Heisenberg models and a particular isotropic model

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The Heisenberg model, a quantum-mechanical analogue of the Ising model, has a large ground-state degeneracy, due to the symmetry generated by the total spin. This symmetry is also responsible for degeneracies in the rest of the spectrum. We discuss the global structure of the spectrum of Heisenberg models with arbitrary couplings, using group-theoretical methods. The Hilbert space breaks up in blocks characterized by the quantum numbers of the total spin, S and M, and each block is shown to constitute the representation space of an explicitly given irreducible representation of the symmetric group S_N, consisting of permutations of the N spins in the system. In the second part of the paper we consider, as a concrete application, the model where each spin is coupled to all the other spins with equal strength. Its partition function is written as a single integral, elucidating its N dependence. This provides a useful framework for studying finite-size effects. We give explicit results for the heat capacity, revealing interesting behavior just around the phase transition.

I. INTRODUCTION

The Ising model is one of the best known models of interacting spins. In its simplest form, with nearest-neighbor interactions only, the Hamiltonian is

$$H_{\text{Ising}} = -J \sum_{\langle ij \rangle} s_i s_j , \tag{1}$$

where the spins take the values $+1$ (up) or -1 (down) and the summation is over nearest-neighbor pairs $\langle ij \rangle$. The ground state of the model depends on the sign of the coupling parameter J. If $J > 0$ (ferromagnetic behavior), the spins tend to align themselves with their neighbors, and the ground state is the configuration with either all the spins up or all down. For $J < 0$ (antiferromagnet) the ground state is the checkerboardlike Néel state, with all the spins up at the even sites [a site $i = (i_1, i_2, \ldots, i_d)$ is called even (odd) when $i_1 + i_2 + \cdots + i_d$ is even (odd)] and down at the odd sites or the other way round. The twofold degeneracy of the ground state in both cases reflects the spontaneous breaking of the Z_2 symmetry of flipping all the spins.

The Heisenberg model is a quantum-mechanical analogue of the Ising model (for an introduction see, e.g., Ref. 1; an early discussion can be found in Ref. 2). The spectrum of this model is not as well understood, in particular the antiferromagnetic ground state is not known. In the Heisenberg model, however, there is a global rotation symmetry, associated to the operator of the total spin, which is very helpful in determining the global structure of the spectrum. This applies to the model in its most general form, i.e., with arbitrary coupling between each pair of spins.

In the first part of this paper we discuss the global spectral structure of Heisenberg models from a group-theoretical point of view. We start with a pedagogical introduction to the Heisenberg model (Sec. II), demonstrating the role of the total-spin operator and writing down explicitly the degenerate ferromagnetic ground states. In Sec. III we consider the consequences of the global rotational symmetry for the rest of the spectrum. It is shown that the spectrum breaks up into blocks labeled by the quantum numbers of the total spin and characterized by an explicitly given representation of S_N, the symmetric group on N elements. Parts of this presentation are well known, but our approach provides an attractive alternative point of view, which exposes clearly the S_N-representation structure of the spectrum.

In Sec. IV we consider the isotropic infinite-range Heisenberg model, with all the spins equally coupled. In this model, knowledge of the global structure of the spectrum is sufficient to write the partition function in the form of a single integral which shows a simple dependence on N. This result is particularly interesting for studying finite-size deviations from the model's thermodynamic ($N \to \infty$) behavior. As a concrete application we present calculations for the heat capacity.

II. THE HEISENBERG MODEL

In the Heisenberg model, the spins are operators in a Hilbert space. The Hamiltonian is

$$H = -J \sum_{\langle ij \rangle} \mathbf{s}_i \cdot \mathbf{s}_j , \tag{2}$$

where the components s_i^x, s_i^y, s_i^z of a single spin $\mathbf{s}_i$ constitute a set of generators of the rotation group SU(2). The spins satisfy the commutation relations

$$[s_i^a, s_j^b] = i \delta_{ij} \varepsilon^{abc} s_i^c . \tag{3}$$

For a single spin, the states are labeled by the quantum numbers (s, m), determined by the eigenvalues $s(s+1)$ and m of $\mathbf{s}^2$ and s^z, respectively. We shall restrict ourselves to the spin-$\frac{1}{2}$ case, which bears a close resemblance to the Ising model. We take $s^a = \sigma^a / 2$, where the σ^a are the Pauli matrices

$$\sigma^x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} , \quad \sigma^y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} , \quad \sigma^z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} , \tag{4}$$

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in terms of which the up state is $\binom{1}{0}$, with quantum numbers $(s=\frac{1}{2}, m=\frac{1}{2})$, and the down state is $\binom{0}{1}$ with $(s=\frac{1}{2}, m=-\frac{1}{2})$.

It is convenient to write the Hamiltonian as

$$H=-J\sum_{\langle ij\rangle}s_i^z s_j^z+\frac{1}{2}(s_i^+ s_j^- +s_i^- s_j^+) , \qquad (5)$$

in terms of the usual ladder operators

$$s^{\pm}=s^x\pm is^y \qquad (6)$$

with the properties

$$s^+\begin{bmatrix}1\\0\end{bmatrix}=0, \quad s^+\begin{bmatrix}0\\1\end{bmatrix}=\begin{bmatrix}1\\0\end{bmatrix} ,$$

$$s^-\begin{bmatrix}1\\0\end{bmatrix}=\begin{bmatrix}0\\1\end{bmatrix}, \quad s^-\begin{bmatrix}0\\1\end{bmatrix}=0 . \qquad (7)$$

The $s_i^z s_j^z$ term in (5) has the same effect as the Ising Hamiltonian (1). It tends to align the neighboring spins (i,j) (anti)parallel in the (anti)ferromagnetic case. The term between parentheses in (5), sometimes called the fluctuation term, is special to the quantum case. It gives zero when acting on parallel neighboring spins, so that the ferromagnetic Ising ground states with all spins up or all down are also ground states of the Heisenberg ferromagnet. Its effect on a pair of opposite spins, however, is to flip both the spins, so that the Néel states are not even

eigenstates of the Heisenberg antiferromagnet. For a two-spin system the solution is of course to take the antisymmetric (singlet) combination

$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle) , \qquad (8)$$

but for a system of many spins the antiferromagnetic ground state is not known.

