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# Low-Temperature Results of the Statistical Theory of Noninteracting Spin Waves

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Low-temperature predictions of a free-spin-wave theory that includes the correct spin-wave kinematics for the $S = 1/2$, quantum Heisenberg ferromagnet, as described in a previous paper, are obtained for three dimensions using analytic and Monte Carlo techniques. The low-temperature propagator is found to be of boson form, and the low-temperature magnetization goes as $T^{3/2}$, which agrees with the interacting theory at lowest order in $T$.

## 1. INTRODUCTION

In a previous paper (Stoller, 1987a), hereafter refered to as I, I analyzed the kinematical problem in quantum spin-wave theory and presented a spin-wave state space that formed a complete basis. This space reflected both the Bose- and Fermi-like properties of spin waves.[2]

The unique feature of this state space is that the number of $k$-space degrees of freedom is a function of the number of excitations. For example, given a multiple excitation state $\Phi(\mathbf{k}_1, \mathbf{k}_2, \ldots, \mathbf{k}_m)$, consisting of $m$ excitations at wave vectors $\mathbf{k}_1, \mathbf{k}_2, \ldots, \mathbf{k}_m$, the volume of $k$ space within which these values of $\mathbf{k}_j$ must be located is a decreasing function of $m$—the greater the number of excitations, the more constricted are the allowable wavevector values to a $k$-space neighborhood about the origin.

In the perturbative thermal field-theoretic approach to the Heisenberg ferromagnet the free-spin-wave distribution serves as the propagator. This thermal distribution function gives the relative population of spin waves at wavevector $\mathbf{k}$ and energy $\varepsilon_{\mathbf{k}}$ as a function of temperature. The propagator

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[2]Bose-like in that excited spin states can have multiple excitations at any given wave vector. Fermi-like because only zero or one spin excitation can reside at any position-space lattice site for spin 1/2.



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plays the crucial role of being the initial (approximate) solution to the problem about which corrections are computed in powers of the interaction Hamiltonian operator. The computation of corrections due to the interaction Hamiltonian constitutes the dynamical problem in spin-wave theory. The dynamical problem is not considered here.

It was noted previously that kinematical and dynamical problems can be treated separately. It should also be noted that the kinematical problem precedes the dynamical problem in that some approximation to spin-wave kinematics must be made in order to phrase the dynamical problem. We need to have state vectors before we can write the eigenvalue equation. On the other hand, we can describe the state space[3] without knowing anything about the interactions.

Having argued that a correct description of the spin-wave state space precedes perturbation theory, it is necessary to show that this particular state space provides a good starting point for perturbation theory. It must be shown that zeroth-order perturbation theory based on this state space provides a reasonably accurate description of long-wavelength phenomena at various temperatures.

In this paper I present analytic and Monte Carlo evidence supporting the validity of the free spin-wave model at low temperatures. At sufficiently low temperatures the spin-wave distribution function generates the observed leading order behavior of the magnetization. This shows that free-spin-wave theory and the harmonic theory that treats free spin waves as noninteracting bosons agree at low temperatures. In a subsequent paper (Stoller, 1987b), I show that the free-spin-wave model also provides a reasonably accurate description of the critical region. The importance of the low-temperature work is twofold. First, it provides a test of the theory, and second, it provides deeper insight into spin systems and a firm foundation for evaluating past results and developing future theory.

In Sections 2.1 and 2.2 the essential properties of the spin-wave state space are developed. In Section 3 I show that the thermal expectation value of the number operator at wave vector $\mathbf{k}$, $\hat{n}_{\mathbf{k}}$, is a boson distribution function for a system with a particle density of $1/2$. In Section 4 this propagator is used to derive the $T^{3/2}$ law for the spontaneous magnetization at low temperatures. The spontaneous magnetization of the ferromagnet is seen to be a quantum phenomenon in the sense of being driven by the condensation of zero-wavenumber spinwaves. These analytic results are shown to agree with Monte Carlo simulations as presented in Section 5.

[3]As described in I, it is found that there is a certain latitude in how one can construct a complete state space. The particular form that I am working with is chosen so as to include most states from the long-wavelength regime. Here is where the best approximate eigenstates are found, due to the weak coupling of spin waves at long wavelengths.

## 2. THE FREE-SPIN-WAVE MODEL

### 2.1. The Boson Hamiltonian and the Sum over States

There are three expressions from I that I use to construct the free-spin-wave model. They are

$$\sum_{\text{reduced state space}} = \sum_{m=0}^{N^d} \left[ \sum_{k_1^x=-Q(m)/2}^{Q(m)/2}, \sum_{k_1^y=-Q(m)/2}^{Q(m)/2} \cdots \right] \cdots \times \cdots \left[ \sum_{k_m^x=-Q(m)/2}^{Q(m)/2}, \sum_{k_m^y=-Q(m)/2}^{Q(m)/2} \cdots \right] \tag{I.28}$$

$$\pm\frac{Q(m)}{2} \approx \pm\frac{(N^d - m + 1)^{1/d}}{2} \tag{I.30}$$

where the approximate equality means that the value of the right-hand side must be adjusted upward or downward to the nearest integer. The relationship becomes an equality in the thermodynamic limit. And,

$$Z_\beta = \sum_{\Phi \in (\text{reduced state space})} (\Phi|\hat{G} \exp(-\beta \hat{H}_B)|\Phi) \tag{I.37}$$

Equation (I.28) says that the sum over states includes all distinguishable ways that $k$-space values can be assigned in an $m$-boson or spin-wave state, where $m$ goes from 0 to $N^d$. Here $N$ is the linear size of the system and $d = 3$ is the number of dimensions. The $k$ space values that can be assigned to the excitations lie in the range $+Q(m)/2$ to $-Q(m)/2$, which is a function of particle number as specified in equation (I.30).

States $\langle\Phi|$ and $|\Phi\rangle$ are multiparticle spin-wave states; $(\Phi|$ and $|\Phi)$ are multiparticle boson states. The operator $\hat{G}$ when sandwiched between boson states is defined so as to generate the inner-product matrix $\langle\Phi'|\Phi\rangle$. What this means is as follows. Given two sets of wavenumbers $\{\mathbf{k}_1, \mathbf{k}_2, \ldots\}$ and $\{\mathbf{k}_1', \mathbf{k}_2', \ldots\}$ specifying the wavenumbers of the particles in two multi-spin-wave states, the inner product $\langle\Phi\{\mathbf{k}_1, \mathbf{k}_2, \ldots\}|\Phi\{\mathbf{k}_1', \mathbf{k}_2', \ldots\}\rangle$ is not a delta function, i.e., multi-spin-wave states are nonorthogonal. Multiboson states, on the other hand, are orthogonal. In order to use them to model spin waves, the inner-product operator $\hat{G}$ is defined with respect to boson states so as to satisfy the condition

$$(\Phi\{\mathbf{k}_1, \mathbf{k}_2, \ldots\}|\hat{G}|\Phi\{\mathbf{k}_1', \mathbf{k}_2', \ldots\}) \equiv \langle\Phi\{\mathbf{k}_1, \mathbf{k}_2, \ldots\}|\Phi\{\mathbf{k}_1', \mathbf{k}_2', \ldots\}\rangle$$

Carets are used to indicate operators. The reader is referred to I for further explanation of these formulas.

