

Higher Random Phase Approximations for the Ising Model. I^{*)}

— *The 2nd-RPA* —

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A self-consistent scheme of random phase approximations, for studying the properties of classical many-body systems, is defined. The case of spin $\frac{1}{2}$ Ising model, with nearest neighbor interaction, is taken as the simplest representative example and the 2nd RPA is worked out in detail. The results agree with the exact high and the low temperature series expansions to the first three terms and are found to be adequate at all intermediate temperatures. These results compare favorably with those of the diagrammatic high density expansions carried to the order $(1/z)$.

§ 1. Introduction

The spin $\frac{1}{2}$ Ising model, with ferromagnetic interaction, serves as a useful approximation for the interpretation of the cooperative magnetic behavior exhibited by certain Dy compounds¹⁾ at low temperatures. In the literature, there exist accounts of many attempts which have been made to obtain approximate solutions^{2),3)} of the three-dimensional Ising model. From among these, the methods of Brout⁴⁾ and Horwitz and Callen⁵⁾ are particularly interesting for the reason that they attempt to evolve a prescription for the evaluation of the system free energy in powers of a small expansion parameter: $(1/z)$, where z is the effective number of spins interacting with any given spin. Such a scheme might in principle be expected to have the advantage that for three-dimensional systems it would converge rapidly (because $z \geq 6$) and thus, in contrast with the low and high temperature expansion methods,³⁾ the system thermodynamics would be known adequately at all temperatures-except possibly in the immediate neighborhood of the phase transition where the relative size of fluctuations could become as large as z itself. Unfortunately, however, the computation of the $(1/z)$ expansion beyond the first order terms turns out to be exceedingly complicated.⁶⁾

The method of Green's function decoupling approximations has been used extensively in the study of the cooperative behavior of many spin systems.⁷⁾ The simplest decoupling, to be called the first RPA, yields reasonable results for the system magnetization. It does not, however, give any correlation between

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the z -components of spatially separated spins and, moreover, it overestimates the position of the transition point.

Improvements beyond the simplest RPA turn out to be hard to achieve. Recently⁸⁾ an attempt was made to go beyond the simplest RPA and, in particular, to incorporate the existence of correlations between the z -components of spins. The upshot of this work was that while some improvement on the simple RPA results is obtained in the form of a modified RPA, the actual computation of the second-order-RPA is prohibitively complicated because of the dynamical nature of the interactions in general spin systems. As the Ising model, in contrast to the quantum mechanical general spin systems, does not include any dynamics, the computation of its thermodynamics, within the second RPA, does not present the same level of difficulty.

In the present paper we formulate the general order RPA and carry out the calculation of the 2nd RPA in some detail. The comparison of the results of such an approach with those following from the diagrammatic high density expansion technique of references 4)-6) is interesting: Both the approaches lead to the molecular field theory (MFA) results as their first approximation. The MFA result is known⁴⁾ to be exact to the order $(1/z)^0$. Moreover, the low-temperature, i.e. $T \ll T_c$ where T_c is the Curie temperature, and the high temperature, i.e. $T \gg T_c$, characteristics of our solution are as good as the results following from the second approximation of references 4) and 5) obtained by summing the $(1/z)$ graphs. In the transition region, however, there seems to be an indication that the results of the present formalism may also suffer from the rather subtle thermodynamic inconsistencies that are known to arise in the diagrammatic high density expansions.⁹⁾ With the increase in the accuracy of the approximations, i.e. when 3rd and higher RPA's are taken into account, the hope is that the region where these inconsistencies are prominent will shrink ever closer towards the transition point.

Section 2 of the present paper is devoted to a brief exposition of the Ising model, and that of the relevant thermodynamic Green's functions. The first RPA is worked out in § 3.

Higher order RPA's are defined in section 4 and the solution for the single spin Green's function is given within the 2nd-RPA. The two-spin Green's function is solved within the 2nd-RPA in § 5. In § 6, solutions for the system magnetization and the spin correlation are investigated. In the limit of high and low temperatures, the results are displayed as convergent series expansions and are compared with the exact ones. The transition region is also discussed. The salient conclusions of this paper are briefly summarized in § 7.

The proof of the temporal symmetry of the RPA decoupling scheme is given in the appendix.

§ 2. The Green's function

The Ising Hamiltonian is

$$\mathcal{H} = -\left(\frac{1}{2}\right) \sum_{f_1, f_2} I(f_1 f_2) S_{f_1}^z S_{f_2}^z - \mu H \sum_f S_f^z, \quad (2.1)$$

where f_1, f_2 denote lattice positions. $I(f_1 f_2)$ is a scalar potential depending on the separation $f_1 - f_2$. For simplicity we shall restrict the range of the interaction potential to the nearest neighbors only. This assumption, however, is not strictly necessary and the procedure of the present paper is also applicable to the case of arbitrary range interaction. The last term in Eq. (2.1) describes the Zeeman energy due to an applied field H .

