

THERMAL BOSON EXPANSION FOR THE HEISENBERG FERROMAGNET

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A boson expansion, which takes into account fluctuations around a mean-field description at finite temperatures, is applied to the Heisenberg model of a $S = \frac{1}{2}$ ferromagnet. The approach incorporates the $T^{3/2}$ -law for the magnetization at low temperatures and, without considering dynamical interactions, provides a better estimate of the critical temperature than the conventional energy renormalized magnon theory and the random-phase approximation.

1. Introduction

The method of boson expansions consists in the replacement of a fermion system by an equivalent system of bosons¹). In its most usual formulation, a mapping of fermion observables into boson operators

$$A \rightarrow (A)_B \quad (1.1)$$

is defined, such that the commutation relations are preserved. Therefore, if

$$[A, B] = C \quad (1.2)$$

then

$$[(A)_B, (B)_B] = (C)_B. \quad (1.3)$$

This condition is complemented by the requirement that the expectation value of the observables in the ground-state $|0\rangle$ of the fermion system are equal to the expectation values of the respective boson images in the boson vacuum $|0\rangle$:

$$\langle 0|A|0\rangle = \langle 0|(A)_B|0\rangle. \quad (1.4)$$

The physics of the problem remains in this way unchanged when going to the boson representation. The Holstein–Primakoff transformation is a well known example of this kind of boson-expansion²⁻⁴). It has been proved to be very useful for the study of the low-temperature properties of magnetically ordered crystals.

The main intent of the boson formalism is to describe fluctuations around a mean-field situation. The generalization to finite temperatures of a mean field and associated bosonic degrees of freedom may be explored with the aid of different techniques⁵⁻⁶).

It is the aim of the method of thermal boson expansions, which we have introduced in refs. 7 and 8, to extend the standard boson expansions to arbitrary temperatures. This objective is achieved replacing the expectation value with respect to the fermion ground-state in the left-hand side of (1.4) by a statistical average taken with an adequate density matrix D_0 , so that

$$\text{Tr}(D_0 A) = \langle 0 | (A)_B | 0 \rangle. \quad (1.5)$$

The prescription indicated by (1.1), (1.3) and (1.5) may be applied to ferromagnetism, allowing to define spin-waves at a finite temperature. The range of application of the Holstein–Primakoff description is hence enlarged up to the vicinity of the critical point.

There are in the literature essentially two kinds of approaches for tackling the problem of temperature-dependent magnons:

1) Renormalization of the magnons with the magnetization⁹⁻¹⁰)

This method, which is referred to as the “Random-Phase Approximation” (RPA), is relying on a decoupling approximation in the equation of motion for a temperature dependent spin Green’s function. It reproduces the $T^{3/2}$ -law for the magnetization at very low temperatures and predicts a critical temperature which, in the case $S = \frac{1}{2}$, is between the value of the mean-field approximation and the exact one. The theory has the drawback of overestimating the decrease of the magnetization at low temperatures, as it does not lead to the T^4 correction discussed by Dyson¹¹).

2) Renormalization of the magnons with the energy¹²⁻¹³).

Since this procedure has been derived by M. Bloch from a variational principle for the Helmholtz free energy of the magnons, it has a more sound theoretical justification than the Green’s function method, where some unclear decoupling must be assumed. The free energy includes anharmonic terms of the hamiltonian for the magnons, so that dynamical interactions between spin-waves are explicitly considered and Dyson’s correction is obtained. Although the method does not give a definite critical point, it breaks down at a specific temperature T_{\max} , which is near the exact phase transition.

The present theory, in the simplest version of taking only harmonic terms, is similar to (1) in the sense that the magnons are kinematically and not dynamically renormalized, but, like (2), is based on a variational principle. The results regarding the evaluation of the critical temperature turn out to be of the same type of those of (2).

The contents of the paper are as follows. In section 2, we apply the general method, presented in this introduction, to the $S = \frac{1}{2}$ Heisenberg ferromagnet in 3 dimensions. In section 3, we use the Peierls variational principle to obtain the renormalization factor. Finally, in section 4, we present the numerical results, compare them with the more usual approaches to temperature-dependent spin-waves and give the conclusions.

