Dynamical Spin Correlations in Many-Spin Systems. I. The Ferromagnetic Case*

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(Received 17 November 1966; revised manuscript received 20 February 1967)

The quantum-statistical mechanics of an anisotropic Heisenberg spin system is studied by a temperature-time-dependent Green's-function formalism. A consistent scheme of higher-order random-phase approximations (RPA) is developed and the second-order (2nd) RPA is examined in detail. It turns out that the 2nd RPA can be defined in two alternative versions, I and II, with equal *a priori* justification. These two versions of the 2nd RPA have then to be supplemented with either a dynamical or a kinematical sum rule, thus leading to four possible alternative descriptions of the problem. Each of these descriptions can in principle be used to determine the spectral functions of both the longitudinal and the transverse dynamical spin-correlation functions. However, upon detailed examination of the 2nd RPA, it is found that only one of these four possible descriptions satisfies all the various consistency requirements. At low temperatures, this description reproduces the spin-wave results. To facilitate analytical solutions, an approximate version of the 2nd RPA, called the modified (mod) RPA, is introduced which leads to a satisfactory expression for the longitudinal correlation function over the entire range of temperatures. Upon examination it is found that the mod RPA determines the longitudinal correlation to the same accuracy, for the case of the isotropic exchange, as the first RPA determines the transverse correlation function. In addition to this mod RPA version of the consistent 2nd RPA, there also appears to be another relatively satisfactory solution for the longitudinal correlation function which follows from one of the less consistent versions of the 2nd RPA. This is treated as a phenomenological result. The system thermodynamics is analyzed in the region of the transition temperature in terms of both the consistent version of the mod RPA, i.e., the I mod RPA, as well as the phenomenological representation, i.e., the II mod RPA, with results which in addition to being an improvement on those following from the first RPA are also free from the inherent inconsistencies of the first RPA. In conclusion, the related work of other authors is discussed and it is shown that all these works suffer from serious internal inconsistencies which render their results for the longitudinal correlation function completely unacceptable and erroneous.

1. INTRODUCTION

THE recent study of the chalcogenides of europium has provided physical relevance to the study of the quantum-statistical mechanics of many-spin systems interacting via the Heisenberg exchange interaction of the form[1–4]

$$\mathcal{H}\sim-\sum_{1,2} I(12)\,\mathbf{S}_1\cdot\mathbf{S}_2. \tag{1.1}$$

Unfortunately, however, the statistical mechanics under the interaction (1.1) cannot be done exactly and one has to resort to making approximations. These approximations fall roughly into the following broad categories: (a) the cluster approximations[5–7]; (b) the high-temperature[8,9] and the low-temperature[10] approximations; (c) those which consist in relaxing certain mathematical constraints[11]; and (d) the Green's-function approximations.[12,13]

While the applicability of most of the results following from approximations (a), (b), and (c) is, in general, restricted to a limited temperature region, the Green's-function technique gives results which are seemingly adequate over the entire range of temperatures. This approximation, however, suffers from a number of serious drawbacks. Firstly, it lacks detailed agreement with both the exact high-temperature and the exact low-temperature results. Secondly, the existing formulation of this approximation neither lends itself to effecting higher-order, i.e., increasingly more accurate, approximations nor adequately determines the longitudinal spin-correlation function.

The purpose of the present work is twofold: Firstly, it is to present a formulation of the theory which lends itself naturally to making higher-order approximations;

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and secondly, to obtain a solution for the longitudinal spin-correlation function which is free from the inadequacies of the earlier results.[14,15]

Section 2 deals with the formulation of the problem. Green's functions are defined and their equations of motion are given.

In Sec. 3, the equations of motion are decoupled according to the first-order (1st) RPA and the analysis is carried out to rederive the results of Ref. 12.

Second-order (2nd) RPA is defined and studied in Sec. 4. It is found that there are two possible versions of the 2nd RPA, both of which satisfy the various space- and time-symmetry requirements.

In Sec. 5, we study the various sum rules that follow from the spin-kinematic requirements, i.e., the kinematic sum rules, and from the dynamic requirements under the given Hamiltonian, i.e., the dynamic sum rules.

Section 6 is devoted to a qualitative discussion of the Green's function $G(11')$ of transverse spin components. It is noted that the introduction of suitable spectral representations for the transverse and the longitudinal Green's functions would lead to a set of four different integral equations for these spectral functions.

In Sec. 7, the sum rules of Sec. 5 are used in conjunction with the expressions for the 2nd RPA and relationships between the longitudinal and the transverse spectral functions are obtained. On combining these results with those of Sec. 6, we can, in principle, determine both the spectral functions.

The results of Sec. 7 are formal in character and solutions for the spectral functions can, in general, only be obtained numerically. An approximation scheme, to be called the modified (mod) RPA, which yields satisfactory results for the longitudinal spectral function, is developed in Sec. 8 and expressions for the longitudinal correlation function obtained. These expressions are analyzed in Sec. 9. The phenomenon of spin diffusion in the critical region is discussed briefly in Sec. 10. In Sec. 11, the 2nd RPA is analyzed for the region of low temperatures and in direct contrast with the results following for the 1st RPA it is found that the 2nd RPA results are completely consistent with the spin-wave theory. Section 12 is devoted to the study of the mod RPA near the Curie temperature. The system thermodynamics is analyzed and the critical energy and the Curie temperature computed. Some of the various calculational and mathematical details not given in the text are discussed in the Appendices.

2. THE FORMULATION

The mathematics of the quantum-statistical Green's functions is by now fairly standard. However, in the literature there exist a number of different formulations of this technique which differ much in detail.[16,17] We have found the imaginary-time-ordered formulation to be particularly convenient for our purposes. (See Ref. 17 for details.)

Let us for the sake of generality work with the following anisotropic Hamiltonian of a slightly more general form than (1.1):

$$\mathcal{H}=\text{const.}-\mu H\sum_{1} S_1^z-\sum_{1,2} I_0(12)\, S_1^z\cdot S_2^z -\sum_{1,2} I_+(12)\, S_1^+\cdot S_2^-. \quad (2.1)$$

Here, H denotes an externally applied field directed along the z axis, $\boldsymbol{\mu}S$ the magnetic moment per ion, $S_1^{x,y,z}$ the Cartesian components of the spin operator $\mathbf{S}_1$ of magnitude S associated with the space point 1, $S_1^{\pm}=S_1^x\pm iS_1^y$, and $I_0(12)$ and $I_+(12)$ the exchange integrals between the space points 1 and 2 for the longitudinal and the transverse components of the spins, respectively. As usual we stipulate that

$$I_0(11)=I_+(11)=0,$$

and choose our units such that $\hbar=1$. [Note that when $I_0=I_+$, interaction (2.1) reduces to that due to Heisenberg and that the case $I_+=0$ refers to the Ising model.]

Let us define a generalized-spin Green's function in the presence of an arbitrary space-time-dependent field u:

$$G[11']=-i\langle\langle S^+(1)\,S^-(1')\rangle\rangle =-i\,\langle T[\mathcal{S}S^+(1)S^-(1')]\rangle/\langle T[\mathcal{S}]\rangle, \quad (2.2)$$

where

$$\Omega(1)=\exp(i\mathcal{H}\tau_1)\Omega_1\exp(-i\mathcal{H}\tau_1), \quad (2.3)$$

$$\langle\cdots\rangle=\text{Tr}[\exp(-\beta\mathcal{H})\cdots]/\text{Tr}[\exp(-\beta\mathcal{H})], \quad (2.4)$$

$$\mathcal{S}=\exp\left[-i\int_0^{-i\beta} d\tau_2\sum_2 u(2)\,S^z(2)\right]. \quad (2.5)$$

In (2.3) Ω_1 denotes an arbitrary Schrödinger operator associated with the space point 1. The times τ are to be purely imaginary and are to be restricted to the interval $[0,-i\beta]$. The time-ordering operation designated

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by T, consists of ordering the product of the operators (on which it acts) from right to left according to increasing distance from the origin towards $-i\beta$ along the negative imaginary axis.

Under the interaction (2.1), the equations of motion of (2.2) are

$$[i(d/d\tau_1)-\mu H+u(1)]G[11']=2\delta(1-1')\langle\langle S^z(1)\rangle\rangle+2\sum_2 I_0(12)\left[\langle\langle S^z(2)\rangle\rangle G[11']+i\frac{\delta G[11']}{\delta u(2)}\right]_{\tau_2=\tau_1}$$
$$-2\sum_2 I_+(12)\left[\langle\langle S^z(1)\rangle\rangle G[21']+i\frac{\delta G[21']}{\delta u(1)}\right]_{\tau_2=\tau_1}, \quad (2.6a)$$

$$[i(d/d\tau_{1'})+\mu H-u(1')]G[11']=-2\delta(1-1')\langle\langle S^z(1')\rangle\rangle-2\sum_{2'} I_0(1'2')\left[\langle\langle S^z(2')\rangle\rangle G[11']+i\frac{\delta G[11']}{\delta u(2')}\right]_{\tau_{2'}=\tau_{1'}}$$
$$+2\sum_{2'} I_+(1'2')\left[\langle\langle S^z(1')\rangle\rangle G[12']+i\frac{\delta G[12']}{\delta u(1')}\right]_{\tau_{2'}=\tau_{1'}}, \quad (2.6b)$$

where $\delta G/\delta u$ denotes functional derivative of G with respect to u.

It should be emphasized here that Eqs. (2.6a) and (2.6b) are exact. If functions of the type $\delta G/\delta u$ did not occur on the right-hand side of (2.6a) and (2.6b), these equations would be exactly soluble in the limit $u=0$ and the Green's function $G(11')$, and consequently the (real) time-dependent correlation function $\langle S_1^+(t_1)S_{1'}^-(t_{1'})\rangle$ would be completely determined. The appearance of the nonlinear terms $\delta G/\delta u$ is a universal feature common to all the interacting many-body systems. Much thought has been given to the problem of constructing suitable solutions for these terms,[18] and it is found that the perturbation-expansion approach is suitable only for conditions much different from those which obtain in the neighborhood of the critical point.[19]

As mentioned earlier, the 1st RPA theories, which in the present formalism are equivalent to ignoring completely the $\delta G/\delta u$ terms occurring on the right-hand side of Eqs. (2.6a) and (2.6b) and solving for the thus linearized equations of motion for $G(11')$, yield results which, in addition to possessing correct limiting behavior for both the limits $\beta=0$ and $\beta=\infty$, also contain information about the transition region. It is therefore tempting to investigate the possibilities of postponing the truncation of the Green's function to a later stage and thus solving for the functional derivative $\delta G/\delta u$. The hope is that, firstly, this solution for $\delta G/\delta u$ would be more accurate than the first-order approximation, which simply ignores it, and, secondly, that upon insertion into (2.6a) and (2.6b) this improved $\delta G/\delta u$ would lead to a more accurate solution of the Green's function $G(11')$.

To this end, we functionally differentiate the equations of motion (2.6a) and (2.6b):

$$\left[i\frac{d}{d\tau_1}-\mu H+u(1)\right]\frac{\delta G[11']}{\delta u(3)}+\delta(1-3)G[11']=2\delta(1-1')\frac{\delta\langle\langle S^z(1)\rangle\rangle}{\delta u(3)}$$
$$+2\sum_2 I_0(12)\left[\frac{\delta\langle\langle S^z(2)\rangle\rangle}{\delta u(3)}G[11']+\langle\langle S^z(2)\rangle\rangle\frac{\delta G[11']}{\delta u(3)}\right]_{\tau_2=\tau_1}$$
$$-2\sum_2 I_+(12)\left[\frac{\delta\langle\langle S^z(1)\rangle\rangle}{\delta u(3)}G[21']+\langle\langle S^z(1)\rangle\rangle\frac{\delta G[21']}{\delta u(3)}\right]_{\tau_2=\tau_1}+F^{(1)}[1;1';3], \quad (2.7a)$$

$$\left[i\frac{d}{d\tau_{1'}}+\mu H-u(1')\right]\frac{\delta G[11']}{\delta u(3)}-\delta(1'-3)G[11']=-2\delta(1-1')\frac{\delta\langle\langle S^z(1')\rangle\rangle}{\delta u(3)}$$
$$-2\sum_{2'} I_0(1'2')\left[\frac{\delta\langle\langle S^z(2')\rangle\rangle}{\delta u(3)}G[11']+\langle\langle S^z(2')\rangle\rangle\frac{\delta G[11']}{\delta u(3)}\right]_{\tau_{2'}=\tau_{1'}}$$
$$+\sum_{2'} I_+(1'2')\left[\frac{\delta\langle\langle S^z(1')\rangle\rangle}{\delta u(3)}G[12']+\langle\langle S^z(1')\rangle\rangle\frac{\delta G[12']}{\delta u(3)}\right]_{\tau_{2'}=\tau_{1'}}+F^{(2)}[1;1';3], \quad (2.7b)$$

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where

$$F^{(1)}[1;1';3]=2i\sum_{2}\left[I_0(12)\frac{\delta^2G[11']}{\delta u(3)\delta u(2)}-I_+(12)\frac{\delta^2G[21']}{\delta u(3)\delta u(1)}\right]_{\tau_2=\tau_1},\tag{2.8}$$

$$F^{(2)}[1;1';3]=-2i\sum_{2'}\left[I_0(1'2')\frac{\delta^2G[11']}{\delta u(3)\delta u(2')}-I_+(1'2')\frac{\delta^2G[12']}{\delta u(3)\delta u(1')}\right]_{\tau_{2'}=\tau_{1'}}.\tag{2.9}$$

Let us now proceed to the limit $u=0$ in Eqs. (2.6a), (2.6b), (2.7a), and (2.7b). The space and time translational invariance of the interaction (2.1) and the canonical, periodic boundary condition [which follows from the fact that Tr $(ABC)=$ Tr (CAB)] are incorporated naturally into the following Fourier representation:

$$G(11')=[G[11']]_{u=0}=(-i\beta N)^{-1}\sum_{\mathbf{k}}{}'\sum_{\nu}G_{\mathbf{k}}(\nu)\exp\{i[\mathbf{k}(1-1')-Z_\nu(\tau_1-\tau_{1'})]\},$$

$$G_{\mathbf{k}}(\nu)=\sum_{(1-1')}\int_0^{-i\beta}G(11')\exp\{i[Z_\nu(\tau_1-\tau_{1'})-\mathbf{k}(1-1')]\}\,d(\tau_1-\tau_{1'}),$$

$$[\delta\langle\langle S^z(1)\rangle\rangle/\delta u(3)]_{u=0}=(-i\beta N)^{-1}\sum_{\lambda}{}'\sum_{\rho}M_\lambda^{(1)}(\rho)\exp\{i[\lambda(1-3)-Z_\rho(\tau_1-\tau_3)]\},$$

$$[\delta G[11']/\delta u(3)]_{u=0}=(1/-i\beta N)^2\sum_{\mathbf{k}_1,\mathbf{k}_2}{}'\sum_{\nu_1,\nu_2}G^{(1)}{}_{\mathbf{k}_1,\mathbf{k}_2}(\nu_1,\nu_2)\exp\{i[\mathbf{k}_1(1-3)+\mathbf{k}_2(1'-3)-Z_{\nu_1}(\tau_1-\tau_3)-Z_{\nu_2}(\tau_{1'}-\tau_3)]\},$$

$$[F^{(l)}[1;1';3]]_{u=0}=(1/-i\beta N)^2\sum_{\mathbf{k}_1,\mathbf{k}_2}{}'\sum_{\nu_1,\nu_2}F^{(l)}{}_{\mathbf{k}_1,\mathbf{k}_2}(\nu_1,\nu_2)\times\exp\{i[\mathbf{k}_1(1-3)+\mathbf{k}_2(1'-3)-Z_{\nu_1}(\tau_1-\tau_3)-Z_{\nu_2}(\tau_{1'}-\tau_3)]\};\qquad l=1,2$$

$$[\delta^2G[11']/\delta u(3)\delta u(4)]_{u=0}\equiv G^{(2)}(1,1';3,4)=G^{(2)}(1,1';4,3)$$
$$=(1/-i\beta N)^3\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3}{}'\sum_{\nu_1,\nu_2,\nu_3}G^{(2)}{}_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3}(\nu_1,\nu_2,\nu_3)\exp\{i[\mathbf{k}_1(1-4)+\mathbf{k}_2(1'-4)+\mathbf{k}_3(3-4)-Z_{\nu_1}(\tau_1-\tau_4)-Z_{\nu_2}(\tau_{1'}-\tau_4)-Z_{\nu_3}(\tau_3-\tau_4)]\}.\tag{2.10}$$

The N-allowed inverse-lattice points within the first Brillouin zone are denoted by $\mathbf{k}$ and λ and the summations by the symbol $\sum'_\lambda$. Moreover,

$$Z_\nu=(\pi\nu/-i\beta);\qquad Z_\rho=(\pi\rho/-i\beta),\tag{2.11}$$

where ν and ρ take on all even integral values, positive and negative, including zero.

Using the Fourier transformations (2.10), Eqs. (2.6a), (2.6b), (2.7a), and (2.7b) take the following form:

$$G_\lambda(\rho)[Z_\rho-E_\lambda]=2\sigma+[2i/(-i\beta N)]\sum_{\lambda_1}{}'\sum_{\rho_1}G^{(1)}{}_{\lambda_1,-\lambda}(\rho_1,-\rho)J_{0+}(\lambda_1-\lambda,\lambda_1),\tag{2.12a}$$

$$G_\lambda(\rho)[Z_\rho-E_\lambda)=2\sigma+(2i/-i\beta N)\sum_{\lambda_1}{}'\sum_{\rho_1}G^{(1)}{}_{\lambda,\lambda_1}(\rho,\rho_1)J_{0+}(\lambda+\lambda_1,\lambda_1),\tag{2.12b}$$

$$G^{(1)}{}_{\lambda_1,\lambda_2}(\rho_1,\rho_2)=[Z_{\rho_1}-E_{\lambda_1}]^{-1}\{F^{(1)}{}_{\lambda_1,\lambda_2}(\rho_1,\rho_2)-G_{-\lambda_2}(-\rho_2)+2M^{(1)}{}_{\lambda_1+\lambda_2}(\rho_1+\rho_2)[1+G_{-\lambda_2}(-\rho_2)J_{0+}(\lambda_1+\lambda_2,\lambda_2)]\},\tag{2.13a}$$

$$G^{(1)}{}_{\lambda_1,\lambda_2}(\rho_1,\rho_2)=[Z_{\rho_2}+E_{\lambda_2}]^{-1}\{F^{(2)}{}_{\lambda_1,\lambda_2}(\rho_1,\rho_2)+G_{\lambda_1}(\rho_1)-2M^{(1)}{}_{\lambda_1+\lambda_2}(\rho_1+\rho_2)[1+G_{\lambda_1}(\rho_1)J_{0+}(\lambda_1+\lambda_2,\lambda_1)]\},\tag{2.13b}$$

where we have used the notation

$$J_p(\mathbf{k})=\sum_1 I_p(12)\exp[i\mathbf{k}(1-2)];$$

$$J_{pp'}(\mathbf{k},\lambda)=J_p(\mathbf{k})-J_{p'}(\lambda);\qquad p,p'=0,+,$$

$$\langle S^z(1)\rangle=\sigma;\qquad E_{\mathbf{k}}=\mu H+2\sigma J_{0+}(0,\mathbf{k}),$$

$$F^{(1)}{}_{\lambda_1,\lambda_2}(\rho_1,\rho_2)=(-2/\beta N)\sum_{\mathbf{k}}{}'\sum_{\nu}G^{(2)}{}_{\mathbf{k},\lambda_2,\lambda_1-\mathbf{k}}(\nu,\rho_2,\rho_1-\nu)J_{0+}(\lambda_1-\mathbf{k},\mathbf{k}),$$

$$F^{(2)}{}_{\lambda_1,\lambda_2}(\rho_1,\rho_2)=(+2/\beta N)\sum_{\mathbf{k}}{}'\sum_{\nu}G^{(2)}{}_{\lambda_1,\mathbf{k},\lambda_2-\mathbf{k}}(\rho_1,\nu,\rho_2-\nu)J_{0+}(\lambda_2-\mathbf{k},\mathbf{k}):\tag{2.14}$$

3. FIRST-ORDER RPA

As mentioned earlier, exact solutions to Eqs. (2.12) and (2.13) cannot be obtained and approximations, therefore, have to be made. A particularly simple approximation is the 1st RPA.[12] This consists in ignoring the variation of G in comparison with G itself. Formally this can be represented as

$$(1/-i\beta N)\sum_{\lambda_1}{}'\sum_{\rho_1}G^{(1)}{}_{\lambda_1,-\lambda}(\rho_1,-\rho)J_{0+}(\lambda_1-\lambda,\lambda_1)$$
$$=(1/-i\beta N)\sum_{\lambda_1}{}'\sum_{\rho_1}G^{(1)}{}_{\lambda,\lambda_1}(\rho,\rho_1)J_{0+}(\lambda+\lambda_1,\lambda_1)\sim 0. \quad (3.1)$$

Physically, the above approximation assumes that the z component of a spin is mostly uncorrelated with its surroundings and that its fluctuations are small. This situation obtains at very low temperatures, where the system is close to its ground state, and approximately at high temperatures, where the randomizing effect of the temperature far outweighs the correlating effect of the exchange interactions. On the other hand, near the critical region, where the fluctuations are large and the system is strongly correlated, we would expect the approximation (3.1) to be unsatisfactory.