The eigenvalues of the operator S_f^z are either $+\frac{1}{2}$ or $-\frac{1}{2}$ (in Dirac's units). This restriction imposes the well-known kinematic constraint:

$$(S_f^+)^2 = (S_f^-)^2 = 0; \quad (S_f^z)^2 = \frac{1}{4}, \quad (2.2a)$$

where

$$S_f^\pm = S_f^x \pm iS_f^y. \quad (2.2b)$$

In combination with the usual spin commutation relations, Eq. (2.2a) leads to the following useful relations:

$$S_f^+ S_f^- + S_f^- S_f^+ = +1; \quad S_f^z S_f^+ = \frac{1}{2} S_f^+. \quad (2.3)$$

It we define a retarded Green's function

$$\langle\langle A(t); B(t') \rangle\rangle \equiv -i\theta(t-t') \langle [A(t), B(t')]_- \rangle, \quad (2.4)$$

where $\theta(x) = +1$ for $x > 0$ and is zero otherwise and where the time dependence of A and B is in the Heisenberg representation with respect to the Hamiltonian \mathcal{H} , its energy Fourier transform

$$\langle\langle A; B \rangle\rangle_{(E)} = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \langle\langle A(t); B(t') \rangle\rangle \exp[iE(t-t')] d(t-t') \quad (2.5)$$

leads to the relevant correlation function:⁷⁾

$$\langle A(t) B(t) \rangle = + \left(2 \lim_{\epsilon \rightarrow +0} \text{Im} \right) \int_{-\infty}^{+\infty} dE [1 - \exp(-\beta E)]^{-1} \langle\langle A; B \rangle\rangle_{(E+i\epsilon)}. \quad (2.6)$$

In Eqs. (2.4) and (2.6) the statistical averages, denoted by the pointed brackets $\langle \dots \rangle$, are assumed to be taken with respect to the canonical ensemble, i.e.

$$\langle \dots \rangle = \text{Tr}[\exp(-\beta \mathcal{H}) \dots] / \text{Tr}[\exp(-\beta \mathcal{H})]. \quad (2.7)$$

The equation of motion of the single spin retarded Green's function, under the Hamiltonian (2.1), is

$$[E - \mu H] \langle\langle S_g^+; S_g^- \rangle\rangle_{(E)} = (\sigma/\pi) + \sum_{f_1} I(f_1 g) \langle\langle S_{f_1}^z S_g^+; S_g^- \rangle\rangle_{(E)}, \quad (2.8a)$$

where

$$\langle S_g^z \rangle = \langle S^z \rangle = \sigma. \tag{2.8b}$$

Equation (2.8a) is readily derived by operating with $i(d/dt)$ on the Green's function $\langle\langle S_g^+(t); S_g^-(t') \rangle\rangle$ and Fourier transforming both sides with respect to the energy via Eq. (2.5). This operation can be performed an arbitrary number of times and we get:

$$\begin{aligned} & [E - \mu H]^n \langle\langle S_g^+; S_g^- \rangle\rangle_{(E)} \\ &= (1/\pi) [(E - \mu H)^{n-1} \sigma + \sum_{f_1} I(g f_1) \langle S_{f_1}^z S_g^z \rangle (E - \mu H)^{n-2} + \dots \\ &+ \sum_{f_1} \dots \sum_{f_{n-1}} I(g f_1) \dots I(g f_{n-1}) \langle S_{f_1}^z \dots S_{f_{n-1}}^z S_g^z \rangle] \\ &+ \sum_{f_1} \dots \sum_{f_n} I(g f_1) \dots I(g f_n) \langle\langle S_{f_1}^z \dots S_{f_n}^z S_g^+; S_g^- \rangle\rangle_{(E)}. \end{aligned} \tag{2.9}$$

In addition to the above equation of motion, we also need to study the equation of motion of the higher order Green's function occurring on the right hand side, i.e. $\langle\langle S_{f_1}^z \dots S_{f_n}^z S_g^+; S_g^- \rangle\rangle$. In this connection we note that due to the kinematic constraints (2.2) and (2.3), the above Green's function reduces to lower order Green's function whenever any two, or more, of the spatial locations f_1, \dots, f_n and g coincide. To deal with this situation we shall use the following procedure:

$$\begin{aligned} \langle\langle S_{f_1}^z \dots S_{f_r}^z S_g^+; S_g^- \rangle\rangle_{(E)} &= \{ [1 - \mathcal{A}(f_1, \dots, f_r, g)] + \mathcal{A}(f_1, \dots, f_r, g) \} \\ &\times \langle\langle S_{f_1}^z \dots S_{f_r}^z S_g^+; S_g^- \rangle\rangle_{(E)}, \end{aligned} \tag{2.10}$$

where the projection operator $[1 - \mathcal{A}(f_1, \dots, f_r, g)] \equiv \widehat{O}(r)$ is such that it has zero eigenvalues whenever any two, or more, of the $(r+1)$ spatial locations f_1, \dots, f_r and g coincide; otherwise its eigenvalues are unity.

In this manner, the right-hand side of Eq. (2.10), will contain Green's functions of all orders, beginning with $\langle\langle S_g^+; S_g^- \rangle\rangle_{(E)}$ and continuing up to $\widehat{O}(r) \langle\langle S_{f_1}^z \dots S_{f_r}^z S_g^+; S_g^- \rangle\rangle_{(E)}$, with the stipulation that now none of the spatial locations, that a given Green's function refers to, coincide.