We shall use throughout the paper $\hbar = 1$.

2. Thermal boson expansion for the Heisenberg ferromagnet

Let us consider the Heisenberg model of a lattice of coupled $S = \frac{1}{2}$ spins, being the interactions restricted to the nearest neighbours. The hamiltonian reads

$$H = -J \sum_{j,l} \mathbf{S}_j \cdot \mathbf{S}_l, \quad (2.1)$$

where J is the exchange integral and \mathbf{S}_j is the spin operator of the electron in lattice site j . The index j runs over all N lattice positions, while l runs only over the z nearest neighbours of j .

Since we are interested in the study of normal modes, we consider the Fourier transform of \mathbf{S}_j ,

$$S_k^\pm = N^{-1/2} \sum_j \exp(\pm i\mathbf{k} \cdot \mathbf{R}_j) S_j^\pm, \quad S_k^z = N^{-1/2} \sum_j \exp(i\mathbf{k} \cdot \mathbf{R}_j) S_j^z, \quad (2.2)$$

where \mathbf{R}_j is the vector taken from the origin to the point j . The operators $S_k^\pm = S_k^x \pm iS_k^y$ satisfy the following commutation relations:

$$[S_k^+, S_{k'}^-] = 2N^{-1/2} S_{k-k}^z, \quad [S_k^z, S_{k'}^\pm] = \pm N^{-1/2} S_{k\pm k'}^\pm. \quad (2.3)$$

With the transformation (2.2) the hamiltonian (2.1) may be written

$$H = -Jz \sum_k \gamma_k \left[\frac{1}{2} (S_k^+ S_k^- + S_k^- S_k^+) + S_k^z S_{-k}^z \right], \quad (2.4)$$

where

$$\gamma_k = \frac{1}{z} \sum_l \exp(ik \cdot \delta_l), \quad (2.5)$$

δ_l being the vector from the atom j to the atom l .

We wish now to map the operators S_k^\pm, S_k^z onto functions of boson operators B_k, B_k^\dagger defined in some bosonic Fock space with vacuum $|0\rangle$. The boson commutators are such that $B_k|0\rangle = 0$ and

$$[B_k, B_{k'}^\dagger] = \delta_{k,k'}, \quad [B_k, B_{k'}] = [B_k^\dagger, B_{k'}^\dagger] = 0. \quad (2.6)$$

The mapping must preserve the commutation relations (2.3), in order to keep track of the spin properties.

Let D_0 be a mean-field density matrix describing the mixed state corresponding to a given temperature. According to (1.5) the following equations hold

$$\text{Tr}(D_0 S_k^\pm) = (0|(S_k^\pm)_B|0), \quad \text{Tr}(D_0 S_k^z) = (0|(S_k^z)_B|0). \quad (2.7)$$

Since we do not know the exact density matrix, which commutes with the hamiltonian (2.1), we assume the so-called independent particle approximation, which consists in taking $\log D_0$ to be a 1-body Hermitean operator. We write the density matrix in the form

$$D_0 = A \exp\left(\alpha \sum_j S_j^z\right) = A \exp(\alpha N^{1/2} S_{k=\theta}^z), \quad (2.8)$$

A and α being constants. The normalization property $\text{Tr} D_0 = 1$ leads to a relationship between A and α . The probabilities of finding a spin up and down are respectively $p = A^{1/N} \exp(\alpha/2)$ and $q = A^{1/N} \exp(-\alpha/2)$, such that $p + q = 1$. We will take the difference between these two probabilities $X = p - q$ as the only parameter which specifies D_0 . This parameter will be determined variationally.

