}(h)$, $j=1,\dots,2^{n-2}$. The ground-state energy is given in the thermodynamic limit by

$$E_{mc}(0)=E_0(0)-|h|\frac{N}{4} \ . \tag{4.3b}$$

If the "magnetic" field is staggered, then the ground state has alternating quantum numbers $c_j=\mathrm{sgn}[h(j)]$, $j=1,\dots,2^{n-2}$, and the same energy as in the uniform case. The manifold of low-lying excitation states is made of two families of states. For a given "magnetic field" $h(j)$, $j=1,\dots,2^{n-2}$, the state obtained from the ground state by "flipping" the quantum number c_k on the kth triangle $(4k-3)(4k-2)(4k-1)$ has the excitation energy $2|h(k)|$. Consequently when the magnitude of the "magnetic field" is uniform, there are $N/4$ independent states with the excitation energy $2|h|$. The second family of low-lying excitations is obtained from the ground state (4.2) by pairing the fourth spin $\frac{1}{2}$ on the kth branch of the tree-like basis with the $s_{123}^{(k)}=\frac{1}{2}$ eigenstate (4.1b) into a triplet. The excitation energy of this state is given in the thermodynamic limit by $1(1+1)\mu_2$ [see (3.10)]. Pairing the fourth spin $\frac{1}{2}$ with the $s_{123}^{(k)}=\frac{3}{2}$ eigenstate costs an extra $|h(k)|$ in energy. We thus conclude that the Hamiltonian (4.3a) has a gap in its excitation spectrum. Depending on the ratio $|h|/\mu_2$ the lowest excitation states are global singlet or global spin-1 chiral states. The chiral ground state is microscopic because the order operator $\chi_{123}^{(j)}$ corresponds geometrically to the circulation around a triangle on whose vertices the smallest possible spins are sitting.

B. Macroscopic chiral state

We want to investigate the possibility of stabilizing a macroscopic, chiral, singlet state, i.e., one which generates a nonvanishing expectation value for the order operator

$$\chi_{ABC} \equiv \mathbf{S}_A \cdot (\mathbf{S}_B \times \mathbf{S}_C) , \tag{4.4a}$$

while belonging to the global, singlet eigenspace of the unperturbed infinite-range Hamiltonian

$$H_0' \equiv J(\mathbf{S}_A + \mathbf{S}_B + \mathbf{S}_C)^2, \quad J > 0 . \tag{4.4b}$$

The macroscopic nature of this state comes about if the spins $\mathbf{S}_{A,B,C}$ are constructed out of $3N$, N even, spin $\frac{1}{2}$ by partitioning those spin $\frac{1}{2}$ into three disjoint subsets $\Omega_{A,B,C}$ which each contain N spin $\frac{1}{2}$.

We show that the operator χ_{ABC} has a nonvanishing and macroscopic (i.e., proportional to N) expectation value for some global singlet states. Our argument goes as follows. We first introduce the raising and lowering spin operators S^+ and S^- in terms of which

$$\chi_{ABC} = \frac{i}{2}(-S_A^- S_B^+ S_C^z + S_A^+ S_B^- S_C^z + S_A^- S_B^z S_C^+ - S_A^+ S_B^z S_C^- - S_A^z S_B^- S_C^+ + S_A^z S_B^+ S_C^-) . \tag{4.5}$$

Now, we note that the quantum number $s_{A,B,C}$ are not arbitrary in the global singlet subspace. If we choose the prescription $\mathbf{S} = (\mathbf{S}_A + \mathbf{S}_B) + \mathbf{S}_C$ for adding the partial spins, a necessary condition to have $s=0$ is that the quantum number s_{AB} (the notation is obvious) equals s_C. For example, for 6 spin $\frac{1}{2}$ the global singlet subspace is five dimensional and its tensorial basis can be labeled with

$$|s_{AB};s_A,s_B,s_C\rangle \in \{ |0;0,0,0\rangle, |0;1,1,0\rangle, |1;1,0,1\rangle, |1;0,1,1\rangle, |1;1,1,1\rangle \} . \tag{4.6a}$$