The relevant equation of motion can now readily be found:

$$\begin{aligned} & \widehat{O}(r) \langle\langle S_{f_1}^z \dots S_{f_r}^z S_g^+; S_g^- \rangle\rangle_{(E)} [E - \mu H]^n \\ &= \left(\frac{1}{\pi}\right) \widehat{O}(r) [(E - \mu H)^{n-1} \langle S_{f_1}^z \dots S_{f_r}^z S_g^z \rangle + (E - \mu H)^{n-2} \sum_{g_1} I(g g_1) \langle S_{f_1}^z \dots S_{f_r}^z S_g^z S_{g_1}^z \rangle \\ &+ \dots + \sum_{g_1} \dots \sum_{g_{n-1}} I(g g_1) \dots I(g g_{n-1}) \langle S_{f_1}^z \dots S_{f_r}^z S_g^z S_{g_1}^z \dots S_{g_{n-1}}^z \rangle] \\ &+ \widehat{O}(r) \sum_{g_1} \dots \sum_{g_n} I(g g_1) \dots I(g g_n) \langle\langle S_{g_1}^z \dots S_{g_n}^z S_{f_1}^z \dots S_{f_r}^z S_g^+; S_g^- \rangle\rangle_{(E)}. \end{aligned} \tag{2.11}$$

§ 3. The first RPA

The simplest approximation to the set of Eqs. (2.9—11) consists in completely ignoring correlations between spatially separated spins. In terms of the Green's function, this amounts to doing the following:

$$\langle\langle S_f^z S_g^+; S_g^- \rangle\rangle_{(E)} = [(1 - \delta_{g,f}) + \delta_{g,f}] \langle\langle S_f^z S_g^+; S_g^- \rangle\rangle_{(E)}, \quad (3.1a)$$

$$\delta_{g,f} \langle\langle S_f^z S_g^+; S_g^- \rangle\rangle_{(E)} = (\frac{1}{2}) \delta_{g,f} \langle\langle S_g^+; S_g^- \rangle\rangle_{(E)}, \quad (3.1b)$$

$$(1 - \delta_{g,f}) \langle\langle S_f^z S_g^+; S_g^- \rangle\rangle_{(E)} \xrightarrow{\text{1st RPA}} (1 - \delta_{g,f}) \sigma \langle\langle S_g^+; S_g^- \rangle\rangle_{(E)}. \quad (3.1c)$$

Using Eq. (2.6) we readily find the implication of the above decoupling:

$$\langle S_f^z S_g^z \rangle - \sigma^2 \equiv L(f, g) = (\frac{1}{4} - \sigma^2) \delta_{g,f}, \quad (3.2)$$

where $L(fg)$ expresses the fluctuation of the S^z operator from its average value. We shall henceforth refer to $L(fg)$ as the system correlation function.

For the single spin Green's function, the approximation (3.1) implies

$$\langle\langle S_g^+; S_g^- \rangle\rangle_{(E)} = \left(\frac{\sigma}{\pi}\right) \left[\frac{1}{E - \mu H - \sigma J(0)} \right], \quad (3.3)$$

and again using Eq. (2.6) we get

$$2\sigma = \tanh \beta \left[\frac{\mu H + \sigma J(0)}{2} \right], \quad (3.4)$$

where $J(0) = \sum_f I(gf)$.

Equations (3.2) and (3.4) are identical to the molecular field theory results and agree with the correct $(1/z)^0$ evaluation of the free energy in the Brout⁴⁾ and Callen and Horwitz⁵⁾ formulations.

In the limit $\mu H \rightarrow +0$, the system is found to be spontaneously magnetized as long as $T < \theta_c$. As the temperature approaches θ_c , the magnetization disappears. We shall call θ_c the MFA Curie temperature:

$$k_B \theta_c = [J(0)/4]. \quad (3.5)$$

Above θ_c , the system is paramagnetic with the susceptibility χ_{MFA} :

$$\chi_{\text{MFA}} = \left(\frac{d\sigma}{d\mu H} \right)_{\text{MFA}} = \frac{\beta/4}{1 - (\theta_c/T)}. \quad (3.6)$$

At temperatures much lower than θ_c , the system is nearly fully aligned and in the limit of zero magnetic field the magnetization is

$$\sigma = \frac{1}{2} - \exp[-\beta J(0)/2] (1 + \epsilon), \quad (3.7)$$

where $\epsilon \ll 1$ and tends to zero exponentially as $T \rightarrow 0$.

The paramagnetic susceptibility and the low temperature magnetization expansions agree with the exact ones to the first two terms. Disagreement with

the exact results, however, appears immediately in the next order terms represented by ϵ .

Although we shall have occasion to discuss the question of the definition of the Curie temperature more fully in a later section (i.e. § 6), it may be remarked here that the above solution is internally inconsistent. While in the limit of vanishing field the system magnetization indeed disappears as $T \rightarrow \theta_c - 0$, and the paramagnetic susceptibility diverges as T approaches θ_c from above, the spin correlation does not portray the existence of the phase transition. The range of the correlation $L(fg)$ is expected to grow inordinately as the Curie point is approached for the reason that the spin fluctuations will become exceedingly large. In contrast, the correlation (3.2) shows no fluctuations at any temperature. (Note that the particular case of $z = \infty$ is rather anomalous and for this case the foregoing result is exact. Here the correlation does not manifest any dominant change in its range with the changing of the system temperature for the reason that the infinite range of the interaction stabilizes the fluctuations.)