The boson Hamiltonian operator $\hat{H}_B = \hat{H}_B^0 + \hat{H}_B^i$, used to model the Heisenberg permutation Hamiltonian, consists of a free and an interacting part. The free-spin-wave model is defined by setting $\hat{H}_B^i$ to zero. Because

there is no interaction term, the partition function reduces to

$$Z_\beta^{\text{free}} = \sum_{\Phi \in (\text{reduced state space})} (\Phi|\hat{G}|\Phi) \exp[-\beta E^0(\Phi)]$$

The free-spin-wave energy of a state $\Phi\{\mathbf{k}_1', \mathbf{k}_2', \ldots\}$ is

$$E^0(\Phi\{\mathbf{k}_1', \mathbf{k}_2', \ldots\}) = \sum_{\mathbf{k}} n_{\mathbf{k}} \varepsilon_{\mathbf{k}}$$

and

$$\varepsilon_{\mathbf{k}} = J \sum_{j=1}^{3} \left(1 - \cos \frac{2\pi k^j}{N}\right)$$

with $n_{\mathbf{k}}$ the number of spin waves at wavenumber $\mathbf{k}$ and $J$ the value of the exchange integral.

Since the spin-wave inner product is normalized, $\langle \Phi | \Phi \rangle = (\Phi|\hat{G}|\Phi) = 1$, and I can ignore the inner-product matrix. This would no longer be the case if I included $H_B^i$; therefore, extending the results obtained here will require more than just the addition of interactions. In what follows the distinction between states constructed using Bose or spin operators is insignificant. In this treatment the Bose operators do little more than define the noninteracting approximation. Their greater purpose is to simplify commutator expressions as arise in higher order perturbation theory.

The operator I am concerned with is $\hat{n}_{\mathbf{k}}$, with respect to which the multiparticle states are diagonal. In the noninteracting model the thermal expectation value of $\hat{n}_{\mathbf{k}}$ is the propagator of thermal field theory, defined for bosons as $\varphi_{\mathbf{k}}^* \varphi_{\mathbf{k}}$, where $\varphi_{\mathbf{k}}^*$ and $\varphi_{\mathbf{k}}$ are boson creation and annihilation operators. The thermal expectation value in the noninteracting approximation is

$$\langle \hat{n}_{\mathbf{k}} \rangle_\beta = Z^{-1} \sum_{\Phi \in (\text{reduced state space})} n_{\mathbf{k}}(\Phi) \exp[-\beta E^0(\Phi)]$$

Note that if we were to consider an operator that was not diagonal in the spin-wave basis, we would have to reintroduce the nondiagonal inner product.

The sum over the reduced state space can be rewritten as a sum over subspaces of fixed particle number,

$$\sum_{\Phi \in (\text{reduced state space})} = \sum_{m=0}^{N^d} \sum_{\{\Phi_m\}} \tag{1}$$

The sum over the set of $m$-particle states $\{\Phi_m\}$ contains all permutationally distinct labelings of $m$ particles with wavenumber values $\mathbf{k}$ such that $|k^{x,y,z}| \leq Q(m)/2$.

### 2.2. Consequences of Symmetry

We now consider a simplification of the sum in equation (1) by returning to the localized spin basis. In position space all spin states can be described

in terms of some combination of up and down spins. From the symmetry of states about the $z$ axis in position space it follows that $k$-space states also have $z$-axis symmetry. Thus, for every subspace of $(N^d/2)-m$ excitations there is a complementary subspace of $(N^d/2)+m$ excitations that contains the same number of states. Due to the spherical symmetry of the Hamiltonian this reflection symmetry also holds for the energies of such multiparticle states. For every state of a given energy in one subspace of $m<N^d/2$ there is a state in the complementary subspace of $m>N^d/2$ with the same energy.

We can picutre the half state space of $m<N^d/2$ particles as constructed by applying $m$ spin-wave raising operators to the totally spin-down ground state, and the half state space of $m>N^d/2$ particles as products of $m$ spin-wave lowering operators acting on the totally spin-up ground state. When we compare the states in any of these subspaces with the states in the complementary subspace we find (1) the correlation properties among different spins in the former state and the correlation properties among different spins in the later state are exactly inverted with respect to the $z$ axis, (2) the energies of the two states are equal, (3) the total $z$ components of their magnetization are equal in value and opposite in sign and (4) complementary states have equal values of total spin squared.

The problem that now arises is, if we call the excitations in the $[(N^d/2)-m]$-particle subspace "spin waves," what do we call the the excitations that comprise the complementary $[(N^d/2)+m]$-particle subspace? To make the problem more concrete, if a state $\Phi_0$ in the $(N^d/2)-m$ subspace contains $v_{\mathbf{k}_0}$ spin waves at wavenumber $\mathbf{k}_0$ is it correct to say that the complementary state $\bar{\Phi}_0$ in the $(N^d/2)+m$ subspace also has $v_{\mathbf{k}_0}$ spin-waves at $\mathbf{k}_0$? The answer is no, because the excitations in the first subspace are not of the same kind as those in the complementary subspace—they cannot be, because the states $\Phi$ and $\bar{\Phi}$ are orthogonal.

If spin-wave states are defined as a product of $m<N^d/2$ spin-wave raising operators $S_K^+$ acting on a spin-down ground state $|0\rangle$, then it can be shown that the complementary states, consisting of $m>N^d/2$ excitations, are constructed as a product of operators $S^-_k$ acting on the state $|\bar{0}\rangle$, where

$$|\bar{0}\rangle=(S^-_{\mathbf{k}=0})^{N^d}|0\rangle$$

If I take the expectation value of $\hat{n}_{\mathbf{k}_0}$ with respect to the previously mentioned states $\langle\Phi_0|$ and $|\Phi_0\rangle$ I get $v_{\mathbf{k}_0}$, but if I take the expectation value of the same operator with respect to the complementary states $\langle\bar{\Phi}_0|$ and $|\bar{\Phi}_0\rangle$ I get zero. This shows that spin-wave quasiparticles and their complements must be considered different species. Calling the complementary particles "anti-spin-waves," I have the following rules for how to treat these subspaces in the state space sum.