However, there is more to the ferromagnetic Heisenberg model as well. Its ground-state degeneracy is not just twofold but $(N+1)$-fold, where N is the number of spins in the system (see Refs. 3 and 4). The reason for this large degeneracy is that the total-spin operator **S** commutes with the Hamiltonian, providing us with the quantum numbers S and M. Since the components $S^{x,y,z}$ do not mutually commute, one can create states with $M=-S+1,-S+2,\ldots,S$, degenerate in energy, by repeated application of S^+ on a state with $M=-S$. Of course, the degeneracy is lifted when the global symmetry is broken by an external magnetic field, through the addition of an interaction term

$$H_B=BS^z=B\sum_i s_i^z \qquad (9)$$

to the Hamiltonian. This causes a "fanning out" of the energy levels, the familiar Zeeman effect.

It is amusing to see what the nontrivial ground states actually look like, using this ladder procedure. Starting from the state with all spins down one obtains the states

$$|0\rangle=|\downarrow\downarrow\cdots\downarrow\rangle ,$$

$$|1\rangle=\frac{1}{\sqrt{N}}(|\uparrow\downarrow\cdots\downarrow\rangle+|\downarrow\uparrow\downarrow\cdots\downarrow\rangle+\cdots+|\downarrow\cdots\downarrow\uparrow\rangle) ,$$

$$|2\rangle=\begin{bmatrix}N\\2\end{bmatrix}^{-1/2}(|\uparrow\uparrow\downarrow\downarrow\cdots\downarrow\rangle+|\uparrow\downarrow\uparrow\downarrow\cdots\downarrow\rangle+\cdots+|\downarrow\cdots\downarrow\downarrow\uparrow\uparrow\rangle) , \qquad (10)$$

$$\vdots$$

$$|N\rangle=|\uparrow\uparrow\cdots\uparrow\rangle .$$

The state $|K\rangle$ is the properly normalized symmetric sum over the $\binom{N}{K}$ states with K spins up and $N-K$ spins down. Its quantum numbers are

$$S=\tfrac{1}{2}N, \quad M=K-\tfrac{1}{2}N , \qquad (11)$$

in terms of which

$$S^{\pm}|K\rangle=\sqrt{(S\pm M+1)(S\mp M)}|K\pm1\rangle . \qquad (12)$$

At first sight it may seem surprising that the states $|K\rangle$, containing antiparallel spin pairs, are ground states of the ferromagnet. A particularly interesting one is $|\frac{1}{2}N\rangle$, a linear combination of states with as many up as down spins (even the Néel states contribute to it!). More generally, for finite N each of the 2^N basis vectors

$|\pm,\pm,\cdots,\pm\rangle$ (where $+=\uparrow$, $-=\downarrow$) has a nonzero projection on one of the $(N+1)$ ground states of the ferromagnet. This indicates that this set of basis vectors is not very suitable to describe the spectrum of the Heisenberg model. The reason is of course that the up and down states are defined with respect to a predefined z axis, obscuring all rotational symmetry.

To illustrate the relation with global rotational symmetry, consider for example the expectation value of the two-point function $\langle s_i^z s_j^z\rangle$ in the different ground states. For the states $|0\rangle$ and $|N\rangle$ one finds

$$\langle s_i^z s_j^z\rangle=\tfrac{1}{4} , \qquad (13)$$

but the other ground states give

$$\langle K | s_i^z s_j^z | K \rangle = \frac{1}{4} \left[1 - 4 \frac{K(N-K)}{N(N-1)} (1 - \delta_{ij}) \right] . \quad (14)$$

Summation over i and j gives $(\frac{1}{2}N - K)^2 = M^2$, confirming the S^z eigenvalue of $|K\rangle$. The average of Eq. (14) over the ground states $|K\rangle$ is

$$_{av}\langle s_i^z s_j^z \rangle_{av} = \frac{1}{12}(1 + 2\delta_{ij}) . \quad (15)$$

For $i \neq j$, this is one-third of the value $\frac{1}{4}$ it attains in the states $|0\rangle$ and $|N\rangle$, as expected from rotational invariance.

The rotational symmetry generated by the total spin is a general feature of Heisenberg models, it is not typical of the nearest-neighbor model with equal interaction strengths we have been considering so far. In fact, the entire spectrum breaks up in blocks labeled by the quantum numbers of the total spin, each block being characterized by a certain irreducible representation of S_N, the symmetric group, or permutation group, on N elements. This is the topic of the next section.

III. STRUCTURE OF THE SPECTRUM

We will start out with a general spin-$\frac{1}{2}$ Hamiltonian for a system of N spins,

$$H = -\sum_{\langle ij \rangle} J_{ij} \mathbf{s}_i \cdot \mathbf{s}_j \quad (16)$$

$$= -\frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}} J_{ij} \left[s_i^z s_j^z + \frac{1}{2}(s_i^+ s_j^- + s_i^- s_j^+) \right] . \quad (17)$$

The arbitrary interaction strengths J_{ij} depend on i and j now and are not restricted to nearest-neighbor pairs. We assume

$$J_{ij} = J_{ji}, \quad J_{ii} = 0 \quad \text{for all } i, j \quad (18)$$

without loss of generality.