Inserting (2.8) in (2.7) we obtain

$$\text{Tr}(D_0 S_k^\pm) = 0 = (0|(S_k^\pm)_B|0) \quad (2.9)$$

and

$$\begin{aligned} N^{1/2} \text{Tr}(D_0 S_{k=\theta}^z) &= \text{Tr}\left(D_0 \sum_j S_j^z\right) = \text{Tr}\left[A \exp\left(\alpha \sum_j S_j^z\right) \sum_j S_j^z\right] \\ &= N \text{Tr}_1[A^{1/N} \exp(\alpha S_1^z) S_1^z] = \frac{N}{2} (p - q) = \frac{N}{2} X \\ &= N^{1/2} (0|(S_{k=\theta}^z)_B|0). \end{aligned} \quad (2.10)$$

On the other hand, the statistical average taken over the commutators (2.3) leads to

$$\begin{aligned} \text{Tr}(D_0[S_k^+, S_{k'}^-]) &= 2N^{-1/2} \text{Tr}(D_0 S_{k-k'}^z) \\ &= \frac{2}{N} \text{Tr} \left\{ A \exp \left(\alpha \sum_j S_j^z \right) \sum_j \exp[i(k-k') \cdot R_j] S_j^z \right\} \\ &= X \delta_{k,k'} = (0|[(S_k^+)_B, (S_{k'}^-)_B]|0) \end{aligned} \quad (2.11)$$

and

$$\text{Tr}(D_0[S_k^z, S_{k'}^\pm]) = 0 = (0|[(S_k^z)_B, (S_{k'}^\pm)_B]|0), \quad (2.12)$$

where use has been made of (2.9) and (2.10).

The following double commutator:

$$N^{1/2} [[S_{k=0}^z, S_k^+], S_{k'}^-] = [S_k^+, S_{k'}^-] \quad (2.13)$$

has as statistical average (see (2.11)):

$$\begin{aligned} N^{1/2} \text{Tr}(D_0 [[S_{k=0}^z, S_k^+], S_{k'}^-]) &= X \delta_{k,k'} \\ &= N^{1/2} (0|[[S_{k=0}^z)_B, (S_k^+)_B], (S_{k'}^-)_B]|0). \end{aligned} \quad (2.14)$$

It is now straightforward to verify that the following boson expansions for S_k^\pm , $S_{k=0}^z$ do preserve the commutation relations, up to the second order in the boson operators,

$$\begin{aligned} (S_k^+)_B &= X^{1/2} B_k + \dots, \quad (S_k^-)_B = X^{1/2} B_k^\dagger + \dots, \\ N^{1/2} (S_{k=0}^z)_B &= \frac{N}{2} X - \sum_k B_k^\dagger B_k. \end{aligned} \quad (2.15)$$

It may be seen for instance that (2.11) follows from (2.15) and (2.6)

$$(0|[(S_k^+)_B, (S_{k'}^-)_B]|0) = X(0|[B_k, B_{k'}^\dagger]|0) = X \delta_{k,k'}. \quad (2.16)$$

Expressions (2.15) are the leading terms of the thermal boson expansion. The bosons are associated to fluctuations around the mean field described by D_0 , whose temperature dependence is contained in the parameter X . We remark that the main difference between (2.15) and the first term of the $T=0$ Holstein–Primakoff series consists in renormalizing the spin $S = \frac{1}{2}$ with the factor X .

To obtain the boson image of the hamiltonian (2.1), we may use the same techniques. The mapping should guarantee that

$$\text{Tr}(D_0 H) = -\frac{1}{4} J N_Z X^2 = (0|(H)_B|0) \quad (2.17)$$

(note that the Heisenberg and the Ising models have the same ground-state energy, in the mean-field approximation).

Using (2.4) we have moreover

$$\text{Tr}(D_0[H, S_k^\pm]) = 0 = (0|[(H)_B, (S_k^\pm)_B]|0), \quad (2.18)$$

$$\begin{aligned} \text{Tr}(D_0[[H, S_k^+], S_{k'}^-]) &= -Jz(1 - \gamma_k) X^2 \delta_{k,k'} \\ &= (0|[[H)_B, (S_k^+)_B], (S_{k'}^-)_B]|0). \end{aligned} \quad (2.19)$$

The conditions (2.17), (2.18) and (2.19) determine the following boson expansion, in leading order in the boson operators, for the hamiltonian:

$$\begin{aligned} (H)_B &= H_0 + (H_2)_B + \dots \\ &= -\frac{1}{4} N J z X^2 + \sum_k J z (1 - \gamma_k) X B_k^\dagger B_k + \dots \end{aligned} \quad (2.20)$$

This hamiltonian, expanded to all orders, gives results perfectly equivalent to the original H .