Introducing Eq. (3.1) into Eq. (2.12) and carrying out the sums over the variable ρ, we readily find

$$iG(11')\underset{\text{1st RPA}}{\sim}\eta(\tau_1-\tau_{1'})\left(\frac{2\sigma}{N}\right)\sum_\lambda{}'\frac{\exp[-iE_\lambda(\tau_1-\tau_{1'})}{[1-\exp(-\beta E_\lambda)]}$$
$$+\eta(\tau_{1'}-\tau_1)\left(\frac{2\sigma}{N}\right)\sum_\lambda{}'\frac{\exp[-iE_\lambda(\tau_1-\tau_{1'})]}{[\exp(\beta E_\lambda)-1]}, \quad (3.2)$$

where

$$\eta(\tau)=1,\quad \text{for } \tau \text{ in } [0,-i\beta]$$
$$=0,\quad \text{otherwise.} \quad (3.3)$$

Analytically continuing to real times, we find the transverse correlation function

$$\langle S_1^+(t_1)S_{1'}^-(t_{1'})\rangle=(2\sigma/N)\sum_\lambda{}'[1-\exp(-\beta E_\lambda)]^{-1}$$
$$\times\exp\{i[\lambda(1-1')-E_\lambda(t_1-t_{1'})]\},$$
$$\langle S_{1'}^-(t_{1'})S_1^+(t_1)\rangle=(2\sigma/N)\sum_\lambda{}'[\exp(\beta E_\lambda)-1]^{-1}$$
$$\times\exp\{i[\lambda(1-1')-E_\lambda(t_1-t_{1'})]\}. \quad (3.4)$$

It should be mentioned here that in spite of the crudeness with which the 1st RPA is expected to represent the physics of the system at general temperatures, it is found that the expressions (3.4) describe the transverse correlation function adequately over the entire range of temperatures.[12]

Let us investigate the behavior of the longitudinal correlation function within the 1st RPA scheme. It is convenient here to treat the case of spin $\frac{1}{2}$. The results for general spin are expected to be similar. From Eq. (3.1) and the discussion preceding it, it is apparent that unlike the case of the transverse correlation function, the first PRA results for the longitudinal correlation function are neighter unique nor satisfactory. For instance, although the following two definitions of the 1st RPA are equivalent:

$$\left[\frac{\delta G[11']}{\delta u(2)}\right]_{\substack{u\to 0\\ \tau 2=\tau 1}}\approx 0,\quad \text{for}\quad 2\neq 1, \quad (3.5)$$

$$\left[\sum_2 I_0(12)\frac{\delta G[11']}{\delta u(2)}-\sum_2 I_+(12)\frac{\delta G[21']}{\delta u(1)}\right]_{\substack{u\to 0\\ \tau 2=\tau 1}}\approx 0, \quad (3.6)$$

and lead directly to Eq. (3.1), and therefore to Eq. (3.4) for the transverse correlation function, yet Eqs. (3.5) and (3.6) lead to different and internally inconsistent results for the longitudinal correlation function. For example, Eq. (3.5) implies

$$T\langle S_f^z(\tau_1)S_g^+(\tau_1)S_l^-(\tau_{1'})\rangle=\sigma T\langle S_g^+(\tau_1)S_l^-(\tau_{1'})\rangle. \quad (3.7)$$

Putting $g=l$ and $\tau_1=\tau_{1'}\pm(i\beta)\Delta$, $\Delta\to+0$ we rapidly get the result

$$\langle S_f^zS_g^z\rangle=\sigma^2. \quad (3.8)$$

Equation (3.6), on the other hand, leads to two different and mutually inconsistent results for the longitudinal correlation function both of which also differ from that given in Eq. (3.8). This can be seen as follows. Equation (3.6) implies

$$\sum_f I_0(g-f)T\langle S_f^z(\tau_1)S_g^+(\tau_1)S_l^-(\tau_{1'})\rangle$$
$$-\sum_f I_+(g-f)T\langle S_g^z(\tau_1)S_f^+(\tau_1)S_l^-(\tau_{1'})\rangle$$
$$=\sigma[\sum_f I_0(g-f)T\langle S_g^+(\tau_1)S_l^-(\tau_{1'})\rangle$$
$$-\sum_f I_+(g-f)T\langle S_f^+(\tau_1)S_l^-(\tau_{1'})\rangle]. \quad (3.9)$$

Putting $g=l$, $\tau_1=\tau_1\pm i\beta\Delta$, and taking the limit $\Delta=+0$ we are led to the following two expressions:

$$\sum_f I_0(fg)\langle S_f^zS_g^z\rangle=J_0(0)\sigma^2$$
$$-\sum_f I_+(fg)[\tfrac{1}{2}\mp\sigma]\langle S_g^+S_f^-\rangle. \quad (3.10)$$

Now, it is readily ascertained that these 1st RPA results for the longitudinal correlation function, i.e., Eqs. (3.8) and (3.10), unlike those for the transverse correlation function, are utterly inadequate and fail even to satisfy the important physical requirement of spatial isotropy, i.e.,

$$[\langle S_1^zS_2^z\rangle]_{H=0,\ I_+=I_0,\ \beta_c\geq\beta}=\langle S_1^iS_2^i\rangle,\qquad i=x,y. \quad (3.11)$$

We conclude, therefore, that without further embellishment the 1st RPA results for the longitudinal correlation are both inadequate as well as internally inconsistent.

In the present paper we seek to achieve improvements on the 1st RPA with the following motivation: Firstly, we need a description of the longitudinal correlation function which should be at least as adequate as the description of the transverse correlation function afforded by the 1st RPA. Secondly, we should like to investigate the possibility of improving on the description of the transverse correlation function already obtained within the 1st RPA.

In conclusion, it might be mentioned that the foregoing discussion also illustrates an important general point: namely, that the Green's-function truncation procedures, of which the 1st RPA is a particularly simple example, in general treat the transverse and the longitudinal components of the spins on different footings. As such in any given approximation the accuracy of the results would in general be different for the spin-correlation functions of the transverse components from that of the longitudinal ones. The best that can, therefore, be hoped for is to find an approximation that describes both the transverse and the longitudinal correlation functions reasonably accurately if not equally accurately.

4. SECOND-ORDER RPA

In order to look for a more accurate solution for the Green's function $G^{(1)}$ than is afforded by the relatively crude but not unreasonable approximation of Eq. (3.1), we turn to the study of the equations of motion of the Green's function $G^{(1)}$ contained in Eqs. (2.13a) and (2.13b). Inevitably, these equations involve the next higher-order Green's function $G^{(2)}$.

An appropriate approximation would naturally consist in linearizing these equations of motion by prescribing a procedure for handling the nonlinear terms containing $G^{(2)}$. For such a procedure to be at all satisfactory, it will have to be consistent with the symmetry requirement that the physics of the problem remain the same irrespective of whether we make our investigations by observing the development of the system in the time variable τ_1 or $\tau_{1'}$.[20] More precisely, this symmetry requirement can be displayed by equating the two exact expressions for the Green's function $G_\lambda(\rho)$ given in Eqs. (2.12a) and (2.12b), i.e.,

$$\sum_{\lambda_1}{}'\sum_{\rho_1}[G^{(1)}{}_{\lambda,\lambda_1}(\rho,\rho_1)J_{0+}(\lambda+\lambda_1,\lambda_1) - G^{(1)}{}_{\lambda_1,-\lambda}(\rho_1,-\rho)J_{0+}(\lambda_1-\lambda,\lambda_1)]=0. \quad (4.1)$$

Moreover, since

$$\delta\langle\langle S^z(1)\rangle\rangle/\delta u(3)=\delta\langle\langle S^z(3)\rangle\rangle/\delta u(1), \quad (4.2)$$

it follows that

$$M_\lambda{}^{(1)}(\rho)=M_{-\lambda}{}^{(1)}(-\rho). \quad (4.3)$$

Similarly, the spatial-inversion symmetry of the Hamiltonian (2.1) guarantees that

$$G_\lambda(\rho)=G_{-\lambda}(+\rho);\qquad M_\lambda{}^{(1)}(\rho)=M_{-\lambda}{}^{(1)}(\rho). \quad (4.4)$$

An unembellished second-order approximation, which simply ignores the $G^{(2)}$ terms in Eqs. (2.13a) and (2.13b), would not satisfy the symmetry requirement of Eq. (4.1), as can easily be confirmed by respectively ignoring the functions $F^{(1)}$ and $F^{(2)}$ (which are equal to zero if $G^{(2)}$ is) in these exact Eqs. (2.13a) and (2.13b).

To achieve a symmetrical approximation, let us combine Eqs. (2.13a) and (2.13b) as follows.

A simple addition of the two equations gives

$$2G^{(1)}{}_{\lambda_1,\lambda_2}(\rho_1,\rho_2)=[Z_{\rho_1}-E_{\lambda_1}]^{-1}\{2M^{(1)}{}_{\lambda_1+\lambda_2}(\rho_1+\rho_2)[1+G_{-\lambda_2}(-\rho_2)J_{0+}(\lambda_1+\lambda_2,\lambda_2)]-G_{-\lambda_2}(-\rho_2)\}$$
$$+[Z_{\rho_2}+E_{\lambda_2}]^{-1}\{-2M^{(1)}{}_{\lambda_1+\lambda_2}(\rho_1+\rho_2)[1+G_{\lambda_1}(\rho_1)J_{0+}(\lambda_1+\lambda_2,\lambda_1)]+G_{\lambda_1}(\rho_1)\}+f^{(1)}{}_{\lambda_1,\lambda_2}(\rho_1,\rho_2), \quad (4.5a)$$

where

$$f^{(1)}{}_{\lambda_1,\lambda_2}(\rho_1,\rho_2)=[Z_{\rho_1}-E_{\lambda_1}]^{-1}F^{(1)}{}_{\lambda_1\lambda_2}(\rho_1,\rho_2)+[Z_{\rho_2}+E_{\lambda_2}]^{-1}F^{(2)}{}_{\lambda_1\lambda_2}(\rho_1,\rho_2). \quad (4.5b)$$

Similarly, multiplying Eqs. (2.13a) and (2.13b) by $[Z_{\rho_1}-E_{\lambda_1}]$ and $[Z_{\rho_2}+E_{\lambda_2}]$, respectively, and adding we get

$$G^{(1)}{}_{\lambda_1,\lambda_2}(\rho_1,\rho_2)[Z_{\rho_1}+Z_{\rho_2}+E_{\lambda_2}-E_{\lambda_1}]$$
$$=2M^{(1)}{}_{\lambda_1+\lambda_2}(\rho_1+\rho_2)[G_{-\lambda_2}(-\rho_2)J_{0+}(\lambda_1+\lambda_2,\lambda_2) - G_{\lambda_1}(\rho_1)J_{0+}(\lambda_1+\lambda_2,\lambda_1)]+G_{\lambda_1}(\rho_1)-G_{-\lambda_2}(-\rho_2) +f^{(2)}{}_{\lambda_1,\lambda_2}(\rho_1,\rho_2), \quad (4.6a)$$

where

$$f^{(2)}{}_{\lambda_1,\lambda_2}(\rho_1,\rho_2)=F^{(1)}{}_{\lambda_1,\lambda_2}(\rho_1,\rho_2)+F^{(2)}{}_{\lambda_1,\lambda_2}(\rho_1,\rho_2). \quad (4.6b)$$

It is clear now that either of the approximations:

$$f^{(1)}{}_{\lambda_1,\lambda_2}(\rho_1,\rho_2)\sim 0;\qquad \text{2nd RPA(I)} \quad (4.7)$$

$$f^{(2)}{}_{\lambda_1,\lambda_2}(\rho_1,\rho_2)\sim 0;\qquad \text{2nd RPA(II)} \quad (4.8)$$

would preserve the symmetries outlined in Eqs. (4.1)–(4.4).

For brevity, Eqs. (4.5a), (4.5b), and (4.7) will henceforth be referred to as the 2nd RPA(I), and the 2nd RPA(II) will denote Eqs. (4.6a), (4.6b), and (4.8).

It should be emphasized here that while both the 2nd RPA approximations, (I) and (II), consist essentially in ignoring the second-order variation of G, i.e., $G^{(2)}$, as compared with the first- and the zeroth-order variations, i.e., $G^{(1)}$ and G; approximations (I) and (II) are not identical. Moreover, it is not possible

[20] Note that the first-order RPA does indeed satisfy this requirement, for when the approximation (3.1) is introduced into either of the equations of motion of the Green's function $G_\lambda(\rho)$, with respect to the variables τ_1 and τ_1', i.e., Eqs. (2.13a) and (2.13b), respectively, the resultant expressions are identical.

to say at this stage which of these would be the better approximation and under what conditions. It might nevertheless be mentioned that from the point of view of consistency, the analysis to be carried out in the succeeding sections favors the 2nd RPA(I) as being the superior approximation of the two.

5. SUM RULES

The kinematics of the spin operators leads to a number of exact relationships between equal-time spin-correlation functions. We shall for convenience call these the kinematic sum rules.

For general spin S, we have

$$S^+(1)S^-(1)=S(S+1)+S^z(1)-[S^z(1)]^2, \quad (5.1\text{a})$$

$$[S_1^{\pm}, S_2^z]_-=\mp\delta_{1,2}S_1^{\pm}; \quad [S_1^+, S^-]_-=\delta_{1,2}2S_1^z; \quad [S_1^z, S_2^z]_-=0, \quad (5.1\text{b})$$

$$\prod_{p=-S}^{+S}[S^z(1)-p]=0 \quad (5.1\text{c})$$

(p is integral or half-odd-integral, depending on whether S is integral or half-odd-integral).

To convert these relationships to sum rules we have to incorporate them into the Green's-function formalism. To this end let us look at the Green's function $G[11']$ in the limit of spatial locations 1 and 1′ identical and $\tau_1=\tau_{1'}\pm(-i\beta)\Delta$; $\Delta\to+0$:

$$\lim_{1=1';\tau_1=\tau_1'\pm(-i\beta\Delta);\Delta\to+0} G[11'] = -i[S(S+1)\pm\langle\langle S^z(1)\rangle\rangle-\langle\langle[S^z(1)]^2\rangle\rangle]. \quad (5.2)$$

Functionally differentiating both sides of Eq. (5.2), and proceeding to the limit $u=0$, we are led to the kinematic sum rule:

$$\lim_{u=0,\tau_1=\tau_1'\pm(-i\beta)\Delta,1=1',\Delta=+0}\frac{\delta\langle\langle S^+(1)S^-(1')\rangle\rangle}{\delta u(3)} =\pm\left[\frac{\delta\langle\langle S^z(1)\rangle\rangle}{\delta u(3)}\right]_{u=0}-\left[\frac{\delta\langle\langle[S^z(1)]^2\rangle\rangle}{\delta u(3)}\right]_{u=0}. \quad (5.3)$$

Fourier transforming both sides of Eq. (5.3) according to the prescription of Eq. (2.10), we get the desired sum rule:

$$(\mp)iM_{\mathbf{k}}^{(1)}(\nu)+i\mathfrak{M}_{\mathbf{k}}^{(1)}(\nu) =(1/-i\beta N)\sum_{\lambda}{}'\sum_{\rho}G^{(1)}{}_{\mathbf{k}-\lambda,\lambda}(\nu-\rho,\rho)\exp(\pm iZ_\rho\epsilon), \quad (5.4)$$

where $\mathfrak{M}_{\mathbf{k}}^{(1)}(\nu)$ is the Fourier transform of the Green's function

$$\delta\langle\langle[S^z(1)]^2\rangle\rangle/\delta u(3)$$

and

$$\epsilon=(-i\beta)\Delta; \qquad \Delta\to+0.$$

The kinematic sum rule of Eq. (5.4) is valid for general spin. Much simplification results, however, for the particular case of $S=\frac{1}{2}$, when

$$\mathfrak{M}_{\mathbf{k}}^{(1)}(\nu)\underset{S=1/2}{=}0. \quad (5.5)$$

Similarly, Eq. (5.1b) readily leads to another set of useful sum rules:

$$\langle[S_1^+(t), S_2^-(t)]_-\rangle=\delta_{1,2}2\sigma, \quad (5.6\text{a})$$

$$\langle[S_1^z(t), S_2^z(t)]_-\rangle=0. \quad (5.6\text{b})$$

We recall that the expression for the transverse correlation function obtained in the 1st RPA [see Eq. (3.4)] does obey this sum rule.

In addition to the foregoing sum rules, which follow directly from the kinematic properties of the spin operators and which are not dependent on the actual form of the interaction in the system, there are others which depend on the dynamic behavior of the spins and as such are dependent on the exchange interactions. A particularly convenient example of such a sum rule is provided by considering the time development of the longitudinal Green's function:

$$i\frac{d}{d\tau_1}\left[\frac{\delta\langle\langle S^z(1)\rangle\rangle}{\delta u(1')}\right]_{u=0}=-i\sum_2 I_+(12) \times\langle T\{[S^+(2)S^-(1)-S^+(1)S^-(2)]\tilde{S}^z(1')\rangle|_{\tau_2=\tau_1}, \quad (5.7)$$

where

$$\tilde{S}^z(n)=S^z(n)-\sigma. \quad (5.8)$$

In the right-hand side of Eq. (5.7) the appearance of the factor $I_+(12)$ guarantees that the spatial arguments of the operators S^+ and S^- are never the same. As such the ordering of these operators is immaterial. This means that the physics of the problem does not depend on how τ_2 tends to τ_1 in each of the two terms on the right-hand side of Eq. (5.7).