As a consequence of the general form of this Hamiltonian, neither the dimensionality of the problem nor the boundary conditions are specified *a priori*. All the information is contained in the set of coupling parameters J_{ij}. In the nearest-neighbor model, for example, the dimension is determined by the number of nearest neighbors of a given spin, which is the number of nonzero couplings J_{ij} for fixed i. Similarly, (anti)periodic or free boundary conditions can be imposed by choosing the J_{ij} appropriately.

It is not difficult to show that H is invariant under global rotations. The N-spin Hilbert space is the tensor product of N single-spin Hilbert spaces. In terms of this tensor product, the operator for the total spin has the form

$$\mathbf{S} = \sum_i \mathbf{s}_i = \mathbf{s} \otimes I \otimes \cdots \otimes I + I \otimes \mathbf{s} \otimes I \otimes \cdots \otimes I$$

$$+ \cdots + I \otimes I \otimes \cdots \otimes I \otimes \mathbf{s} , \quad (19)$$

where the ith factor in each term acts on the ith spin. The commutator of a single-spin component with the

Hamiltonian is

$$[s_i^a, H] = i \varepsilon^{abc} \sum_j J_{ij} s_i^b s_j^c . \quad (20)$$

From this it is clear that

$$[\mathbf{S}, H] = 0 \quad (21)$$

since each term on the right-hand side of Eq. (20) is canceled by a similar contribution from $[s_j^a, H]$. This means conservation of total spin $\mathbf{S}$. Its components satisfy the commutation relations

$$[S^a, S^b] = i \varepsilon^{abc} S^c \quad (22)$$

so the states in the spectrum carry the quantum numbers S and M.

We will follow a different approach, though. The Hamiltonian can be interpreted as an element of the group algebra of S_N, the symmetric group on N elements. From this point of view, the Hilbert space is the representation space for an S_N representation on which H acts. This space will be shown to break up into blocks and S and M will arise as natural labels on these blocks. The states in each block constitute an irreducible representation of S_N which is given explicitly.

First, we will show that the Hamiltonian can be viewed as an element of the group algebra of S_N. The group algebra of a group G is set of formal sums $\sum_{g \in G} x_g \cdot g$, where the x_g are numbers, with the obvious addition and multiplication rules. The group algebra plays an important role in the representation theory of finite groups. Now consider a term $\langle ij \rangle$ in H,

$$H_{\langle ij \rangle} = s_i^z s_j^z + \frac{1}{2}(s_i^+ s_j^- + s_i^- s_j^+) \quad (23)$$

(ignoring the prefactor for the moment). Its action only depends on the spins i and j of the state in Hilbert space on which it acts. Denoting the values of these spins by $|i,j\rangle$, we have

$$H_{\langle ij \rangle} | \uparrow \uparrow \rangle = \frac{1}{4} | \uparrow \uparrow \rangle ,$$

$$H_{\langle ij \rangle} | \downarrow \downarrow \rangle = \frac{1}{4} | \downarrow \downarrow \rangle ,$$

$$H_{\langle ij \rangle} | \uparrow \downarrow \rangle = \frac{1}{4}(-1 | \uparrow \downarrow \rangle + 2 | \downarrow \uparrow \rangle) , \quad (24)$$

$$H_{\langle ij \rangle} | \downarrow \uparrow \rangle = \frac{1}{4}(-1 | \downarrow \uparrow \rangle + 2 | \uparrow \downarrow \rangle) .$$

This can be written in a general form as

$$H_{\langle ij \rangle} |i,j\rangle = \frac{1}{4}(-1 |i,j\rangle + 2 |j,i\rangle)$$

$$= \frac{1}{4}(2(ij) - I) |i,j\rangle , \quad (25)$$

where $(ij) \in S_N$ is the two-cycle permutation or transposition interchanging the spins at sites i and j. The contribution of the identity operator I, which is the unit element of S_N, can be removed by adding a constant to the Hamiltonian (16), and will be neglected. The Hamiltoni-

an is a linear combination of terms of the form (25), with coefficients proportional to J_{ij},

$$H = -\frac{1}{2} \sum_{\langle ij \rangle} J_{ij}(ij) \ . \tag{26}$$

As such, it is an element of the group algebra of S_N. Note that it is restricted to the subspace of this algebra spanned by the conjugacy class of transpositions (two-cycles). In the calculation of the partition function, however, one needs the exponential Hamiltonian $\exp[-\beta H]$ which is not restricted to this conjugacy class.

The 2^N-dimensional Hilbert space of the spin model can thus be viewed as the representation space of a representation of S_N. It is clear that this representation is reducible. Any permutation leaves the numbers of up and down spins unchanged, so the representation space decomposes into a sum of invariant subspaces W_K of dimension $\binom{N}{K}$, corresponding to the sectors of different S^z eigenvalues $M = K - \frac{1}{2}N$. Each basis element of the subspace W_K can be labeled by the K sites where the up spins are located,

$$W_0 = \{( ) = |0\rangle\} \ ,$$

$$W_1 = \{(1),(2),(3), \cdots ,(N)\} \ ,$$

$$\vdots$$

$$W_K = \{(i_1,i_2,\ldots,i_K)|1 \leq i_1 < i_2 < \cdots < i_K \leq N\} \ ,$$

$$\vdots$$

$$W_N = \{(1,2,3,\ldots,N) = |N\rangle\} \ . \tag{27}$$

By taking the symmetric sum of all the states in W_K, for a fixed value of K, one recovers the state $|K\rangle$ of Eq. (10), which is a singlet under S_N.