First, the state space sum is broken into two parts—the $m < N^d/2$ half and the $m > N^d/2$ half. The first half consists of the spin-wave states and the second half of anti-spin-wave states. The number of spin waves or anti-spin waves is always less than or equal to $N^d/2$. Second, if $\hat{n}_{\mathbf{k}}$ is the number operator for spin waves and $\bar{n}_{\mathbf{k}}$ that for anti-spin waves, then $\hat{n}_{\mathbf{k}}$ has a zero expectation value when evaluated with respect to anti-spin-wave states, and $\bar{n}_{\mathbf{k}}$ has zero expectation value when evaluated with respect to spin-wave states. Finally, with regard to an operator that is symmetric about the $z$ axis, such as the total spin $\mathcal{S}^2 = [\sum_{\mathbf{j}} \hat{\mathbf{S}}_j]^2$, the thermal expectation over spin and anti-spin waves is twice that of the expectation value of $\mathcal{S}^2$ taken over only one of these subspaces. These distinctions between spin and anti-spin waves are time-independent because there is no coupling between states of different numbers of excitations.

The rules given above reduce the size of the state space at the expense of introducing occasional factors of two. They translate directly into an identical set of conditions for the boson representation. Without these rules spin-wave perturbation theory would always get wrong answers. That is because although the reduction scheme of (I.30) does preserve the equality in the number of states in complementary subspaces, it does not preserve the symmetry in their energies, as shown in the following example.

Consider the situation that exists if I do not distinguish spin and anti-spin-waves and instead just impose the wavenumber cutoff of equation (I.30). I examine the spectra of the two subspaces of $m = 1$ and $m = N^d - 1$ spin-wave states in one dimension. Equation (I.30) says that a single spin wave can have any wavenumber between $-N/2$ and $+N/2$, that is, any value in the first Brillouin zone. On the other hand, spin waves in the $(N^d - 1)$-particle subspace must carry wavenumber 0 or 1 [$\pm Q(N^d - 1)/2$ is shifted by $+1/2$ in order to apply to the finite system in this case]. The spectrum of the one-spin-wave space goes as $\varepsilon_k$, which is proportional to the cosine of $k$, while the spectrum of the $N^d - 1$ subspace goes as $n_{k=1}\varepsilon_1$, which is linear. The spectral symmetry of these two subspaces has not been preserved. As a result, the thermal expectation value of a symmetric quantity will be skewed in the positive or negative $z$ direction.

By applying the rules given above, I generate the following formulas:

$$\sum_{\Phi \in (\text{reduced state space})} = \sum_{m=0}^{N^d/2} \sum_{\{\Phi_m\}} + \sum_{\bar{m}=0}^{N^d/2} \sum_{\{\bar{\Phi}_{\bar{m}}\}} \tag{2}$$

$$\langle n_{\mathbf{k}\neq 0} \rangle_\beta = \left\{ \sum_{m=0}^{N^d/2} \sum_{\{\Phi_m\}} n_{\mathbf{k}}(\Phi_m) \exp[-\beta E(\Phi_m)] \right\} \times \left\{ 2 \sum_{m=0}^{N^d/2} \sum_{\{\Phi_m\}} \exp[-\beta E(\Phi_m)] \right\}^{-1} \tag{3}$$

$$\sum_{\mathbf{k}\neq 0}\left[\langle n_{\mathbf{k}}\rangle_\beta + \langle \bar{n}_{\mathbf{k}}\rangle_\beta\right] = 2\sum_{\mathbf{k}\neq 0}\langle n_{\mathbf{k}}\rangle_\beta \tag{4}$$

The summations are taken with respect to states in either spin or Bose representations.

## 3. THE ANALYTIC FORM OF THE PROPAGATOR AT LOW TEMPERATURES

I approximate the value of the sum over states at low temperature by replacing the sum with the single state that contributes most. This technique, borrowed from ensemble theory, gives accurate results when the total additional contributions from other states is small. This will be seen to be the case at low temperatures.

Begin the reduction by considering just spin waves and dividing the state sum into subsums over states with fixed total energy $G$ and particle number $m < N^d/2$. Note that I shall always neglect contributions to the summation limits that go as $N^{-1}$, such as occur depending on whether the number of spins is odd or even. These effects vanish in the thermodynamic limit. We have

$$\left\langle \sum_{\mathbf{k}\neq 0} n_{\mathbf{k}} \right\rangle_\beta = Z^{-1}\sum_G e^{-\beta G}\sum_{m=0}^{N^d/2}\sum_{\{\Phi_{Gm}\}}\sum_{\mathbf{k}\neq 0}\langle n_{\mathbf{k}}\rangle_{Gm} \tag{5}$$

where $E(\Phi_{GM}) \equiv G$ and $\langle n_{\mathbf{k}}\rangle_{Gm} = \langle \Phi_{GM}|\hat{n}_{\mathbf{k}}|\Phi_{GM}\rangle$. The sum of $\langle n_{\mathbf{k}}\rangle_{Gm}$ over $\{\Phi_{Gm}\}$ will be replaced with the expectation value of $\hat{n}_{\mathbf{k}}$ taken with respect to that state $\tilde{\Phi}_{Gm}$ that dominates the sum. This state is found using the standard combinatoric arguments for a boson microcanonical ensemble (Huang, 1963). The energy spectrum is divided into cells $j = 1, 2, \ldots$ containing $g_1, g_2, \ldots$ $k$-levels each cell is assigned an energy that is the average of the free-spin-wave energies over the wavenumbers in that cell. I assume that (1) energy differences between cells are much smaller than the energies of the cells, (2) the sum of the energies of the spin waves in a cell for any state in the set $\{\Phi_{Gm}\}$ is much less than the total energy of the state $G$, and (3) for states in $\{\Phi_{Gm}\}$ the total number of spin waves for $k$ values within any of the cells is much less than $m$, except for occupation numbers at $\mathbf{k} = 0$. These conditions hold generally in the thermodynamic limit.