Fourier transforming Eq. (5.7) according to Eq. (2.10) we get

$$M_{\mathbf{k}}^{(1)}(\nu)Z_\nu=\lim_{\epsilon=-i\beta\Delta;\Delta\to+0}-(1/\beta N)\sum_{\lambda}{}'\sum_{\rho}G^{(1)}{}_{\lambda,\mathbf{k}-\lambda}(\rho,\nu-\rho) \times[J_+(\lambda)\exp(\pm iz_\rho\epsilon)-J_+(\mathbf{k}-\lambda)\exp(\pm iZ_\rho\epsilon)], \quad (5.9)$$

where any of the four possible combinations of the signs of the exponents on the right-hand side of Eq. (5.9) should lead to the same physical result. This situation is analogous to that already encountered in connection with the kinematic sum rule: that in Eq. (5.3) the physical consequences of either of the limits, $\tau_1=\tau_{1'}\pm0$, are to be identical and as such the two alternative versions of Eq. (5.4) should yield the same results.

Equation (5.9) provides us with a dynamical sum rule which is valid for all values of the spin S. A further consequence of this sum rule is the symmetry requirement that

$$\sum_{\lambda}' \sum_{\rho} [G^{(1)}{}_{\lambda,\mathbf{k}-\lambda}(\rho,\nu-\rho)J_{++}(\lambda,\mathbf{k}-\lambda)$$
$$+G^{(1)}{}_{\lambda,-\mathbf{k}-\lambda}(\rho,-\nu-\rho)J_{++}(\lambda,-\mathbf{k}-\lambda)]=0, \quad (5.10)$$

where we have used the information that $M_{\mathbf{k}}^{(1)}(\nu)=M_{-\mathbf{k}}^{(1)}(-\nu)$.

The physical content of the foregoing dynamical sum rule is analogous to that of the current-conservation laws for particle systems, e.g.,

$$[\partial n(r,t)/\partial t]+\nabla\cdot\mathcal{J}(r,t)=0, \quad (5.11)$$

where $\mathcal{J}(\mathbf{r},t)$ is the particle or the electrical current, depending on whether a $n(\mathbf{r},t)$ is the particle or the charge density in the neighborhood of the space-time point $(\mathbf{r},t)$. The sum rules and the symmetry requirements of Eqs. (5.7)–(5.10) may therefore be called the spin-current conservation laws.

It is with satisfaction that we note that inasmuch as both the 2nd RPA expressions, i.e., (I) and (II), satisfy the dynamical symmetry condition of Eq. (5.10), they both obey the current-conservation laws.

6. FORMAL SOLUTION FOR G(11′)

In this section, we shall discuss the two alternative solutions for the Green's function $G(11')$, which follow as a result of substituting the two 2nd RPA expressions for $G^{(1)}{}_{\lambda1,\lambda2}(\rho_1,\rho_2)$ into the original equation of motion (2.12):

$$G_\lambda(\rho)[Z_\rho-E_\lambda]-2\sigma \underset{\text{2nd RPA(I)}}{\approx} \left(\frac{i}{-i\beta N}\right)\sum_{\lambda_1}'\sum_{\rho_1} J_{0+}(\lambda_1-\lambda,\lambda_1)\left\{\frac{2M^{(1)}{}_{\lambda_1-\lambda}(\rho_1-\rho)[1+G_\lambda(\rho)J_{0+}(\lambda_1-\lambda,\lambda)]-G_\lambda(\rho)}{Z_{\rho_1}-E_{\lambda_1}}\right.$$
$$\left.+[Z_\rho-E_\lambda]^{-1}[-G_{\lambda_1}(\rho_1)+2M^{(1)}{}_{\lambda_1-\lambda}(\rho_1-\rho)[1+G_{\lambda_1}(\rho_1)J_{0+}(\lambda_1-\lambda,\lambda_1)]]\right\} \quad (6.1\text{a})$$

and

$$G_\lambda(\rho)[Z_\rho-E_\lambda]-2\sigma \underset{\text{2nd RPA(II)}}{\approx} \left(\frac{2}{-\beta N}\right)\sum_{\lambda_1}'\sum_{\rho_1} J_{0+}(\lambda_1-\lambda,\lambda_1)[Z_{\rho_1}-Z_\rho+E_\lambda-E_{\lambda_1}]^{-1}$$
$$\times\{[G_{\lambda_1}(\rho_1)-G_\lambda(\rho)]+2M^{(1)}{}_{\lambda_1-\lambda}(\rho_1-\rho)[J_{0+}(\lambda_1-\lambda,\lambda)G_\lambda(\rho)-J_{0+}(\lambda_1-\lambda,\lambda_1)G_{\lambda_1}(\rho_1)]\}. \quad (6.1\text{b})$$

Equations (6.1a) and (6.1b) provide the two alternative 2nd RPA expressions for the transverse Green's function $G(11')$. Again it is clear that except for carrying out the relevant calculations there is no obvious *a priori* way of deciding as to which of the two Eqs. (6.1a) and (6.1b) would lead to a more satisfactory solution.

It should be mentioned here that an alternative procedure could have been to equate the two 2nd RPA expressions for the Green's function $G^{(1)}$, and to establish thereby different independent relationship between $M^{(1)}$ and G. This procedure would have the further virtue in that equations (6.1a) and (6.1b) would then be identical to each other. There is, however, a serious drawback in following this procedure. As already mentioned, the two approximations, 2nd RPA(I) and (II), are not identical and any predictions based on a procedure which effectively subtracts one from the other may lead to serious error. Moreover, the present scheme of deriving an independent relationship between G and $M^{(1)}$, using a rigorous sum rule, has the added advantage that the results then automatically conserve the sum rule in question. Moreover, as a general rule, in approximate treatments of many-body systems, the results obtained are the more satisfactory, the greater the number of rigorous sum rules satisfied by the approximations involved.[21] Similarly, the preservation of the physical symmetry requirements is also of paramount importance.

In both the expressions, (6.1a) and (6.1b), the transverse Green's function $G(11')$ is coupled to the longitudinal Green's function $M_\lambda^{(1)}(\rho)$. In order, therefore, that a complete solution be achieved we need an additional relationship between the Green's functions G and $M^{(1)}$. The various sum rules discussed in the foregoing section provide just such relationships. For present purposes, however, it suffices to know that there exist suitable spectral representations for G and $M^{(1)}$ (see Appendix A) with the help of which the 2nd RPA expressions (I) and (II) can straightforwardly be transformed into integral equations connecting the transverse spectral function with the longitudinal one. In a similar fashion the sum rules of the preceding section can be made to yield additional relations between the two spectral functions (e.g., see the following section). When this is done, we have, in principle, four corresponding sets of integral equations for each of the two spectral functions. The reason there are four sets of equations is that there are two versions of the 2nd RPA each of which can be combined with either the kinematical or the dynamical sum rule. Not surprisingly at general temperatures these integral equations do not turn out to be amenable to analytical solution and must as such be studied by numerical methods.

We might add here that only one of the four possible integral equations for each of the two spectral functions

[21] G. Baym, Phys. Rev. **127**, 1391 (1962).

turns out to be completely satisfactory. This is so firstly because the 2nd RPA(II) leads to internal inconsistencies under both the kinematic and the dynamic sum rules. Moreover, the results of the 2nd RPA(I) under the dynamic sum rule are not found to be satisfactory near the transition point. Thus only the 2nd RPA(I), calculated under the kinematic sum rule, is a completely consistent approximation. It is to be noted that since both the 2nd RPA expressions are spin current-conserving approximations, the application of the kinematic sum rule to the 2nd RPA(I) should lead to an approximation which embodies aspects of both a current-conservation symmetry and the spin kinematics.

7. LONGITUDINAL GREEN'S FUNCTION M(1)

While a detailed study of both the longitudinal and the transverse correlation functions as well as their inter-relationship must await a numerical analysis, it is instructive to investigate the form of the dependence of the longitudinal Green's function on that of the transverse one.

It has already been noted in the preceding section that the 2nd RPA manifests an implicit connection between the Green's functions G and $M^{(1)}$. Our task in the present section is to investigate the additional relationships between these Green's functions which result as a consequence of the kinematic and the current-conserving sum rules. Once this is done, the program of the preceding section will also be completed and a set of closed integral equations for the spectral functions of the transverse and the longitudinal components can then be achieved.

It has already been mentioned that the 2nd RPA(II) is an unsatisfactory approximation because it leads to some internal inconsistencies. [The appropriate analysis for this case is rather instructive and is briefly discussed in Appendix B. The rationale for including this analysis is that it is only after carrying it out that the internal inconsistencies of the 2nd RPA(II) are discovered]. As such in the present section we shall only study the 2nd RPA(I).

Let us consider first the dynamical sum rule of Eq. (5.9). Introducing Eqs. (4.5) and (4.7) into (5.9) we get

$$-M_{\mathbf{k}}^{(1)}(\nu)Z_\nu=\lim_{\epsilon\to(-i\beta)0} M_{\mathbf{k}}^{(1)}(\nu)(1/\beta N)\sum_\lambda{}'\sum_\rho[J_+(\lambda)\exp(\pm iZ_\rho\epsilon)-J_+(\mathbf{k}-\lambda)\exp(\pm iZ_\rho\epsilon)]$$
$$\times\{[Z_\rho-E_\lambda]^{-1}+[Z_\rho-Z_\nu-E_{\mathbf{k}-\lambda}]^{-1}+[Z_\rho-E_\lambda]^{-1}J_{0+}(\mathbf{k},\mathbf{k}-\lambda)G_{-\mathbf{k}+\lambda}(-\nu+\rho)$$
$$+[Z_\rho-Z_\nu-E_{\mathbf{k}-\lambda}]^{-1}G_\lambda(\rho)J_{0+}(\mathbf{k},\lambda)\}+(1/2\beta N)\sum_\lambda{}'\sum_\rho J_{++}(\lambda,\mathbf{k}-\lambda)$$
$$\times\{G_\lambda(\rho)[Z_\nu-Z_\rho+E_{\mathbf{k}-\lambda}]^{-1}-G_{\lambda-\mathbf{k}}(\rho-\nu)[Z_\rho-E_\lambda]^{-1}\}. \quad (7.1)$$

Using the spectral representation of Eq. (A5) for the Green's function G, and summing over ρ, Eq. (7.1) readily leads to the following result:

$$[M_{\mathbf{k}}^{(1)}(\nu)]_{\text{dynamic sum rule}}^{\text{2nd RPA(I)}}=a_{\mathbf{k}}(\nu)[b_{\mathbf{k}}(\nu)]^{-1}, \quad (7.2\text{a})$$

where

$$a_{\mathbf{k}}(\nu)=(2N)^{-1}\sum_\lambda{}'\int_{-\infty}^{+\infty}f_\lambda(\omega)J_{++}(\mathbf{k}-\lambda,\lambda)[n(E_{\mathbf{k}-\lambda})-n(\omega)]\{[E_{\mathbf{k}-\lambda}-\omega+Z_\nu]^{-1}-[E_{\mathbf{k}-\lambda}-\omega-Z_\nu]^{-1}\}\,d\omega, \quad (7.2\text{b})$$

$$b_{\mathbf{k}}(\nu)=Z_\nu+N^{-1}\sum_\lambda{}'\int_{-\infty}^{+\infty}f_\lambda(\omega)J_{0+}(\mathbf{k},\lambda)J_{++}(\mathbf{k}-\lambda,\lambda)[n(E_{\mathbf{k}-\lambda})-n(\omega)]$$
$$\times\{[E_{\mathbf{k}-\lambda}-\omega+Z_\nu]^{-1}-[E_{\mathbf{k}-\lambda}-\omega-Z_\nu]^{-1}\}\,d\omega. \quad (7.2\text{c})$$

Note that all the four sign combinations in the exponents on the right-hand side of Eq. (7.1) lead, as they should, to the same result given in Eq. (7.2) above.

Using the procedure outlined in Appendix A, Eq. (7.2) leads to the following expression for the longitudinal spectral function:

$$F_{\mathbf{k}}(\omega_0)\Big|_{\text{dynamical sum rule}}^{\text{2nd RPA(I)}}=[y^{(1)}(\omega_0)x^{(2)}(\omega_0)-x^{(1)}(\omega_0)y^{(2)}(\omega_0)]\{[x^{(2)}(\omega_0)]^2+\pi^2[y^{(2)}(\omega_0)]^2\}^{-1}, \quad (7.3\text{a})$$

where

$$x^{(1)}(\omega_0)=-x^{(1)}(-\omega_0)$$

$$=-\omega_0\frac{\mathcal{P}}{N}\sum_\lambda{}'\int_{-\infty}^{+\infty}f_\lambda(\omega)J_{++}(\mathbf{k}-\lambda,\lambda)[n(E_{\mathbf{k}-\lambda})-n(\omega)]\{[E_{\mathbf{k}-\lambda}-\omega]^2-\omega_0^2\}^{-1}\,d\omega, \quad (7.3b)$$

$$x^{(2)}=-x^{(2)}(\omega_0)=\omega_0\left\{1-\frac{2}{N}\mathcal{P}\sum_\lambda{}'\int_{-\infty}^{+\infty}f_\lambda(\omega)J_{0+}(\mathbf{k},\lambda)J_{++}(\mathbf{k}-\lambda,\lambda)\right.$$

$$\left.\times[n(E_{\mathbf{k}-\lambda})-n(\omega)][(E_{\mathbf{k}-\lambda}-\omega)^2-\omega_0^2]^{-1}\,d\omega\right\}, \quad (7.3c)$$

$$y^{(2)}(\omega_0)=+y^{(2)}(-\omega_0)=N^{-1}\sum_\lambda{}'\int_{-\infty}^{+\infty}f_\lambda(\omega)J_{0+}(\mathbf{k},\lambda)J_{++}(\mathbf{k}-\lambda,\lambda)$$

$$\times[n(E_{\mathbf{k}-\lambda})-n(\omega)][\delta(E_{\mathbf{k}-\lambda}-\omega+\omega_0)+\delta(E_{\mathbf{k}-\lambda}-\omega-\omega_0)]\,d\omega, \quad (7.3d)$$

$$y^{(1)}(\omega_0)=+y^{(1)}(-\omega_0)$$

$$=(2N)^{-1}\sum_\lambda{}'\int_{-\infty}^{+\infty}f_\lambda(\omega)J_{++}(\mathbf{k}-\lambda,\lambda)[n(E_{\mathbf{k}-\lambda})-n(\omega)][\delta(E_{\mathbf{k}-\lambda}-\omega+\omega_0)+\delta(E_{\mathbf{k}-\lambda}-\omega-\omega_0)]\,d\omega. \quad (7.3e)$$

We notice that since

$$F_{\mathbf{k}}(\omega_0)=-F_{\mathbf{k}}(-\omega_0), \quad (7.4)$$

as such the longitudinal spectral function satisfies the sum rule (5.6b). [See Eq. (A4b).]

Let us use next the kinematic sum rule. Introducing the 2nd RPA (I) expression for $G^{(1)}{}_{\mathbf{k}-\lambda,\lambda}(\nu-\rho,\rho)$ into the kinematic sum rule of Eq. (5.4) we get

$$\pm iM_{\mathbf{k}}^{(1)}(\nu)+i\mathfrak{M}_{\mathbf{k}}^{(1)}(\nu)=\lim_{\epsilon=(-i\beta)\Delta;\Delta=+0}(-1/2i\beta N)\sum_\lambda\sum_\rho{}'\exp(\mp iZ_\rho\epsilon)\{G_{\mathbf{k}-\lambda}(\nu-\rho)[Z_\rho+E_\lambda]^{-1}$$

$$\times[1-2M_{\mathbf{k}}^{(1)}(\nu)J_{0+}(\mathbf{k},\mathbf{k}-\lambda)]-2M_{\mathbf{k}}^{(1)}(\nu)[Z_\rho+E_\lambda]^{-1}+2M_{\mathbf{k}}^{(1)}(\nu)[Z_\nu-Z_\rho-E_{\mathbf{k}-\lambda}]^{-1}$$

$$-G_{-\lambda}(-\rho)[1-2M_{\mathbf{k}}^{(1)}(\nu)J_{0+}(\mathbf{k},\lambda)][Z_\nu-Z_\rho-E_{\mathbf{k}-\lambda}]^{-1}\}. \quad (7.5)$$

The ρ sums are performed as usual by introducing the spectral representation for the Green's function G. We get

$$\mathfrak{M}_{\mathbf{k}}^{(1)}(\nu)=\frac{1}{2N}\sum_\lambda{}'\int_{-\infty}^{+\infty}f_\lambda(\omega)[n(E_{\mathbf{k}-\lambda})-n(\omega)]\{[E_{\mathbf{k}-\lambda}-\omega+Z_\nu]^{-1}+[E_{\mathbf{k}-\lambda}-\omega-Z_\nu]^{-1}\}\,d\omega$$

$$-M_{\mathbf{k}}^{(1)}(\nu)\left\{1+2\bar{n}+N^{-1}\sum_\lambda{}'J_{0+}(\mathbf{k},\lambda)\int_{-\infty}^{+\infty}f_\lambda(\omega)[n(E_{\mathbf{k}-\lambda})-n(\omega)]\right.$$

$$\left.\times[(E_{\mathbf{k}-\lambda}-\omega+Z_\nu)^{-1}+(E_{\mathbf{k}-\lambda}-\omega-Z_\nu)^{-1}]\,d\omega\right\}, \quad (7.6a)$$

where

$$\bar{n}=(1/N)\sum_\lambda{}'n(E_\lambda). \quad (7.6b)$$

It should be emphasized here that both the ρ sums in Eq. (7.5), i.e., involving the expressions $\exp(\pm iZ_\rho\epsilon)$, respectively, lead as they should to the same relationship between the Green's functions $M_{\mathbf{k}}^{(1)}(\nu)$ and $\mathfrak{M}_{\mathbf{k}}^{(1)}(\nu)$:

For $S=\frac{1}{2}$, $\mathfrak{M}_{\mathbf{k}}^{(1)}(\nu)=0$ and we get

$$M_{\mathbf{k}}^{(1)}(\nu)=c_{\mathbf{k}}(\nu)[d_{\mathbf{k}}(\nu)]^{-1}, \quad (7.7a)$$

$$c_{\mathbf{k}}(\nu)=(2N)^{-1}\sum_\lambda{}'\int_{-\infty}^{+\infty}f_\lambda(\omega)[n(E_{\mathbf{k}-\lambda})-n(\omega)][(E_{\mathbf{k}-\lambda}-\omega+Z_\nu)^{-1}+(E_{\mathbf{k}-\lambda}-\omega-Z_\nu)^{-1}]\,d\omega, \quad (7.7b)$$

$$d_{\mathbf{k}}(\nu)=\eta+N^{-1}\sum_\lambda{}'J_{0+}(\mathbf{k},\lambda)\int_{-\infty}^{+\infty}f_\lambda(\omega)[n(E_{\mathbf{k}-\lambda})-n(\omega)][(E_{\mathbf{k}-\lambda}-\omega+Z_\nu)^{-1}+(E_{\mathbf{k}-\lambda}-\omega-Z_\nu)^{-1}]\,d\omega. \quad (7.7c)$$

It is shown in Appendix E that the above equation holds even for the case of general spin, where η is given by Eq. (E15). Of course, for $S=\frac{1}{2}$, $\eta=1+2\bar{n}$.