If we now compare (2.20) with the Holstein–Primakoff hamiltonian, we notice that the factor $S = \frac{1}{2}$ has been replaced by $S = X/2$.

In the harmonic term of (2.20) we identify the energy of the thermal spin-waves

$$\omega_k(X) = Jz(1 - \gamma_k)X. \quad (2.21)$$

The relationship between X and T is the object of the next section.

3. Variational determination of the renormalization factor

In order to know the function $X = X(T)$ and therefore the way how the dispersion relation is affected by the temperature, we assume the existence of thermal equilibrium. The free energy should then be minimized with respect to the parameter X .

The free energy is divided into two parts, one corresponding to the mean field and the other to an ensemble of thermal magnons,

$$F = F_0 + F_2, \quad (3.1)$$

with

$$\begin{aligned} F_0 &= E_0 - TS_0 \\ &= -\frac{1}{4} NJzX^2 + N \frac{k_B T}{2} [(1+X) \log(1+X) + (1-X) \log(1-X)] \end{aligned} \quad (3.2)$$

(the entropy of the mean field is defined as $S = -k_B \text{Tr}(D_0 \log D_0)$, with k_B the Boltzmann constant),

$$\begin{aligned} F_2 = E_2 - TS_2 &= \sum_k \omega_k(X) n_k(X) + k_B T \sum_k \{n_k(X) \log n_k(X) \\ &\quad - [1 + n_k(X)] \log[1 + n_k(X)]\}, \end{aligned} \quad (3.3)$$

where $n_k(X) = 1/\{\exp[\beta\omega_k(X)] - 1\}$, with $\beta = 1/k_B T$, are the occupancy numbers of the renormalized magnons.

In order that F has a minimum, it is necessary that (for the s.c. lattice, $z = 6$)

$$\begin{aligned} \frac{dF}{dX} &= -3NJX + \frac{Nk_B T}{2} \log \frac{1+X}{1-X} \\ &\quad + \sum_k \omega_k n_k(X) + \beta X \sum_k \omega_k^2 n_k(X) [n_k(X) + 1] \\ &\quad - k_B T \beta^2 X \sum_k \omega_k^2 n_k(X) [n_k(X) + 1] \\ &= -3NJX + \frac{Nk_B T}{2} \log \frac{1+X}{1-X} + \sum_k \omega_k n_k(X) = 0, \end{aligned} \quad (3.4)$$

where $\omega_k = \omega_k(X=1)$ is the spin-wave energy at absolute zero.

The eq. (3.4) may still be put into the form

$$X = \text{th} \left\{ \frac{T_C}{T} \left[X - \frac{1}{3JN} \sum_k \omega_k n_k(X) \right] \right\}, \quad (3.5)$$

with $T_C = 3J/k_B$ the Curie temperature provided by the mean-field approximation. The second term in brackets, which has a simple form due to a cancellation between contributions arising from the magnon energy and entropy in (3.4), is precisely the term used by M. Bloch¹²⁻¹³) to renormalize the spin-wave energy. In fact, her X , which is to be inserted in eq. (2.21), in the case of cubic lattices is given by

$$X = 1 - \frac{1}{3JN} \sum_k \omega_k n_k(X). \quad (3.6)$$

It should be emphasized however that the second term of (3.6) results from the first anharmonic term in the conventional Holstein–Primakoff hamiltonian, in contrast to (3.5), which follows from the harmonic truncation of the modified Holstein–Primakoff expansion.

The renormalization factor of the presented method, indicated in (3.5), is independent of the wavefactor k , for all types of lattices. This result contrasts with the theory of energy renormalized magnons, where this k -independence of X is only valid for simple cubic lattices.