§ 4. Higher order RPA's

The natural generalization⁸⁾ of the first RPA of Eq. (3.1c) is the n th order RPA defined in the following way. Let us express the $(n+1)$ th-order semi-invariants⁹⁾

$$\text{and } \left. \begin{aligned} O(n) (S_{f_1}^z \cdots S_{f_n}^z S_g^-(t') S_g^+(t))_c \\ O(n) (S_{f_1}^z \cdots S_{f_n}^z S_g^+(t) S_g^-(t'))_c \end{aligned} \right\} \quad (4.1)$$

in terms of the correlation functions. (Note that $(\cdots)_c$ denotes the semi-invariant which treats the $(n+1)$ operators $S_{f_1}^z, \cdots, S_{f_n}^z, (S_g^- S_g^+)$ and $S_{f_1}^z, \cdots, S_{f_n}^z, (S_g^+ S_g^-)$ as the relevant statistical operators. Moreover the presence of the projection operators $O(n)$ insures that no two, or more, of the $(n+1)$ spatial locations f_1, \cdots, f_n and g coincide.) The difference of these two $(n+1)$ th order semi-invariants, multiplied by the function $-i\theta(t-t')$, then defines the n th order RPA. Note that this approximation expresses the Green's function $O(n) \langle\langle S_{f_1}^z \cdots S_{f_n}^z S_g^+; S_g^- \rangle\rangle_{(E)}$ in terms of all the lower order Green's functions.

This prescription is illustrated below for the case of the first and the second RPA's. As the first few semi-invariants are

$$\begin{aligned} (xy)_c &= \langle xy \rangle - \langle x \rangle \langle y \rangle, \\ (xyz)_c &= \langle xyz \rangle - \langle xy \rangle \langle z \rangle - \langle xz \rangle \langle y \rangle - \langle yz \rangle \langle x \rangle + 2\langle x \rangle \langle y \rangle \langle z \rangle, \end{aligned} \quad (4.2)$$

therefore the first and the 2nd RPA's respectively are as given in Eq. (3.1c) and the following:

$$\widehat{O}(2) \langle\langle S_{f_1}^z S_{f_2}^z S_g^+; S_g^- \rangle\rangle_{(E)} \xrightarrow{\text{2nd RPA}}$$

$$\widehat{O}(2) [\sigma \langle\langle S_{f_1}^z S_g^+; S_g^- \rangle\rangle_{(E)} + \sigma \langle\langle S_{f_2}^z S_g^+; S_g^- \rangle\rangle_{(E)} + L(f_1 f_2) \langle\langle S_g^+; S_g^- \rangle\rangle_{(E)} - \sigma^2 \langle\langle S_g^+; S_g^- \rangle\rangle_{(E)}]. \tag{4.3}$$

Note that according to the statement defining $\Delta(\dots)$ in § 2, the projection operator $\Delta(f_1, f_2, g)$ is given by the following relation:

$$\widehat{O}(2) = 1 + 2(\delta_{f_1, f_2} \delta_{f_1, g}) - [\delta_{f_1, f_2} + \delta_{f_1, g} + \delta_{f_2, g}] = 1 - \Delta(f_1, f_2, g). \tag{4.4}$$

Having defined the 2nd-RPA, it is now necessary to introduce it as an approximation in the equations of motion. For the single-spin Green's function, this entails using Eq. (2.9) with $n=2$ which we re-write in the following more convenient form:

$$\begin{aligned} [E - \mu H]^2 \langle\langle S_g^+; S_g^- \rangle\rangle_{(E)} &= \left(\frac{1}{\pi}\right) [(E - \mu H) \sigma + \sum_{f_1} I(g f_1) \langle S_{f_1}^z S_g^z \rangle] \\ &+ \frac{J^2(0)}{4z} \langle\langle S_g^+; S_g^- \rangle\rangle_{(E)} + \sum_{f_1} \sum_{f_2} I(g f_1) I(g f_2) [1 - \delta_{f_1 f_2}] \\ &\times \langle\langle S_{f_1}^z S_{f_2}^z S_g^+; S_g^- \rangle\rangle_{(E)}, \end{aligned} \tag{4.5a}$$

where we note the fact that

$$1 = (1 - \delta_{f_1 f_2}) + \delta_{f_1 f_2}, \tag{4.5b}$$

and the kinematic condition (2.2a). As

$$I(g f_1) I(g f_2) (1 - \delta_{f_1 f_2}) \equiv I(g f_1) I(g f_2) (1 - \delta_{f_1 f_2}) 0(2), \tag{4.5c}$$

therefore the last term on the right hand of Eq. (4.5a) can be decoupled as noted in Eq. (4.3). Proceeding in this manner and eliminating the terms containing $\sum_f I(g f) \langle\langle S_f^z S_g^+; S_g^- \rangle\rangle_{(E)}$ by using the identity

$$[E - \mu H] \langle\langle S_g^+; S_g^- \rangle\rangle_{(E)} - \left(\frac{\sigma}{\pi}\right) = \sum_f I(g f) \langle\langle S_f^z S_g^+; S_g^- \rangle\rangle_{(E)}, \tag{4.5d}$$

(compare Eq. (2.9) for $n=1$), we readily find:

$$\langle\langle S_g^+; S_g^- \rangle\rangle_{(E)} = \left(\frac{1}{\pi}\right) \frac{[A + \sigma(E - E(0)) + \sigma x]}{[E - E(+)] [E - E(-)]}, \tag{4.5e}$$

where for convenience we have introduced the notation

$$E(0) = \mu H + \sigma J(0) \left(\frac{z-1}{z}\right), \tag{4.6a}$$

$$x = [\sigma J(0) / z], \tag{4.6b}$$

$$E(\pm) = E(0) \pm \Phi, \tag{4.6c}$$

$$\Phi^2 - x^2 = \sum_{f_1} \sum_{f_2} I(f_1 g) I(f_2 g) L(f_1 f_2) \equiv \Psi, \tag{4.6d}$$

$$A = \sum I(f g) L(f g), \tag{4.6e}$$

and where we have used the following reduction resulting from the nearest neighbor approximation:

$$\sum_f [I(gf)]^n = z[J(0)/z]^n. \tag{4.7}$$

The use of Eq. (2.6) now leads us to the expression relating the system magnetization to the function Φ defined above, i.e.