Indeed, the representation subspaces W_K are not irreducible under S_N either. Not surprisingly, they decompose into irreducible sectors with different total-spin quantum number S. This decomposition, described nicely in Wigner's book,[5] can be summarized as follows. Within each subspace W_K (for $K \leq \frac{1}{2}N$) there is a subset of states which transform as W_{K-1}. This gives a decomposition of W_K as

$$W_K = W_{K-1} \oplus D_K \ , \tag{28}$$

where D_K can be shown to be an irreducible subspace. Subsequently, one applies the same decomposition for W_{K-1} and so on until one ends up with the full decomposition

$$W_K = D_0 \oplus D_1 \oplus D_2 \oplus \cdots \oplus D_K \ . \tag{29}$$

Finally, the decomposition of W_K for $K > \frac{1}{2}N$ is found by

noting that

$$W_{N-K} \simeq W_K \ . \tag{30}$$

Before discussing the representation spaces D_K, let us say something more about this recursive decomposition of W_K. Since W_{K-1} can be regarded as a subspace of W_K according to Eq. (28), it is interesting to see how the corresponding states in the two spaces are mapped on each other. For every state with $K-1$ up spins we want to determine the corresponding state in the space spanned by basis vectors with K up spins. Let $|\psi_{(K-1)}\rangle = (i_1,i_2,\ldots,i_{K-1})$ be an arbitrary state in W_{K-1}. Then the corresponding state $|\psi_{(K)}\rangle \in W_K$ is given by the sum over the $N-K+1$ states $(j_1,j_2,\ldots,j_K) \in W_K$ satisfying the condition that the set of numbers $\{j_\alpha, \alpha = 1,\ldots,K\}$ consists of the numbers $\{i_\beta, \beta = 1,\ldots,K-1\}$ supplemented by one other number. In other words, $|\psi_{(K)}\rangle$ is the state given by the sum over all the states for which all the spins i_α as well as one additional spin are up spins. This is exactly the state obtained by acting on $|\psi_{(K-1)}\rangle$ with the ladder operator S^+.

In terms of Young tableaux, the decomposition of W_K can be visualized as follows (see Ref. 6). The reducible representation of S_N on the space W_K is a permutation representation corresponding to the so-called skew Young diagram
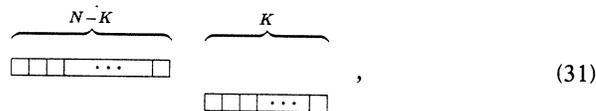
which decomposes into the following Young diagrams for irreducible representations:
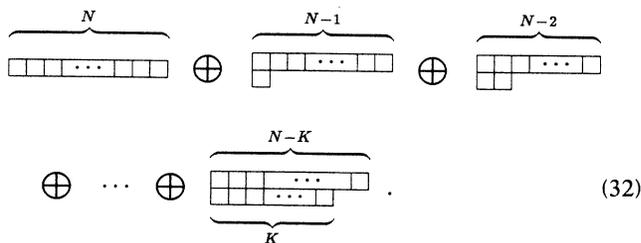
The irreducible representation D_K (we use the same notation D_K for the representation itself and for its representation space) is identified as

Schematically, the Hilbert space decomposes under S_N as follows:

$$
\begin{array}{l}
D_0 \\
D_0 \; D_1 \\
D_0 \; D_1 \; D_2 \\
\quad \vdots \\
D_0 \; D_1 \; D_2 \; \cdots \; D_{(1/2)(N-1)} \\
D_0 \; D_1 \; D_2 \; \cdots \; D_{(1/2)(N-1)} \\
\quad \vdots \\
D_0 \; D_1 \; D_2 \\
D_0 \; D_1 \\
D_0
\end{array}
\quad \text{and} \quad
\begin{array}{l}
D_0 \\
D_0 \; D_1 \\
D_0 \; D_1 \; D_2 \\
\quad \vdots \\
D_0 \; D_1 \; D_2 \; \cdots \; D_{(1/2)N} \\
\quad \vdots \\
D_0 \; D_1 \; D_2 \\
D_0 \; D_1 \\
D_0
\end{array}
\tag{34}
$$

for odd and even N, respectively. In this diagram, the quantum number S increases from right to left, while M runs vertically. The dimension of D_K is $\binom{N}{K}-\binom{N}{K-1}$, with the convention $\binom{N}{-1}=0$. It is easily checked that the dimensions of the subspaces in this decomposition add up to 2^N. In the limit $N\rightarrow\infty$, $D_{(1/2)N}$ has dimension $2^N \cdot 4/N\sqrt{2\pi N}$, while the largest D_K is the one for $K=\frac{1}{2}N-\frac{1}{2}\sqrt{N}$, whose dimension is $\sqrt{N/e}$ times as large.

This ends our discussion of the global spectral structure. To investigate the spectrum in more detail one has to consider the representation theory of the S_N group algebra element H of Eq. (26) in each of the representations D_K. This will depend on the specific form of the Hamiltonian, i.e., on the couplings J_{ij}. In practical applications, these couplings will not be arbitrary as in Eq. (16) but related by symmetries. For example, the nearest-neighbor model on an L^d lattice with periodic boundary conditions and equal couplings $J_{ij}=J$ for all nearest-neighbor pairs has additional translational, rotational, and reflection invariance properties. The exploitation of these extra symmetries, regarded as a subgroup of $S_N=S_{L^d}$, will be important for solving the model.