Note that the last state on the right-hand side (RHS) of (4.6a) is the tensorial representation of the semiclassical triangular Néel state for which an alternative representation is given in terms of a Young tableau by Ma.[14] An explicit calculation yields, for this basis,

$$\langle i|\chi_{ABC}|j\rangle = \frac{2}{3} \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & i & -i & 0 \\ 0 & -i & 0 & i & 0 \\ 0 & i & -i & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} . \tag{4.6b}$$

This example partly confirms our prediction, but it can be misleading in that it is too simple. For $N>2$, the quantum numbers $s_{AB};s_A,s_B,s_C$ do not uniquely specifiy the tensorial basis elements of the global singlet subspace as a consequence of the permutation symmetry in each of the subsets $\Omega_{A,B,C}$. More disturbingly, nearly all of the tensorial basis elements of the singlet subspace are mixed by χ_{ABC}. Nevertheless, the simple mixing found in (4.6b) partly survives for larger N. The extension of the basis elments (4.6a) to a set of three global singlet states characterized by two of the spin quantum numbers sitting on the vertices of the triangle ABC with the same arbitrary integer value l, $l=1,\ldots,N/2$, while the third spin is in a singlet state, is

$$\{ |1\rangle, |2\rangle, |3\rangle \} \equiv \{ (2l+1)^{-1/2} \times \sum_{m=-1}^{l} (-1)^{l+m} |m,-m,0\rangle , \text{ and c.p.}(0) \} \tag{4.7a}$$

where c.p(0) represents the cyclic permutation of the 0. Explicit calculation for the matrix elements for these three state gives

$$\langle i|\chi_{ABC}|j\rangle = (-1)^{l+1} \frac{l(l+1)}{2l+1} \begin{bmatrix} 0 & i & -i \\ -i & 0 & i \\ i & -i & 0 \end{bmatrix} . \tag{4.7b}$$

Consequently, some matrix elements of χ_{ABC} in the tensorial basis of the singlet subspace are proportional to $N/4$ in the thermodynamic limit. This suggests that χ_{ABC} can have extensive eigenvalues in the global singlet subspace. But, in any case, we have proven the weaker statement that there exists a global singlet state for which χ_{ABC} has a macroscopic expectation value, namely, either one of the two linear combinations of the states (4.7a) which are eigenstates of the Hermitean matrix on the RHS of (4.7b) with nonvanishing eigenvalues.

Let $\mathcal{H}_{123}$ be the subspace which is spanned by the normalized and orthogonal basis (4.7a). The corresponding truncated chiral operator which is represented by (4.7b) has the normalized eigenstates

$$\begin{aligned} |-\rangle &= 3^{-1/2}(-e^{-i\pi/3}|1\rangle + |2\rangle - e^{+i\pi/3}|3\rangle) , \\ |0\rangle &= 3^{-1/2}(|1\rangle + |2\rangle + |3\rangle) , \\ |+\rangle &= 3^{-1/2}(-e^{+i\pi/3}|1\rangle + |2\rangle - e^{-i\pi/3}|3\rangle) , \end{aligned} \tag{4.8a}$$

with the corresponding eigenvalues

$$-\sqrt{3}(-1)^{l+1}\frac{l(l+1)}{2l+1}, \ 0, \ , +\sqrt{3}(-1)^{l+1}\frac{l(l+1)}{2l+1} . \tag{4.8b}$$

We note that the eigenstates of the truncated chiral operator are linear superpositions of the basis (4.7a) with coefficients of uniform magnitude and that state $|-\rangle$ is the complex conjugate of state $|+\rangle$. The linear combination corresponding to the largest possible eigenvalue in (4.8b) is a generic state for all those spin-$\frac{1}{2}$ configurations for which one of the quantum numbers among s_A, s_B, s_C vanishes while the other two are in the largest possible spin state $l=N/2$. This linear combination has the same degeneracy as the global singlet subspace of N spin $\frac{1}{2}$. When $N=2^n$, we know how to stabilize the bipartite Néel state of, say, the subset Ω_C. Therefore, the perturbation made of the appropriate function of χ_{ABC} added to the appropriate class of Hamiltonian (3.2) could in principle stablize a macroscopic, chiral, singlet state. The state is pictured as a triangle ABC on whose vertices two macroscopic spins, which correspond to a ferromagnetic configuration of spin $\frac{1}{2}$, are resonating with a singlet corresponding to a bipartite Néel-type configuration of the underlying spin $\frac{1}{2}$. It is precisely the fact that χ_{ABC} and the class of perturbation (3.2) do not commute that causes the resonance. But this absence of commutativity makes it more difficult to construct the appropriate perturbation.