Expressions (7.7) now readily lead to the following relationship between the spectral functions $F_\lambda(\omega)$ and $f_\lambda(\omega)$:

$$[F_{\mathbf{k}}(\omega_0)]^{\text{2nd RPA (I)}}_{\text{kinematic sum rule}}=[y^{(3)}(\omega_0)x^{(4)}(\omega_0)-y^{(4)}(\omega_0)x^{(3)}(\omega_0)]\{[x^{(4)}(\omega_0)]^2+\pi^2[y^{(4)}(\omega_0)]^2\}^{-1}, \tag{7.8a}$$

where

$$x^{(3)}(\omega_0)=+x^{(3)}(-\omega_0)=N^{-1}\mathcal{P}\sum_\lambda{}'\int_{-\infty}^{+\infty}f_\lambda(\omega)[n(E_{\mathbf{k}-\lambda})-n(\omega)][E_{\mathbf{k}-\lambda}-\omega]\{[E_{\mathbf{k}-\lambda}-\omega]^2-\omega_0^2\}^{-1}\,d\omega, \tag{7.8b}$$

$$y^{(3)}(\omega_0)=-y^{(3)}(-\omega_0)$$
$$=(2N)^{-1}\sum_\lambda{}'\int_{-\infty}^{+\infty}f_\lambda(\omega)[n(E_{\mathbf{k}-\lambda})-n(\omega)][\delta(E_{\mathbf{k}-\lambda}-\omega+\omega_0)-\delta(E_{\mathbf{k}-\lambda}-\omega-\omega_0)]\,d\omega, \tag{7.8c}$$

$$x^{(4)}(\omega_0)=x^{(4)}(-\omega_0)=\eta+\frac{2}{N}\mathcal{P}\sum_\lambda{}'J_{0+}(\mathbf{k},\lambda)\int_{-\infty}^{+\infty}f_\lambda(\omega)[n(E_{\mathbf{k}-\lambda})-n(\omega)][E_{\mathbf{k}-\lambda}-\omega]\{[E_{\mathbf{k}-\lambda}-\omega]^2-\omega_0^2\}^{-1}\,d\omega, \tag{7.8d}$$

$$y^{(4)}(\omega_0)=-y^{(4)}(-\omega_0)=N^{-1}\sum_\lambda{}'J_{0+}(\mathbf{k},\lambda)\int_{-\infty}^{+\infty}f_\lambda(\omega)[n(E_{\mathbf{k}-\lambda})-n(\omega)][\delta(E_{\mathbf{k}-\lambda}-\omega+\omega_0)-\delta(E_{\mathbf{k}-\lambda}-\omega-\omega_0)]\,d\omega. \tag{7.8e}$$

Once again the above expressions for the longitudinal spectral function obey the relation $F_k(\omega)=-F_k(-\omega)$ and as such preserve the kinematic sum rule (5.6b).

The fact that the foregoing solutions for $F_k(\omega)$, i.e., Eqs. (7.3) and (7.8), differ and would possibly yield results which would be different in detail, is a demonstration of the difficulty which usually arises with approximate treatments of the many-body problem where complete internal dynamic and statistical consistency is not attained. Indeed, the two approximations, (7.3) and (7.8), emphasize different aspects of the dynamics of the interacting many-spin system and their results would differ as likely from each other as they certainly must do from the exact result.

It might be mentioned here that from the results of the present section an approximation scheme to be called the modified RPA is developed in the following sections. The mod RPA provides an expression for the longitudinal correlation function, following from Eqs. (7.6)–(7.8), which seems to describe the equilibrium thermodynamics reasonably adequately over the entire range of temperatures. The Eqs. (7.2)–(7.3), on the other hand, do not yield such a satisfactory representation of the longitudinal correlation function in the modified RPA (see Appendix D).

In Appendix B, during the course of the study of the 2nd RPA(II), it is discovered that in spite of the inherent weaknesses of the 2nd RPA(II) due to internal inconsistencies, it leads to at least one expression for the Green's function $M^{(1)}$ which yields satisfactory results in the mod RPA for the longitudinal correlation function [see Eq. (B5)]. As such, in the following sections the 2nd RPA longitudinal correlation functions will be analyzed following from both Eqs. (7.6)–(7.8) as well as the phenomenological Eq. (B5). For the sake of brevity these approximations will, respectively, be called the (I)mod RPA and the (II)mod RPA.

8. MODIFIED RPA AND THE LONGITUDINAL CORRELATION

We have observed in the preceding sections that formal expressions for the transverse spectral functions can be obtained by a self-consistent application of the second-order RPA when some exact relationships, i.e., the sum rules, expressing the longitudinal spectral function in terms of the transverse one, are invoked. As these expressions are in the form of complicated integral equations to which analytical solutions are hard to find, it is therefore necessary to look for an approximation scheme, based preferrably on physically meaningful considerations, whereby the resultant expressions would be easy to handle mathematically. One such scheme is the mod RPA, which consists in inserting the 1st RPA result for the transverse spectral function, i.e. $f_\lambda^{(1)}(\omega)$, where

$$f_\lambda^{(1)}(\omega)=2\sigma\delta(\omega-E_\lambda)\approx f_\lambda(\omega), \tag{8.1}$$

into the 2nd RPA expressions relating the longitudinal spectral function to the transverse one and thus obtaining an approximate, i.e., mod RPA, expression for the longitudinal spectral function. While we cannot at this stage predict how satisfactory this approximation procedure would really be for the description of the longitudinal correlation function, we can anticipate that this description would not include relaxation effects, much as the 1st RPA did not include these effects.

It is convenient to represent the mod RPA procedure schematically as follows:

$$F_\lambda^{(2i)}(\omega)\xrightarrow[\text{Eqs. (7.6)–(7.8); (B5)}]{}F_\lambda^{(2i)}(\omega)[f_{\mathbf{k}}^{(2i)}(\omega_0)], \tag{8.2a}$$

$$f_\lambda^{(2i)}(\omega)\xrightarrow[\text{Eqs. (6.1a)(6.1b)}]{}f_\lambda^{(2i)}(\omega)[f_{\mathbf{k}_1}^{(2i)}(\omega_1);F_{\mathbf{k}_2}^{(2i)}(\omega_2)], \tag{8.2b}$$

where $F_\lambda^{(2i)}(\omega)$ and $f_\lambda^{(2i)}(\omega)$ denote the consistent second-RPA solutions for the spectral functions $F_\lambda(\omega)$ and $f_\lambda(\omega)$, respectively.

The mod RPA is defined as

$$F_\lambda^{(i\text{ mod})}(\omega) \xrightarrow[\text{Eq. (8.2a)}]{} F_\lambda^{(2i)}(\omega)[f_{\mathbf{k}}^{(1)}(\omega_0)], \quad (8.3a)$$

where $i=(\text{I})$ or (II), depending on whether we use Eqs. (7.6)–(7.8) or (B5) in the relation (8.2a).

It should be emphasized here that the mod RPA, defined in Eq. (8.3a), is not the first step of a logical iteration procedure and any further iteration, e.g.,

$$f_\lambda(\omega) \to f_\lambda(\omega)[f_{\mathbf{k}_1}^{(1)}(\omega_1);\, F_{\mathbf{k}_2}^{(i\text{ mod})}(\omega_2)], \quad (8.3b)$$

or indeed

$$f_\lambda(\omega) \to f_\lambda(\omega)[f_{\mathbf{k}_1}(\omega_1);\, F_{\mathbf{k}_2}^{(i\text{ mod})}(\omega_2)] \quad (8.3c)$$

is completely inadmissible. The methods of the present section are therefore, strictly speaking, not suitable for the study of the transverse correlation function in any form of the 2nd RPA.

Introducing, according to the prescription (8.3a), the expression (8.1) for the spectral function $f_\lambda(\omega)$ into the right-hand side of Eqs. (7.8) and (B5), we obtain, respectively, the following expressions for $F_{\mathbf{k}}^{(i\text{ mod})}(\omega_0)$:

$$F_{\mathbf{k}}^{(\text{I mod})}(\omega_0) = [Y^{(1)}(\omega_0)X^{(2)}(\omega_0) - X^{(1)}(\omega_0)Y^{(2)}(\omega_0)]\{[X^{(2)}(\omega_0)]^2 + \pi^2[Y^{(2)}(\omega_0)]^2\}^{-1}, \quad (8.4a)$$

$$F_{\mathbf{k}}^{(\text{II mod})}(\omega_0) = [Y^{(3)}(\omega_0)X^{(4)}(\omega_0) - X^{(3)}(\omega_0)Y^{(4)}(\omega_0)]\{[X^{(4)}(\omega_0)]^2 + \pi^2[Y^{(4)}(\omega_0)]^2\}^{-1}, \quad (8.5a)$$

$$X^{(1)}(\omega_0) = X^{(1)}(-\omega_0) = (2\sigma/N)\sum_\lambda{}' [n(E_{\mathbf{k}-\lambda}) - n(E_\lambda)][E_{\mathbf{k}-\lambda} - E_\lambda][(E_{\mathbf{k}-\lambda} - E_\lambda)^2 - \omega_0^2]^{-1}, \quad (8.4b)$$

$$Y^{(1)}(\omega_0) = -Y^{(1)}(-\omega_0) = (\sigma/N)\sum_\lambda{}' [n(E_{\mathbf{k}-\lambda}) - n(E_\lambda)][\delta(E_{\mathbf{k}-\lambda} - E_\lambda + \omega_0) - \delta(E_{\mathbf{k}-\lambda} - E_\lambda - \omega_0)], \quad (8.4c)$$

$$X^{(2)}(\omega_0) = X^{(2)}(-\omega_0) = \eta + (4\sigma/N)\sum_\lambda{}' J_{0+}(\mathbf{k}, \lambda)[n(E_{\mathbf{k}-\lambda}) - n(E_\lambda)][E_{\mathbf{k}-\lambda} - E_\lambda][(E_{\mathbf{k}-\lambda} - E_\lambda)^2 - \omega_0^2]^{-1}, \quad (8.4d)$$

$$Y^{(2)}(\omega_0) = -Y^{(2)}(-\omega_0) = (2\sigma/N)\sum_\lambda{}' J_{0+}(\mathbf{k}, \lambda)[n(E_{\mathbf{k}-\lambda}) - n(E_\lambda)][\delta(E_{\mathbf{k}-\lambda} - E_\lambda + \omega_0) - \delta(E_{\mathbf{k}-\lambda} - E_\lambda - \omega_0)], \quad (8.4e)$$

$$X^{(3)}(\omega_0) = -X^{(3)}(-\omega_0)$$
$$= (2\sigma/N)\sum_\lambda{}' J_{++}(\lambda, \mathbf{k}-\lambda)[n(E_\lambda) - n(E_{\mathbf{k}-\lambda})][\omega_0 + E_{\mathbf{k}-\lambda} - E_\lambda]^{-1}, \quad (8.5b)$$

$$Y^{(3)}(\omega_0) = +Y^{(3)}(-\omega_0) = (2\sigma/N)\sum_\lambda{}' J_{++}(\lambda, \mathbf{k}-\lambda)[n(E_\lambda) - n(E_{\mathbf{k}-\lambda})]\delta(\omega_0 + E_{\mathbf{k}-\lambda} - E_\lambda), \quad (8.5c)$$

$$X^{(4)}(\omega_0) = -X^{(4)}(-\omega_0) = \omega_0 + (4\sigma/N)\sum_\lambda{}' J_{++}(\lambda, \mathbf{k}-\lambda)[\omega_0 + E_{\mathbf{k}-\lambda} - E_\lambda]^{-1}$$
$$\times\{J_{0+}(\mathbf{k}, \lambda)n(E_\lambda) - J_{0+}(\mathbf{k}, \mathbf{k}-\lambda)n(E_{\mathbf{k}-\lambda})\}, \quad (8.5d)$$

$$Y^{(4)}(\omega_0) = Y^{(4)}(-\omega_0) = (4\sigma/N)\sum_\lambda{}' J_{++}(\lambda, \mathbf{k}-\lambda)\delta(\omega_0 + E_{\mathbf{k}-\lambda} - E_\lambda)\{J_{0+}(\mathbf{k}, \lambda)n(E_\lambda) - J_{0+}(\mathbf{k}, \mathbf{k}-\lambda)n(E_{\mathbf{k}-\lambda})\}. \quad (8.5e)$$

The above modified-RPA solutions for the longitudinal spectral function $F_{\mathbf{k}}(\omega)$ are in a form suitable for computing the time-dependent, longitudinal spin correlation $\langle S_1^z(t_1)S_2^z(t_2)\rangle$ [see Eqs. (A7)]. While a detailed computation will be given elsewhere at a later time, we give such analysis as can be carried out analytically in the following sections.

9. THE CRITICAL FLUCTUATIONS

The ferromagnetic-paramagnetic phase transition, occurring at the Curie point, is an example of a second-order phase transition; the study of the system thermodynamics in the critical region is therefore of much physical interest. The phenomenon of magnetic critical scattering,[22] analogously to the scattering of light from a liquid near its critical state, i.e., opalescence, and the scattering of x rays from a metallic alloy in the vicinity of its ordering temperature, embodies vital information about the critical region through its dependence on the dynamical spin-correlation functions. In the present section we shall analyze the mod RPA correlation functions with a view to studying their behavior in the critical region and to relating it to the critical magnetic scattering of neutrons.

[22] L. van Hove, Phys. Rev. **93**, 268 (1954); **95**, 249 (1954); **95**, 1374 (1954).

Let us recast Eqs. (8.4) and (8.5) into a form more convenient for analytical analysis, i.e.,

$$[M_k^{(1)}(\nu)]^{(\mathrm{I\ mod})}=A_k(Z_\nu)[B_k(Z_\nu)]^{-1}, \tag{9.1a}$$

$$[M_k^{(1)}(\nu)]^{(\mathrm{II\ mod})}=C_k(Z_\nu)[D_k(Z_\nu)]^{-1}, \tag{9.2a}$$

$$A_k(Z_\nu)=A_k(-Z_\nu)=(2\sigma/N)\sum_\lambda{}' \times[n(E_{k-\lambda})-n(E_\lambda)][E_{k-\lambda}-E_\lambda+Z_\nu]^{-1} \tag{9.1b}$$

$$B_k(Z_\nu)=B_k(-Z_\nu)=\eta+(2\sigma/N)\sum_\lambda{}' \times[J_{0+}(\mathbf{k},\lambda)+J_{0+}(\mathbf{k},\mathbf{k}-\lambda)][n(E_{k-\lambda})-n(E_\lambda)] \times[E_{k-\lambda}-E_\lambda+Z_\nu]^{-1}, \tag{9.1c}$$

$$C_k(Z_\nu)=-C_k(-Z_\nu) =(2\sigma/N)\sum_\lambda{}' J_{++}(\lambda,\mathbf{k}-\lambda)[n(E_\lambda)-n(E_{k-\lambda})] \times[E_{k-\lambda}-E_\lambda+Z_\nu]^{-1}, \tag{9.2b}$$

$$D_k(Z_\nu)=-D_k(-Z_\nu) =Z_\nu+(4\sigma/N)\sum_\lambda{}' J_{++}(\lambda,\mathbf{k}-\lambda)[E_{k-\lambda}-E_\lambda+Z_\nu]^{-1} \times\{[n(E_\lambda)]J_{0+}(\mathbf{k},\lambda)-[n(E_{k-\lambda})]J_{0+}(\mathbf{k},\mathbf{k}-\lambda)\}. \tag{9.2c}$$

Equations (9.1) and (9.2) correspond, respectively, to Eqs. (8.4) and (8.5) and η is as given in Eq. (E15).

In the critical region, i.e., $|\beta_c-\beta|\ll\beta_c$, if the applied field H is vanishingly small, the magnetization σ is much less than the saturation value S. Then

$$n(E_k)=(1/2\sigma\beta)\{[\zeta+\xi_k]^{-1}-\sigma\beta +\tfrac{1}{3}(\sigma\beta)^2[\zeta+\xi_k]-O(\sigma\beta)^4\}, \tag{9.3}$$

where

$$\lim_{H=0}[\mu H/2\sigma]=\zeta;\qquad \xi_k=J_{0+}(0,\mathbf{k}). \tag{9.4}$$

Let us study the situation obtaining at and beyond the Curie point where $\sigma\to0$ as $H\to0$:

$$\eta=\frac{2S(S+1)}{3\sigma}\left\{1+\frac{81\sigma^2}{20S^2(S+1)^2} \times[\tfrac{4}{3}S(S+1)-1]+O(\sigma^3)\right\}, \tag{9.5}$$

$$[M_k^{(1)}(\nu)]^{(\mathrm{I\ mod})}=[\delta_{\nu,0}+0(\sigma^2/Z_\nu^2)] \times\{-2[\zeta+\xi_k^{(0)}]+O[\sigma^2\gamma(\mathbf{k})]\}^{-1}, \tag{9.6}$$

$$[M_k^{(1)}(\nu)]^{(\mathrm{II\ mod})}=\alpha_k[1+0(\sigma)] \times\{Z_\nu^2-2[\zeta+\xi_k^{(0)}]\alpha_k\}^{-1}, \tag{9.7}$$

$$\alpha_k=(2/N\beta)\sum_\lambda{}'[\xi_{k-\lambda}-\xi_\lambda][\zeta+\xi_\lambda]^{-1};$$

$$\xi_k^{(0)}=J_0(0)-J_0(\mathbf{k}), \tag{9.8}$$

where $\gamma(\mathbf{k})$ is the same as in Eq. (D5c).