It is a usual approximation to replace the sum over k by an integral, whose upper limit corresponds to the boundary of the first Brillouin zone,

$$\sum_k \omega_k n_k(X) = \frac{V}{(2\pi)^3} \int_0^{k_{\max}} \frac{\omega_k}{\exp[\beta\omega_k(X)] - 1} 4\pi k^2 dk, \quad (3.7)$$

with V the volume of the sample. The temperature dependence of (3.7) may be estimated for low enough temperatures, when mainly long wavelength magnons are excited. We approximate the exact dispersion relation by its power expansion in k and extend to infinity the upper limit of the integral. The result reads

$$\sum_k \omega_k n_k(X) \approx \frac{N}{f} \frac{0.237}{(3J)^{3/2}} \left(\frac{k_B T}{X} \right)^{5/2}, \quad (3.8)$$

with $f = 1, 2, 4$ for s.c., b.c.c. and f.c.c. lattices respectively, so that

$$\frac{1}{3JN} \sum_k \omega_k n_k(X) \approx \frac{0.237}{f} \left(\frac{T}{T_C X} \right)^{5/2}. \quad (3.9)$$

If we replace (3.9) in (3.5) and (3.6) we do not find in the first case any power series dependence of X on T (the argument of the hyperbolic tangent is not small enough to allow for a truncation of the respective series), while in the second case we find a $T^{5/2}$ -law for the renormalization factor.

The insertion of the approximation (3.9) in (3.5) allows to draw the conclusion that in the limit $T/T_C \rightarrow 0$ the first term of the argument of th, which is due to the mean field, dominates, leading to

$$X \approx \exp(T_C X/T) \approx 1 - \exp(-2T_C X/T) \quad (3.10)$$

and, therefore, to the well-known spin-wave energy at $T = 0$ and the corresponding C. Bloch's law. With the increase of T/T_c , the second term, due to the magnons, gains importance, until a certain point $T = T_{\max}$ is reached. For $T > T_{\max}$, the transcendental equation (3.5) does not have any solution more. The same kind of behaviour has been found by M. Bloch in her numerical solution of (3.6)¹²⁻¹³).

4. Results and conclusions

We have solved eq. (3.5) considering the exact dispersion relation and taking full account of the finite size of the first Brillouin zone. For the simple cubic lattice, $z = 6$ and the dispersion relation may be written

$$\omega_k(X) = 6J[1 - \cos(ka/\sqrt{3})]X, \quad (4.1)$$

with a the lattice constant.