Using the average energy of a cell as $\varepsilon_j = g_j^{-1}\sum_{\mathbf{k}\in\{j\}}\varepsilon_{\mathbf{k}}$, where $g_j$ is the number of levels in the $j$th cell and $\{j\}$ is the set of $k$-levels in the $j$th cell, we obtain for these conditions

$$\begin{aligned}
&|\varepsilon_j - \varepsilon_{j+1}| \ll \varepsilon_j \\
&\sum_{\mathbf{k}\in\{j\}} n_{\mathbf{k}}\varepsilon_{\mathbf{k}} \ll G \text{for all } n_{\mathbf{k}} \text{ specified by } \Phi \in \{\Phi_{Gm}\} \\
&\sum_{\mathbf{k}\in\{j\}} n_{\mathbf{k}} \ll m \text{for all } \Phi \in \{\Phi_{Gm}\} \text{ and } \mathbf{k} \neq 0
\end{aligned} \tag{6}$$

Given a spin-wave distribution with $n_j$ spin waves in cell $j$, the number $\omega_j$ of distinct quantum states that can be obtained by different assignments of the $n_j$ spin waves to the $g_j$ levels is

$$\omega_j = \frac{(n_j + g_j - 1)!}{n_j!(g_j - 1)!}$$

The total number of different quantum states that can be constructed from a set of $n_j$ is $W\{n_j\} = \prod_j \omega_j$. The set of values of $n_j$ that contributes with the greatest number of states, $\{\tilde{n}_j\}$, is obtained by maximizing $\ln[W\{n_j\}]$ subject to the constraints $\sum_j n_j = m$ and $\sum_j n_j \varepsilon_j = G$. The factorials are approximated using Stirling's formula. The variation of

$$\left[\ln W\{n_j\} + \alpha\left(\sum_j n_j \varepsilon_j - G\right) + \gamma\left(\sum_j n_j - m\right)\right]$$

is taken with respect to $n_j$, and set to zero. The result, as found in many statistical mechanics textbooks (e.g., Huang, 1963, p. 193), for the occupation number in the $j$'th cell that characterizes the most strongly contributing partition is

$$\tilde{n}_j(Gm) = \frac{g_j}{e^{\gamma + \alpha \varepsilon_j} - 1}$$

where $\gamma$ and $\alpha$ are Lagrange multipliers determined by $\sum_j \tilde{n}_j(Gm) = m$, and $\sum_j \tilde{n}_j(Gm)\varepsilon_j = G$. The energies $\varepsilon_{\mathbf{k}}$ are taken to be equal in this approximation for all $\mathbf{k}$'s in the $j$th group. The $\tilde{n}_{\mathbf{k}}(Gm)$ are then evenly distributed within the cell and $\tilde{n}_k(Gm) = g_j^{-1}\tilde{n}_j(Gm)$. As a result, I have

$$\tilde{n}_{\mathbf{k}}(Gm) = \frac{1}{e^{\gamma + \alpha \varepsilon_{\mathbf{k}}} - 1} \tag{7}$$

with

$$\sum_{\mathbf{k}=0} \tilde{n}_{\mathbf{k}}(Gm) = m, \qquad \sum_{\mathbf{k}=0} \tilde{n}_{\mathbf{k}}(Gm)\varepsilon_{\mathbf{k}} = G \tag{8}$$

Equation (7) is the boson distribution for a system of $m$ particles at a temperature $\alpha$. The sums over $\mathbf{k}$ in (8) are bounded by $-Q(m)/2$ and $+Q(m)/2$ in accordance with the reduced $k$-space condition of equation (I.30).

Replacing the sum of expectation value with the expectation value in the most probable state is justified by the strong peak in contributions about the most probable value. The smallness of contributions away from this peak is the property that justifies the Bose distribution for a microcanonical system away from a phase transition. Equation (7) is a valid approximation as long as $\alpha$ is not near a critical point for the present model, which is

found numerically to occur at $1.95J/k_B$. Therefore, it is safe to use the most-probable-state approximation for the propagator at low temperatures. In the critical region, however, the thermal expectation value *does* receive large contributions from states whose phase space points are outside the neighborhood of the most probable state. The neglect of these states, or fluctuations as they are referred to in ensemble theory, makes the most-probable-state propagator inaccurate near $T_c$.

Before replacing the sums $\langle n_{\mathbf{k}} \rangle_{Gm}$ over $\{\Phi_{Gm}\}$ with $\tilde{n}_{\mathbf{k}}(Gm)$ the contributions from different values of $G$ and $m$ must be weighted to account for the different number of states in these subsets. For instance, if there are twice as many states in the sum over $\{\Phi_{Gm}\}$ as in the sum over $\{\Phi_{G'm'}\}$, then the contribution of $\tilde{n}_{\mathbf{k}}(Gm)$ must be twice that of $\tilde{n}_{\mathbf{k}}(G'm')$. The relative weight for each term is the proportion of states in the $(G, m)$ subspace relative to the total number of states; this ratio is given by $R_{Gm/\text{all}}$,

$$R_{\text{Gm/all}} = \frac{\sum_{\{\Phi_{Gm}\}}}{\sum_{Gm} \sum_{\{\Phi_{Gm}\}}}$$

$$= \frac{\sum_{G} \sum_{\{\Phi_{Gm}\}}}{\sum_{Gm} \sum_{\{\Phi_{Gm}\}}} \frac{\sum_{\{\Phi_{Gm}\}}}{\sum_{G} \sum_{\{\Phi_{Gm}\}}}$$

$$= R_{m/\text{all}} R_{Gm/m} \tag{9}$$

The factoring of $R_{Gm/\text{all}}$ is accomplished by multiplying and dividing by the total number of states of fixed total particle number $m$. Using this ratio enables me to rewrite equation (5) as

$$\left\langle \sum_{\mathbf{k}\neq 0} n_{\mathbf{k}} \right\rangle_{\beta} = Z^{-1} \sum_{\mathbf{k}\neq 0} \sum_{m} R_{m/\text{all}} \sum_{G} e^{-\beta G} R_{Gm/m} \tilde{n}_{\mathbf{k}}(Gm) \tag{10}$$

I next determine the energy $\tilde{G}$ that makes the largest contribution to the sum over $G$.

Instead of the sum over $G$ as written, consider for a moment the normalized sum over all states $\{\Phi_m\}$ each contributing an amount $e^{-\beta G} \sum_{\mathbf{k}\neq 0} \tilde{n}_{\mathbf{k}}(Gm)$, where $G = E^0(\Phi_m)$ is a variable. This ensemble average is given by

$$\sum_{\{\Phi_m\}} e^{-\beta G} \left[ \sum_{\mathbf{k}\neq 0} \tilde{n}_{\mathbf{k}}(Gm) \right] \Big/ \sum_{\{\Phi_m\}} \tag{11}$$

This avearge is taken over an ensemble of occupation numbers $\{\xi_{\mathbf{k}}\}$ that describe the states $\Phi_m \in \{\Phi_m\}$. I am using $\xi_{\mathbf{k}}$ instead of $n_{\mathbf{k}}$ to emphasize the

independence of these occupation numbers. Each state contributes to the average with a weight $e^{-\beta G}[\sum_{\mathbf{k}\neq 0}\tilde{n}_{\mathbf{k}}(Gm)]$. By dividing the sum over $\{\Phi_m\}$ into sums over $G$ of sets $\{\Phi_{Gm}\}$, I get

$$\frac{\sum_{\{\Phi_m\}} e^{-\beta G}\left[\sum_{\mathbf{k}\neq 0}\tilde{n}_{\mathbf{k}}(Gm)\right]}{\sum_{\{\Phi_m\}}} = \sum_G e^{-\beta G}\left[\sum_{\mathbf{k}\neq 0}\tilde{n}_{\mathbf{k}}(Gm)\right]\frac{\sum_{\{\Phi_{Gm}\}}}{\sum_{\{\Phi_m\}}}$$

$$= \sum_G R_{Gm/m} e^{-\beta G}\sum_{k\neq 0}\tilde{n}_{\mathbf{k}}(Gm) \tag{12}$$

It follows that the sum over $G$ in equation (10) can be replaced by an evaluation of the ensemble average of equation (11).

