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Magnon renormalization in the Heisenberg ferromagnet

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An analysis of the concept of renormalization of magnons is presented in view of a recently developed Bose expansion of spin operators. The advantages as well as the limitations of this concept are discussed. It is shown how the kinematic interaction becomes crucial in the critical region. In our renormalized magnon picture it turns out that the phase transition of the Heisenberg ferromagnet can be described as a generalized Bose condensation in the "kinematic space". Finally, our formalism is used to calculate the magnetization curve of the Heisenberg ferromagnet, yielding T_c in excellent agreement with high-temperature expansions.

I. INTRODUCTION

The fundamental work of Dyson[1] produced a clear picture of the low-temperature behavior of ferromagnets. Their elementary excitations were shown to be Bose-like weakly interacting species — the magnons. Later it was realized[2–8] that the same picture could be used for temperatures comparable with the critical temperature, provided the energy of the magnon was "renormalized". This renormalization represents the dressing effect of the interaction on the bare (free) magnon spectrum, the latter being exact with only one magnon present. Practically speaking the renormalization in most works consisted of a temperature-dependent factor multiplying the bare-magnon energy. This is purely a renormalization of the magnon "mass".

Two main nonperturbative techniques were used for the calculation of the renormalization of magnons: the Green-function approach[2–5] and a variational technique[6–8] (see, however, Ref. 9). In the latter approach the diagonal part of the Dyson-Maleev[1,10] Hamiltonian was used to calculate a free energy that was subsequently minimized with respect to the magnon (Boson) occupation number. The nondiagonal part as well as the kinematic interaction[1] were neglected.

In the present work we use the exact Bose expansion that was developed in Refs. 11 and 12 (based on Ref. 13). It consists of the following expressions:

$$S_i^+ = B_i^\dagger \frac{1}{(1+\hat{N}_i)^{1/2}} \frac{1+(-1)^{\hat{N}_i}}{2} ,$$
$$S_i^- = \frac{1+(-1)^{\hat{N}_i}}{2} \frac{1}{(1+N_i)^{1/2}} B_i , \quad (1)$$
$$S_i^z = -\tfrac{1}{2}(-1)^{\hat{N}_i} ,$$

where S_i^+, S_i^-, S_i^z are the usual three spin operators (for $s=\frac{1}{2}$) and $B, B^\dagger$ are Bose operators

$$[B_j, B_i^\dagger] = \delta_{ji} \quad (2)$$

and $\hat{N} = B^\dagger B$ is the number operator in the Bose space. Alternatively one can use the following expressions[12]:

$$S^+ = B^\dagger \Big(\sum_{n=0}^{\infty} b_n B^{\dagger n} B^n \Big) ,$$
$$S^- = \Big(\sum_{n=0}^{\infty} b_n B^{\dagger n} B^n \Big) B , \quad (3)$$
$$S^z = \sum_{n=0}^{\infty} C_n B^{\dagger n} B^n ,$$

where

$$b_n = (-1)^n \frac{1}{n!} \sum_{\substack{\mu=0 \\ \text{even}}}^{n} \binom{n}{\mu} (1+\mu)^{-1/2}$$
$$C_n = (-1)^{n+1} 2^{n-1}/n! . \quad (4)$$

Expressions (3) and (1) are equivalent in the sense that their matrix elements are equal in the Bose space. They constitute an exact Bose expansion of the spin operators. The Heisenberg Hamiltonian

$$H = -\sum_{ij} J_{ij} (S_i^+ S_j^- + S_i^z S_j^z) ,$$
$$J_{ij} = \begin{cases} J, & i,j, \text{ nearest neighbors} \\ 0, & \text{otherwise} \end{cases} , \quad (5)$$

where i,j denote the $\mathfrak{N}$ lattice sites ($i \neq j$) can be written in terms of the Bose operators. This is simply done by replacing S_i^+, S_i^-, S_i^z by the appropriate expression in $B_i^\dagger, B_i$

$$H=-\sum_{ij} J_{ij} B_i^\dagger \left(\sum_{n,m} b_n b_m B_i^{\dagger n} B_i^n B_j^{\dagger m} B_j^m\right) B_j - \sum_{ij} J_{ij} \sum_{n,m} C_n C_m B_i^{\dagger n} B_i^n B_j^{\dagger m} B_j^m \ . \tag{6}$$

Since i,j are different lattice sites and $[B_i, B_j^\dagger]=0$ for $i \neq j$ one can write

$$H=-\sum_{\substack{i,j\\n,m}} J_{ij} b_n b_m B_i^{\dagger n+1} B_j^{\dagger m} B_i^n B_j^{m+1} - \sum_{\substack{i,j\\n,m}} J_{ij} C_n C_m B_i^{\dagger n} B_j^{\dagger m} B_i^n B_j^m \ . \tag{7}$$

This is the Bosonized Hamiltonian we are going to use in this paper. As shown in Ref. 12 the representation of Eq. (7) in the Bose space is one of repeating blocks of size $2^{\mathfrak{N}} \times 2^{\mathfrak{N}}$, each block being equal to the matrix representing H in the spin space. The operator $\sum_i [2\hat{N}_i + (-1)^{\hat{N}_i}]$ is an invariant of the blocks, i.e., it is a c number inside each block.

In this work we use a variational approach based on the Peierls-Bogolubov[14] inequality in order to find an effective free-Bose Hamiltonian whose free energy is optimally close (in the sense defined below) to the exact free energy of the Heisenberg model. In contrast to previous work[6–8] our Bosonized Hamiltonian is Hermitean and thus the use of the Peierls-Bogolubov inequality is justified. In addition the kinematic interaction[1] is not neglected in the Hamiltonian[6] and its effect is shown to be very important in the critical region.

The structure of the paper is as follows: The variational approach is presented in Sec. II. Section III presents the calculations and the results. The reader who is uninterested in technical details can skip it. Section IV is devoted to a discussion of the results and a brief summary of the paper.