The simplest guess for the class of Hamiltonian stabilizing a macroscopic, chiral, singlet state is

$$H'\equiv H_0'-V_A(\{\lambda_i\})-V_B(\{\lambda_i\})-V_C(\{\lambda_i\})-\chi_{ABC} \ . \tag{4.9}$$

The positive parameters J and λ_i, $i=1,\ldots,n$, satisfy conditions (3.6). (We are implicitly assuming that χ_{ABS} has an extensive spectrum.) The matrix elements of H' with respect to the basis elements (4.7a) are the same as in (4.7b) except for the vanishing diagonal elements being replaced by the parameter [see (3.3b)] $-3V^{\text{Néel}}$. Consequently, the eigenvalues of this 3×3 matrix become $-3V^{\text{Néel}}$ and

$$-3V^{\text{Néel}}\pm\sqrt{3}(-1)^{l+1}\frac{l(l+1)}{(2l+1)} \ ,$$

where $l=N/2$. The lowest eigenvalue

$$-3V^{\text{Néel}}-\sqrt{3}\frac{l(l+1)}{(2l+1)}$$

of the truncated Hamiltonian H' acting on the three-dimensional subspace $\mathcal{H}_{123}$ is an upper bound to the true ground-state energy. The true ground state must necessarily be a macroscopic, chiral, singlet state since $-3V^{\text{Néel}}$ is the lowest eigenvalue of $-V_A(\{\lambda_i\})-V_B(\{\lambda_i\})-V_C(\{\lambda_i\})$.

To study the properties of the eigenstate (4.8a), we compare them to the ground state of the infinite-range Hamiltonian

$$\begin{aligned} H_0''&=J(\mathbf{S}_A\cdot\mathbf{S}_B+\mathbf{S}_A\cdot\mathbf{S}_C+\mathbf{S}_B\cdot\mathbf{S}_C)\\ &=\tfrac{1}{2}(H_0'-J\mathbf{S}_A^2-J\mathbf{S}_B^2-J\mathbf{S}_C^2) \ . \end{aligned} \tag{4.10a}$$

The ground state has the energy

$$E_0''(0)=-\tfrac{3}{2}Jl(l+1), \quad \text{where } l=\frac{N}{2} \ , \tag{4.10b}$$

and can be given a semiclassical interpretation since

$$\begin{aligned} \langle\mathbf{S}_A\cdot\mathbf{S}_B\rangle&=\langle\mathbf{S}_A\cdot\mathbf{S}_C\rangle\\ &=\langle\mathbf{S}_B\cdot\mathbf{S}_C\rangle=\cos\left[\frac{2\pi}{3}\right]l(l+1) \ . \end{aligned} \tag{4.10c}$$

This ground state mimics the configuration of three two-dimensional vectors of magnitude $l^2+O(1/l)$ which minimizes the classical version of (4.10) (see Refs. 1–3 and 14). Hence, we call this ground state the semiclassical Néel state for a tripartite partition of $3N$ spin $\frac{1}{2}$ and denote it with $|\psi_{\text{Néel}}\rangle_3^{\text{cl}}$. With respect to the tensorial basis[16] (the notation is obvious)

$$\begin{aligned} |\psi_{\text{Néel}}\rangle_3^{\text{cl}}&=(2l+1)^{-1/2}\\ &\quad\times\sum_{m=-l}^{l}(-1)^{l+1}|l;m\rangle_{l\otimes l}\otimes|l;-m\rangle \ ,\\ l&=\frac{N}{2} \ . \end{aligned}$$