The expressions for the longitudinal correlation function are now obtained by summing over ν and by analytically continuing to real times:

$$\langle\tilde{S}_1{}^z(t_1)\tilde{S}_{1'}{}^z(t_1)\rangle \underset{\mathrm{I\ mod}}{=} (1/N)\sum_k{}'\{2\beta[\zeta+\xi_k^{(0)}]\}^{-1} \times\exp[i\mathbf{k}(1-1')], \tag{9.9}$$

$$\langle\tilde{S}_1{}^z(t_1)\tilde{S}_{1'}{}^z(t_{1'})\rangle \underset{\mathrm{II\ mod}}{=} (1/N) \times\sum_k{}'\exp[i\mathbf{k}(1-1')][\alpha_k/2\omega_k]\{[n(\omega_k)+1] \times\exp[-i\omega_k(t_1-t_{1'})]+n(\omega_k)\exp[i\omega_k(t_1-t_{1'})]\}, \tag{9.10a}$$

$$\langle[S_1{}^z(t_1),S_{1'}{}^z(t_{1'})]_-\rangle \underset{\mathrm{II\ mod}}{=} (1/N) \times\sum_k{}'\exp[i\mathbf{k}(1-1')][\alpha_k/2\omega_k]\{\exp[-i\omega_k(t_1-t_{1'})] -\exp[i\omega_k(t_1-t_{1'})]\}, \tag{9.10b}$$

where

$$\omega_k=+[2(\zeta+\xi_k^{(0)})\alpha_k]^{1/2}. \tag{9.10c}$$

Because of the cooperative nature of the problem, the critical region is known to be characterized mainly by the long-ranged part of the correlation functions, and is therefore manifested in their small-$\mathbf{k}$ transforms. Moreover, it is believed[23] that much of the critical scattering is elastic in character and is as such described adequately by the equal-time correlations, i.e., by $\tilde{F}_k$, where $\tilde{F}_k$ is as defined in Eq. (C7):

$$[\tilde{F}_k] \underset{\beta_c\geq\beta;\sigma=0}{=} [2\beta(\zeta+\xi_k^{(0)})]^{-1}, \tag{9.11a}$$

$$[\tilde{F}_k] \underset{\beta_c\geq\beta;\sigma=0}{=} [\alpha_k/2\omega_k]\coth(\beta\omega_k/2). \tag{9.11b}$$

When $\mathbf{k}\ll1$, the above expressions have the limit

$$\tilde{F}_k \underset{k\ll1}{\approx} \{2\beta[\zeta+I_0\mathbf{k}^2]\}^{-1}. \tag{9.12}$$

Equation (9.12), being similar to that obtained by Elliott and Marshall,[24] displays an important fact, namely that in the immediate vicinity of the critical point, when $\zeta\ll1$—note that at $\beta=\beta_c$, $\zeta=0$—the correlations become extremely long ranged. As the correlation function is a measure of the magnetization density fluctuations δS^z around the statistical average σ, a sharp increase in the range of the correlation function is a manifestation of the phenomenon of critical fluctuations.

We conclude this section by emphasizing the fact that near and beyond the Curie temperature, the mod RPA results for the static longitudinal correlation function are found to be fairly satisfactory; they lead to an explanation of the critical fluctuations and

[23] See Ref. 22, notwithstanding the recent objections by M. E. Fisher, in the *Proceedings of the International Conference on Magnetism, Nottingham 1964*, (The Institute of Physics and the Physical Society, London, 1965), p. 79; also L. Passel, K. Blinowski, P. Neilson, and T. Brun, *ibid.*, p. 99.

[24] R. J. Elliott and W. Marshall, Rev. Mod. Phys. **30**, 75 (1958).

moreover obey the spatial isotropy requirements of Eq. (3.11). This is in obvious contrast to the behavior of the 1st RPA results (see Sec. 3).

10. SPIN DIFFUSION

The conservation of the total magnetization, i.e.,

$$\frac{d}{dt}\int \sigma(\mathbf{r}, t)\, d\mathbf{r}=0, \tag{10.1}$$

where $\sigma(\mathbf{r}, t)$ describes the local magnetization density at a space-time point (r, t), can also be expressed in the differential form:

$$(\partial/\partial t)\sigma(r, t)+\nabla\cdot\mathbf{j}(\mathbf{r}, t)=0, \tag{10.2}$$

where $\mathbf{j}(\mathbf{r}, t)$ is a spin current. In the hydrodynamic limit, when all properties of the system vary slowly in space and time,[25] the spin current is related to the derivative of the magnetization density, i.e.,

$$\mathbf{j}(\mathbf{r}, t)\sim -D[\nabla\sigma(\mathbf{r}, t)], \tag{10.3}$$

and as such the magnetization density obeys a diffusion equation:

$$\partial\sigma(\mathbf{r}, t)/\partial t=D\nabla^2\sigma(\mathbf{r}, t). \tag{10.4}$$

Whereas the form of Eq. (10.4) has been suggested by general phenomenological arguments, to find the value of the diffusion constant D we have to refer to the microscopic dynamics of the system. It is natural therefore to look for a description of the diffusion constant in the dynamical correlation functions.

Following Kadanoff and Martin,[25] a generalized diffusion spectral function $\mathfrak{D}(\mathbf{k}, \omega)$ can be defined, the high-frequency moments of which are related to similar moments of the longitudinal spectral function $F_{\mathbf{k}}(\omega)$ [refer to Appendix C, Eqs. (C3)–(C6) for details]. According to Bennett and Martin,[26] a sufficient approximation to the spectral function $\mathfrak{D}(\mathbf{k}, \omega)$ is the two-parameter representation:

$$\mathfrak{D}(\mathbf{k}, \omega)\sim\Delta(\mathbf{k})\Gamma(\mathbf{k})\exp\{-\omega[\Gamma(\mathbf{k})]^2\}, \tag{10.5}$$

where $\Gamma(\mathbf{k})$ is interpreted as a collision time for processes involving wave-vector transfer $\mathbf{k}$. The diffusion constant D is the hydrodynamic limit of $\mathfrak{D}(\mathbf{k}, \omega)$, i.e., $D=\Delta(0)\Gamma(0)$.

The relation (10.5) readily leads to the result

$$\Delta(\mathbf{k})=\sqrt{\pi}\mathfrak{D}_{\mathbf{k}}^{(0)}; \qquad \Gamma(\mathbf{k})=[\mathfrak{D}_{\mathbf{k}}^{(0)}/2\mathfrak{D}_{\mathbf{k}}^{(2)}]^{1/2}, \tag{10.6}$$

where $\mathfrak{D}^{(n)}$ is the nth-order frequency moment of the spectral function $\mathfrak{D}(\mathbf{k}, \omega)$ and is, in general, related to the $(n+1)$th-order frequency moments of the spectral function $F_{\mathbf{k}}(\omega)$ [refer Eq. (C6)], i.e.,

$$\mathbf{k}^2\mathfrak{D}_{\mathbf{k}}^{(0)}=F_{\mathbf{k}}^{(1)}; \qquad k^2\mathfrak{D}_{\mathbf{k}}^{(2)}=F_{\mathbf{k}}^{(3)}-[F_{\mathbf{k}}^{(1)}]^2, \tag{10.7}$$

$$F_{\mathbf{k}}^{(2n-1)}=[-M_{\mathbf{k}}^{(1)}(0)]^{-1}\int_{-\infty}^{+\infty}F_{\mathbf{k}}(\omega)\omega^{2n-1}\,d\omega =[-M_{\mathbf{k}}^{(1)}(0)]^{-1}m_{\mathbf{k}}^{(2n)}, \tag{10.8}$$

where $m_{\mathbf{k}}^{(2n)}$ are defined as the large-Z expansion coefficients of the Green's function $M_{\mathbf{k}}^{(1)}(Z)$ [see Eqs. (C1)–(C2)]. The moments $\mathfrak{D}_{\mathbf{k}}^{(0)}$ and $\mathfrak{D}_{\mathbf{k}}^{(2)}$ are now calculated readily from Eqs. (9.6) and (9.7) and in the limit $\beta_c\geq\beta$ and $H=0$ we get, respectively,

$$\mathfrak{D}_{\mathbf{k}}^{(2n)}=0, \qquad n=0, 1, 2, \cdots \tag{10.9a}$$

$$\mathbf{k}^2\mathfrak{D}_{\mathbf{k}}^{(0)}=2[\zeta+\xi_{\mathbf{k}}^{(0)}]\alpha_{\mathbf{k}};$$

$$\mathfrak{D}_{\mathbf{k}}^{(2n)}=0, \qquad n=1, 2, 3\cdots \tag{10.9b}$$

Equations (10.9a) and (10.9b) display the result already anticipated that the modified RPA description of the longitudinal correlation function does not include any relaxation effects and leads to a vanishing spin-diffusion coefficient. For a satisfactory description of these effects, it is presumably necessary to solve for the longitudinal spectral function in the self-consistent second RPA, i.e., solve Eqs. (8.2) without the approximation (8.1).

It should be mentioned that Bennett and Martin[26] have recently given a Green's-function treatment for the paramagnetic region of a Heisenberg many-spin system. On comparing our results with Ref. 26, it is established that while the first moment of the spectral function $F_{\mathbf{k}}(\omega)$—or equivalently the zeroth moment of the function $\mathfrak{D}(\mathbf{k}, \omega)$—is given correctly in the (II) mod RPA, the third moment of $F_{\mathbf{k}}(\omega)$—or the second moment of $\mathfrak{D}(\mathbf{k}, \omega)$—is in error. The reason for the success of the truncated sum-rule procedure[27] of Bennett and Martin in the calculation of the third moment of $F_{\mathbf{k}}(\omega)$—which uses an approximation similar in spirit to our 2nd RPA—seems to be that, as they study only the paramagnetic region, they are able to carry out analytical evaluation of the hydrodynamic behavior—i.e., the limiting behavior for $\mathbf{k}=0$ and $\omega=0$—through the use of the exact relation

$$G_\lambda(\rho)\underset{\beta_c\geq\beta;H=0}{=}2M_\lambda^{(1)}(\rho). \tag{10.10}$$

In conclusion it may be mentioned that Eq. (10.9a) is identical to the result that would have been obtained by invoking the spatial isotropy and assuming that the resultant longitudinal correlation at $\beta_c\geq\beta$ and $H=0$ would be the same as the transverse correlation function found in the 1st RPA. This means that the (I) mod RPA expression for the longitudinal correlation function, in contrast with (II) mod RPA, is for all intents and purposes at the same level of approximation

[25] L. P. Kadanoff and P. C. Martin, Ann. Phys. (N.Y.) **24**, 419 (1963).

[26] H. S. Bennett and P. C. Martin, Phys. Rev. **138**, A608 (1965).

[27] Reference 26, Eqs. (71), (72), and (74).

as the 1st RPA expression for the transverse correlation function.

11. SOLUTION OF 2ND RPA AT LOW TEMPERATURES

While, as has already been noted in Sec. 6, it is true that self-consistent solutions to the 2nd RPA cannot be obtained analytically at general temperatures, the situation at low temperatures is radically different. Here a rapidly convergent iteration scheme can be designed whereby the low-temperature system thermodynamics can be determined, within the self-consistent 2nd RPA scheme, as a power-series expansion in terms of a small dimensionless parameter θ proportional to the ratio of the system temperature and that referring to the transition point.

Before we proceed with this analysis it is helpful to remind ourselves of a few relevant details known from Refs. 12 and 13. The 1st RPA solution for the transverse Green's function G describes the low-temperature system thermodynamics correctly up to and including the second dominant power of θ. Moreover, from the last of the three papers referred to in Ref. 13 we know that in the regime of low temperatures, i.e., $\theta\ll 1$, a valid first step in an iteration procedure is to replace the less dominant terms in the equation of motion of the Green's function G by the approximate 1st RPA results for the relevant terms and thereby to obtain a more accurate expression for the Green's function G which, in turn, can then be used to improve on the 1st RPA results for the less dominant terms on the right-hand side of the equation of motion of G. A second iteration can now be started by inserting these improved results on the right-hand side of the original equation of motion of G and proceeding therefrom to the computation of an even more accurate solution for the Green's function G. In what follows we carry out an explicit solution of the 2nd RPA(I) along these lines.

Representing the 2nd RPA(I), described completely by Eqs. (6.1a) and (7.7), schematically as follows:

$$G \underset{\text{Eq. (6.1a)}}{=} G_{(0)}+\Psi[G, M^{(1)}], \qquad (11.1\text{a})$$

$$M^{(1)} \underset{\text{Eq. (7.7)}}{=} M^{(1)}[G], \qquad (11.1\text{b})$$

where $G_{(0)}$ denotes the 1st RPA solution for the transverse Green's function G and where the function Ψ is the less dominant part of G referred to earlier. Clearly, since the transverse Green's function $M^{(1)}$ is much less than unity in the low-temperature regime, it therefore suffices to use, for the first iteration, the (I) mod RPA expression for $M^{(1)}$, i.e.,

$$M^{(1)}=M^{(1)}[G_{(0)}]=M_{(0)}{}^{(1)}, \qquad (11.2)$$

and as such the 1st iteration is

$$G\simeq G_{(1)}=G_{(0)}+\Psi[G_{(0)}, M_{(0)}{}^{(1)}]. \qquad (11.3)$$

The consistent nth iteration would therefore simply be

$$G\simeq G_{(n)}=G_{(0)}+\Psi[G_{(n-1)}, M_{(n-1)}{}^{(1)}], \qquad (11.4\text{a})$$

where

$$M_{(n-1)}{}^{(1)}=M^{(1)}[G_{(n-1)}]. \qquad (11.4\text{b})$$

The above is a succinct description of the program to be followed for the computation of the self-consistent 2nd RPA. The relevant algebraic details, albeit tedious, are rather straightforward and do not at all warrant recording in their entirety. In our opinion, the following outline is both instructive as well as adequate.

Let us consider the special case of Heisenberg isotropic exchange in lattices of cubic symmetry where the range of interaction is limited to nearest neighbors only. According to the analysis of Appendix E, the parameter η occurring in the expression for $M^{(1)}$ can be expanded in powers of the small parameter θ as follows

$$\eta \underset{\theta\ll 1}{=} 2S-2\bar{n}+4\bar{n}\delta_{S,1/2}+o(\theta^3), \qquad (11.5)$$

where $\bar{n}$ is of order $\theta^{3/2}$. As such, we have

$$M_{\mathbf{k}}{}^{(1)}(\nu)=[1+o(\theta^{3/2})]N^{-1}\sum_{\lambda}{}' [n(E_{\mathbf{k}-\lambda})-n(E_\lambda)] \times[E_{\mathbf{k}-\lambda}-E_\lambda+Z_\nu]^{-1}. \qquad (11.6)$$

Equation (6.1a) for the Green's function G can now be rewritten as follows:

$$G_\lambda(\rho)[Z_\rho-E_\lambda]\simeq 2\sigma+\Delta(\lambda)G_\lambda(\rho) +[2i/(-i\beta N)]\sum_{\lambda_1}{}'\sum_{\rho_1} J(\lambda_1-\lambda, \lambda_1)M_{\lambda_1-\lambda}{}^{(1)}(\rho_1-\rho) \times[(Z_{\rho_1}-E_{\lambda_1})^{-1}+(Z_\rho-E_\lambda)^{-1}]+X(\lambda, \rho), \qquad (11.7\text{a})$$

where

$$\Delta(\lambda)=-2i(-i\beta N)^{-1}\sum_{\lambda_1}{}'\sum_{\rho_1} J(\lambda_1-\lambda, \lambda_1)[Z_{\rho_1}-E_{\lambda_1}]^{-1}, \qquad (11.7\text{b})$$

and where $X(\lambda, \rho)$ is of order $\theta^{3/2}$ of the terms retained on the right-hand side of Eq. (11.7a).

The second term on the right-hand side of (11.7a) causes the poles of the the Green's function G to shift from E_λ to $\tilde{E}_\lambda$, where

$$\tilde{E}_\lambda=E_\lambda+\Delta(\lambda)=\mu H+2SJ(0,\mathbf{k}) \times[1-(\pi\nu_0/S)Z(\tfrac{5}{2})\theta^{5/2}+o(\theta^3)], \qquad (11.8)$$

where $\nu_0=1$, for simple cubic; $=(\frac{3}{4})(2)^{2/3}$ for bcc; $=(2)^{1/3}$, for fcc

$$\theta=[3/4\pi\nu_0 S\beta J(0)];$$

$$Z(n)=\sum_{r=1}^{\infty}(r)^{-n}\exp[-\mu\beta Hr]. \qquad (11.9)$$

Inserting Eq. (11.6) into the right-hand side of Eq.

(11.7a) and carrying the sums over the variables ρ and ρ_1, we find

$$\sigma = S - a_0\theta^{3/2} - a_1\theta^{5/2} - a_2\theta^{7/2} - a_3\theta^4 - o(\theta^{9/2}), \quad (11.10)$$

where a_0, a_1, a_2, and a_3 are the well-known coefficients given by the spin-wave theory. It should be emphasized that while Eq. (11.10) is strictly speaking the result of the first iteration only, i.e., it corresponds to $G_{(1)}$ of Eq. (11.3), it turns out that no further iteration is necessary because the dominant difference between $G_{(2)}$ and $G_{(1)}$ is in the order $X(\lambda, \rho)$, which contributes to the system thermodynamics in the order $\theta^{3/2}$ higher than the terms retained. Moreover, it is important to note that the results of Eq. (11.10) are obtained correctly only up to the second power of the fugacity $\exp(-\mu\beta H)$, thereby emphasizing the correspondence of the 2nd RPA with the second virial expansion developed elsewhere.[13,19]

It will be recalled that the anomalous θ^3 contribution in the 1st RPA expression for the low-temperature magnetization had two origins: Firstly it arises because of the incorrect normalization of the elementary excitation energies, i.e., $E_{\mathbf{k}}$ instead of $\tilde{E}_{\mathbf{k}}$; and secondly for the special case of $S=\frac{1}{2}$ there is an additional contribution of the form θ^3 which results because of the first term on the right-hand side of Eq. (11.7a) being equal to 2σ rather than $2S$. This latter type of θ^3 contribution is in effect cancelled by the second set of terms on the right-hand side of Eq. (11.7a) while the contribution from the $X(\lambda, \rho)$ terms is at least in the order $\theta^{3/2}$ higher. These results are in agreement with those following from the application of spin-wave theory.

Finally let us say a few words about the longitudinal correlation function in the limit of low temperatures. Inserting the approximate expression for $M_\lambda^{(1)}(\rho)$ given in Eq. (11.6) into the relation

$$\langle S_g^z S_l^z \rangle = \sigma^2 - (1/\beta N) \sum_{\mathbf{k}}{}' \sum_{\nu} M_{\mathbf{k}}^{(1)}(\nu) \exp[i\mathbf{k}(g-l)], \quad (11.11)$$

we readily find

$$\langle S_g^z S_l^z \rangle = \sigma^2 + \delta_{g,l}[S-\sigma] + R(g-l), \quad (11.12)$$

where $R(g-l)$ is a function of the vector $(g-l)$ and is at least of the order θ^3. We shall not carry out an explicit evaluation of the function $R(g-l)$ here. It is clear, however, that at low temperatures the expression (11.12) would be satisfactory. Moreover, it evidently preserves the sum rule:

$$\langle S_g^z S_l^z \rangle = \langle [S^z]^2 \rangle, \qquad g=l \quad (11.13)$$

which most unembellished spin-wave theories do not.

12. THERMODYNAMICS—CRITICAL REGION

In this section we analyze the critical properties of the interacting many-spin system in the mod RPA representation and compare the results with those obtained in the 1st RPA and by the high-temperature series expansion techniques of Refs. 8 and 28.

To illustrate the nature of the problem of calculating, from the expressions for the spin-correlation functions obtained in the present paper, the equilibrium thermodynamics for temperatures in the vicinity of, and higher than, the transition temperature we consider first the (I) mod RPA [see Eq. (9.1)]. It has already been noted that while the longitudinal correlation function is determined via the mod RPA, we do not have a prescription for the calculation of the transverse correlation function within the mod RPA scheme. Nevertheless it is recalled that the 1st RPA results for the transverse correlation function were found to be reasonable over the entire range of temperatures. Therefore, as a working arrangement, the system thermodynamics may be studied within the following scheme—to be called the scheme (Ia)—which consists in using the 1st RPA expressions for the transverse correlation function, i.e., Eq. (3.4), and the (I) mod RPA results for the longitudinal correlation function. In order for this scheme to be satisfactory, it is greatly desirable that the level of approximation for the transverse and the longitudinal correlations be the same. While in general it is true that the Green's-function truncation procedures do not automatically insure such an equality of the level of approximation, it turns out, through perhaps a chance coincidence, that the scheme (I*a*) does possess the equality in question for the particular case of isotropic exchange interaction. Moreover, as long as the exchange anisotropy is small, i.e., $I_+ \simeq I_0$, the level of approximation of the longitudinal and the transverse correlations is substantially the same.