II. VARIATIONAL APPROACH

In this section it is assumed that the free energy of the Heisenberg model can be represented by using a free-Bose Hamiltonian H_0 with a temperature-dependent interaction (renormalized Bosons)

$$H_0=\sum_{\vec{k}} \epsilon(\vec{k},T) B_{\vec{k}}^\dagger B_{\vec{k}} \ . \tag{8}$$

Let

$$\tilde{H}=H+(1/\beta)\mu W \ , \tag{9}$$

where μ is a positive constant, $\beta=1/k_B T$, and W is the block invariant. Since W commutes with H, one can write $Z_{\tilde{H}}$, the partition function of $\tilde{H}$,

$$Z_{\tilde{H}}=\mathrm{Tr}(e^{-\beta H} e^{-\mu W}) \ . \tag{10}$$

$e^{-\mu W}$ is a c number inside each block, which we denote by $e^{-\mu W_{\text{block}}}$.

$$Z_{\tilde{H}}=\sum_{\text{all blocks}} (\mathrm{Tr}_{\text{block}} e^{-\beta H}) e^{-\mu W_{\text{block}}} \tag{11}$$

$\mathrm{Tr}_{\text{block}} e^{-\beta H}$ is the partition function Z_H of the Heisenberg model, for any block. In the mth block of a spin $S_i^z=-\frac{1}{2}$, W is given by $\sum_i (4m_i+1)$. Hence

$$Z_{\tilde{H}}=Z_H \sum_{\text{all } m_i=0}^{\infty} \exp\left(-\mu \sum_i (4m_i+1)\right) \ . \tag{12}$$

Defining: $F_{\tilde{H}}=-(1/\mathfrak{N}) T \ln Z_{\tilde{H}}$ and $F_H=-(1/\mathfrak{N}) T \ln Z_H$ one obtains a relation between those two free energies

$$F_{\tilde{H}}=F_H - T \ln\left(\frac{e^{-\mu}}{1-e^{-4\mu}}\right) \ . \tag{13}$$

Using the Peierls-Bogolubov inequality[14]

$$F_{\tilde{H}} \leq F_{H_0} + \frac{1}{\mathfrak{N}} \langle \tilde{H}-H_0 \rangle_0 \ , \tag{14}$$

where $\langle \ \rangle_0$ means averaging with respect to H_0. From Eqs. (9), (13), and (14)

$$F_H \leq F_{H_0} + \frac{1}{\mathfrak{N}} \langle H-H_0 \rangle_0 + \frac{\mu T}{\mathfrak{N}} \langle W \rangle_0 + T \ln\left(\frac{e^{-\mu}}{1-e^{-4\mu}}\right) . \tag{15}$$

Thus the free energy of the Heisenberg ferromagnet is bounded from above by the expression on the right-hand side of Eq. (15), which will be denoted henceforth as F_{mod}. The minimal value of this upper bound is our "best estimate" of F_H. F_{mod} depends on μ and the n's

$$n_{\vec{k}}=\langle B_{\vec{k}}^\dagger B_{\vec{k}} \rangle_0 = (e^{+\beta\epsilon(\vec{k},T)}-1)^{-1} \ . \tag{16}$$

In an exact theory the value of μ is irrelevant (see Ref. 12). Here, however, we choose the μ that minimizes F_{mod}. Doing so we get from Eq. (15)

$$\frac{1}{\mathfrak{N}} \langle W \rangle_0 = \frac{1+3e^{-4\mu}}{1-e^{-4\mu}} \ . \tag{17}$$

The right-hand side of Eq. (17) is the average of W with respect to $\tilde{H}$, $\langle W \rangle_{\tilde{H}}$, that is the original average of W

$$\frac{1}{\mathfrak{N}} \langle W \rangle_{\tilde{H}} = \left(\sum_{\text{blocks}} W e^{-\mu W_{\text{blocks}}} \Big/ \sum_{\text{blocks}} e^{-\mu W_{\text{block}}}\right) \ . \tag{18}$$

Thus the variational principle leads to the result that the average of W must be kept equal to its "real" average. W plays the role of a conserved quantity (like the number of particles in a usual Bose system) and μ is its associated "chemical potential".

As is shown below, the averages $\langle H\rangle_0$ and $\langle W\rangle_0$ depend only on two parameters, N and L, defined through relations

$$N=\frac{1}{\mathfrak{N}}\sum_{\vec{k}}n_{\vec{k}},\quad L=\frac{1}{\mathfrak{N}}\sum_{\vec{k}}\alpha(\vec{k})n_{\vec{k}}\ , \tag{19}$$

where

$$\alpha(\vec{k})=\tfrac{1}{3}(\cos k_xa+\cos k_ya+\cos k_za)$$

for the sc lattice and a equals the lattice constant. In addition, F_{mod} depends on the $n_{\vec{k}}$'s directly. Therefore we find the minimum of F_{mod} by using two Lagrange multipliers g_1 and g_2 so that we can independently vary N, L, and the $n_{\vec{k}}$'s. The function to minimize is

$$\begin{aligned}\mathcal{L}=&-\frac{T}{\mathfrak{N}}\sum_{k}[(n_{\vec{k}}+1)\ln(n_{\vec{k}}+1)-n_{\vec{k}}\ln n_{\vec{k}}]\\&+\frac{1}{\mathfrak{N}}\langle H\rangle_0+T\ln\frac{e^{-\mu}}{1-e^{-4\mu}}\\&+\frac{\mu T}{\mathfrak{N}}\langle W\rangle_0-g_1\left(N-\frac{1}{\mathfrak{N}}\sum_{\vec{k}}n_{\vec{k}}\right)\\&-g_2\left(L-\frac{1}{\mathfrak{N}}\sum_{\vec{k}}\alpha(\vec{k})n_{\vec{k}}\right)\ .\end{aligned} \tag{20}$$

The first term in Eq. (20) is the entropy of a free-Bose gas. Performing the derivatives with respect to N, L, and the $n_{\vec{k}}$'s one obtains

$$g_1=\frac{1}{\mathfrak{N}}\frac{\partial}{\partial N}\langle H\rangle_0+\frac{\mu T}{\mathfrak{N}}\frac{\partial}{\partial N}\langle W\rangle_0\ , \tag{21}$$

$$g_2=\frac{1}{\mathfrak{N}}\frac{\partial}{\partial L}\langle H\rangle_0\ , \tag{22}$$

$$\ln\frac{n_{\vec{k}}+1}{n_{\vec{k}}}=g_1+\alpha(\vec{k})g_2\ . \tag{23}$$

From Eqs. (16) and (23),

$$\epsilon(\vec{k},T)=g_1(T)+g_2(T)\alpha(\vec{k})\ , \tag{24}$$

where the fact that g_1 and g_2 are temperature dependent has been made explicit. The magnon renormalization in our case consists of a multiplicative factor g_2 and an additive one, g_1.

Equations (16) and (21)–(24) enable one to express the $n_{\vec{k}}$'s in terms of N, L; and Eq. (19) expresses N, L as functions of the $n_{\vec{k}}$'s. The resulting two self-consistent equations are then solved numerically.

III. CALCULATIONS AND RESULTS

This section is mainly devoted to the calculation of the averages $\langle H\rangle_0$ and $\langle W\rangle_0$ (Secs. III A–III C). After completing these calculations, we can find $\partial\langle H\rangle_0/\partial N$, $\partial\langle H\rangle_0/\partial L$ and $\partial\langle W\rangle_0/\partial N$ and formulate the self-consistent equations and their numerical solution (Sec. III D).