The expectation value of H_0'' and the analog of (4.10c) for the eigenstates (4.8a) of the truncated chiral operator are easily obtained from the fact that the states $|1,2,3\rangle$ are all eignestates of $\mathbf{S}_A\cdot\mathbf{S}_B$, $\mathbf{S}_A\cdot\mathbf{S}_C$, and $\mathbf{S}_B\cdot\mathbf{S}_C$ with the eigenvalues $-l(l+1)$ or 0. More precisely, in the subspace $\mathcal{H}_{123}$

$$\begin{aligned} \mathbf{S}_A\cdot\mathbf{S}_B&=-l(l+1)|1\rangle\langle1| \ ,\\ \mathbf{S}_A\cdot\mathbf{S}_C&=-l(l+1)|2\rangle\langle2| \ ,\\ \mathbf{S}_B\cdot\mathbf{S}_C&=-l(l+1)|3\rangle\langle3| \ . \end{aligned} \tag{4.11}$$

To understand (4.11), recall that the basis states (4.7a) are the tensorial product of a semiclassical Néel state $|\psi_{\text{Néel}}\rangle_2^{\text{cl}}$ for a bipartition of $2N=4l$ spin $\frac{1}{2}$ with a singlet state for N spin $\frac{1}{2}$ (see Ref. 16). Henceforth,

$$\mathbf{S}_I\cdot\mathbf{S}_J=\tfrac{1}{2}(S_I^+S_J^-+S_I^-S_J^+)+S_I^zS_J^z \ , \quad I,J\in\{A,B,C\} \ ,$$

when acting on the state with Ω_I and Ω_J in the bipartite Néel state gives the eigenvalue $-l(l+1)$, $l=N/2$, but when acting on Ω_I or Ω_J in the singlet state gives the eigenvalue 0. This fact and the unitarity of the transformation relating (4.7a) to (4.8a) allows us to write

$$\begin{aligned} H_0''&=-Jl(l+1)(|1\rangle\langle1|+|2\rangle\langle2|+|3\rangle\langle3|+\cdots)\\ &=-Jl(l+1)(|-\rangle\langle-|+|0\rangle\langle0|+|+\rangle\langle+|+\cdots) \ . \end{aligned} \tag{4.12a}$$

The eigenstates (4.8a) are degenerate with the energy

$$E_c''(0)=-Jl(l+1) \ , \tag{4.12b}$$

and give the expectation value

$$\begin{aligned} \langle I|\mathbf{S}_A\cdot\mathbf{S}_B|I\rangle&=\langle I|\mathbf{S}_A\cdot\mathbf{S}_C I\rangle\\ &=\langle I|\mathbf{S}_B\cdot\mathbf{S}_C|I\rangle=-\tfrac{1}{3}l(l+1) \ , \end{aligned} \tag{4.12c}$$

where $I\in\{-,0,+\}$ and $l=N/2$. This shows that the states $|-\rangle$ and $|+\rangle$ for which the chiral operator χ_{ABC}

develops a macroscopic expectation value, are excited states of the infinite-range antiferromagnetic Hamiltonian on a tripartite sublattice and that they possess a tripartite Néel order. The classical analog of these states is the configuration of three three-dimensional vectors of magnitude $l^2+O(1/l)$ such that they are directed along the edges of a regular, triangular wedge with the angle $\arccos(-1/3)$ between any pair of edges.

V. CONCLUSIONS

In this paper we have considered the infinite-range quantum Heisenberg model. We showed that by simple generalizations of this Hamiltonian it is possible to lift the (infinite) degeneracy of the singlet subspace. We formed, for the ground state, various Néel states as well as VB and chiral states. We found the low-lying spectrum for the Néel, VB, and chiral phases. This work shows that, contrary to common belief, it is possible to think of VB's and even chiral states in a mean-field sense. They are classical limits of states based on a singlet description, such as quantum dimers and others. We find that the Néel states have a gapless spectrum. This result, while natural for local Hamiltonian, is far from obvious in this singular limit. Conversely, we found that VB states have a nonzero energy gap. The microscopic chiral state was also shown to develop a gap. The macroscopic chiral state is likely to retain some tripartite Néel order and it is possible that it is gapless. We expect that these results may help to elucidate the nature of mean-field theory for these states. Finally, it would be quite interesting to relate this study to the large d limit (d being the dimension of space) of a local Heisenberg model.

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