To make this discussion precise let us define the transition temperature for a vanishing applied field H. (The case for finite H—which can easily be handled in an alternative fashion within the correlation function scheme—will not be discussed here). As the spin-kinematic requirement $\mathbf{S}(2)\cdot\mathbf{S}(2)=S(S+1)$ holds for all space-time points 2, the following is a rigorous sum rule:

$$\lim_{2=2'} [\langle \mathbf{S}(2)\cdot\mathbf{S}(2')\rangle] = [\tfrac{1}{2}\langle \mathbf{S}^+(2)\cdot\mathbf{S}^-(2)\rangle + \tfrac{1}{2}\langle \mathbf{S}^-(2)\cdot\mathbf{S}^+(2)\rangle + \langle \mathbf{S}^z(2)\cdot\mathbf{S}^z(2)\rangle] = S(S+1), \quad (12.1)$$

and as such should obtain for all temperatures. We remind ourselves here that excluding the immediate neighborhood of the transition point the spontaneous magnetization σ is nonzero throughout the ferromagnetic region and the parameter ζ, being proportional to the inverse of the static parallel susceptibility, is zero (except at the trivial point $\beta=\infty$). The para-

[28] C. Domb and A. R. Miedema, in *Progress in Low Temperature Physics*, edited by C. Gorter (North-Holland Publishing Company, Amsterdam, 1964), Vol. 4, p. 296.

TABLE I. Critical parameters of a simple cubic lattice with nearest-neighbor Heisenberg interaction. Column headings are identified as follows:

(Ia); (IIa) $=\beta_c J_0(0)$, in the (Ia) and the (IIa) schemes.
(Il); (IIl) $=\beta_c J_0(0)$ of the longitudinal correlation in the (I) and (II) mod RPA.
(t) $=\beta_c J_0(0)$ of the 1st RPA transverse correlation.
(RW) $=\beta_c J_0(0)$ due to Rushbrooke and Wood.
(Ib); (IIb) $=-\epsilon_c\beta_c$, in the (I) and (II) mod RPA pictures according to the procedure explained in Sec. 12.
(1st RPA b) $=-\epsilon_c\beta_c$, in the 1st RPA picture with the longitudinal correlation function given by Eq. (3.8).
(TK b) $=-\epsilon_c\beta_c$ found by the interpolation procedure due to Tahir-Kheli, Ref. 13.

Spin	(Ia); (Il); (t)	(IIa)	(IIl)	RW	(Ib)	(IIb)	(1st RPA b)	(TK b)
$\frac{1}{2}$	3.03	3.37	4.25	3.53	0.775	0.737	0.517	0.626
1	1.14	1.19	1.29	1.14	0.775	0.760	0.517	0.651
$\frac{3}{2}$	0.607	0.620	0.650	0.588	0.775	0.766	0.517	0.664
$\frac{5}{2}$	0.260	0.262	0.265	0.242	0.775	0.771	0.517	0.674
$\frac{7}{2}$	0.144	0.145	0.147	0.134	0.775	0.773	0.517	

magnetic region, on the other hand, is characterized by the requirement that in the absence of an applied field H the magnetization σ be zero and ζ be finite except in the neighborhood of the Curie point. Thus, the Curie point is simply characterized by the requirement that for $H=0$, Eq. (12.1) should hold when both ζ and σ are simultaneously zero, i.e.,

$$\lim_{2=2',\sigma=0,\zeta=0}[\langle \mathbf{S}(2)\cdot\mathbf{S}(2')\rangle]=S(S+1), \quad \text{only for } \beta=\beta_c. \tag{12.2}$$

For the isotropic exchange case—i.e., the Heisenberg case—in addition to Eq. (12.2) the following sum rules also obtain:

$$\lim_{2=2';\sigma=0;\zeta=0;I_+=I_0}[\langle S^x(2)\cdot S^x(2')\rangle=\langle S^y(2)\cdot S^y(2')\rangle =\langle S^z(2)\cdot S^z(2')\rangle] =\tfrac{1}{3}[S(S+1)]. \tag{12.3}$$

[Note that for $S=\frac{1}{2}$ the sum rule (12.3) should obtain for arbitrary values of H, σ, ζ, and the exchange interaction. Even for this case, however, the stated limit refers only to the Curie temperature.]

Since for the Heisenberg case the individual sum rules of Eq. (12.3) are obeyed, the scheme (Ia) has complete internal consistency when $I_0=I_+$ and for this particular case the various alternative procedures for the determination of the Curie temperature all lead to a unique result. (Note that while this result for the Curie temperature is necessarily identical to that given by the 1st RPA of Ref. 12, the essential difference here is that we now have achieved a satisfactory description of all the relevant correlation functions.)

The behavior of the nonisotropic case, within the scheme (Ia), is in direct contrast with that of the isotropic exchange case discussed above. Here the longitudinal and the transverse correlation functions are not at the same level of approximation (the difference in the accuracy of the two correlations becoming the more marked the smaller the ratio I_+/I_0) and this situation in effect ensures that different numerical values for the transition temperature are obtained when only one of the two correlation functions is used for its calculation. To illustrate this point further we consider the two correlation functions separately. As the transverse correlation function refers to the 1st RPA, the procedure of Ref. 12 provides a unique way of determing its Curie point, and we get

$$\frac{2S(S+1)}{3}=\beta_c^{-1}(N)^{-1}\sum_{\mathbf{k}}{}'[J_0(0)-J_+(\mathbf{k})]^{-1}. \tag{12.4}$$

For convenience these results will be referred to as (t). The Curie temperature from the longitudinal correla-

TABLE II. Critical parameters of a body-centered cubic (bcc) lattice with nearest-neighbor Heisenberg interaction. Column headings are identified in the caption of Table I.

Spin	(Ia); (Il); (t)	(IIa)	(IIl)	RW	(Ib)	(IIb)	(1st RPA b)	(TK b)
$\frac{1}{2}$	2.79	3.03	3.64	3.08	0.590	0.570	0.393	0.487
1	1.04	1.08	1.15	1.06	0.590	0.582	0.393	0.508
$\frac{3}{2}$	0.557	0.567	0.587	0.544	0.590	0.585	0.393	0.517
$\frac{5}{2}$	0.239	0.241	0.265	0.227	0.590	0.588	0.393	0.525
$\frac{7}{2}$	0.133	0.134	0.135	0.127	0.590	0.589	0.393	

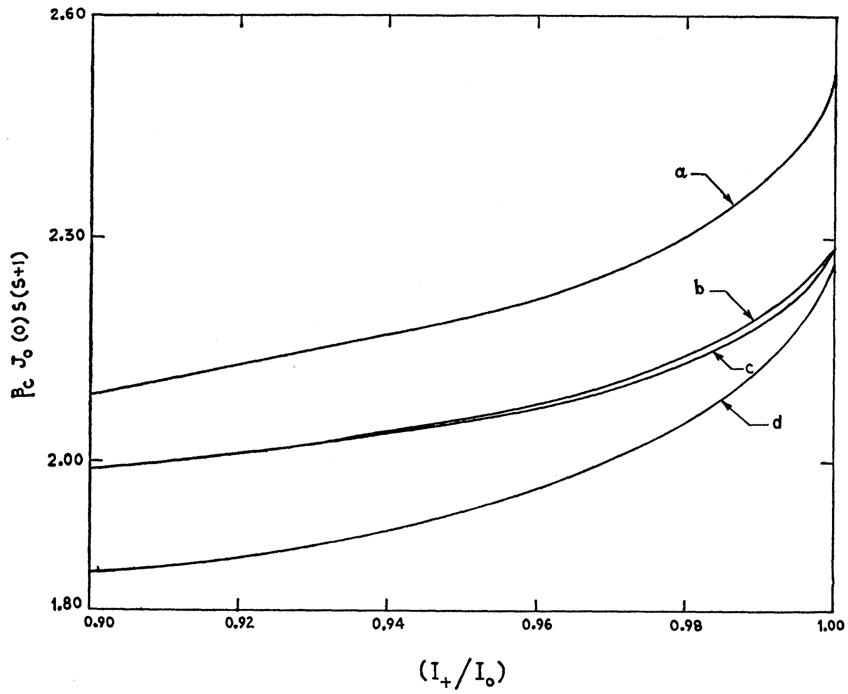

FIG. 1. A plot of $\beta_c J_0(0)S(S+1)$ against the ratio of the transverse and the longitudinal components of the exchange interaction, i.e., I_+/I_0, for a simple cubic lattice with nearest-neighbor exchange. Curve a: (IIa) scheme for spin $\frac{1}{2}$; curve b: (IIa) scheme for spin $\frac{7}{2}$; curve c: (Ia) scheme for all spins; curve d: (t) scheme for all spins.

TABLE III. Critical parameters of a face-centered cubic (fcc) lattice with nearest-neighbor Heisenberg interaction. Column headings are identified in the caption of Table I with the following addition:

(Domb-Sykes b) $= -\epsilon_c\beta_c$, found by Domb and Sykes, Ref. 8.

Spin	(Ia); (II); (t)	(IIa)	(III)	RW	(Ib)	(IIb)	(1st RPA b)	(TK b)	(Domb–Sykes b)
$\frac{1}{2}$	2.69	2.90	3.41	2.89	0.517	0.505	0.345	0.433	0.439
1	1.01	1.04	1.10	1.00	0.517	0.512	0.345	0.450	0.449
$\frac{3}{2}$	0.538	0.546	0.563	0.522	0.517	0.515	0.345	0.458	
$\frac{5}{2}$	0.231	0.233	0.237	0.219	0.517	0.516	0.345	0.465	
$\frac{7}{2}$	0.128	0.129	0.129	0.122	0.517	0.517	0.345		

TABLE IV. Critical parameters of a simple cubic lattice with nearest-neighbor Ising interaction. Column headings are identified in Table I and as follows:

(MF) $=\beta_c J_0(0)$, in the molecular field-approximation.
(MF b) $= -\beta_c\epsilon_c$, in the molecular field-approximation.
(Series); (Series b) = the high-temperature series method results for $\beta_c J_0(0)$ and $-\epsilon_c\beta_c$, respectively.

Spin	(Ia); (IIa)	(II)	(t): (MF)	(Series)	(Ib); (IIb)	(1st RPA b); (MF b)	(Series b)
$\frac{1}{2}$	2.34	3.03	2.00	2.66	0.258	0	0.218
1	0.879	1.14	0.750		0.258	0	
$\frac{3}{2}$	0.469	0.607	0.400		0.258	0	
$\frac{5}{2}$	0.201	0.260	0.171		0.258	0	
$\frac{7}{2}$	0.112	0.144	0.095		0.258	0	

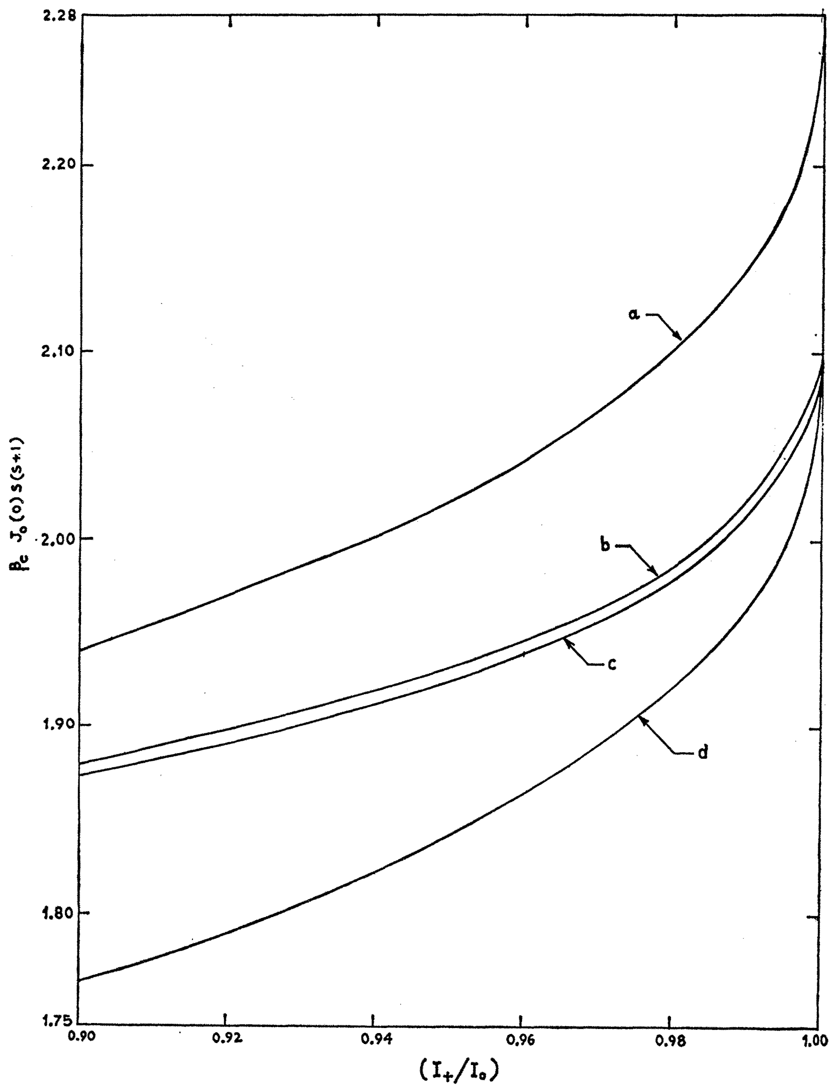

FIG. 2. A plot of $\beta_c J_0(0) S(S+1)$ against the ratio I_+/I_0 for a bcc lattice with nearest-neighbor exchange. Curve a:(IIa) scheme for spin $\frac{1}{2}$; curve b:(IIa) scheme for spin $\frac{7}{2}$; curve c:(Ia) scheme for all spins; curve d:(t) scheme for all spins.

tion function can also be found simply from the following requirement: As the Curie temperature is approached (from either side), the correlation range lengthens and approaches infinity at $\beta=\beta_c$ for $H=0$. We refer to these results as (Il). Finally, for the anisotropic exchange case, the Curie temperature can also be determined in an analogous manner to that of Eq. (12.2). These results will therefore also be referred to as (Ia).

We emphasize here that while strictly speaking the set of results (t) are exclusively the 1st RPA results and the set (Il) pertains only to the (I) mod RPA, in

TABLE V. Critical parameters of a bcc lattice with nearest-neighbor Ising interaction. Column headings are identified in the captions of Tables I and IV.

Spin	(Ia); (IIa)	(Il)	(t); (MF)	(Series)	(Ib); (IIb)	(1st RPA b); (MF b)	(Series b)
$\frac{1}{2}$	2.26	2.79	2.00	2.52	0.197	0	0.169
1	0.848	1.04	0.75		0.197	0	
$\frac{3}{2}$	0.452	0.557	0.400		0.197	0	
$\frac{5}{2}$	0.194	0.239	0.171		0.197	0	
$\frac{7}{2}$	0.108	0.133	0.095		0.197	0	

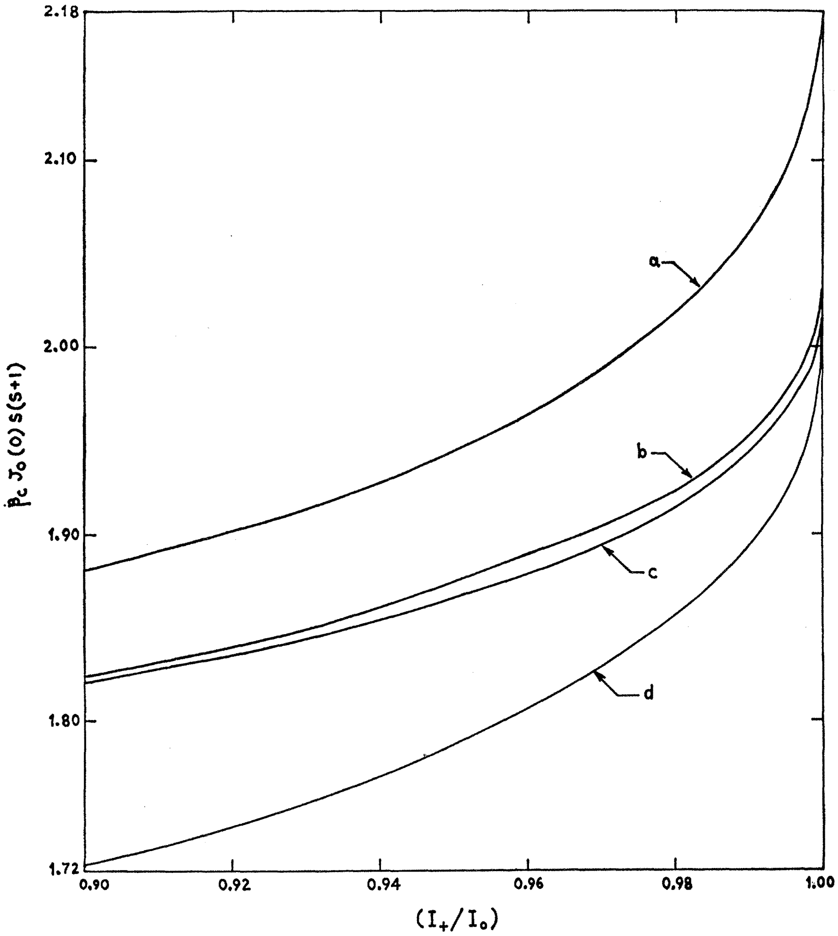

FIG. 3. A plot of $\beta_c J_0(0)\, S(S+1)$ against the ratio I_+/I_0 for a fcc lattice with nearest-neighbor exchange. Curve a: (IIa) scheme for spin $\frac{1}{2}$; curve b: (IIa) scheme for spin $\frac{7}{2}$; curve c: (Ia) scheme for all spins; curve d: (t) scheme for all spins.

the present paper we prefer to regard the set of results (Ia) as being the averaged (I) mod RPA results.

Let us turn next to the discussion of the (II) mod RPA. In this representation even the isotropic case does not lead to a unique result for the Curie temperature for the reason that the level of approximation of the 1st RPA transverse correlation function results is quite different from that of the longitudinal results obtained within the (II) mod RPA. However, in view of the fact that Eq. (12.2) leads to an acceptable compromise, we have again computed the Curie temperature using this relation and we refer to these results as (IIa). The longitudinal correlation is also analyzed in a similar fashion to that explained previously and its Curie temperatures for this case are denoted as (IIl).

Let us consider next the calculation of the exchange

TABLE VI. Critical parameters of a bcc lattice with nearest-neighbor Ising interaction. Column headings are identified in the captions of Tables I and IV.