A. Calculation of $\langle W\rangle_0$ and $\langle(-1)^{N_i}\rangle_0=\langle S^z\rangle_0$

Using Eqs. (3) and (4) one obtains

$$\langle(-1)^{\hat{N}_i}\rangle_0=\sum_{\nu=0}^{\infty}\frac{(-2)^\nu}{\nu!}\langle B_i^{\dagger\nu}B_i^{\nu}\rangle_0\ . \tag{25}$$

Going over to Fourier representation

$$B_i=\frac{1}{\sqrt{N}}\sum_{\vec{k}}B_{\vec{k}}e^{i\vec{k}\cdot\vec{r}_i} \tag{26}$$

and using Wick's theorem[16] we obtain

$$\langle(-1)^{N_i}\rangle_0=\sum_{\nu=0}^{\infty}\frac{(-2)^\nu}{\nu!}\frac{1}{\mathfrak{N}^\nu}\sum_{\vec{k}_1}\cdots\sum_{\vec{k}_\nu}\cdots\sum_{\vec{q}_1}\cdots\sum_{\vec{q}_\nu}n_{\vec{k}_1}n_{\vec{k}_2}\cdots n_{\vec{k}_\nu}\sum_{\sigma}\prod_{j=1}^{\nu}\delta_{\vec{k}_{\sigma(j)}\vec{q}_j}\ ,$$

σ denotes a permutation of $\{1,\ldots,\nu\}$. The summations over the q's yields one when acting on the product of Kronecker δ's. Then, using $\sum_\sigma 1=\nu!$, the number of permutations of ν objects, and using the fact that the summations are decoupled we obtain

$$\langle(-1)^{\hat{N}_i}\rangle_0=\sum_{\nu=0}^{\infty}(-2)^\nu N^\nu\ . \tag{28}$$

For $N<\frac{1}{2}$ the sum in Eq. (28) is

$$\langle(-1)^{\hat{N}_i}\rangle_0=\frac{1}{1+2N}\ . \tag{29}$$

One can easily be convinced that Eq. (29) is correct for any N. This is essentially due to the fact that $\langle(-1)^{\hat{N}_i}\rangle_0$ is bounded in absolute value by 1 and cannot be a singular object.

Using the definition of W (see the Introduction)

$$\langle W\rangle_0=2N+\frac{1}{1+2N}\ . \tag{30}$$

B. Calculation of $\langle(-1)^{N_i}(-1)^{N_j}\rangle_0$

The term $\langle(-1)^{\hat{N}_i}(-1)^{\hat{N}_j}\rangle_0$ corresponds to the $(-\sum_{ij}J_{ij}S_i^zS_j^z)$ part of H.

Expanding $(-1)^{N_i}$, like in Eq. (25), we get for $i \neq j$

$$\langle(-1)^{\hat{N}_i}(-1)^{\hat{N}_j}\rangle_0 = \sum_{n,m=0}^{\infty} \frac{(-2)^n}{n!}\frac{(-2)^m}{m!}\langle B_i^{\dagger n} B_j^{\dagger m} B_i^n B_j^m\rangle_0 \quad . \tag{31}$$

We have used $[B_i,B_j^\dagger]=0$ for $i \neq j$. Going to the Fourier transformed representation and using Wick's theorem

$$\langle(-1)^{\hat{N}_i}(-1)^{\hat{N}_j}\rangle_0 = \sum_{m,n=0}^{\infty} \frac{(-2)^n}{n!\mathfrak{N}^n}\frac{(-2)^m}{m!\mathfrak{N}^m}\sum_{\vec{k}_1}\cdots\sum_{\vec{k}_{n+m}}\sum_{\vec{q}_1}\cdots\sum_{\vec{q}_{n+m}}\exp\left(i\sum_{\nu=1}^{n}(\vec{k}_\nu-\vec{q}_\nu)\cdot\vec{\Delta}_{ij}\right)n_{\vec{k}_1}n_{\vec{k}_2}\cdots n_{\vec{k}_{n+m}} \times\sum_{\sigma}\sum_{\lambda=1}^{n+m}\delta_{\vec{k}_{\sigma(\lambda)},\vec{q}_\lambda} \quad , \tag{32}$$

where

$$\vec{\Delta}_{ij} \equiv \vec{r}_i - \vec{r}_j \quad . \tag{33}$$

When $1 \leq \nu \leq n$ the sum over $\vec{q}_\nu$ in Eq. (32) is

$$\sum_{\vec{q}_\lambda} e^{-i\vec{q}_\lambda\cdot\vec{\Delta}_{ij}}\delta_{\vec{k}_{\sigma(\lambda)},\vec{q}_\lambda} = \exp(-i\vec{k}_{\sigma(\lambda)}\cdot\vec{\Delta}_{ij}) \quad , \tag{34}$$

when $n+1 \leq \nu \leq n+m$ the sum over $\vec{q}$ in Eq. (32) is

$$\sum_{\vec{q}_\nu}\delta_{\vec{k}_{\sigma(\nu)},\vec{q}_\nu} = 1 \tag{35}$$

Consequently, summing over all $\vec{q}_\nu$ yields

$$\langle(-1)^{\hat{N}_i}(-1)^{N_j}\rangle_0 = \sum_{m,n=0}^{\infty} \frac{(-2)^n}{\mathfrak{N}^n n!}\frac{(-2)^m}{\mathfrak{N}^m m!}\sum_{\vec{k}_1}\cdots\sum_{\vec{k}_{n+m}}\exp\left(i\sum_{\nu=1}^{n}\vec{k}_\nu\cdot\vec{\Delta}_{ij}\right)n_{\vec{k}_1}n_{\vec{k}_2}\cdots n_{\vec{k}_{n+m}}\sum_{\sigma}\prod_{\lambda=1}^{n}\exp(i\vec{k}_{\sigma(\lambda)}\cdot\vec{\Delta}_{ij}) \quad . \tag{36}$$

The sum over all permutations σ is equal to the following expression

$$\sum_{\sigma}\prod_{\lambda=1}^{n} e^{-i\vec{k}_{\sigma(\lambda)}\cdot\vec{\Delta}_{ij}} = \frac{n!m!}{2\pi}\int_0^{2\pi} d\phi\, e^{i\phi n}\prod_{\lambda=1}^{n+m}(1+e^{-i\phi}e^{-i\vec{k}_j\cdot\vec{\Delta}_{ij}}) \quad . \tag{37}$$

This is so because

$$\frac{1}{2\pi}\int_0^{2\pi} d\phi\, e^{i\phi m} = \delta_{m,0} \quad ,$$

so the integral in Eq. (37) picks up all possible products of n terms of type $e^{i\vec{k}_j\cdot\vec{\Delta}_{ij}}$, each product appearing only once. Hence

$$\langle(-1)^{\hat{N}_i}(-1)^{\hat{N}_j}\rangle_0 = \sum_{n,m=0}^{\infty} \frac{(-2)^n}{\mathfrak{N}^n}\frac{(-2)^m}{\mathfrak{N}^m}\sum_{\vec{k}_1}\cdots\sum_{\vec{k}_{n+m}}\frac{1}{2\pi}\int_0^{2\pi} d\phi\, e^{i\phi n} \times\exp\left(i\sum_{\nu=1}^{n}\vec{k}_\nu\cdot\vec{\Delta}_{ij}\right)\prod_{\nu=1}^{n+m}(1+e^{-i\phi}e^{-i\vec{k}_\nu\cdot\vec{\Delta}_{ij}})n_{\vec{k}_1}\cdots n_{\vec{k}_{n+m}} \quad . \tag{38}$$