$$1 = \sigma[\tau(+)+\tau(-)] + \left[\frac{A+\sigma x}{\Phi} \right] [\tau(+)-\tau(-)], \tag{4.8a}$$

where

$$\tau(\alpha) = \coth \left[\frac{\beta E(\alpha)}{2} \right]; \quad \alpha = +, - . \tag{4.8b}$$

Equations (4.8) constitute the 2nd-RPA result for the system magnetization. Analogously to the first RPA result, it is a transcendental relation but unlike the 1st RPA it contains an additional, unknown, parameter Φ . The computation of Φ in effect requires the knowledge of the correlation function $L(f_1 f_2)$.

We might mention here that in the extreme limit of $z \rightarrow \infty$, the above result reduces to the previous one because then both x and Φ are self-consistently zero. Thus in a certain sense the 2nd RPA result, (4.8), includes some of the additional $(1/z)$ effects which are ignored in the 1st RPA. We shall return to the discussion of this point in a later section.

§ 5. The correlation

To determine the correlation $L(fg)$ we need to study the equation of motion of the Green's function $\langle\langle S_f^z S_g^+; S_g^- \rangle\rangle_{(E)}$. [See the appendix for additional remarks.] From Eq. (2.11) we get:

$$\begin{aligned} [E - \mu H] \langle\langle S_{f_1}^z S_g^+; S_g^- \rangle\rangle_{(E)} &= [E - \mu H] \langle\langle S_{f_1}^z S_g^+; S_g^- \rangle\rangle_{(E)} [1 - \delta_{g,f_1} + \delta_{g,f_1}] \\ &= [(E - \mu H) \left(\frac{1}{2}\right) \delta_{g,f_1} + \left(\frac{1}{4}\right) I(gf_1)] \langle\langle S_g^+; S_g^- \rangle\rangle_{(E)} \\ &\quad + (1 - \delta_{g,f_1}) \left(\frac{1}{\pi}\right) [L(f_1 g) + \sigma^2] \\ &\quad + (1 - \delta_{gf_1}) \sum_{f_2} I(gf_2) (1 - \delta_{f_1,f_2}) \langle\langle S_{f_1}^z S_{f_2}^z S_g^+; S_g^- \rangle\rangle_{(E)}. \end{aligned} \tag{5.1}$$

The last term on the right-hand side of Eq. (5.1) contains the Green's function $\langle\langle S_{f_2}^z S_{f_1}^z S_g^+; S_g^- \rangle\rangle$ with the stipulation that none of the spatial positions labelled by g, f_1 and f_2 coincide. As such we can directly introduce the 2nd-RPA of Eq. (4.3) into Eq. (5.1) just as it was done in the preceding section. After some algebra, we arrive at the result

$$\begin{aligned} &[\langle\langle S_{f_1}^z S_g^+; S_g^- \rangle\rangle_{(E)} - \sigma \langle\langle S_g^+; S_g^- \rangle\rangle_{(E)}] [E - E(3)] \\ &= \left(\frac{1}{\pi}\right) \left[L(gf_1) - \delta_{g,f_1} \left(\frac{1}{4} - \sigma^2\right) \right] \end{aligned}$$

$$\begin{aligned}
& + \delta_{g,f_1} \left(\frac{1}{2} - \sigma \right) \langle\langle S_g^+; S_g^- \rangle\rangle_{(E)} [E - E(3)] \\
& + [A(gf_1) - \delta_{g,f_1} A] \langle\langle S_g^+; S_g^- \rangle\rangle_{(E)} \\
& - 2\sigma I(gf_1) [\langle\langle S_{f_1}^z S_g^+; S_g^- \rangle\rangle_{(E)} - \sigma \langle\langle S_g^+; S_g^- \rangle\rangle_{(E)}], \quad (5.2a)
\end{aligned}$$

where

$$E(3) = E(0) + x = \mu H + \sigma J(0), \quad (5.2b)$$

$$A(gf_1) = \sum_{f_2} I(gf_2) L(f_1 f_2); \quad A(gg) = A. \quad (5.2c)$$

The above equation can now be combined with Eq. (4.5e) and solved. This procedure, however, would seem to result in an integral representation for the Green's function, because of the presence of the $I(f_1 g)$ terms on the right-hand side of Eq. (5.2a). The kernel of this integral equation, given in the inverse-lattice summation representation, is, however, trivially separable. This separability is a direct consequence of the translational invariance of the system.

A much more transparent procedure for solving Eq. (5.2a) is to stay in the real lattice representation and treat $I(f_1 g)$ as an operator with the eigenvalues $+I = J(0)/z$, whenever g and f_1 are nearest neighbors, and zero otherwise.