IV. THE ISOTROPIC INFINITE RANGE HEISENBERG MODEL

As an example, we shall consider the model in which each spin interacts with every other spin with equal strength. (For a discussion of the Ising analogue of this model see, e.g., Ref. 7.) This model can be viewed as a system of N spins on the vertices of an $(N-1)$-dimensional simplex (the higher-dimensional generalization of a tetraeder), interacting along its edges. With this picture in mind, the model is effectively infinite-dimensional for $N\rightarrow\infty$. The ferromagnetic version of this model was studied by Kittel and Shore[8] a long time ago. They derived expressions for the $N\rightarrow\infty$ limit and presented numerical results for various finite N. A remarkable finding was that the phase transition develops very slowly as N is increased.

Here, instead of taking the $N\rightarrow\infty$ limit at the begin-

ning, we first derive an expression for the partition function in terms of a single integral, elucidating its N dependence. Large-N results can be recovered subsequently by calculating this integral in the saddle-point approximation. We will briefly mention the antiferromagnetic case too.

The partition function is

$$
Z=\frac{\text{Tr}\exp[-\beta H]}{\text{Tr}I}
\tag{35}
$$

with Hamiltonian

$$
-\frac{1}{2}J\sum_{i,j=1}^{N}\mathbf{s}_i\cdot\mathbf{s}_j\rightarrow H
$$
$$
=-\frac{1}{2}J\mathbf{S}^2+\frac{1}{2}J\frac{1}{2}N\left[\frac{1}{2}N+1\right] \quad (J>0),
\tag{36}
$$

where a constant has been added to normalize the ground-state energy to zero, and $\beta=1/k_B T$.

For this Hamiltonian, the energy of a state is entirely determined by its quantum number S. Calculation of the partition function thus reduces to counting the number of states with this quantum number. The states in the representation D_K in the scheme (34) have $S=\frac{1}{2}N-K$, and there are $2S+1$ such blocks, each consisting of $\binom{N}{K}-\binom{N}{K-1}=\binom{N}{(1/2)N-S}-\binom{N}{(1/2)N-(S+1)}$ states. Hence one gets

$$
Z=\exp\left[-\frac{1}{8}\beta JN(N+2)\right]\frac{1}{2^N}
$$
$$
\times\sum_{S}^{(1/2)N}(2S+1)\left\{\left[\begin{array}{c}N\\\frac{1}{2}N-S\end{array}\right]-\left[\begin{array}{c}N\\\frac{1}{2}N-(S+1)\end{array}\right]\right\}
$$
$$
\times\exp\left[\frac{1}{2}\beta JS(S+1)\right],
\tag{37}
$$

adopting the convention $\left[\begin{array}{c}N\\-1\end{array}\right]=0$. Here the summation runs over integers $S=0,1,\ldots,\frac{1}{2}N$ for even N and over half-integers $S=\frac{1}{2},\frac{3}{2},\ldots,\frac{1}{2}N$ for odd N. In the Appendix it is shown that Z can be rewritten in terms of an integral,

$$Z = 2\exp\left[-\frac{1}{2}a(N+1)\right]\frac{\partial}{\partial a}\int_{-\infty}^{\infty}\frac{d\eta}{\sqrt{2\pi/a(N+1)}}\left[\exp\left[-\frac{1}{2}a\eta^2\right]\cosh a\eta\right]^{N+1} \tag{38}$$

$$= \exp\left[-\frac{1}{2}a(N+1)\right]\int_{-\infty}^{\infty}\frac{(N+1)d\eta}{\sqrt{2\pi/a(N+1)}}\eta\tanh a\eta\left[\exp\left[-\frac{1}{2}a\eta^2\right]\cosh a\eta\right]^{N+1}, \tag{39}$$

where

$$a = \tfrac{1}{4}\beta J(N+1). \tag{40}$$

The advantage of these expressions is that they exhibit clearly how Z depends on N. It is interesting to note that the integral occurring in Eq. (38) is very similar to the analogous expression for the corresponding model for classical spins, see, e.g., Ref. 7.

For large N, η can be interpreted as the order parameter defined by the spin fraction, in the sense that

$$\langle\eta^2\rangle = \left\langle\frac{S(S+1)}{\tfrac{1}{2}N(\tfrac{1}{2}N+1)}\right\rangle \tag{41}$$

(up to a $1/N$ correction). Here the expectation value on the left-hand side is calculated with Eq. (38) and the right-hand side with Eq. (37). This means that our η is essentially the same as the one defined by Kittle and Shore,[8] even though their η is a discrete quantity taking values in the interval $[0,1]$. In fact, from Eq. (39) we recover their result that for $a=1$ (i.e., $T=T_c$) the most probable value of η is $(6/N)^{1/4}$, and below we shall see [Eq. (43)] that a similar correspondence holds in the general case ($a\neq1$).

We shall focus on the large-N limit of the partition function and the heat capacity C_V. For comparison we have displayed C_V for $N=2000$ in Fig. 1, which is adapted from Ref. 8. Guided by the prominent appearance of the number $(N+1)$ in Eq. (38) we perform an expansion in $1/(N+1)$, keeping $a=\tfrac{1}{4}\beta J(N+1)$ fixed; the corresponding expansion in $1/N$, at fixed $a_0=\tfrac{1}{4}\beta JN$, is easily

derived from this. For $(N+1)$ large, the integrand in Eq. (38) is dominated by the value of η at which the exponent

$$-\tfrac{1}{2}\eta^2 + \log\cosh a\eta \tag{42}$$

is maximal. The value $\tilde{\eta}$ is given by the familiar condition

$$\tanh a\tilde{\eta} = \tilde{\eta}, \tag{43}$$

signaling a phase transition at $a=1$. Recall from (40) that a is inversely proportional to the temperature, so $a=T_c/T$.