In fig. 1 we represent the solution X of (3.5) as a function of the reduced

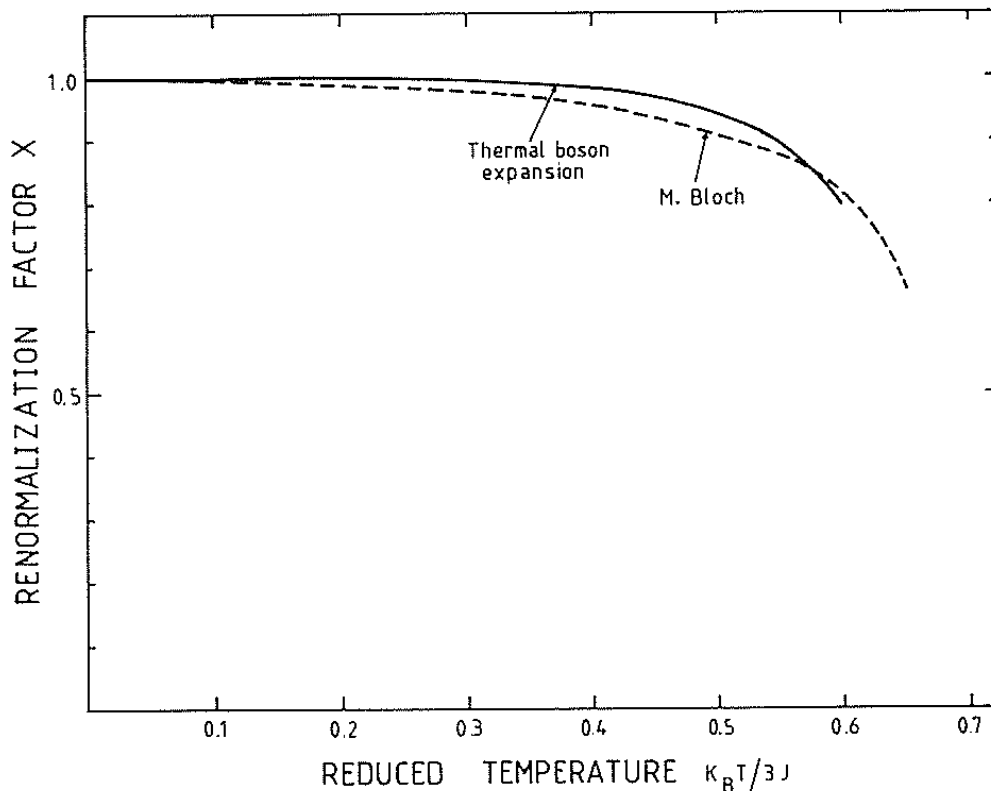


Fig. 1. Renormalization factor for the spin-wave energy, as a function of the reduced temperature $k_B T/3J$, obtained with the thermal boson expansion and with M. Bloch's approach.

temperature $t = T/T_C = k_B T/3J$, compared with M. Bloch's results. The conclusion is that the maximal temperature in the thermal boson method is $t = 0.60$, which is very near the most accurate value $t = 0.56^{14}$, obtained with the aid of a high temperature series expansion. In contrast with our method, the energy renormalized magnon method provides $t = 0.65$, which is out of the right value by 16%, while the RPA leads to $t = 0.66$.

Just before $T = T_{\max}$, we have found a lower branch of X -solutions. We have however not displayed them, since they are unphysical (see however the discussion in ref.¹⁵).

We call attention to the fact that the curve for X in the thermal boson method runs over the curve obtained by M. Bloch¹²⁻¹³), in the regime of low temperatures, crossing it at $t = 0.57$. Our method shows up, therefore, a very wide range of applicability for the concept of magnons.

The decrease of the spin-wave energy with the temperature has been observed directly by neutron-scattering experiments on, for instance, EuO and EuS¹⁶⁻¹⁷), which are good examples of a $S = \frac{7}{2}$ ferromagnet with second nearest interactions. Unfortunately, nature does not give us a good representative of a simple Heisenberg ferromagnet with $S = \frac{1}{2}$ (salts like $K_2CuCl_4 \cdot 2H_2O$ have spin $\frac{1}{2}$, but further neighbour interactions are relevant).

Two properties which depend directly on the excitation of the elementary magnetic modes are the magnetic specific heat and the magnetization. The former results from the energy corresponding to the hamiltonian (2.20):

$$E = -\frac{1}{4}NJzX^2 + \sum_k \omega_k(X)n_k(X). \quad (4.2)$$

We obtain

$$c_V = \left(\frac{dE}{dT}\right)_V = \left(\frac{dE}{dX}\right)_V \frac{dX}{dT}, \quad (4.3)$$

with

$$\left(\frac{dE}{dX}\right)_V = -\frac{1}{2}NJzX + \sum_k \omega_k n_k(X) + \beta X \sum_k \omega_k^2 n_k(X)[n_k(X) + 1]. \quad (4.4)$$

The derivative dX/dT may be obtained from (3.5) by numerical differentiation.

On the other hand, the magnetization is the expectation value with respect to a statistical set of magnons of the operator

$$(M)_B = \frac{g\mu_B}{V} \left(\sum_j S_j^z\right)_B = \frac{g\mu_B}{V} \left(\frac{N}{2} X - \sum_k B_k^\dagger B_k\right), \quad (4.5)$$

where g is the Landé factor and μ_B the Bohr magneton. The reduced magnetization is

$$\frac{M}{M_0} = \frac{M(X)}{M(1)} = X - \sum_k n_k(X) = X - \frac{V}{(2\pi)^3} \int_0^{k_{\max}} \frac{4\pi k^2 dk}{\exp[\beta\omega_k(X)] - 1}. \quad (4.6)$$

This quantity is plotted in fig. 2, as a function of the reduced temperature $k_B T/3J$. The results of M. Bloch and of the RPA are represented for comparison. The reduced magnetization obeys, in all approaches, the celebrated $T^{3/2}$ -law, for very low temperatures. Our approach, as well as the RPA, do not reproduce Dyson's term, arising from the dynamical interactions between magnons. Near the real critical point, the magnetization is more steep in our method, if compared with the other two, in agreement with the real situation. The magnetization at the maximal attainable temperature does not vanish, being about 30% of the saturation value.