In this manner we are led to the 2nd-RPA solution for the longitudinal Green's function, i.e.

$$\begin{aligned}
& \langle\langle S_{f_1}^z S_g^+; S_g^- \rangle\rangle_{(E)} = \sigma \langle\langle S_g^+; S_g^- \rangle\rangle_{(E)} + \left(\frac{1}{\pi} \right) \left[\frac{L(gf_1) - \delta_{g,f_1} L(gg)}{E - E(3)} \right] \\
& + \left[\delta_{g,f_1} \left(\frac{1}{2} - \sigma \right) + \frac{A(gf_1) - \delta_{g,f_1} A}{E - E(3)} \right] \langle\langle S_g^+; S_g^- \rangle\rangle_{(E)} \\
& - \frac{2\sigma}{[E - E(3)][E - E(4)]} \left[\frac{L(gf_1) I(gf_1)}{\pi} + A(gf_1) I(gf_1) \langle\langle S_g^+; S_g^- \rangle\rangle_{(E)} \right], \quad (5.3)
\end{aligned}$$

where

$$E(4) = E(0) - x. \quad (5.4)$$

The correlation function is now computed in the usual manner and after some straightforward algebra we find

$$L(gf) = \left[\left(\frac{1}{4} - \sigma^2 \right) - UR \right] \delta_{g,f} + \frac{U}{N} \sum_{\mathbf{K}} \left[\frac{\exp[i\mathbf{K}(g-f)]}{1 - VJ(\mathbf{K})} \right], \quad (5.5a)$$

where the inverse lattice sum is over the first Brillouin zone and where

$$\begin{aligned}
U = & \left(\frac{1}{4} - \sigma^2 \right) + \left[\frac{A^2}{\phi\tau(3)} \right] \left[\frac{n(+)}{\phi - x} + \frac{n(-)}{\phi + x} - \frac{2\phi n(3)}{\psi} \right] \\
& + \left[\frac{\sigma A}{\phi\tau(3)} \right] \left[\left(\frac{\phi + x}{\phi - x} \right) n(+) - \left(\frac{\phi - x}{\phi + x} \right) n(-) - \frac{4\phi x n(3)}{\psi} \right]
\end{aligned}$$

$$\begin{aligned}
 & - \left\{ \left(\frac{2\sigma^2}{\Phi J(0)} \right) \Psi \left[\frac{n(+)}{\Phi-x} + \frac{n(-)}{\Phi+x} - \frac{2\Phi n(3)}{\Psi} \right] + \left(\frac{2\sigma A}{\Phi J(0)} \right) [n(+)-n(-)] \right\} \\
 & \times \left\{ \left(\frac{A}{\Phi} \right) \left[\frac{n(+)}{\Phi-x} + \frac{n(-)}{\Phi+x} - \frac{2\Phi n(3)}{\Psi} \right] \right. \\
 & \quad \left. + \left(\frac{\sigma}{\phi} \right) \left[\left(\frac{\Phi+x}{\Phi-x} \right) n(+)-\left(\frac{\Phi-x}{\Phi+x} \right) n(-) - \frac{4\Phi x n(3)}{\Psi} \right] \right\}^{-1}, \quad (5.5b)
 \end{aligned}$$

$$\begin{aligned}
 V = & \left(\frac{A}{\Phi \tau(3)} \right) \left[\frac{2\Phi n(3)}{\Psi} - \frac{n(+)}{\Phi-x} - \frac{n(-)}{\Phi+x} \right] \\
 & + \left[\frac{\sigma}{\Phi \tau(3)} \right] \left[\frac{4\Phi x n(3)}{\Psi} + \left(\frac{\Phi-x}{\Phi+x} \right) n(-) - \left(\frac{\Phi+x}{\Phi-x} \right) n(+), \right] \quad (5.5c)
 \end{aligned}$$

$$R = \frac{1}{N} \sum_K [1 - VJ(K)]^{-1}, \quad (5.5d)$$

$$n(\alpha) = [\exp(\beta E(\alpha)) - 1]^{-1}; \quad \alpha = +, -, 3. \quad (5.5e)$$

Here $\tau(\alpha)$ is defined as in Eq. (4.8b) with α given by Eq. (5.5e) and Ψ is as given in Eq. (4.6d).

In deriving Eqs. (5.5) we have made use of the well-known relation¹⁰⁾ for spatially isotropic nearest-neighbor interactions (e.g. in lattices of cubic symmetry):

$$\frac{1}{N} \sum_K J(K-\lambda) f(\lambda) = \left[\frac{J(K)}{J(0)} \right] \frac{1}{N} \sum_K J(\lambda) f(\lambda), \quad (5.6)$$

which follows whenever $f(\lambda) = f(-\lambda)$.

We note that since U and V are functions of σ , A and Φ , and since A and Φ are themselves determined in terms of U and V through the relations

$$AV = U[R-1], \quad (5.7)$$

$$\Phi^2 = x^2 + \left(\frac{U}{V^2} \right) [R-1] + \left[\frac{1}{4} - \sigma^2 - UR \right] \frac{J^2(0)}{z}, \quad (5.8)$$

thus the set of Eqs. (4.8), (5.5), (5.7) and (5.8) are a coupled transcendental set. Their self-consistent solution determines both the magnetization σ and the correlation $L(gf)$.

§ 6 . Solution

The set of Eqs. (4.8), (5.5), (5.7) and (5.8) cannot be solved analytically at general temperature and as such the solution will have to be computed numerically. (Note that this is also true of the much simpler result of the first RPA, i.e. Eq. (3.4).) However, in certain ranges of temperature rapidly convergent iteration procedures can be used which yield the result as a self-consistent solution in terms of suitable series expansions.