The summation over the $n_{\vec{k}}$'s is now decoupled, so we can perform it. The result is

$$\langle(-1)^{\hat{N}_i}(-1)^{\hat{N}_j}\rangle_0 = \int_0^{2\pi}\frac{d\phi}{2\pi}\sum_{n,m=0}^{\infty}(-2)^n(-2)^m(e^{i\phi}L_{ij}+N)^n(N+e^{-i\phi}L_{ij})^m \quad , \tag{39}$$

where

$$L_{ij} \equiv \frac{1}{\mathfrak{N}}\sum_{\vec{k}_\lambda} e^{i\vec{k}_\lambda\cdot\vec{\Delta}_{ij}}n_{\vec{k}_\lambda} = \frac{1}{\mathfrak{N}}\sum_{\vec{k}_\lambda} e^{-i\vec{k}_\lambda\cdot\vec{\Delta}_{ij}}n_{\vec{k}} \quad . \tag{40}$$

For (i,j) nearest neighbors $L_{ij}=(1/\mathfrak{N})\sum_{\vec{k}}\alpha(\vec{k}_\lambda)n_{\vec{k}}$ [see Eq. (19)]. Hence, after performing the summation in Eq. (39) we have to calculate the integral over ϕ. To do so we define $z=e^{i\phi}$ and $z^{-1}=e^{-i\phi}$ and we obtain a contour integral on the unit circle

$$\langle(-1)^{\hat{N}_i}(-1)^{\hat{N}_j}\rangle_0=\int\frac{dz}{2\pi i}\frac{1}{1+2(N+L_{ij}z)}\frac{1}{z(1+2N)+2L_{ij}} . \tag{41}$$

Since clearly $|2L_{ij}/(1+2N)|<1$ only the pole at $z=-2L_{ij}/(1+2N)$ contributes to Eq. (41). Hence

$$\langle(-1)^{\hat{N}_i}(-1)^{\hat{N}_j}\rangle_0=[(1+2N)^2-4L_{ij}^2]^{-1} . \tag{42}$$

C. Calculation of $\langle S_i^+S_j^-\rangle_0$

First we use expression (3) to express $\langle S_i^+S_j^-\rangle_0$ in terms of Bosons

$$\langle S_i^+S_j^-\rangle_0=\sum_{n,m=0}^{\infty}b_nb_m\langle B_i^{\dagger\,n+1}B_j^{\dagger m}B_i^nB_j^{m+1}\rangle_0 . \tag{43}$$

The fact that $i\neq j$ has already been used in Eq. (43).

Next we go to the Fourier transformed variables and use Wick's theorem

$$\langle S_i^+S_j^-\rangle_0=\sum_{m,n=0}^{\infty}b_nb_m\frac{1}{\mathfrak{N}^{n+m}}\sum_{\vec{k}_1}\cdots\sum_{\vec{k}_{n+m+1}}\sum_{\vec{p}_1}\cdots\sum_{\vec{p}_{n+m+1}}\exp\left(i\sum_{\nu=1}^{n+1}\vec{k}_\nu\cdot\vec{\Delta}_{ij}-i\sum_{\nu=1}^{n}\vec{p}_\nu\cdot\vec{\Delta}_{ij}\right)n_{\vec{k}_1}\cdots n_{\vec{k}_{n+m+1}}$$
$$\times\sum_{\sigma}\prod_{\lambda=1}^{n+m+1}\delta_{\vec{k}_{\sigma(\lambda)},\vec{p}_\lambda} , \tag{44}$$

where σ denotes a permutation of $\{1,\dots,n+m+1\}$. Summing over the ρ's

$$\langle S_i^+S_j^-\rangle_0=\sum_{m,n=0}^{\infty}b_nb_m\frac{1}{\mathfrak{N}^{n+m+1}}\sum_{\vec{k}_1}\cdots\sum_{\vec{k}_{n+m+1}}\exp\left(i\sum_{\nu=1}^{n+1}\vec{k}_\nu\cdot\vec{\Delta}_{ij}\right)n_{\vec{k}_1}\cdots n_{\vec{k}_{n+m+1}}\sum_{\sigma}\prod_{\lambda=1}^{n}e^{-i\vec{k}_{\sigma(\lambda)}\cdot\vec{\Delta}_{ij}} \tag{45}$$

where we used Eqs. (34) and (35).

As in Sec. III B we express the sum over the permutations σ as an integral

$$\sum_{\sigma}\prod_{\nu=1}^{n}e^{-i\vec{k}_{\sigma(\nu)}\cdot\vec{\Delta}_{ij}}=n!(m+1)!\int_0^{2\pi}\frac{d\phi}{2\pi}e^{i\phi n}\sum_{\nu=1}^{n+m+1}(1+e^{-i\vec{k}_\nu\cdot\vec{\Delta}_{ij}-i\phi}) . \tag{46}$$

Proceeding as in Sec. III B we get

$$\langle S_i^+S_j^-\rangle_0=\sum_{n,m=0}^{\infty}b_nb_mn!(m+1)!\int_0^{\pi}\frac{d\phi}{2\pi}e^{-i\phi}(N+Le^{i\phi})^{n+1}(N+Le^{-i\phi})^m . \tag{47}$$

In order to perform the summation over n and over m in Eq. (47), we use the following representation of the coefficients b_n [see Eq. (4)]:

$$b_n=\frac{(-1)^n}{n!2\sqrt{\pi}}\int_{-\infty}^{\infty}dx\,e^{-x^2}[(1+e^{-x^2})^n+(1-e^{-x^2})^n] . \tag{48}$$

The equality of Eqs. (48) and (4) can be easily checked (see the Appendix of Ref. 12). Next we perform the n,m summation and calculate the integral over ϕ by the substitution $z=e^{i\phi}$ and use of Cauchy's theorem. The result is

$$\langle S_i^+S_j^-\rangle_0=\frac{L_{ij}}{4\pi}\int_{\infty}^{\infty}dx\int_{\infty}^{\infty}dy\,e^{-x^2-y^2}\sum_{\sigma_1=\pm1}\sum_{\sigma_2=\pm1}\{[1+N(1+\sigma_1e^{-x^2})][1+N(1+\sigma_2e^{-y^2})]$$
$$-L_{ij}^2(1+\sigma_1e^{-x^2})(1+\sigma_2e^{-y^2})\}^{-2} . \tag{49}$$