It is clear that all methods based on boson expansions should break down near the critical point, where fluctuations of all orders of magnitude are known to be important. We do not consider therefore the finite value of the magnetiz-

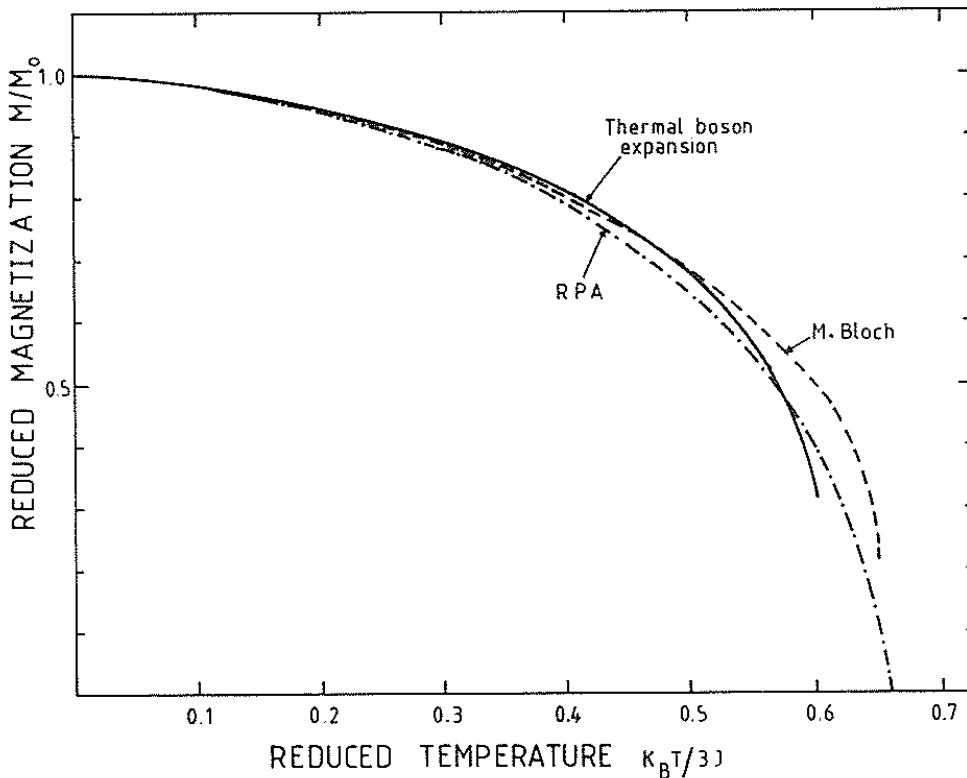


Fig. 2. Reduced magnetization M/M_0 , as a function of the reduced temperature $k_B T/3J$, obtained with the thermal boson expansion, with M. Bloch's approach and with the RPA.

ation at the maximal temperature as a serious drawback. The calculations of ref. 15 show that the inclusion of higher order anharmonicities in the method of energy renormalized magnons does not modify this situation.

The RPA leads, on the contrary, to a well defined critical point. The behaviour of the reduced magnetization, when going to zero, is ruled by the critical exponent characteristic of the mean-field theory, although the phase transition is predicted to occur at a different temperature (the critical point is the same as that of the spherical model).

We may now summarize our conclusions as follows:

1) The method of boson expansions allows for an unified framework of the mean-field and fluctuations around it, for a given many-body system at a finite temperature.

2) A theoretical description of thermal magnons in terms of a self-consistent renormalization of the magnons at $T > 0$ has been given. This renormalization is governed by the mean-field for $T/T_C \ll 1$ and by the magnons themselves for $T/T_C \approx \frac{1}{2}$.

3) The non-interacting thermal bosons lead to results which reproduce the main features of the anharmonic approach developed by M. Bloch. A better determination of the critical point for the simple cubic lattice with $S = \frac{1}{2}$, in comparison with M. Bloch's theory and with the RPA, has been made.

The role of anharmonic terms in the thermal boson expansion should be investigated, in order to make contact with Dyson's treatment. The independent particle approximation, which neglects two-body correlations in the density matrix, might also be improved.

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