Let us first investigate the situation at very high temperatures. Here the

magnetization is much smaller than unity (as long as $\mu H \ll kT$). In the limit of vanishing applied field, the system susceptibility is readily found from Eq. (5.5) using the well-known thermodynamic relation:

$$[L(K)]_{\lim K=0} = \beta\chi, \quad (6.1a)$$

where $L(K)$ is the inverse lattice Fourier transform of the correlation, i.e.

$$L(gf) = \frac{1}{N} \sum_{\mathbf{K}} L(K) \exp[i\mathbf{K}(g-f)]. \quad (6.1b)$$

Note that the equivalence of the susceptibility χ defined by Eq. (6.1a) and the relation,

$$\chi = \left(\frac{d\sigma}{d\mu H} \right), \quad (6.1c)$$

is in the nature of a thermodynamic Ward identity. The satisfaction of such identities in approximate statistical mechanical treatments is by no means automatic. Indeed, the high density expansion treatments of references 4) and 5) suffer from the drawback that such Ward identities are exceedingly difficult to conserve.¹¹⁾

Now, in the limit of high temperatures and vanishing field we have

$$n(\alpha) = [e^{\alpha\beta\theta} - 1]^{-1} - 0(\beta\mu H); \quad \alpha = +, -. \quad (6.2)$$

Therefore from Eq. (4.8) we get

$$\frac{2A}{\Phi} \Big|_{\mu H=0; T \geq T_c} = \tanh[\beta\Phi/2]. \quad (6.3a)$$

Similarly Eqs. (5.5b) and (5.5c) give

$$U \Big|_{\mu H=0; T \geq T_c} = \left[\frac{1}{4} - (A^2/\Phi^2) \right], \quad (6.3b)$$

$$V \Big|_{\mu H=0; T \geq T_c} = (A/\Phi^2). \quad (6.3c)$$

Combining Eqs. (6.3) with the Fourier transform of Eq. (5.5a), i.e.

$$L(K) = \left(\frac{1}{4} - \sigma^2 \right) - UR + \left[\frac{U}{1 - VJ(K)} \right], \quad (6.4)$$

we readily get

$$L(K) = \left[\frac{1}{1 - V(T)J(K)} \right] \left[\left(\frac{4}{N} \right) \sum_{\lambda} \frac{1}{1 - V(T)J(\lambda)} \right]^{-1}, \quad (6.5a)$$

where

$$V(T) = (\beta/4) - (\beta^3/48z)J^2(0) + 0(\beta)^4. \quad (6.5b)$$

Using Eq. (6.1a) we now rapidly find the susceptibility:

$$\begin{aligned} \chi = (\beta/4) & \left[1 + (\beta/4)J(0) + (\beta/4)^2 J^2(0) \left(\frac{z-1}{z} \right) \right] \\ & + (\beta/4)^4 J^3(0) \left[1 - \frac{7}{3z} - \frac{a}{36} \right] + O(\beta)^5, \end{aligned} \quad (6.6)$$

where $a=0$, for s.c. and b.c.c. lattices and is equal to $+1$ for the f.c.c. lattice.

The above result agrees with the exact one to the order β^3 but the β^4 term is only approximately correct.

The specific heat, C_v , can also be similarly computed and we find:

$$C_v = \frac{d\langle \mathcal{H} \rangle}{dT} = \left(\frac{\beta J(0)}{4} \right)^2 (Nk_B) \left[\frac{1}{2z} + \left(\frac{a}{36} \right) \left(\frac{\beta J(0)}{4} \right) \right] + O(\beta)^4. \quad (6.7)$$

Once again the above expression agrees with the exact result to the order β^3 and the β^4 term is again only approximately correct.

Thus the high temperature behavior of the 2nd RPA represents an improvement over that of the 1st RPA. In fact, within this temperature range, the 2nd RPA results seem to be equivalent to the diagrammatic, high density expansion¹²⁾ results computed to the order $(1/z)$.

Let us look next at the low-temperature region. Once again rapidly convergent series expansion, in powers of $\exp(-\beta J(0)/2)$, is feasible. We emphasize that both this expansion and the preceding high-temperature expansion are achieved self-consistently through the coupled relations for the system magnetization and the longitudinal correlation. For $T \ll T_c$ (where T_c is the RPA Curie temperature) and $\mu H=0$ we find

$$V = \beta \exp[-\beta J(0)/2] (1 + \epsilon), \quad (6.8a)$$

$$U = \exp[-\beta J(0)/2] (1 + \epsilon), \quad (6.8b)$$

$$\Phi = x + \exp[-\beta J(0)/2] J(0) (1 + \epsilon), \quad (6.8c)$$

$$A = \beta \exp[-\beta J(0)] (J^2(0)/z) (1 + \epsilon) \quad (6.8d)$$

and

$$\sigma = \frac{1}{2} - \exp\left[-\frac{\beta J(0)}{2}\right] - z \exp\left[-\beta J(0) \frac{(z-1)}{z}\right] (1 + \epsilon), \quad (6.9)$$

where ϵ is exponentially vanishing as $\beta \rightarrow \infty$.

The expression (6.9) agrees with the exact result of the low temperature series expansions to the order given.³⁾ Once again this result is an improvement over the 1st RPA result given in § 3.