D. Self-consistent equations and the magnetization curve

Using the results of Secs. III A–III C we can write $\langle H\rangle_0$ in terms of N,L, and the parameters J [see Eq. (5)] and T

$$\frac{1}{\mathfrak{N}}\langle H\rangle_0=-\frac{Jz}{2}\langle S_i^+S_j^-\rangle_0-\frac{Jz}{8}\langle(-1)^{\hat{N}_i}(-i)^{\hat{N}_j}\rangle_0 \ , \quad (50)$$

where i,j are any pair of nearest neighbors (due to the cubic symmetry of the problem it does not matter which pair), z is the number of nearest neighbors and the factor $\frac{1}{2}$ is there to avoid double counting. The two averages in Eq. (50) are given in Eqs. (42) and (49) as functions of N and L. The parameter μ can be expressed in terms of N, using Eqs. (30) and (17)

$$\mu=\frac{1}{2}\ln\left(\frac{N+1}{N}\right) \ . \quad (51)$$

Using Eq. (30) we obtain

$$\frac{\partial\langle W\rangle_0}{\partial N}=2-\frac{2}{(1+2N)^2} \ . \quad (52)$$

Hence the substitution of Eqs. (50) [with the averages as given in Eqs. (42) and (49)], (51), and (52) in Eqs. (21) and (22) yields g_1 and g_2 as functions of N and L for every temperature.

The effective spectrum $\epsilon(\vec{k},T)$ is, according to Eq. (24)

$$\epsilon(\vec{k},T)=g_1(N,L,T)+\alpha(\vec{k})g_2(N,L,T) \ , \quad (53)$$

where the N,L dependence of the g's has been stressed.

Now using Eqs. (16) and (19) we have

$$N=\frac{1}{\mathfrak{N}}\sum_{\vec{k}}\{\exp[g_1(N,L,T)+\alpha(\vec{k})g_2(N,L,T)]-1\}^{-1} \ , \quad (54)$$

$$L=\frac{1}{\mathfrak{N}}\sum_{\vec{k}}\alpha(\vec{k})\{\exp[g_1(N,L,T)+\alpha(\vec{k})g_2(N,L,T)]-1\}^{-1} \ . \quad (55)$$

For numerical purposes it is more convenient to use the following expressions, derived by going to an integral in Eqs. (54) and (55)

$$N=\sum_{m=1}^{\infty}e^{-\beta m g_1}I_0^3\left(\frac{-\beta m g_2}{3}\right) \ ,$$
$$L=\sum_{m=1}^{\infty}e^{-\beta m g_1}I_1\left(\frac{-\beta m g_2}{2}\right)I_0^2\left(\frac{-\beta m g_2}{3}\right) \ , \quad (56)$$

where I_0 and I_1 are Bessel functions of imaginary arguments. Equations (54) and (55) are a couple of self-consistent equations for N and L for every temperature T. Their solution has been found numerically. The magnetization M can be found using Eqs.

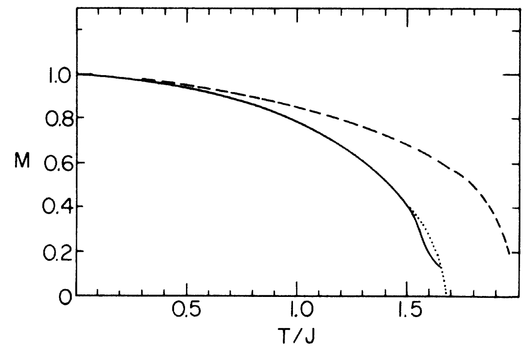

FIG. 1. Magnetization curve. The solid line represents the magnetization M vs the scaled temperature T/J, the dashed line represents the result of M. Bloch (Ref. 6) rescaled to our units and the dotted line is the extrapolation of the $M\sim(T_c-T)^{1/2}$ behavior we get up to $T/J\sim1.5$.

(54) and (29):

$$M=\frac{1}{2}\frac{1}{1+2N} \ . \quad (57)$$

The solid line in Fig. 1 is a plot of M versus the temperature measured in units of J. The broken line represents the results of Bloch.[6,7] Figure 2 is a plot of M^2 versus the temperature. For $1<T/J<1.5$ we get a straight line. Hence

$$M\sim|T-1.68J|^{1/2} \quad (58)$$

in the critical region. Thus the critical exponent β,[17] is mean-field-like. This should come as no surprise since we have essentially used a random-phase approach. In the region where T/J is bigger than 1.5, the magnetization deviates from Eq. (58). As explained in Sec. IV, this is due to the fact that in a noninteraction Bose model [Eq. (8)] there is no transition to the paramagnetic phase. To obtain this transition one has to add a nonlinear term in the $n_{\vec{k}}$'s to the Hamiltonian. This term will presumably influence the results only for $T/J>1.5$. The extrapolation of the straight line in Fig. 2 to the $M^2=0$ axis yields $T_c/J\sim1.68$ for the critical temperature. The

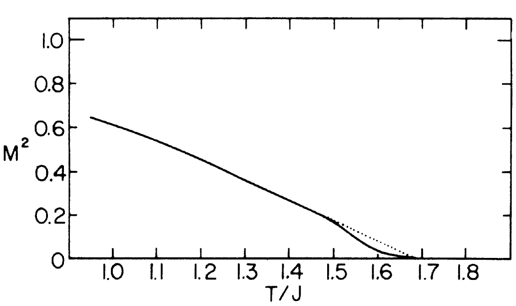

FIG. 2. Squared magnetization vs the temperature. The meaning of the different lines is as in Fig. 1.

extrapolated part is denoted by dotted lines in Figs. 1 and 2. Our result for T_c is in excellent agreement with the results obtained from high-temperature expansions.[18]

IV. DISCUSSIONS AND SUMMARY

This section is concerned with analysis of the results obtained in Secs. I–III. Section IV A deals with effective diagonal Hamiltonians in general. Section IV B is devoted to an analysis of the meaning of the results. In Sec. IV C we treat the special case of an effective noninteracting Bose Hamiltonian. Section IV D summarizes the paper.

A. General diagonal Hamiltonian: the existence problem

The main question to which we address ourselves in this subsection is: Can one find a diagonal Hamiltonian H_0, such that averaging entitities of physical interest (such as S^z) with respect to it [e.g., $\mathrm{Tr}(S_i^z e^{-\beta H_0})/\mathrm{Tr}\, e^{-\beta H_0}$] one obtains the same (or close) results one would have obtained by averaging with respect to the original Heisenberg Hamiltonian? By "diagonal" we mean, as defined in Sec. 1, a Hamiltonian H_0 that depends only on the operators $\hat{n}_k = B_k^\dagger B_k$. This question is related but not equivalent to the question whether H_0 can be reached from H through some kind of renormalization-group (RG) transformation.[19] The reason is the fact we want to average the original (like S^z) operators with respect to H_0, whereas in an RG approach one has to transform the operators too (which may be a very difficult task).

The reason we are able to analyze such a problem is the fact that all averages in Sec. III are correct for any decoupled diagonal Hamiltonian H_0 (see Appendix A).