Equation (11) is evaluated by again partitioning the energy spectrum into cells with $g_j$ $k$-space levels per cell. A set of ensemble configurations is described by a set of cell occupation numbers $\{\xi_j\}$. The number of distinct states that satisfy this partitioning of spin waves is $W\{\xi_j\}$, as given before. The contribution to the sum made by states described by this partition is $W\{\xi_j\}\, e^{-\beta G}\sum_{\mathbf{k}\neq 0}\tilde{n}_{\mathbf{k}}(Gm)$. Since $G$ is not fixed in the ensemble, I maximize this expression subject only to $\sum_j \xi_j = m$. This maximum is found by solving for $\xi_a$ in the following variational expression:

$$\delta\xi_a \frac{\partial}{\partial \xi_a}\left(\ln\left(W\{\xi_j\}e^{-\beta G}\sum_{\mathbf{k}\neq 0}\tilde{n}_{\mathbf{k}}(Gm)\right) + \gamma'\left(\sum \xi_j - m\right)\right) = 0 \tag{13}$$

where $G = \sum_j \xi_j\varepsilon_j$ and $\delta\xi_j$ is arbitrary. Notice that when the derivative of $e^{-\beta G}$ is taken, the same factor of $-\beta$ enters the expression as would if there was a constraint on the energy with $\beta$ the undetermined multiplier, except in this case $\beta$ is known to be the inverse temperature. In order to evaluate the variation of $\sum_{\mathbf{k}\neq 0}\tilde{n}_{\mathbf{k}}(Gm)$ I need its explicit functional dependence on $G$. This is obtained in the Appendix, with the result

$$\sum_{\mathbf{k}\neq 0}\tilde{n}_{\mathbf{k}}(Gm) = \left(\frac{R_m(4)}{G}\right)^{-3/2} R_m(2)$$

where $R_m(i)$ is defined in the Appendix. With this I obtain

$$\frac{\partial}{\partial\xi_a}\ln W\{\xi_j\} + \frac{\partial}{\partial\xi_a}\left[-\beta\sum_j \xi_j\varepsilon_j\right] + \frac{\partial}{\partial\xi_a}\left[\frac{3}{5}\ln G\right] + \gamma'$$

$$= \ln\left[\frac{\xi_a + g_a - 1}{\xi_a}\right] - \varepsilon_a(\beta - G^{-1}) + \gamma' = 0 \tag{14}$$

This is a transcendental equation for $\xi_a$, which I cannot solve in general. It is simplified by the following approximation. At low temperatures I only need the distribution of low-energy states. Therefore, I can solve (14) subject

to the condition that $\xi_a$ is the occupation number for particles at a wavevector value $a$ that is large compared to the lattice spacing. For $a$ labeling a low-energy state ($\varepsilon_a < k_B T$), $\xi_a$ will be greater than one and I can take $\varepsilon_a < \xi_a \varepsilon_a$. In light of the additional condition $\xi_a \varepsilon_a \ll G$ from equation (6), I set $\varepsilon_a G^{-1}$ to zero and get

$$-\beta\varepsilon_a + \ln\left[\frac{\tilde{\xi}_a + g_a - 1}{\tilde{\xi}_a}\right] - \gamma' = 0$$

Hence,

$$\tilde{\xi}_{\mathbf{k}}(m) = \frac{1}{\exp(\beta\varepsilon_{\mathbf{k}} + \gamma') - 1}$$

where $\beta$ is the actual inverse temperature and $\gamma'$ is determined by $\sum_{\mathbf{k}} \tilde{\xi}_{\mathbf{k}} = m$. The largest contribution to the energy sum comes from $\tilde{G}_m = \sum_{\mathbf{k}} \tilde{\xi}_{\mathbf{k}}(m)\varepsilon_{\mathbf{k}}$. As is typical of the ensemble method, selecting the value $\tilde{G}_m$ from the sum over energies neglects fluctuations about the most probable value. The error is expected to be negligible at low temperatures.

Equation (10) becomes

$$\left\langle \sum_{\mathbf{k}\neq 0} n_{\mathbf{k}} \right\rangle_\beta = Z^{-1} \sum_m R_{m/\text{all}}[\exp(-\beta\tilde{G}_m)] \sum_{\mathbf{k}\neq 0} \tilde{n}_{\mathbf{k}}(\tilde{G}_m, m) \tag{15}$$

Next, I replace the sum over $m$ with the largest value of the summand. The ratio of the number of states of $m$ spin waves to the total number of states is

$$R_{m/\text{all}} = \frac{(m + N^d - 1)!}{m!(N^d - 1)!} 2^{-N^d} \tag{16}$$

Using results from the theory of Bose condensation, I will now show that $\tilde{n}_{\mathbf{k}}$ and $\tilde{G}$ are essentially constant at low temperatures with respect to variations in $m$. Making the low-temperature approximations for the energy, $\varepsilon_{\mathbf{k}} \approx J\mathbf{k}^2$, and the cutoff, $Q(m) = \infty$, I can write the constraint conditions that determine the chemical potentials $\gamma$ and $\gamma'$ as (Huang, 1963, p. 200)

$$\begin{aligned}\frac{N^d}{m} &= \pi^{-3} \int_0^\infty \frac{k^2\, dk}{\lambda_m e^{\beta J k^2} - 1} + \frac{1}{N^d} \frac{1}{\lambda_m - 1} \\ &= \left[\frac{JT}{2\pi}\right]^{3/2} g_{3/2}(\lambda_m^{-1}) + \frac{1}{N^d} \frac{1}{\lambda_m - 1}\end{aligned} \tag{17}$$

where $\lambda_m = e^\alpha$, $g_n(z) = \sum_{r=1}^\infty (z^r / r^n)$, and $g_{3/2}(z \leq 1) \leq g_{3/2}(1) = 2.612\ldots$.