If $a\leq1$ the only solution to (43) is $\tilde{\eta}=0$. For $a>1$, two additional solutions appear, and the integrand is maximal for these nontrivial values of $\tilde{\eta}$, see Fig. 2. A Taylor expansion of the integrand of Eq. (38) around $\eta=\tilde{\eta}$ now gives rise to an expansion in $1/(N+1)$. We shall give results to lowest nontrivial order in $1/N$ only, although higher-order corrections are obtained easily. For $a<1$ one finds

$$Z = 2\exp\left[-\frac{1}{2}a(N+1)\right]\frac{\partial}{\partial a}\frac{1}{\sqrt{1-a}}\left[1+\mathcal{O}\left[\frac{1}{N}\right]\right] \tag{44}$$

$$= \exp\left[-\frac{1}{2}a(N+1)\right]\frac{1}{(1-a)^{3/2}}\left[1+\mathcal{O}\left[\frac{1}{N}\right]\right], \tag{45}$$

from which it follows that the lowest-order correction to the value zero of the heat capacity per spin

$$C_V = \frac{1}{N}\beta^2\frac{\partial^2}{\partial\beta^2}\ln Z \tag{46}$$

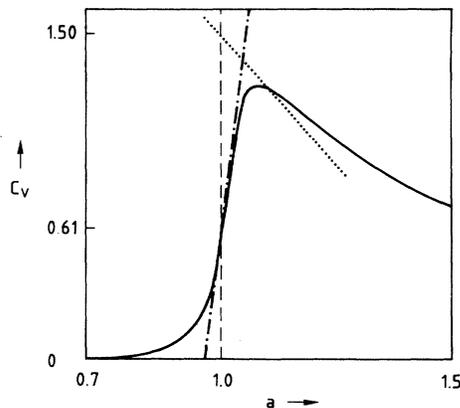in the high-temperature phase is [for small $\tau=(T-T_c)/T_c=(1-a)/a$]

FIG. 1. Heat capacity per spin for the isotropic model ($N=2000$) as a function of $a=\tfrac{1}{4}\beta J(N+1)$ (adapted from Ref. 8). The dotted line is $\tfrac{3}{2}-\tfrac{12}{5}(a-1)$, see Eq. (50), the dash-dotted line is Eq. (55): $0.61+0.36\sqrt{2000}(a-1)$.
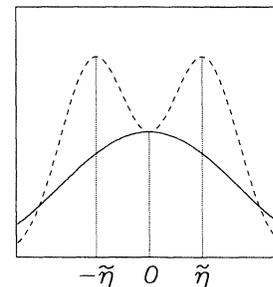

FIG. 2. The integrand in Eq. (39) for $a<1$ (solid line) and $a>1$ (dashed line).

$$C_V^{(N)}(\tau > 0) = \frac{1}{N}\left[\frac{3}{2}\frac{1}{\tau^2} + \mathcal{O}(\tau^0)\right] + \mathcal{O}\left[\frac{1}{N^2}\right] . \qquad (47)$$

For $a > 1$, expansion of the integrand around $\pm\tilde{\eta}$ gives

$$Z = 4\exp\left[-\frac{1}{2}a(N+1)\right]\frac{\partial}{\partial a}$$

$$\times \frac{(\exp[-\frac{1}{2}a\tilde{\eta}^2]\cosh a\tilde{\eta})^{N+1}}{\sqrt{1-a(1-\tilde{\eta}^2)}}\left[1+\mathcal{O}\left[\frac{1}{N}\right]\right] , \qquad (48)$$

which can be evaluated using

$$\frac{d\tilde{\eta}}{da} = \frac{\tilde{\eta}(1-\tilde{\eta}^2)}{1-a(1-\tilde{\eta}^2)} . \qquad (49)$$

For small $|\tau| = (T_c - T)/T_c = (a-1)/a$ this gives for the heat capacity in the low-temperature phase

$$C_V^{(N)}(\tau < 0) = \frac{3}{2} - \frac{12}{5}|\tau| + \mathcal{O}(|\tau|^2)$$

$$- \frac{1}{N}\left[\frac{1}{|\tau|^2} + \mathcal{O}(|\tau|^0)\right] + \mathcal{O}\left[\frac{1}{N^2}\right] . \qquad (50)$$

This behavior of the heat capacity, Eqs. (47) and (50), seems compatible with the finite-size data of Ref. 8, see also Fig. 1.

These results are valid for a not too close to 1, in fact we must have $|a-1| \approx |\tau| \gg 1/\sqrt{N}$, otherwise the derivations of Eqs. (45) and (48) and the subsequent results for the heat capacity lose validity. In the thermodynamic limit $N \to \infty$, this means that only the phase transition point $a = 1$ itself is not described by these formulas, but for finite N there is a finite interval of a values around $a = 1$ in which the theory behaves qualitatively different. The width of this interval is $\mathcal{O}(1/\sqrt{N})$ and can be regarded as a measure of the "width of the phase transition" for finite N (for convenience we keep using the term "phase transition" although strictly speaking there is no phase transition in a finite system).