We start with the magnetization M (defined as $2\langle S^z\rangle_0$). According to Eq. (29) it is given by $M = 1/(1+2N)$. Hence in the critical region below the critical temperature T_c, N must be very big. At and above T_c, N must be infinite. One can easily see that it is possible to find an H_0 that reproduces the exact (or any other) magnetization curve, given the curve $M(T)$ choose H_0 to be a nonintegrating Bose gas [see Eq. (8)], with

$$\epsilon(\vec{k},T) = T \ln \frac{\bar{N}(T)+1}{\bar{N}(T)} \quad , \tag{59}$$

where $\bar{N}$ satisfies

$$M(T) = \frac{1}{1+2\bar{N}(T)} \quad .$$

Then, according to Eq. (16)

$$n_k = \bar{N}(T) \quad . \tag{60}$$

Consequently: $N(T) = \bar{N}(T)$, which is what we wanted to have.

The next question is whether one can reproduce both the magnetization and the spin-spin correlation functions. The answer to this question is negative, at least in the critical region. The reason is the fact that the denominator in Eq. (42) tends to infinity when N does [L_{ij} is always smaller than N, see its definition Eq. (40)]. Hence

$$\langle S_i^z S_j^z \rangle_0 \underset{N\to\infty}{\longrightarrow} 0 \quad . \tag{61}$$

For any pair (i,j) such that $i \neq j$. Since it is clear that the nearest-neighbor correlation function cannot go to zero at T_c, we conclude that no decoupled diagonal Hamiltonian (however complicated) can correctly reproduce both M and the longitudinal spin-spin correlation functions. The correct treatment of the longitudinal correlation function poses problems in the Green-function approach too.[5] On the other hand, the asymptotic behavior of the transverse correlation function, Eq. (49), in the limit $N \to \infty$ is

$$\langle S_i^+ S_j^- \rangle_0 \underset{N>>1}{\sim} \frac{L_{ij}}{N} \quad . \tag{62}$$

If $n_{\vec{k}} = N$ for every $\vec{k}$, $L_{ij} = 0$ and if one chooses $n_{\vec{k}}$ to be a sharply peaked functions at $\vec{k} \sim 0$ and very small for other $\vec{k}$'s, L_{ij} can be made as close to 1 as one wishes.

Thus any intermediate value can be attained. The same holds for the exact expression, Eq. (49).

Since Eqs. (42) and (49) are correct for any pair of lattice points $i \neq i$, we can find the asymptotic behavior of the longitudinal and transverse correlation functions in our model. Using Eqs. (40) and (62) we obtain (for $N >> 1$)

$$\langle S_{\vec{k}}^{\pm} S_{\vec{k}}^{\mp} \rangle_0 \propto n_{\vec{k}} \quad , \tag{63}$$

for small k.

In the same limit, assuming $L_{ij} << N$, we get from Eq. (42)

$$\langle S_{\vec{k}}^z S_{-\vec{k}}^z \rangle_0 \propto \sum_{\vec{q}} n_{\vec{k}-\vec{q}} n_{\vec{q}} \tag{64}$$

$n_{\vec{k}}$ cannot be $1/k^2$ even for small k, otherwise the longitudinal correlation diverges for finite k.

The conclusions from this subsection are:

(a) A renormalized magnon model cannot reproduce the spin-spin correlation function for high temperatures and small momenta. This conclusion is intuitively clear since at high enough temperatures (close to T_c) the longitudinal correlations become very important, whereas in renormalized magnon model one mainly concentrates on the transverse correlations. Perhaps a model that is in the nature of van Kranendonk's[20] for high k and of a renormalized magnon type for low $\vec{k}$ is a good description. For an attempt in this spirit see Sokoloff (Ref. 21).

(b) The fact that $M=1/(1+2N)$ explains why one may obtain "wrong" powers of T in the approximate temperature expansions when one uses the approximate formula $M=1-2N$. This is so because substitution of Dyson's expansion[1] in Eq. (29) leads to

$$\tfrac{1}{2}-N=\tfrac{1}{2}-2a_0\theta^{3/2}-2a_1\theta^{5/2}+4a_0^2\theta^3+\cdots \ , \quad (65)$$

where a_0, a_1 etc. are given in Ref. 18. The appearance of the "spurious" θ^3 merely indicates that one has used the wrong formula for the magnetization.

(c) It is possible that by using a model in which only high-$\vec{k}$ spin-wave operators are bosonized one can get a better description of the ferromagnet (including correlations).

B. Kinematic condensation

Formula (29) teaches us that if our model has a phase transition to a paramagnetic phase than the number of bosons N is infinite at the transition point T_c and beyond it. It is interesting to note that one arrives at a similar formula using the method of Tyablikov and Callen.[2,9] In their work N does not have the meaning of a number of bosons. It merely arises from the fluctuation-dissipation theorem. Attempts to interpret their result in terms of bosons meet with difficulties if one restricts oneself to the first block[12] of the bosonized Hamiltonian, as is usually done. This is so since $N\leq 1$ in the first block. In our approach this result creates no difficulties at all and as we shall show, it has a physical interpretation. On the other hand it becomes clear that the bosons we are dealing with are not the physical magnons — at least in the high-temperature limit, because the number of magnons is clearly restricted to one (at most) per lattice site.

When N tends to infinity we see from Eq. (51) that

$$\mu\sim 1/2N \ . \quad (66)$$

Thus μ tends to zero as $N\rightarrow\infty$. In this respect μ behaves like a chemical potential of a free-Bose gas. As $\mu\rightarrow 0$, more and more blocks contribute to the partition function, until at $\mu=0$ all blocks contribute to the partition function, which yields an infinite N and an infinite partition function.

On the other hand, at low temperatures, when $N\rightarrow 0$, we obtain from Eq. (51)

$$\mu\sim -\tfrac{1}{2}\ln N \ . \quad (67)$$

In this limit $\mu\rightarrow\infty$, effectively projecting out the first block only.

When one works in the first block only, one effectively disregards the kinematic interaction. The mere existence of higher blocks reflects the fact that there is a kinematic interaction. This inclusion of more and more blocks as the temperature approaches T_c means that the kinematic interaction becomes increasingly more important. Hence in the picture we describe, the phase transition is kind of a generalized Bose condensation, where the object that becomes singular is the number of contributing blocks. We call this phenomenon kinematic condensation.

It is possible that our picture overemphasizes the role of the kinematic interaction. In this sense it is complementary to the magnon renormalization theories, in which this effect is neglected.

In order to clarify our result further we note that from Eq. (51) it follows that:

$$N=1/(e^{2\mu}-1) \ , \quad (68)$$

which has the appearance of a Bose distribution in the "kinematic space".

We can actually regard the Bose space as a direct product of the "dynamical space" and the "kinematic space". Assume the "Hamiltonian" of the "kinematic space" is

$$H_{\text{kin}}=-\mu W \ . \quad (69)$$

Then the corresponding free energy is

$$F_{\text{kin}}=-T\ln\frac{e^{-\mu}}{1-e^{-4\mu}} \ ,$$

as is clear from Eqs. (12) and (13).