Since $\tilde{\xi}_{\mathbf{k}}(\gamma')$ is the same function of $\gamma'$ as $\tilde{n}_{\mathbf{k}}(\gamma)$ is of $\gamma$, and since $\gamma$ and $\gamma'$ are both determined by the same condition, it follows that $\gamma = \gamma'$, $\alpha = \beta$

(i.e., $\alpha$ equals inverse temperature), and $\tilde{\xi}_{\mathbf{k}}(\alpha, \gamma') = \tilde{n}_{\mathbf{k}}(\beta, \gamma)$. Since $g_{3/2}(z) \leq g_{3/2}(1)$ and $g_{3/2}(1)$ is finite, the first term in (17) vanishes as $T \to 0$. There remains

$$\lim_{T\to 0} \frac{N^d}{m} = \frac{1}{N^d} \frac{1}{\lambda_m - 1}$$

In the thermodynamic limit $N^d \to \infty$, while $N^d/m$ remains finite. This implies that $\lambda_m$ goes to 1 to keep the right-hand side from vanishing. This, in turn, implies that $\gamma(m)$ is approximately zero for all finite particle densities:

$$\lim_{N\to\infty} \lim_{T\to 0} \lambda_m = 1 \qquad \text{for all} \quad mN^{-d} \neq 0 \tag{18}$$

This is the behavior we expect, for the following reason. $\lambda_m = 1 + \text{order}(N^{-d})$ indicates a finite contribution to the density of states in (17) from those states at $\mathbf{k} = 0$, that is, spin-wave condensation is occurring. The thermal expectation value of the amount of condensation is, ignoring weighting factors, the sum of the amount of condensation occurring at each density. Since a completely ordered state at $T = 0$ requires 100% condensation, condensation must occur at all densities ($\lambda_m \to 1$ for all $m$) as $T \to 0$. This is the physical meaning of equation (18).

Putting $\gamma_m = \ln \lambda_m \approx 0$ in equation (15) allows me to consider $\tilde{G}_m$ and $\tilde{n}_{\mathbf{k}}(\tilde{G}_m, m)$ independent of $m$. Once I take the weighting factor $\exp(-\beta \tilde{G}_m) \sum_{\mathbf{k}\neq 0} \tilde{n}_{\mathbf{k}}(\tilde{G}_m, m)$ to be a constant, the value of $m$ at which the greatest contribution is made is determined solely on the basis of $R_{m/\text{all}}$. Now, $R_{m/\text{all}}$ is proportional to the binomial coefficient of $(m + N^d)$ by $m$, which is strongly peaked at $m = N^d/2$. That is, there are far more ways to construct $(N^d/2)$-spin-wave states than there are for any other subspace. The expectation value becomes

$$\left\langle \sum_{\mathbf{k}\neq 0} n_{\mathbf{k}} \right\rangle_\beta = Z^{-1}\{\exp[-\beta \tilde{G}(N^d/2)]\} \sum_{\mathbf{k}\neq 0} \tilde{n}_{\mathbf{k}}(\beta, \gamma(N^d/2))$$

where I have replaced $\tilde{n}_{\mathbf{k}}(\tilde{G}(N^d/2), N^d/2)$ with $\tilde{n}_{\mathbf{k}}(\beta, \gamma(N^d/2))$.

The normalization factor $Z^{-1}$ remains to be evaluated. This is done by replacing the sum over states in $Z$ with the single largest term,

$$Z = 2 \sum_m \sum_G e^{-\beta G} \sum_{\{\Phi_{Gm}\}}$$

The sum extends over the $m$-particle spin-wave states, for $m = 0, \ldots, N^d/2$. The factor of 2 is a consequence of the symmetry between spin- and anti-spin-wave states [cf. equation (3)]. The sum $\{\Phi_{Gm}\}$ is dominated by the state with occupation numbers given by $\tilde{n}_{\mathbf{k}}(G, m)$, as before. The relative contribution of states in subspaces of different $G$ is greatest at $\tilde{G} = \sum \tilde{\xi}_{\mathbf{k}}(m)\varepsilon_{\mathbf{k}}$, and the sum over $m$ again reduces to the single term at $m = N^d/2$.

Thus, $2Z^{-1} \approx \exp[\beta\tilde{G}(N^d/2)]$, and I am left with

$$\left\langle \sum_{\mathbf{k}\neq 0} n_{\mathbf{k}} \right\rangle_{\beta} = \tfrac{1}{2} \sum_{\mathbf{k}\neq 0} \tilde{n}_{\mathbf{k}}(\beta, \gamma(N^d/2))$$

It is now necessary to solve for $\gamma$. A graph of $\gamma$ as a function of density and temperature, based the numerical solution of the constraint equation, is shown in Figure 1. It can be seen that $\gamma = 0$ for all $T < T_c' = 1.95J/k_B$, which is to be expected from equation (18). Here $T_c'$ is the critical temperature as predicted by this low-temperature approximation (not the actual critical temperature) and represents the region near which the steepest-descent method that I have used is expected to give erroneous results. Setting $\gamma = 0$, the final result is

$$\lim_{N\to\infty} \lim_{T\to 0} \left\langle \sum_{\mathbf{k}\neq 0} n_{\mathbf{k}} \right\rangle_{\beta} = \sum_{\mathbf{k}\neq 0} \frac{\tilde{n}_{\mathbf{k}}(\beta, 0)}{2} = \sum_{\mathbf{k}\neq 0} \frac{1/2}{\exp(\beta\varepsilon_{\mathbf{k}}) - 1} \tag{19}$$

and the low-temperature spin-wave (or anti-spin-wave) propagator is

$$\langle n_{\mathbf{k}} \rangle_{\beta} = \frac{1/2}{\exp(\beta\varepsilon_{\mathbf{k}}) - 1}$$

## 4. ANALYTIC DERIVATION OF THE LOW TEMPERATURE MAGNETIZATION IN THE NONINTERACTING APPROXIMATION

Consider the thermal average of the expectation value of the total spin component squared:

$$\langle \Phi | \left( \sum_{\mathbf{j}} \mathbf{S}_{\mathbf{j}} \right)^2 | \Phi \rangle = \frac{N^d}{2}\left[ \frac{N^d}{2} + 1 \right] - \left( \sum_{\mathbf{k}\neq 0} [n_{\mathbf{k}} + \bar{n}_{\mathbf{k}}] \right)\left( N^d - \sum_{\mathbf{k}\neq 0} [n_{\mathbf{k}} + \bar{n}_{\mathbf{k}}] + 1 \right) \tag{20}$$

$n_{\mathbf{k}}$ and $\bar{n}_{\mathbf{k}}$ are evaluated with respect to the state $\Phi$. Here $\mathbf{S}_{\mathbf{j}}$ is the three-component spin operator at a position site $\mathbf{j} = (j^x, j^y, j^z)$ and the $z$ component

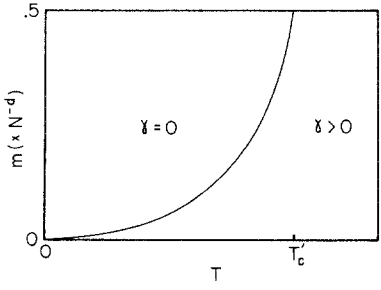


**Fig. 1.** Schematic of the two regimes $\gamma = 0$ and $\gamma > 0$ of the chemical potential as a function of temperature and density based on the numerical solution of the constraint equation.