Finally, let us consider the region in the immediate vicinity of the phase transition. Here, in the absence of the field H , the system magnetization vanishes and simultaneously the spatial range of the correlation $L(gf)$ becomes macroscopically long. In other words, the Fourier transform $L(K)$ becomes large as $K \rightarrow 0$. From Eq. (5.5a) it is obvious that when this happens:

$$V \rightarrow V(c) = [J(0)]^{-1}. \quad (6.10)$$

Now proceeding to the limit $\mu H=0$, $T=T_c$ and $\sigma=0$ in Eqs. (6.2) and (6.3) (or directly using Eqs. (4.8) and (5.5)) we get

$$V(c) = A(c)/\Phi^2(c), \quad (6.11a)$$

$$U(c) = \frac{1}{4} - A^2(c)/\Phi^2(c), \quad (6.11b)$$

$$2[A(c)/\Phi(c)] = \tanh\left(\frac{\Phi(c)}{2k_B T_c}\right). \quad (6.11c)$$

Combining Eqs.(6.10) and (6.11), the Curie temperature T_c is found to obey the following relation:

$$\tanh\left[\left(\frac{J(0)}{4k_B T_c}\right)\left(\frac{F(-1)-1}{F(-1)}\right)^{1/2}\right] = \left(\frac{F(-1)-1}{F(-1)}\right)^{1/2}, \quad (6.12)$$

where $F(-1)$ is the well-known Watson¹³⁾ sum; i.e. $F(-1)=1.51638$ for s.c.; = 1.39320 for b.c.c. and = 1.34466 for f.c.c. The solution of Eq. (6.12) leads to the result:

$$k_B T_c = \left[\frac{J(0)}{4}\right] y, \quad (6.13)$$

Table.

The Curie Temperature is given as $k_B T_c = (J(0)/4)y$. The system energy at the critical point, i.e. $\mu H=0$, $T=T_c$, is $\langle \mathcal{H} \rangle = E(c)$.

Lattice	(y) 2nd RPA	(y) Padé	(y) ref. 4)	(y) ref. 5)	$-(E(c)8/NJ(0))$ 2nd RPA	$(-8E(c)/NJ(0))$ Padé
s.c.	0.875	0.752	0.660	0.656	0.360	
b.c.c.	0.898	0.794	0.718	0.712	0.282	
f.c.c.	0.908	0.816	0.740	0.739	0.256	0.245

where y is less than unity and is listed in the table. For comparison, the results of the Padé approximant, high temperature series extrapolation scheme,¹⁴⁾ and those following from references 4) and 5), are also included. The 2nd RPA result for the Curie temperature is seen to be about 10% higher than the Padé estimate, while the estimates of references 4) and 5) are about 10% too low.

The system energy, $\langle \mathcal{H} \rangle$, at the transition point can now also be readily evaluated and we get

$$\langle \mathcal{H} \rangle_{T=T_c, \mu H=0} = -\frac{NJ(0)}{8} \left(\frac{F(-1)-1}{F(-1)}\right). \quad (6.14)$$

These results are included in the table and are compared with the available Padé estimates.

Perhaps it is worth emphasizing that the Curie temperature, T_c , given in Eq. (6.13) has been computed on the assumption that the range of the correlation, in the absence of an applied field, becomes infinite as T approaches the transition temperature from above. Thermodynamically this statement is identical to that relating to the divergence of zero field susceptibility at the Curie point. In any given approximation, however, the exact equivalence of the two statements is not necessarily true. For instance, in the words of Englert,¹¹⁾ there is no "guarantee that the Curie point obtained by the divergence in the long-range order (or in the specific heat) coincides with the infinity of the susceptibility."

§ 7. Conclusions

The 2nd RPA has been shown to represent a considerable improvement over the 1st RPA—i.e. the molecular field approximation. Both at low temperatures as well as at high temperatures its behavior agrees more accurately with the exact low and high temperature series expansions.

In the vicinity of the phase transition the situation is also an improvement over the molecular field results. Unlike in the first RPA, the longitudinal correlation is shown to be non-zero even when the spins are spatially separated.

The feature which in our opinion particularly recommends the use of the general random phase approximation scheme presented in this paper, is its simplicity coupled with its relatively reasonable validity in the entire range of temperatures.

Finally it may be mentioned that the RPA scheme presented here is readily applicable to the study of other classical, many-body systems.¹⁶⁾ Some of these applications, as well as the study of the third order RPA, will be the subject of our future investigations.

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Appendix

The preservation of the temporal symmetry, which is essential in constructing a conserving approximation,^{8),15)} is achieved trivially in the Ising model Green's functions. To prove this we show below that the equations of motion relevant to the 2nd RPA, are manifestly time-symmetrical. For instance, we should either use the equation

$$\begin{aligned} \left(\frac{id}{dt}\right) \left(\frac{id}{dt'}\right) \langle\langle S_g^+(t); S_g^-(t') \rangle\rangle &= \frac{id}{dt'} [\delta(t-t')] (2\sigma) \\ &+ \sum_{f_1} \sum_{f_2} I(f_1 g) I(f_2 g) \langle\langle S_{f_1}^z S_g^+(t); S_{f_2}^z S_g^-(t') \rangle\rangle. \end{aligned} \quad (\text{A}\cdot 1)$$

Or, alternatively a suitable combination¹⁷⁾ of the equations of motion $(i(d/dt))^2 \ll S_g^+(t); S_g^-(t') \gg$ and $(i(d/dt'))^2 \ll S_g^+(t); S_g^-(t') \gg$ is needed to maintain the temporal symmetry. In view, however, of the fact that

$$S_f^z(t) = S_f^z(t') = S_f^z(0), \quad (\text{A}\cdot 2)$$

all these equations of motion are identical. Therefore, the operation of the 2nd RPA on either of these time-symmetrized equations of motion leads to identical results to those given in the text.

An obvious extension of the above argument demonstrates the time-symmetry of the general order RPA described in the text whenever it refers to a classical many-body system such as the Ising model.

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