This region very close to the phase transition appears to show interesting behavior. Consider expression (39) for the partition function with $\tau = (1-a)/a = \delta/\sqrt{N+1}$, where $0 \le |\delta| \ll 1$. The leading terms in the exponent of the integrand are

$$(N+1)\left[-\frac{1}{2}\frac{\delta}{\sqrt{N+1}}\eta^2 - \frac{1}{12}a^4\eta^4\right] , \qquad (51)$$

which both appear to be of leading order in N, after making the substitution $a\eta \to y/(N+1)^{1/4}$. Since $|\delta| \ll 1$, however, we can consider the δ-dependent exponential as a perturbation. We find

$$Z = \exp\left[-\frac{1}{2}a(N+1)\right]\frac{(N+1)^{3/4}}{a\sqrt{2\pi a}}\int_{-\infty}^{\infty} dy\, y^2 \exp\left[-\frac{1}{2}\delta y^2 - \frac{1}{12}y^4\right]\left[1+\mathcal{O}\left[\frac{1}{\sqrt{N+1}}\right]\right] , \qquad (52)$$

$$= \exp\left[-\frac{1}{2}a(N+1)\right]\frac{(N+1)^{3/4}}{a\sqrt{2\pi a}}$$

$$\times \left[6(12)^{-1/4}\Gamma\left[\frac{3}{4}\right] - \frac{1}{2}\delta 6(12)^{1/4}\Gamma\left[\frac{5}{4}\right] + \frac{1}{8}\delta^2 6(12)^{3/4}\Gamma\left[\frac{7}{4}\right] - \frac{1}{48}\delta^3 6(12)^{5/4}\Gamma\left[\frac{9}{4}\right] + \mathcal{O}(\delta^4)\right]$$

$$\times \left[1+\mathcal{O}\left[\frac{1}{\sqrt{N}}\right]\right] . \qquad (53)$$

This leads to

$$C_V^{(N)}\left[|\tau| \ll \frac{1}{\sqrt{N}}\right] = 2\left[\frac{9}{8} - \frac{3}{2}\frac{\Gamma^2(\frac{5}{4})}{\Gamma^2(\frac{3}{4})}\right] - 6\sqrt{3}\frac{\Gamma(\frac{5}{4})}{\Gamma(\frac{3}{4})}\left[\frac{\Gamma^2(\frac{5}{4})}{\Gamma^2(\frac{3}{4})} - \frac{1}{2}\right]\delta + \mathcal{O}(\delta^2) + \mathcal{O}\left[\frac{1}{\sqrt{N}}\right] \qquad (54)$$

$$= 0.61 - 0.36\sqrt{N}\,\tau + \text{ higher-order corrections .} \qquad (55)$$

Thus we have explicitly found the value of the heat capacity and its slope *at* the phase transition in a finite system. The fact that the slope is proportional to $\sqrt{N}$ confirms the earlier remark that the width of the phase transition is of order $1/\sqrt{N}$. The behavior (55) appears to be in qualitative and quantitative accordance with the numerical results for C_V of Kittle and Shore,[8] see Fig. 1 (recall that $-\tau \approx a - 1$).

For completeness we mention the antiferromagnetic case [see Eq. (69) in the Appendix] as well, although it is not very interesting. It might seem appropriate to

redefine the normalization of the Hamiltonian (36) such that the antiferromagnetic ground-state energy becomes zero, but we stick to the original normalization for continuity reasons. The integrand is maximal at $\tilde{\eta} = 0$ and the partition function becomes [here $a = -\frac{1}{4}\beta J(N+1) > 0$]

$$Z = \exp\left[\frac{1}{2}a(N+1)\right]\frac{1}{(1+a)^{3/2}}\left[1+\mathcal{O}\left[\frac{1}{N}\right]\right] , \qquad (56)$$

which is just the ferromagnetic result (45) with $a \to -a$.

The partition function has continuous behavior around $a=0$ so we can regard the antiferromagnetic case as an extension of the high-temperature phase of the ferromagnet.

V. CONCLUSION

In the first part of this paper we have discussed Heisenberg models with arbitrary couplings. The global structure of the spectrum of such models is determined by the well-known global rotational symmetry provided by the total spin, which causes the spectrum to break up into blocks of states labeled by the quantum numbers S and M of the total spin. The group-theoretical approach pursued here shows that the states within one such block transform according to explicitly given irreducible representations of the symmetric group S_N.

In an attempt to diagonalize the Hamiltonian in the representations D_K, one might try to proceed by applying representation theory for the S_N group algebra, in terms of the Schur functions, for example. In practice, one is usually interested in Heisenberg models satisfying extra relations between the coupling parameters J_{ij}, such as the nearest-neighbor model with equal couplings between each pair of neighboring spins. Consideration of the additional symmetries following from these relations, regarded as subgroups of S_N, is probably essential. Another possible extension of this work would be a generalization to spins in higher-dimensional representations of SU(2). There, one expects the appearance of S_N representations other than the ones discussed here. Furthermore, it would be interesting to give a description of spin waves in the present framework.

In the second part of this paper we studied the infinite-range Heisenberg model with equal couplings between all the N spins. We have presented a compact formulation of the partition function which clearly exhibits the dependence on N and a allows for a straightforward study of deviations from the $N \to \infty$ behavior. As an example, we calculated finite-size corrections to the heat capacity. These calculations reveal interesting behavior close to the phase transition and are in quantitative agreement with numerical data for finite systems.

APPENDIX: REWRITING THE PARTITION FUNCTION

In this appendix we present the derivation of the integral representation (38) and (39) of the partition function Eq. (37),

$$
Z = \exp\left[-\frac{1}{8}\beta J N(N+2)\right]\frac{1}{2^N}
$$

$$
\times \sum_{S}^{(1/2)N}(2S+1)\left\{\begin{bmatrix} N \\ \frac{1}{2}N-S \end{bmatrix} - \begin{bmatrix} N \\ \frac{1}{2}N-(S+1) \end{bmatrix}\right\}
$$

$$
\times \exp\left[\frac{1}{2}\beta J S(S+1)\right] . \tag{57}
$$

We will concentrate on the ferromagnetic case, $J > 0$. After that we will summarize the results for the antiferromagnet and briefly discuss the inclusion of an external field.