The corresponding entropy S_{kin} is

$$S_{\text{kin}}=\frac{1}{\mathfrak{N}}\langle\mu W\rangle+\ln\frac{e^{-\mu}}{1-e^{-4\mu}} \ . \quad (70)$$

Hence F_{mod} [see Eq. (15)] can be expressed as

$$F_{\text{mod}}=-TS_0+TS_{\text{kin}}-\frac{1}{\mathfrak{N}}\langle H\rangle_0 \ , \quad (71)$$

where S_0 is the free-Bose-gas entropy.

Thus, our model is such that includes a correction to the entropy of the effective Hamiltonian in the form of S_{kin}. When $\mu\rightarrow 0$ the kinematic entropy becomes far more important than the S_0 entropy and determines the fact that the system undergoes a continuous transition. In models where the kinematic part is absent, it is not clear that such a transition occurs and indeed in the usual magnon renormalization, there is a first-order transition.

Finally, we should mention that a noninteracting Bose Hamiltonian gives no transition at all, (see Appendix B) but N goes practically to zero at a well defined temperature). We believe that even a small nonlinearity will make the transition occur at finite T.

C. Case of effective noninteracting Bose model

In the case of an effective noninteracting Bose model [see Eq. (8)] one obtains a spectrum [Eq. (24)]

$$\epsilon(\vec{k},T)=g_1+g_2\alpha(\vec{k}) \ ,$$

where g_1 and g_2 depend on the temperature only and $\alpha(\vec{k})$ is as in Eq. (19), and depends only on $\vec{k}$. g_1 turns out to be positive and g_2 negative. The unrenormalized spectrum of the Heisenberg model[22] (or the coefficient of the $B^{\dagger}_{\vec{k}}B_{\vec{k}}$ term in the Bose expansion) is proportional to $\alpha(\vec{k})$ given by

$$\omega(\vec{k})=1-\alpha(\vec{k}) \ . \tag{72}$$

Hence, one can rewrite $\epsilon(\vec{k},T)$

$$\epsilon(\vec{k},T)=g_1+g_2+(-g_2)\omega(\vec{k}) \ . \tag{73}$$

Thus the fact that $g_2<0$ is consistent with our understanding that the $k=0$ magnons have the lowest energy. g_1+g_2 must be positive, otherwise the $n_{\vec{k}}$'s are infinite. Consequently g_1 itself is positive. The term g_1+g_2 may be considered as a chemical potential where as $-g_2\omega(\vec{k})$ can be regarded as the energy spectrum of the effective Bose model.

The operator $S^{\pm}_{\vec{k}\to 0}$ creates Godstone excitations[23] in the Heisenberg model. Since $B^{\dagger}_{\vec{k}\to 0}$ is different from $S^{\pm}_{\vec{k}\to 0}$, it does not necessarily create zero energy excitations. Hence its spectrum does not have to go to zero as k tends to zero — and indeed $\epsilon(0,T)\neq 0$, except for zero temperature. However, if one accepts g_1+g_2 as a chemical potential, the spectrum $-g_2\omega(\vec{k})$ goes to zero as $\vec{k}\to 0$. Thus $B^{\dagger}_{\vec{k}\to 0}$ creates an "effective Goldstone Boson" if the effective Bose system is described in an appropriate grand canonical ensemble.

As seen in Fig. 1 and described in Sec. III, the magnetization curve does not reach the $M=0$ axis. This property is correct for any finite temperature in our approximation (a proof of this fact appears in Appendix B). Thus either the variational approach breaks down close to T_c or H_0 is a too simple effective Hamiltonian.

The magnetization curve shows a clear tendency (i.e., $M\sim|T-T_c|^{1/2}$ for $T<1.5$. Hence only the region that is very close to T_c has to be changed. This can be done by adding a nonlinear term with a small coefficient to H_0. Only when N becomes very big, or close enough to T_c, will such a nonlinear term show its presence and bend the magnetization curve towards the $M=0$ line.

D. Concluding remarks

(a) The concept of renormalized magnons is both elegant and fruitful. It leads to an elegant picture of what is happening in the ferromagnet on one hand — and it enables one to calculate physical quantities like the magnetization curve and the critical temperature on the other hand.

(b) An analysis of the role of the kinematic interaction in the critical region is presented here for the first time. It is possible that we have overestimated the importance of this interaction, being complementary to other approaches who neglect this interaction altogether.

(c) Bound state have not been taken into account, as our main interest was the critical region and three-dimensional systems.

(d) It would be interesting to generalize our approach by introducing more constraints (such as a correct low-T behavior[5]) and by adding the critical fluctuations.

(e) Using a Bose expansion for general spin, developed by one of the authors,[24] one can generalize the present work to any spin.

(f) It seems possible to construct a theory of renormalized magnons in the critical region and in the paramagnetic region. The basic idea involved in such a construction is the fact that close to T_c there exist big regions in space, of the size of the correlation length, in which the spins are strongly correlated for long times.[17] Thus the magnetization inside such a correlated region is slowly varying both in space and time. Consequently for high enough $\vec{k}$, one can find spin waves inside this correlated *droplet.* An attempt in this direction is the work of Sokoloff.[21]

(g) It seems possible to use ideas similar to those that appear in this work, for the investigation of dynamical properties of ferromagnets.

APPENDIX A: WICK'S THEOREM FROM A GENERAL DECOUPLED DIAGONAL HAMILTONIAN

Let H_0 be a general decoupled diagonal Hamiltonian, i.e., H_0 is of the following form:

$$H_0=\sum_{\vec{k}} f_{\vec{k}}(\hat{n}_{\vec{k}}) \ , \tag{A1}$$

where the $f_{\vec{k}}$'s are any set of functions and $\hat{n}_{\vec{k}}$ is the usual Bose-number operator. Let $|\{\tilde{n}_{\vec{k}}\}\rangle$ denote a state, defined by the eigenvalues $\hat{n}_{\vec{k}}$ of the corresponding $n_{\vec{k}}$'s. H_0 and $e^{-\beta H_0}$ are diagonal in this representation. When all $\vec{p}_i$ are different from each other

$$\langle\{\tilde{n}_k\}|B^{\dagger}_{\vec{p}_1}\cdots B^{\dagger}_{\vec{p}_r}B_{\vec{q}_1}\cdots B_{\vec{q}_r}e^{-\beta H_0}|\{\tilde{n}_{\vec{k}}\}\rangle=\langle\{\tilde{n}_{\vec{k}}\}|B^{\dagger}_{\vec{p}_1}\cdots B^{\dagger}_{\vec{p}_r}B_{\vec{q}_1}\cdots B_{\vec{q}_r}|\{\tilde{n}_{\vec{k}}\}\rangle\exp\left[-\beta\sum_{\vec{k}} f_{\vec{k}}(\tilde{n}_{\vec{k}})\right] \ . \tag{A2}$$