Spin	(Ia); (IIa)	(Il)	(t); (MF)	(Series)	(Ib); (IIb)	(1st RPA b); (MF b)	(Series b)
$\frac{1}{2}$	2.23	2.69	2.00	2.45	0.72	0	0.159
1	0.836	1.01	0.75	0.881	0.172	0	0.160
$\frac{3}{2}$	0.446	0.538	0.400		0.172	0	
$\frac{5}{2}$	0.191	0.231	0.171		0.172	0	
$\frac{7}{2}$	0.106	0.128	0.095		0.172	0	
					0.172	0	0.175

energy at the Curie point, i.e.,

$$\langle \mathcal{H} \rangle_{H=0;\beta=\beta_c} = -N\epsilon_c. \qquad (12.5)$$

Rather than discuss the contributions to ϵ_c arising from the longitudinal and the transverse correlations separately, we have found it more convenient to analyze the quantity $\beta_c\epsilon_c$—where β_c is close to, but in general not identical with, the corresponding results (Ia) and (IIa)—as follows: Expand the correlation functions in powers of σ and proceed to the limit $H=0$, $\sigma=0$, replacing all β's occurring in the expressions by β_c. We

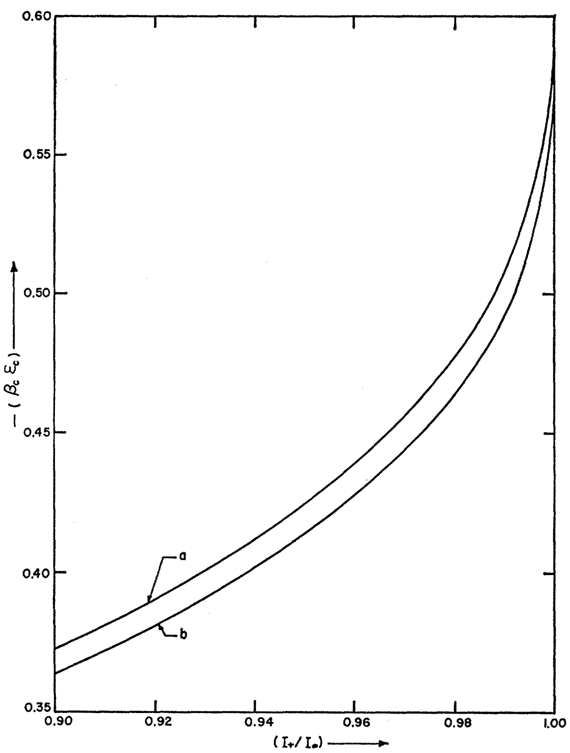

FIG. 4. Plot of the critical energy per spin measured in the units of critical temperature for a simple cubic lattice with nearest-neighbor exchange. Curve a: $-\beta_c\epsilon_c$ in the mod RPA(I) scheme for all spins; curve b: $-\beta_c\epsilon_c$ in the mod RPA(II) scheme for $S=\frac{1}{2}$. (For spins $>\frac{1}{2}$, the relevant curves would lie between a and b and would be practically indistinguishable from curve a for $S\geq\frac{7}{2}$.)

refer to these results as (Ib) and (IIb), respectively, depending on whether the longitudinal correlation is given in the (I) mod RPA or the (II) mod RPA representation.

The foregoing results are tabulated in Tables I–VI for the Heisenberg and the Ising cases and are displayed on graphs in Figs. 1–6 for intermediate values of the exchange couplings.

The high-temperature behavior of the present theory [i.e., mod RPA (I) and (II)] is similar to that of the 1st RPA and the susceptibility agrees with the exact one[29] to the order β^2.

[29] H. A. Brown and J. M. Luttinger, Phys. Rev. **100**, 685 (1955).

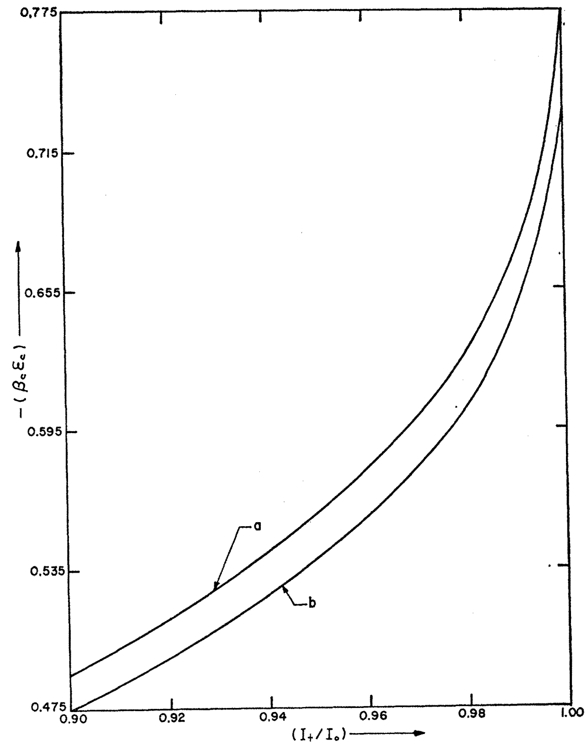

FIG. 5. Plot of $-\beta_c\epsilon_c$ for a bcc lattice with nearest-neighbor exchange. Curve a: $-\beta_c\epsilon_c$ in the mod RPA(I) scheme for all spins; curve b: $-\beta_c\epsilon_c$ in the mod RPA(II) scheme for $S=\frac{1}{2}$. (For spins $>\frac{1}{2}$, the curves would lie between a and b and would practically coincide with curve a for $S\geq 3$.)

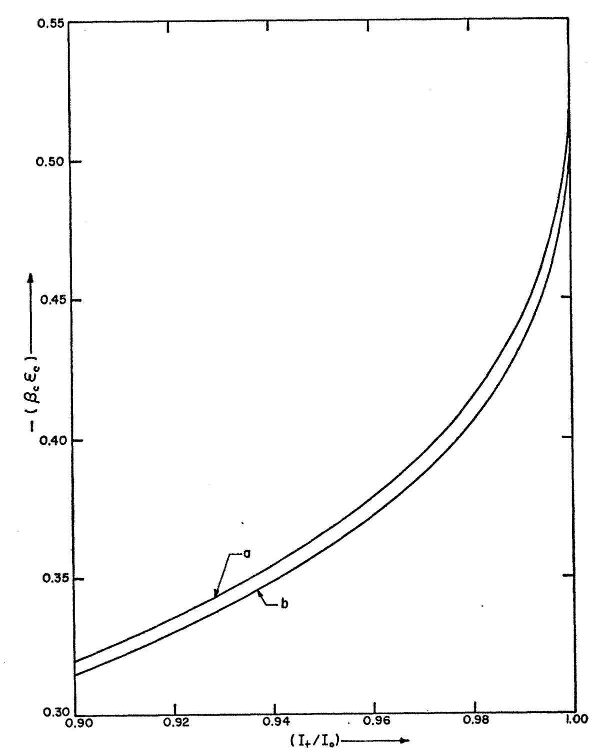

FIG. 6. Plot of $-\beta_c\epsilon_c$ for a fcc lattice with nearest-neighbor exchange. Curve a: $-\beta_c\epsilon_c$ in the mod RPA(I) scheme for all spins; curve b: $-\beta_c\epsilon_c$ in the RPA(II) scheme for $S=\frac{1}{2}$. (For spins $>\frac{1}{2}$, the curves lie between a and b and are indistinguishable from curve a for $S\geq\frac{5}{2}$.)

APPENDIX A

In this Appendix we outline a procedure for analyzing the Green's functions $G(11')$ and $M^{(1)}(1, 1')$ into suitable spectral representations.

Let us assume the following spectral representation:

$$iG(11')=\eta(\tau_1-\tau_{1'})N^{-1}\sum_{\mathbf{k}}{}'\int_{-\infty}^{+\infty}f_{\mathbf{k}}(\omega)[n(\omega)+1]\times\exp[i\mathbf{k}(1-1')-i\omega(\tau_1-\tau_{1'})]\,d\omega+\eta(\tau_{1'}-\tau_1)N^{-1}\sum_{\mathbf{k}}{}'\int_{-\infty}^{+\infty}f_{\mathbf{k}}(\omega)n(\omega)\times\exp[i\mathbf{k}(1-1')-i\omega(\tau_1-\tau_{1'})]\,d\omega, \tag{A1a}$$

$$iM(1,1')=N^{-1}\sum_{\mathbf{k}}{}'\int_{-\infty}^{+\infty}F_{\mathbf{k}}(\omega)\times\exp[i\mathbf{k}(1-1')-i\omega(\tau_1-\tau_1')]\times\{[n(\omega)+1]\eta(\tau_1-\tau_{1'})+n(\omega)\eta(\tau_{1'}-\tau_1)\}\,d\omega=\langle T[\tilde{S}^z(1)\tilde{S}^z(1')]\rangle, \tag{A1b}$$

where $\tilde{S}_{(1)}{}^z$ is defined as in Eq. (5.9) and where

$$n(\omega)=[\exp(\beta\omega)-1]^{-1}. \tag{A2}$$

As long as the spectral functions $f_{\mathbf{k}}(\omega)$, $F_{\mathbf{k}}(\omega)$ are real, satisfy the positivity conditions $\omega f_{\mathbf{k}}(\omega)\geq 0$, $\omega F_{\mathbf{k}}(\omega)\geq 0$, and the integrals of their absolute values, i.e., $\int|f_{\mathbf{k}}(\omega)|\,d\omega$, $\int|F_{\mathbf{k}}(\omega)|\,d\omega$ exist, the representation (A1a) and (A1b) is legitimate.[25] It should be mentioned that Eqs. (A1a) and (A1b) also satisfy the fundamental property of periodicity, with the period $-i\beta$ in the variables τ_1 and $\tau_{1'}$.

Moreover, from the spin-commutation relations

$$[S_1^+(\tau),S_{1'}^-(\tau)]_-=2\delta_{1,1'}S_1^z(\tau);\qquad [S_1^z(\tau),S_{1'}^z(\tau)]_-=0 \tag{A3}$$

it follows that

$$\int_{-\infty}^{+\infty}f_{\mathbf{k}}(\omega)\,d\omega=2\sigma; \tag{A4a}$$

$$\int_{-\infty}^{+\infty}F_{\mathbf{k}}(\omega)\,d\omega=0. \tag{A4b}$$

Note that because of Eqs. (2.10) the representation (A1a) and (A1b) can also be equivalently expressed as follows:

$$G(11')=(-i\beta N)^{-1}\sum_{\mathbf{k}}{}'\sum_{\nu}\exp[i\mathbf{k}(1-1')-iZ_\nu(\tau_1-\tau_1')]\int_{-\infty}^{+\infty}f_{\mathbf{k}}(\omega)[Z_\nu-\omega]^{-1}\,d\omega, \tag{A5a}$$

$$M^{(1)}(1,1')=(-i\beta N)^{-1}\sum_{\mathbf{k}}{}'\sum_{\nu}\exp[i\mathbf{k}(1-1')-iZ_\nu(\tau_1-\tau_{1'})]\int_{-\infty}^{+\infty}F_{\mathbf{k}}(\omega)[Z_\nu-\omega]^{-1}\,d\omega. \tag{A5b}$$

The representation (A1) provides an immediate relationship between the Green's functions for imaginary times and the physically relevant correlation functions. For instance, analytically continuing (A1) to real times we readily get the results

$$\langle S_1^+(t_1)\bar{S}_{1'}(t_{1'})\rangle=N^{-1}\sum_{\mathbf{k}}{}'\int_{-\infty}^{+\infty}f_{\mathbf{k}}(\omega)[n(\omega)+1]\exp[i\mathbf{k}(1-1')-i\omega(t_1-t_{1'})]\,d\omega,$$

$$\langle\bar{S}_1'(t_1')S_1^+(t_1)\rangle=N^{-1}\sum_{\mathbf{k}}{}'\int_{-\infty}^{+\infty}f_{\mathbf{k}}(\omega)n(\omega)\exp[i\mathbf{k}(1-1')-i\omega(t_1-t_{1'})]\,d\omega, \tag{A6}$$

and similarly

$$\langle\tilde{S}_1^z(t_1)\tilde{S}_{1'}{}^z(t_{1'})\rangle=N^{-1}\sum_{\mathbf{k}}{}'\int_{-\infty}^{+\infty}F_{\mathbf{k}}(\omega)[n(\omega)+1]\exp[i\mathbf{k}(1-1')-i\omega(t_1-t_{1'})]\,d\omega, \tag{A7a}$$

$$\langle[\tilde{S}_1^z(t_1),\tilde{S}_{1'}{}^z(t_{1'})]_-\rangle=N^{-1}\sum_{\mathbf{k}}{}'\int_{-\infty}^{+\infty}F_{\mathbf{k}}(\omega)\exp[i\mathbf{k}(1-1')-i\omega(t_1-t_{1'})]\,d\omega, \tag{A7b}$$

$$\langle[\tilde{S}_1^z(t_1),\tilde{S}_{1'}{}^z(t_{1'})]_+\rangle=N^{-1}\sum_{\mathbf{k}}{}'\int_{-\infty}^{+\infty}F_{\mathbf{k}}(\omega)\coth(\beta\omega/2)\exp[i\mathbf{k}(1-1')-i\omega(t_1-t_{1'})]\,d\omega. \tag{A7c}$$

Note that the expressions (A7b) and (A7c) express the well-known fluctuation-dissipation theorem, which relates the system fluctuations (characterized by the statistical average of an anticommutator of the dynamical operators) with the dissipation characterized by the imaginary part $F_{\mathbf{k}}(\omega)$ of the frequency wave-dependent susceptibility.

There now remains to establish a similar direct relationship between the Green's functions and the spectral functions. This is provided by the representation (A5). To this end, let us study the following functions:

$$G_k(Z)=\int_{-\infty}^{+\infty} f_k(\omega)[Z-\omega]^{-1}\,d\omega, \tag{A8a}$$

$$M_k^{(1)}(Z)=\int_{-\infty}^{+\infty} F_k(\omega)[Z-\omega]^{-1}\,d\omega, \tag{A8b}$$

where Z is an arbitrary, complex variable. We note that firstly

$$G_k(Z)\,|_{Z=Z_\nu}=G_k(Z_\nu),$$
$$M_k^{(1)}(Z)\,|_{Z=Z_\nu}=M_k^{(1)}(Z_\nu). \tag{A9}$$

Secondly, $G_k(Z)$, $M_k^{(1)}(Z)$ are analytic functions of the variable Z when Z does not lie on the real axis and thirdly that both $G_k(Z)$ and $M_k^{(1)}(Z)$ approach zero in the limit that $|Z|\to\infty$. It can be shown that under these conditions, the extension of the Fourier transforms $G_k(Z_\nu)$ from a set of discrete points at the imaginary axis to the whole of the complex Z plane as $G_k(Z)$ and $M_k^{(1)}(Z)$, is unique.[30]

Equations (A8a) and (A8b) now readily lead to the desired relationships:

$$f_k(\omega)=\lim_{\Delta\to+0}(2\pi i)^{-1}[G_k(\omega-i\Delta)-G_k(\omega+i\Delta)], \tag{A10a}$$

$$F_k(\omega)=\lim_{\Delta\to+0}(2\pi i)^{-1}[M_k^{(1)}(\omega-i\Delta)-M_k^{(1)}(\omega+i\Delta)]. \tag{A10b}$$

APPENDIX B

In this Appendix we shall study the 2nd RPA (II) expressions for the longitudinal Green's function. Let us first use the dynamic sum rule of Eq. (5.9). We get

$$M_k^{(1)}(\nu)Z_\nu=\lim_{\epsilon=-i\beta\Delta,\Delta=+0}\left(\frac{-1}{\beta N}\right)\sum_\lambda{}'\sum_\rho[J_+(\lambda)\exp(\pm iZ_\rho\epsilon)-J_+(\mathbf{k}-\lambda)\exp(\pm iZ_\rho\epsilon)][Z_\nu+E_{k-\lambda}-E_\lambda]^{-1}$$
$$\times\{2M_k^{(1)}(\nu)[G_{\lambda-k}(\rho-\nu)J_{0+}(\mathbf{k},\mathbf{k}-\lambda)-G_\lambda(\rho)J_{0+}(\mathbf{k},\lambda)]+G_\lambda(\rho)-G_{\lambda-k}(\rho-\nu)\}. \tag{B1}$$

In the right-hand side of Eq. (B1) all the four possible combinations of the signs of the exponents should lead to the same result for $M_k^{(1)}(\nu)$. We find, however, that this is not so, the results being the following:

$$[M_k^{(1)}(\nu)]^{\text{2nd RPA (II)}}_{\text{dynamical sum rule}}=A_k(\nu)/B_k^{(j)}(\nu), \tag{B2}$$

where

$$A_k(\nu)=(1/N)\sum_\lambda{}'J_{++}(\lambda,\mathbf{k}-\lambda)[Z_\nu+E_{k-\lambda}-E_\lambda]^{-1}\int_{-\infty}^{+\infty}n(\omega)[f_\lambda(\omega)-f_{k-\lambda}(\omega)]\,d\omega, \tag{B3}$$

$$\underset{(j=1,2)}{B_k^{(j)}(\nu)}=Z_\nu+(2/N)\sum_\lambda{}'J_{++}(\lambda,\mathbf{k}-\lambda)[Z_\nu+E_{k-\lambda}-E_\lambda]^{-1}$$
$$\times\int[n(\omega)+j-1][f_\lambda(\omega)J_{0+}(\mathbf{k},\lambda)-f_{k-\lambda}(\omega)J_{0+}(\mathbf{k},\mathbf{k}-\lambda)]\,d\omega, \tag{B4a}$$

$$\underset{(j=3,4)}{B_k^{(j)}(\nu)}=Z_\nu+(2/N)\sum_\lambda{}'J_{++}(\lambda,\mathbf{k}-\lambda)[Z_\nu+E_{k-\lambda}-E_\lambda]^{-1}$$
$$\times\int_{-\infty}^{+\infty}n(\omega)[f_\lambda(\omega)J_{0+}(\mathbf{k},\lambda)-f_{k-\lambda}(\omega)J_{0+}(\mathbf{k},\mathbf{k}-\lambda)]\,d\omega+C(j),$$

$$C(j)=(2\sigma/N)\sum_\lambda{}'J_+(\lambda)[Z_\nu+E_{k-\lambda}-E_\lambda]^{-1}J_{++}(\mathbf{k}-\lambda,\lambda),\qquad j=3$$
$$=(2\sigma/N)\sum_\lambda{}'J_+(\mathbf{k}-\lambda)[Z_\nu+E_{k-\lambda}-E_\lambda]^{-1}J_{++}(\lambda,\mathbf{k}-\lambda),\qquad j=4. \tag{B4b}$$

The above expressions are all different unless $\nu=0$.

While it is clear that due to these internal inconsistencies the 2nd RPA (II) dynamic-sum-rule results are suspect, it should nevertheless be mentioned that one of these four expressions given in Eqs. (B2)–(B4), i.e.

$$M_k^{(1)}(\nu)=A_k(\nu)[B_k^{(1)}(\nu)]^{-1}, \tag{B5}$$

leads to a surprisingly good result for the longitudinal correlation function in the mod RPA representation. We shall therefore treat this expression as though it were obtained phenomenologically and use it for the study of the longitudinal correlation function whenever necessary.

[30] G. Baym and N. D. Mermin, J. Math. Phys. 2, 232 (1961).