The negative terms in (57) can be rewritten using the equality

$$
-(2S+1)\begin{bmatrix} N \\ \frac{1}{2}N-(S+1) \end{bmatrix}\exp\left[\frac{1}{2}\beta J S(S+1)\right]
$$

$$
=(2S'+1)\begin{bmatrix} N \\ \frac{1}{2}N-S' \end{bmatrix}\exp\left[\frac{1}{2}\beta J S'(S'+1)\right] , \tag{58}
$$

where $S'=-(S+1)$ and we have used that $\binom{N}{\frac{1}{2}N+S'}=\binom{N}{\frac{1}{2}N-S'}$. Equation (57) now reduces to the rather elegant expression

$$
Z = \exp\left[-\frac{1}{8}\beta J(N+1)^2\right]
$$

$$
\times \frac{1}{2^N}\sum_{S=-(1/2)N}^{(1/2)N}(2S+1)\begin{bmatrix} N \\ \frac{1}{2}N-S \end{bmatrix}
$$

$$
\times \exp\left[\frac{1}{2}\left[\frac{1}{4}\beta J\right](2S+1)^2\right] . \tag{59}
$$

We rewrite the last exponential by applying

$$
\exp\left[\frac{1}{2}qp^2\right] = \frac{1}{\sqrt{2\pi q}}\int_{-\infty}^{\infty}dt\,\exp\left[-\frac{1}{2q}t^2+pt\right] \tag{60}
$$

for $p=2S+1$, $q=\frac{1}{4}\beta J$, and obtain

$$
Z = \exp\left[-\frac{1}{2}a(N+1)\right]\int_{-\infty}^{\infty}\frac{dt}{\sqrt{2\pi a/(N+1)}}\exp\left[-\frac{1}{2a}(N+1)t^2\right]\frac{\partial}{\partial t}\frac{1}{2^N}\sum_{S=-(1/2)N}^{(1/2N)}\begin{bmatrix} N \\ \frac{1}{2}N-S \end{bmatrix}\exp[(2S+1)t] , \tag{61}
$$

where we have introduced

$$
a = \frac{1}{4}\beta J(N+1) . \tag{62}
$$

Now the summation over S can be carried out, leading to

$$
Z = \exp\left[-\frac{1}{2}a(N+1)\right]\int_{-\infty}^{\infty}\frac{dt}{\sqrt{2\pi a/(N+1)}}\exp\left[-\frac{1}{2a}(N+1)t^2\right]\frac{\partial}{\partial t}(\exp t\,\cosh^N t) . \tag{63}
$$

Upon using the $t \rightarrow -t$ symmetry of the integrand, introducing an additional derivative, and performing partial integration, we get

$$Z = \exp\left[-\frac{1}{2}a(N+1)\right] \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi a/(N+1)}} \cosh^{N+1} t \frac{1}{N+1} \frac{\partial^2}{\partial t^2} \exp\left[-\frac{1}{2a}(N+1)t^2\right].$$ (64)

With the equality

$$\frac{\partial^2}{\partial t^2} \frac{\exp[-(1/2a)(N+1)t^2]}{\sqrt{2\pi a/(N+1)}} = 2(N+1) \frac{\partial}{\partial a} \frac{\exp[-(1/2a)(N+1)t^2]}{\sqrt{2\pi a/(N+1)}}$$ (65)

this turns into

$$Z = 2\exp\left[-\frac{1}{2}a(N+1)\right] \frac{\partial}{\partial a} \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi a/(N+1)}} \left[\exp\left[-\frac{1}{2a}t^2\right] \cosh t\right]^{N+1}$$ (66)

$$= \exp\left[-\frac{1}{2}a(N+1)\right] \int_{-\infty}^{\infty} \frac{(N+1)d\eta}{\sqrt{2\pi/a(N+1)}} \eta \tanh a\eta \left[\exp\left[-\frac{1}{2}a\eta^2\right] \cosh a\eta\right]^{N+1}.$$ (67)

[Equation (67) is obtained by computing $\partial/\partial a$ after substituting $t \rightarrow t'\sqrt{a}$ in Eq. (66).]

In the antiferromagnetic case, $J < 0$, the derivation is the same up to Eq. (59). Instead of Eq. (60) we then apply

$$\exp\left[-\frac{1}{2}qp^2\right] = \frac{1}{\sqrt{2\pi q}} \int_{-\infty}^{\infty} dt \exp\left[-\frac{1}{2q}t^2 + ipt\right]$$ (68)

and the remainder of the derivation proceeds analogously to the ferromagnetic case, leading to

$$Z = -2\exp\left[\frac{1}{2}a(N+1)\right] \frac{\partial}{\partial a} \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi a/(N+1)}} \left[\exp\left[-\frac{1}{2a}t^2\right] \cos t\right]^{N+1}$$ (69)

[where now $a = -\frac{1}{4}\beta J(N+1) > 0$]. This expression is related to (66) by $a \rightarrow -a$, $t \rightarrow it$.

For completeness we also mention the inclusion of an external field. If we add a coupling term $-BS_3$ to the Hamiltonian, the factor $(2S+1)$ in Eq. (57) is replaced by

$$\sum_{M=-S}^{S} \exp[-\beta BM] = \frac{\sinh\frac{1}{2}\beta B(2S+1)}{\sinh\frac{1}{2}\beta B}.$$ (70)

Proceeding along the lines of the derivation given above one obtains (with $t_0 = \frac{1}{2}\beta B$)

$$Z = \frac{\exp[-\frac{1}{2}a(N+1)]}{\sinh t_0} \frac{1}{N+1} \frac{\partial}{\partial t_0} \int_{-\infty}^{\infty} \frac{dt}{\sqrt{2\pi a/(N+1)}} \left[\exp\left[-\frac{1}{2a}t^2\right] \cosh(t+t_0)\right]^{N+1}$$ (71)

in the ferromagnetic case, with a similar result for the antiferromagnet.

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