Hence

$$\langle B^\dagger_{\vec{p}_1} \cdots B^\dagger_{\vec{p}_r} B_{\vec{q}_1} \cdots B_{\vec{q}_r} \rangle_0$$

$$= n_{\vec{p}_1} n_{\vec{p}_2} \cdots n_{\vec{p}_2} \sum_\sigma \prod_{i=1}^{r} \delta_{\vec{p}_i, \vec{q}_{\sigma(i)}} , \quad \text{(A3)}$$

where σ is a permutation of $\{1,\ldots,r\}$. $\langle \ \rangle_0$ means thermal averaging with respect to H_0 and $n_{\vec{p}}$ is the thermal average of $\hat{n}_{\vec{p}}$, namely,

$$\left[\sum_{\hat{n}_{\vec{p}}=0} \hat{n}_{\vec{p}} e^{-\beta f(\hat{n}_{\vec{p}})} \Big/ \sum_{\hat{n}_{\vec{p}}=0} e^{-\beta f(\hat{n}_{\vec{p}})} \right] . \quad \text{(A4)}$$

APPENDIX B: UNATTAINABILITY OF ZERO MAGNETIZATION IN AN EFFECTIVE FREE-BOSE MODEL

The aim of this Appendix is to show that our approach, where H_0 describes a noninteracting Bose gas[8] cannot lead to a second-order transition at a finite temperature. This is done by proving that the assumption of a finite critical temperature leads to an inconsistency.

Let us assume that our model has a finite transition temperature, T_c. The total number of Bosons is [see Eqs. (16), (19), and (24)]

$$N = \int\int\int_{\pi}^{\pi} \frac{d^3k}{(2\pi)^3} \frac{1}{e^{\beta[g_1 + g_2 \alpha(\vec{k})]} - 1} . \quad \text{(B1)}$$

Since $-1 \leq \alpha(\vec{k}) \leq 1$, it is not difficult to show from Eq. (B1) that N can tend to infinity as $T \to T_c$ if and only if both g_1 and g_2 tend to zero as $T \to T_c$ at most as $1/N$. Let L denote L_{ij} for (i,j) nearest neighbors.

Using Eq. (B1) and the corresponding integral expression for L [see Eq. (19)] we obtain

$$\beta(g_1 N + g_2 L) \sim \int\int\int_{\pi}^{\pi} \frac{d^3k}{(2\pi)^3} \frac{1}{1 + \frac{1}{2}\beta[g_1 + g_2 \alpha(\vec{k})]} . \quad \text{(B2)}$$

Hence, to order $1/N^2$:

$$1 - \frac{L}{N} \sim \frac{T - \frac{1}{2} g_1}{N(-g_2)} - \left[\frac{g_1}{-g_2} - 1 \right] . \quad \text{(B3)}$$

Let us define

$$u = \frac{g_1}{-g_2} - 1 . \quad \text{(B4)}$$

From Eqs. (21), (22), and Sec. III it follows that $g_1 > 0$ and $g_2 < 0$. Since necessarily $n_k > 0$ for all k one must have $g_1 > |g_2|$. From those properties of g_1 and g_2 it follows that $u > 0$.

From Eqs. (B3) and (B4)

$$1 - \frac{L}{N} \sim \frac{T}{N|g_2|} - u + O\left[\frac{1}{N} \right] , \quad \text{(B5)}$$

where we have neglected g_1 with respect to T. To the same order it follows from Eq. (B1)

$$\frac{|g_2| N}{T} \sim \int\int\int_{-\pi}^{\pi} \frac{1}{u + 1 - \alpha(\vec{k})} \frac{d^3k}{(2\pi)^3} . \quad \text{(B6)}$$

When $u = 0$ the integral $W(u)$ in Eq. (B6) is Watson's integral[22] $W = 1.516\ldots$. It can be shown that

$$0.659 \cdots \leq \frac{1}{W(u)} - u \leq 1 \quad \text{for } u > 0 .$$

Hence using Eq. (B6)

$$\frac{1}{u+1} < \frac{|g_2| N}{T} < \frac{1}{u + 0.659 \cdots} . \quad \text{(B7)}$$

Substitution of Eq. (B7) into Eq. (B5) yields

$$0 < \frac{L}{N} < 0.34 \cdots . \quad \text{(B8)}$$

The result (B8) is crucial to our proof since it enables us to find the asymptotic behavior of g_1 and g_2. To understand this point let us examine [see Eq. (42)]

$$\frac{\partial \langle S_i^z S_j^z \rangle_0}{\partial N} = -\frac{1 + 2N}{[(1+2N)^2 - 4L^2]^2} . \quad \text{(B9)}$$

Equation (B9) contributes to g_1. If $L/N \sim 1$ was possible, the contribution of this term to g_1 could be of order $1/N$, whereas using restriction Eq. (B8) it follows that this term is of order $1/N^3$. In order to examine the contribution of $\langle S_i^+ S_j^- \rangle_0$ to g_1 and g_2 in the limit of very big N, it is enough to take only the contribution of $\sigma_1 = \sigma_2 = 1$ in Eq. (49) and to replace $1 - e^{-x^2}$ by x^2 and $1 - e^{-y^2}$ by y^2. Then one rescales the new variables $\bar{x} = x\sqrt{N}$ and $\bar{y} = y\sqrt{N}$. The result is that in the limit $N \to \infty$ one can write

$$\frac{1}{\mathfrak{N}} \frac{\partial \langle H \rangle_0}{\partial N} \sim \frac{qa}{N} , \quad \text{(B10)}$$

$$\frac{1}{\mathfrak{N}} \frac{\partial \langle H \rangle_0}{\partial L} \sim -\frac{a}{N} , \quad \text{(B11)}$$

where $q \equiv L/N$ and

$$a = \frac{Jz}{2} \int_0^\infty du \int_0^\infty dv \frac{1 + u^2 + v^2 + (1+3q^2) u^2 v^2}{[1 + u^2 + v^2 + (1-q^2) u^2 v^2]^3} \quad \text{(B12)}$$

a is clearly of order unity.

Using Eqs. (51) and (52) it follows that

$$\mu \frac{\partial \langle W \rangle_0}{\partial N} = \frac{1}{N} - \frac{1}{2N^2} + O\left[\frac{1}{N^3} \right] . \quad \text{(B13)}$$

From Eqs. (21) and (22)

$$\frac{N+1/2}{T}\frac{qa}{N} \sim \frac{qa}{TN} \ . \qquad \text{(B14)}$$

If $q \to 0$ at T_c, it follows from Eq. (B14) that N is of order one in contradiction to our assumptions.

$q \to 0$ at T_c, corresponds to [see Eq. (B5)] the equality on the right-hand side of Eq. (B17) which is correct only in the limit $u \to \infty$. Hence from Eq. (B6): $|g_2|N \to 0$ at T_c. But from Eq. (B11) $|g_2|N \to a$ at T_c and $a \neq 0$. So in this case we have a contradiction too.

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