of the spin at each site is 1/2. Normalizing the expectation value and neglecting terms of order $N^{-d}$, I get

$$\langle \mathfrak{S}^2 \rangle = 1 - 4\left( N^{-d} \sum_{\mathbf{k}\neq 0} [n_{\mathbf{k}} + \bar{n}_{\mathbf{k}}] \right)\left( 1 - N^{-d} \sum_{\mathbf{k}\neq 0} [n_{\mathbf{k}} + \bar{n}_{\mathbf{k}}] \right)$$

Take the magnetization $M_\beta$ to be the positive square root of $\langle \mathfrak{S}^2 \rangle_\beta$ measured in normalized magnetic units. Since

$$\left\langle \sum_{\mathbf{k}\neq 0} \bar{n}_{\mathbf{k}} e \right\rangle_\beta = \left\langle \sum_{\mathbf{k}\neq 0} n_{\mathbf{k}} \right\rangle_\beta = \sum_{\mathbf{k}\neq 0} \tilde{n}_{\mathbf{k}}(\beta, 0)$$

and, in the present approximation,[4] $\langle \sum_{\mathbf{k}\neq 0} n_{\mathbf{k}}^2 \rangle_\beta = \sum_{\mathbf{k}\neq 0} \tilde{n}_{\mathbf{k}}^2(\beta, 0)$, I have

$$\langle M \rangle_\beta = \left\{ 1 - 4\left[ 2N^{-d} \sum_{\mathbf{k}\neq 0} \tilde{n}_{\mathbf{k}}(\beta, 0) \right]\left[ 1 - 2N^{-d} \sum_{\mathbf{k}\neq 0} \tilde{n}_{\mathbf{k}}(\beta, 0) \right] \right\}^{1/2}$$

Making the low-temperature approximations $\varepsilon_{\mathbf{k}} \approx J\mathbf{k}^2$ and $Q(N^d/2) \to \infty$ and replacing the sums with integrations gives

$$\begin{aligned} \langle M \rangle_\beta &= \left[ 1 - 4\left( \frac{\pi^{-3}}{4} \int_0^\infty \frac{k^2\, dk}{e^{\beta J k^2} - 1} \right)\left( 1 - \frac{\pi^{-3}}{4} \int_0^\infty \frac{k^2\, dk}{e^{\beta J k^2} - 1} \right) \right]^{1/2} \\ &= \{ 1 - 4(J\beta)^{-3/2} R_{N^{-d}/2}(2)[1 - (J\beta)^{-3/2} R_{N^d/2}(2)] \}^{1/2} \\ &\approx [1 - 2(J\beta)^{-3/2} R_{N^d/2}(2)] \\ &= 1 - CT^{3/2} \end{aligned} \tag{21}$$

$C$ is given by

$$2(J/k_B)^{-3/2} R_{N^d/2}(2) = (J/k_B)^{-3/2} \zeta(3/2)/4$$

Equation (21) takes into account all features of the free spin-wave model and reproduces the coefficient and power of $T$ in the Bloch law for low temperature magnetization (Bloch, 1930, 1932; Wagner, 1972, p. 180).

## 5. NUMERICAL INVESTIGATION OF THE LOW-TEMPERATURE MAGNETIZATION

The expectation value of $M_\beta$ to first order in $\sum_{\mathbf{k}\neq 0} \hat{n}_{\mathbf{k}}$ is evaluated using Monte Carlo methods,

$$M_\beta \approx \left\langle N^d - 2 \sum_{\mathbf{k}\neq 0} \hat{n}_{\mathbf{k}} \right\rangle_\beta$$

[4]The variational equation for determining the term that contributes the most to the expectation value $\langle n_{\mathbf{k}}^2 \rangle_\beta$ differs from that for $\langle n_{\mathbf{k}} \rangle_\beta$ in that the former contains the term $2 \ln[n_{\mathbf{k}}(\Phi)]$, while the latter contains only $\ln[n_{\mathbf{k}}(\Phi)]$. Terms of this order are neglected, however, in comparison to terms of order $n_{\mathbf{k}}(\Phi) \ln[n_{\mathbf{k}}(\Phi)]$ from Stirlings approximation. As a result of this approximation the same state $\tilde{\Phi}(\beta)$ makes the largest contribution to both expectation values. Consequently $\langle n_{\mathbf{k}}^2 \rangle_\beta \approx n_{\mathbf{k}}(\tilde{\Phi}(\beta))^2 = [\langle n_{\mathbf{k}} \rangle_\beta^2]_{\text{ensemble approx.}}$

Since the Monte Carlo result is built of contributions from all the sums over subspaces rather than just a single term, obtaining the $T^{3/2}$ behavior from a Monte Carlo simulation substantiates the ensemble approximations of Sections 3 and 4.

The magnetization values I obtain for finite systems are accurate to an estimated 0.1%. However, the Monte Carlo technique cannot deal with infinite-size systems and as a consequence the $N=\infty$ extrapolations are subject to additional uncertainties. These uncertainties are of three kinds. First, since it is necessary to extrapolate to values of $N$ outside the range that can be explored numerically, the errors at $N=\infty$ are larger than the errors of the computed values. Second, the size dependence of the results is not known exactly and is arrived at by fitting the data to a straight line in $1/N$. Errors are introduced if the exact size dependence is not linear in $1/N$. Third, finite-size effects are manifested in the energy spectrum, which I now discuss.

In a finite-size quantum system the energy levels are discrete. In particular, we have a gap between the ground and the first excited states given by $\varepsilon_1 = J[1-\cos(2\pi/N)]$, which goes to zero as $N^{-2}$. As a result, for $k_B T < \varepsilon_1(N)$ the population of the ground state is greater, and the population of the excited states less, than what would be the case in the infinite-size system. Since the magnetization at low temperatures varies directly with the number of excited states, this means that $M_\beta(N)$ goes to its saturated value more rapidly for smaller values of $N$. At $T \ll \varepsilon_1(N)/k_B$ the number of excited states goes to zero as $\exp[-\beta\varepsilon_1(N)]$ and the reduced magnetization differs from one by an exponentially small amount. In this region, finite-size effects are dominant and the power-law behavior I hope to observe is lost. To avoid being misled by this effect, the analysis only includes magnetization values at $T \geq \varepsilon_1(N)/k_B$.

The validity of the lowest order in $T$ approximation requires $k_B T/J \ll 1$. As $T$ approaches $J/k_B$, nonlinearities will appear in $M_\beta(N)$. However, these nonlinearities are weak because, as will be seen, the data fit the linear approximation to within statistical accuracy up to temperatures of $0.6J/k_B$.

The details of the Monte Carlo algorithm I have used are discussed elsewhere (Stoller, 1987b), so it will suffice to note the tests used to check the algorithm and results. A version of the algorithm was written in position space, using the classical Hamiltonian, and reproduced magnetization curves for finite classical Heisenberg systems (Binder and Müller-Krumbhaar, 1973). The present results were obtained by updating in wavenumber space. The wavenumber algorithm reproduced the magnetization and susceptibility curves for a quantum model with a simpler cutoff than that of equation (I.30), which was solved exactly for $N=3$. The results passed standard tests for equilibration and ergodicity, which consist in

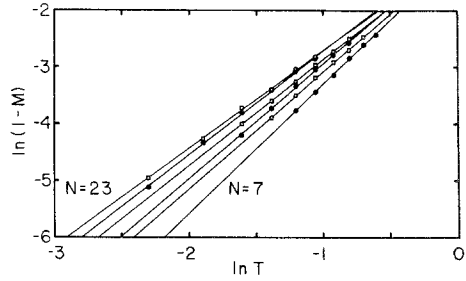


**Fig. 2.** Low-temperature magnetization as a function of temperature. Lines of the linear least squares fits begin with the largest systems on the left and go to the smallest systems on the right.

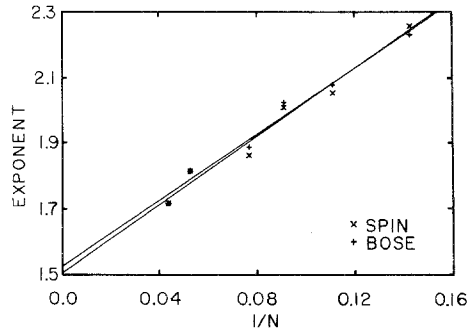


**Fig. 3.** Extrapolation of the low-temperature magnetization exponent based on the finite-size results.

checking for correlations among sections of a single long run. The simulation was run until the magnitudes of relaxation effects, based on the mean and dispersion in the magnetization, indicated that longer runs would not lead to values different from those I am reporting by more than the errors given.

The exponent $x$ from $T^x$ in equation (21) is converted to a slope by taking the logarithm of equation (21):

$$\ln(1-M) = \ln C + x \ln T$$

**Table I.** Comparison of the Analytic and Monte Carlo Results for the Low Temperature Magnetization Exponents in the Thermodynamic Limit

| Analytic: Bose and spin wave | Monte Carlo | |
|---|---|---|
| | Boson state space | Spin-wave state space |
| 1.5 | $1.525 \pm 0.030$ | $1.506 \pm 0.035$ |

where $M$ is obtained by dividing the magnetization at $T$ by its value at $T=0$. The data for $\ln(1-M)$ versus $\ln T$ are plotted in Figure 2 for cubes of $N=7$, 9, 11, 13, 19, and 23 sites per side. Each data point represents between 5000 (for $N=23$) and 40,000 (for $N=7$) system updates, giving magnetization values to estimated accuracies of 0.01% at the lowest temperatures to 0.07% at the highest temperatures.

Computations were also carried out on a purely boson system that had no constraints on the state space. In this case we know that the exact exponent is 3/2 and the results serve as another means of verifying the accuracy of the algorithm. In total, the computations required 25 hr (after debuging) on the Control Data Dual Cyber computer at the University of Texas at Austin.

The values of the exponent at $N=\infty$ are obtained by extrapolating in $1/N$ from the exponents for finite systems, as shown in Figure 3 for both the Bose and spin systems.

The extrapolated are listed in Table 1. The error bounds of one standard deviation are obtained by assuming that the nonlinearities in the dispersion of the exponents about the regression lines of figure 3 are due to normally distributed, random errors.

## APPENDIX. THE ENERGY DEPENDENCE OF $\tilde{n}_{\mathbf{k}}$ AT LOW TEMPERATURE

The calculation determining the Lagrange multiplier $\alpha(G)$ is

$$\left(\prod_{a=x,y,z} \sum_{k^a=-Q(m)/2}^{+Q(m)/2}\right) \varepsilon_{\mathbf{k}} \tilde{n}_{\mathbf{k}}(\alpha, \gamma(m)) = G$$

Separating out the contribution from $\mathbf{k}=0$ and taking the thermodynamic limit, we can write the remaining sum as an integral over $k$ space:

$$= \varepsilon_{\mathbf{k}=0} \tilde{n}_{\mathbf{k}=0}(\alpha, \gamma(m)) + (2\pi)^{-3} \iiint_{k=-Q(m)/2}^{Q(m)/2} \frac{\varepsilon_{\mathbf{k}}\, d^3k}{e^{\gamma} e^{\alpha \varepsilon_{\mathbf{k}}} - 1}$$

When $\alpha \gg J$, large values of $k$ are effectively surpressed, so I can use a small-$k$ approximation to the energy, $\varepsilon_{\mathbf{k}} \approx J\mathbf{k}^2$, and take $Q(m)/2$ to infinity. Since $\gamma$ is a function of $m$, I write $e^{\gamma} = \lambda_m$. Making a substitution of variables gives

$$G \approx (J\alpha)^{-5/2} \left[ \frac{\pi^{-2}}{2} \int_{k=0}^{\infty} \frac{x^4\, dx}{\lambda_m e^{x^2} - 1} \right]$$

$$\equiv (J\alpha)^{-5/2} R_m(4)$$

Hence,

$$\alpha = J^{-1}\left(\frac{R_m(4)}{G}\right)^{2/5}$$

This shows that the approximation of large $\alpha$ is good for sufficiently small $G$, which is realized at low temperatures. That is, as $T \to 0$, the value of $G$ that contributes most to the thermal expectation value goes to 0.

Applying this to $\sum_{\mathbf{k}\neq 0} \tilde{n}_{\mathbf{k}}(G, m)$ gives

$$\begin{aligned}\sum_{\mathbf{k}\neq 0} \tilde{n}_{\mathbf{k}}(G, m) &\approx \frac{\pi^{-2}}{2} \int_{k=0}^{\infty} \frac{k^2\, dk}{\lambda_m e^{\alpha(G)Jk^2} - 1} \\ &= (J\alpha)^{-3/2}\left(\frac{\pi^{-2}}{2} \int_{k=0}^{\infty} \frac{x^4\, dx}{\lambda_m e^{x^2} - 1}\right) \\ &\equiv [J\alpha(G)]^{-3/2} R_m(2)\end{aligned}$$

Finally,

$$\sum_{\mathbf{k}\neq 0} \tilde{n}_{\mathbf{k}}(G, m) \approx \left(\frac{R_m(4)}{G}\right)^{-3/5} R_m(2)$$

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