Finally, let us study the consequences of imposing the kinematic sum rule of Eq. (5.4) on the 2nd RPA (II). For simplicity let us consider $S=\frac{1}{2}$; the results are expected to be similar for general spin [see Eq. (E15)]:

$$[M_{\mathbf{k}}^{(1)}(\nu)]^{\text{2nd RPA (II)}}_{\text{kinematical sum rule}} \underset{S=1/2}{=} \lim_{\epsilon=-i\beta\Delta,\Delta=+0} (\pm i)(-i\beta N)^{-1} \sum_{\lambda}{}' \sum_{\rho \geq} G^{(1)}{}_{\mathbf{k}-\lambda,\lambda}(\nu-\rho,\rho) \exp(\pm iZ_\rho\epsilon). \quad \text{(B6)}$$

Let us first do the ρ sums on the right-hand side of Eq. (B6). Taking into account the upper signs first we get

$$M_{\mathbf{k}}^{(1)}(\nu) = e_{\mathbf{k}}(\nu)[h_{\mathbf{k}}^{(+)}(\nu)]^{-1}, \quad \text{(B7a)}$$

where

$$e_{\mathbf{k}}(\nu) = \left(\frac{1}{N}\right) \sum_{\lambda}{}' \int_{-\infty}^{+\infty} n(\omega)[f_\lambda(\omega) - f_{\mathbf{k}-\lambda}(\omega)][Z_\nu + E_\lambda - E_{\mathbf{k}-\lambda}]^{-1} d\omega, \quad \text{(B7b)}$$

$$h_{\mathbf{k}}^{(+)}(\nu) = 1 + \left(\frac{2}{N}\right) \sum_{\lambda}{}' \int_{-\infty}^{+\infty} n(\omega)[Z_\nu + E_\lambda - E_{\mathbf{k}-\lambda}]^{-1}[f_\lambda(\omega) J_{0+}(\mathbf{k}, \boldsymbol{\lambda}) - f_{\mathbf{k}-\lambda}(\omega) J_{0+}(\mathbf{k}, \mathbf{k}-\boldsymbol{\lambda})] d\omega. \quad \text{(B7c)}$$

Analogously, treating the lower signs, the result is

$$M_{\mathbf{k}}^{(1)}(\nu) = e_{\mathbf{k}}(\nu)[h_{\mathbf{k}}^{(-)}(\nu)]^{-1}, \quad \text{(B8a)}$$

where

$$h_{\mathbf{k}}^{(-)} = h_{\mathbf{k}}^{(+)} - 2Z_\nu(1/N) \sum_{\lambda}{}' [Z_\nu + E_\lambda - E_{\mathbf{k}-\lambda}]^{-1}. \quad \text{(B8b)}$$

So, once again we find that except for the trivial case of $\nu=0$, the results following from the 2nd RPA (II) are internally inconsistent. [We recall that no such obvious difficulty arose with the 2nd RPA (I).]

APPENDIX C

In this Appendix we establish some general relationships between the high-frequency moments of the longitudinal spectral function and the large-Z expansion coefficients of the Green's function $M_{\mathbf{k}}^{(1)}(Z)$. These relations are exploited in the study of the longitudinal correlation function in general, and of the critical fluctuations and the spin diffusion in particular (refer to Secs. 9 and 10). Expanding both sides of Eq. (A8b) in inverse powers of Z we get

$$M_{\mathbf{k}}^{(1)}(Z) \underset{|z|\gg 1}{=} \sum_{p=0}^{\infty} \mathbf{m}_{\mathbf{k}}^{(p)}(Z)^{-p}$$

$$= \sum_{n=1}^{\infty} \left[\int_{-\infty}^{+\infty} F_{\mathbf{k}}(\omega)\omega^{2n-1} d\omega\right](Z)^{-2n}. \quad \text{(C1)}$$

Comparing coefficients, it follows that

$$\mathbf{m}_{\mathbf{k}}^{(0)} = 0; \qquad \mathbf{m}_{\mathbf{k}}^{(2n-1)} = 0, \qquad n = 1, 2, 3, \cdots,$$

$$\mathbf{m}_{\mathbf{k}}^{(2n)} = \int_{-\infty}^{+\infty} F_{\mathbf{k}}(\omega)\omega^{2n-1} d\omega. \quad \text{(C2)}$$

The above relations are exact whenever the high-frequency moments of the spectral function exist.

The Green's function $M_{\mathbf{k}}^{(1)}(Z)$, being even and analytic in the variable Z off the real axis, admits the following spectral representation[25,26]:

$$1 - M_{\mathbf{k}}^{(1)}(Z)[M_{\mathbf{k}}^{(1)}(0)]^{-1}$$

$$= \left[1 - \frac{\mathbf{k}^2}{\pi} \int_{-\infty}^{+\infty} \mathfrak{D}_{\mathbf{k}}(\omega)[Z^2 - \omega^2]^{-1} d\omega\right]^{-1}, \quad \text{(C3)}$$

where the spectral function $\mathfrak{D}_{\mathbf{k}}(\omega)$ is a generalized frequency wave-dependent diffusion constant. In the hydrodynamic limit, $\mathfrak{D}_{\mathbf{k}}(\omega)$ reduces to the diffusion constant D, i.e.,

$$\mathfrak{D}_{\mathbf{k}}(\omega) \underset{\lim \mathbf{k}\to 0;\omega\to 0}{=} D. \quad \text{(C4)}$$

Expanding both sides of Eq. (C3) in inverse powers of Z and comparing coefficients, we establish the following relations between the moments of the spectral functions $F_{\mathbf{k}}(\omega)$ and $\mathfrak{D}_{\mathbf{k}}(\omega)$:

$$\mathbf{k}^2\mathfrak{D}_{\mathbf{k}}^{(0)} = F_{\mathbf{k}}^{(1)}; \ \mathbf{k}^4\mathfrak{D}_{\mathbf{k}}^{(2)} + \mathbf{k}^4[\mathfrak{D}_{\mathbf{k}}^{(0)}]^2 = F_{\mathbf{k}}^{(3)},$$

$$\mathbf{k}^2\mathfrak{D}_{\mathbf{k}}^{(4)} + 2\mathbf{k}^4\mathfrak{D}_{\mathbf{k}}^{(0)}\mathfrak{D}_{\mathbf{k}}^{(2)} + \mathbf{k}^6[\mathfrak{D}_{\mathbf{k}}^{(0)}]^3 = F_{\mathbf{k}}^{(5)}; \cdots, \quad \text{(C5)}$$

where

$$\mathfrak{D}_{\mathbf{k}}^{(n)} = (\pi)^{-1} \int_{-\infty}^{+\infty} \mathfrak{D}_{\mathbf{k}}(\omega)\omega^n d\omega,$$

$$F_{\mathbf{k}}^{(n)} = [-M_{\mathbf{k}}^{(1)}(0)]^{-1} \int_{-\infty}^{+\infty} F_{\mathbf{k}}(\omega)\omega^n d\omega. \quad \text{(C6)}$$

Finally, let us analyze the equal-time longitudinal correlation function $\langle \tilde{S}_1^z(t)\tilde{S}_2^z(t)\rangle$. Fourier transforming with respect to the inverse lattice, i.e.,

$$\tilde{F}_{\mathbf{k}} = \sum_{(1-2)} \langle \tilde{S}_1^z(t)\tilde{S}_2^z(t)\rangle \exp[-i\mathbf{k}\cdot(1-2)], \quad \text{(C7)}$$

and using the relation (A9b), we get

$$\tilde{F}_{\mathbf{k}} = \beta^{-1} \int_{-\infty}^{+\infty} \frac{d\omega}{\omega} F_{\mathbf{k}}(\omega)$$

$$\times [1 + \sum_{n=1}^{\infty} (-1)^{n-1} B_{2n-1}(\beta\omega)^{2n}/(2n)!], \quad \text{(C8)}$$

where B_{2n-1} are the Bernoulli numbers $B_1=\frac{1}{6}$, $B_3=\frac{1}{30}$, $B_5=\frac{1}{42}$, etc. While the first term on the right-hand side of Eq. (C8) is proportional to the wave-dependent susceptibility and is easily expressed in terms of $M_{\mathbf{k}}^{(1)}(0)$ via the relation

$$-M_{\mathbf{k}}^{(1)}(0) = \int_{-\infty}^{+\infty} \frac{F_{\mathbf{k}}(\omega)}{\omega} d\omega \quad \text{(C9)}$$

[refer to Eq. (A5b)], the remaining terms are expressible in terms of the large-Z expansion coefficients of the Green's function $M_{\mathbf{k}}^{(1)}(Z)$ [see Eq. (C2) above].

Therefore

$$\tilde{F}_k = -\beta^{-1}M_k^{(1)}(0) + \sum_{n=1}^{\infty} (-1)^{n-1}B_{2n-1}(\beta)^{2n-1}\mathbf{m}_k^{(2n)}/(2n)!. \quad \text{(C10)}$$

APPENDIX D

It was stated in Sec. 9 that the dynamic sum-rule solution of the 2nd RPA (I), as evidenced from its result for the longitudinal correlation function in the mod RPA, is unsatisfactory. The reason for this is the following. A rigorous physical requirement is that when the system is spatially isotropic, i.e., $I_0 = I_+$; $H=0$, and is in a phase other than the condensed one (i.e., paramagnetic rather than ferromagnetic) the spin correlations should display spatial isotropy. The behavior of the Fourier transform of the equal-time (transverse) spin correlation is known in the paramagnetic region to be of the form[31]

$$\tilde{f}_k = \sum_{(1-2)} \langle S_1^+(t) S_2^-(t) \rangle \exp[i\mathbf{k}(1-2)] \underset{k\ll 1}{=} \text{const}[\mathbf{k}^2 + e^2]^{-1}, \quad \text{(D1a)}$$

where

$$\tilde{f}_k \underset{\lim \beta_c \geq \beta; H=0; I_0=I_+}{=} \tilde{F}_k, \quad \text{(D1b)}$$

and where e^2 is inversely proportional to the susceptibility and is as such $\ll 1$ when $|\beta_c - \beta| \ll \beta_c$ and is $\gg 1$ when $\beta \ll \beta_c$.

In the mod RPA, the 2nd RPA (I) can be equivalently written as

$$[M_k^{(1)}(Z)]^{\text{(I) mod}}_{\text{dynamic sum rule}} = A_k(Z)[B_k(Z)]^{-1}, \quad \text{(D2)}$$

where

$$A_k(Z) = (2\sigma/N) \sum_{\lambda} J(\mathbf{k}-\lambda, \lambda)[n(E_{k-\lambda}) - n(E_\lambda)] \times [E_{k-\lambda} - E_\lambda + Z]^{-1}, \quad \text{(D3)}$$

$$B_k(Z) = Z + (2\sigma/N) \sum_{\lambda}{}' J(\mathbf{k}-\lambda, \lambda) \times [J(\mathbf{k}, \lambda) + J(\mathbf{k}, \mathbf{k}-\lambda)] \times [n(E_{k-\lambda}) - n(E_\lambda)][E_{k-\lambda} - E_\lambda + Z]^{-1}. \quad \text{(D4)}$$

In the paramagnetic region when the applied field H is vanishingly small, the magnetization σ is much less than the saturation value S, and therefore

$$M_k^{(1)}(0) = \{-2[\zeta + J(0, \mathbf{k})] + \gamma(\mathbf{k})\}^{-1} + 0(\sigma), \quad \text{(D5a)}$$

where

$$\gamma(\mathbf{k}) = \{(2/N) \sum_{\lambda}{}' [\zeta + J(0, \lambda)]^{-1}\} \times \{N^{-1} \sum_{\lambda}{}' [\zeta + J(0, \lambda)]^{-1}[\zeta + J(0, \mathbf{k}-\lambda)]^{-1}\}^{-1}. \quad \text{(D5b)}$$

Similarly,

$$M_k^{(1)}(Z) \underset{Z\neq 0}{=} X(\mathbf{k})[Z^2 - Y(\mathbf{k})]^{-1}, \quad \text{(D6a)}$$

$$X(\mathbf{k}) = (2/\beta N) \sum_{\lambda}{}' [J(0, \mathbf{k}-\lambda) - J(0, \lambda)] \times [\zeta + J(0, \lambda)]^{-1}, \quad \text{(D6b)}$$

$$Y(\mathbf{k}) = 2[\zeta + J(0, \mathbf{k})]X(\mathbf{k}) - (2/\beta N) \sum_{\lambda}{}' [J(0, \mathbf{k}-\lambda) - J(0, \lambda)]^2 \times [\zeta + J(0, \lambda)]^{-1}. \quad \text{(D6c)}$$

For simplicity let us assume the lattice to be simple cubic and the range of $I(12)$ to be restricted to the nearest neighbors only. Then,

$$X(\mathbf{k}) = c(\beta)J(0, \mathbf{k});$$
$$Y(\mathbf{k}) = 2[\zeta + J(0, \mathbf{k})]c(\beta)J(0, \mathbf{k}) - d(\beta)[J(0, \mathbf{k})]^2, \quad \text{(D7a)}$$

where

$$c(\beta) = (2/\beta N)(1/J(0)) \sum_{\lambda}{}' J(\lambda)[\zeta + J(0, \lambda)]^{-1}, \quad \text{(D7b)}$$

$$d(\beta) = (2/\beta N)[1/J(0)]^2 \sum_{\lambda}{}' J^2(\lambda)[\zeta + J(0, \lambda)]^{-1}, \quad \text{(D7c)}$$

$C(\beta)$ and $d(\beta)$ depend only on β, I, and the crystal structure.[32]

Let us now look at the limiting behavior of the functions $\gamma(\mathbf{k})$, $X(\mathbf{k})$, and $Y(\mathbf{k})$ when $\mathbf{k} \ll 1$. For the study of the function $\gamma(\mathbf{k})$ we only need the sum in the denominator of Eq. (D5b). For small $\mathbf{k}$,

$$(1/N) \sum_{\lambda}{}' [\zeta + J(0, \lambda)]^{-1}[\zeta + J(0, \mathbf{k}-\lambda)]^{-1} \underset{k\ll 1}{\approx} (1/N) \sum_{\lambda}{}' [\zeta + I\lambda^2 + o(\lambda)^4]^{-1} \times [\zeta + I(\mathbf{k}^2 + \lambda^2 - 2\mathbf{k}\lambda\cos\theta) + o(\mathbf{k}-\lambda)^4]^{-1}. \quad \text{(D8)}$$

For a system of macroscopic dimensions, the sum over λ is well approximated by an integral, e.g.,

$$N^{-1} \sum_{\lambda}{}' (\cdots) \to (2\pi)^{-3} \int \int_{-\pi}^{+\pi} \int d\lambda_x\, d\lambda_y\, d\lambda_z (\cdots), \quad \text{(D9)}$$

and since for sufficiently small ζ—which is the case in the neighborhood of the critical point—the major contribution to the integral comes from small values of λ, we can extend the range of integration to the whole of the λ space, and Eq. (D8) becomes

$$\approx (2\pi)^{-3}(2I^2\mathbf{k})^{-1} \int_0^\infty \lambda\, d\lambda [(\zeta/I) + \lambda^2]^{-1} \times \{\ln[(\zeta/I) + (\mathbf{k}+\lambda)^2 - \ln[(\zeta/I) + (\mathbf{k}-\lambda)^2]\}. \quad \text{(D10)}$$

In the limit that $\zeta/I \ll 1$, Eqs. (D5b) and (D10)

[31] See Refs. 23 and 24.

[32] Inverse lattice sums of the form (D7) etc. can be easily obtained from the well-known extended Watson sums which have been extensively tabulated for crystals of cubic symmetry with nearest-neighbor interactions; see, e.g., I. Mannari and C. Kawabata, Okayama University, Department of Physics Research Note No. 15, 1964 (unpublished).

readily lead to the result

$$\gamma(\mathbf{k})\cong\gamma_0\mathbf{k}+o(\mathbf{k}^2), \quad \text{(D11)}$$

where γ_0 is a constant depending on β and I. Similarly,

$$X(\mathbf{k}) \underset{\mathbf{k}\langle\langle 1}{=} x_0\mathbf{k}^2+o(\mathbf{k}^4),$$

$$Y(\mathbf{k}) \underset{\mathbf{k}\langle\langle 1}{=} y_0\mathbf{k}^2+o(\mathbf{k}^4).$$

Thus

$$\tilde{F}_{\mathbf{k}} \underset{\mathbf{k}\langle\langle 1}{\approx} [2\beta(\zeta+J(0,\mathbf{k}))-\beta\gamma_0\mathbf{k}+o(\mathbf{k}^2)]^{-1}+o(\mathbf{k}^2). \quad \text{(D12)}$$

The above result differs markedly from the generally accepted one given by Eq. (D1). As such the expression (D2) for the Green's function $M_{\mathbf{k}}^{(1)}(Z)$ is to be considered unsatisfactory.

APPENDIX E

In this Appendix we extend the kinematic sum-rule treatment to general spin (see Secs. 7 and 8). To this end, let us define a generalized transverse Green's function of the form

$$g[11']=-i\langle\langle S^+(1)\,\exp[xS^z(1')]S^-(1')\rangle\rangle, \quad \text{(E1)}$$

where x is an arbitrary variable. Within the 1st RPA, $g[11']$ satisfies the following approximate equations of motion:

$$[i(d/d\tau_1)-\mu H+u(1)]g[11'] \underset{\text{1st RPA}}{\approx} 2\delta(1-1')\Theta(1)+2\sum_2[I_0(12)\langle\langle S^z(2)\rangle\rangle g[11'] -I_+(12)\langle\langle S^z(1)\rangle\rangle g[21']]_{\tau_2=\tau}, \quad \text{(E2a)}$$

$$[i(d/d\tau_{1'})+\mu H-u(1')]g[11'] =-2\delta(1-1')\Theta(1')-2\sum_{2'}[I_0(1'2')\langle\langle S^z(2')\rangle\rangle g[11'] -I_+(1'2')\langle\langle S^z(1')\rangle\rangle g[12']]_{\tau_{2'}=\tau_{1'}}, \quad \text{(E2b)}$$

where

$$\Theta(1)=\langle\langle[S^+(1),\exp[xS^z(1)]S^-(1)]_-\rangle\rangle. \quad \text{(E3)}$$

Note that the given form of Eq. (E2b) is the result of an implicit 1st RPA assumption, without which the symmetry of Eqs. (E2a) and (E2b) would not be maintained.

Functionally differentiating both the Eqs. (E2a) and (E2b) with respect to $u(3)$, Fourier-transforming in a manner analogous to Eqs. (2.10) and performing an addition similar to that done in 2nd RPA (I), we get

$$g^{(1)}{}_{\lambda_1,\lambda_2}(\rho_1,\rho_2)=[Z_{\rho_1}-E_{\lambda_1}]^{-1}\{\Theta_{\lambda_1+\lambda_2}(\rho_1+\rho_2)-g_{-\lambda_2}(-\rho_2) \times[1-2M^{(1)}{}_{\lambda_1+\lambda_2}(\rho_1+\rho_2)J_{0+}(\lambda_1+\lambda_2,\lambda_2)]\} +[Z_{\rho_2}+E_{\lambda_2}]^{-1} \times\{g_{\lambda_1}(\rho_1)[1-2M^{(1)}{}_{\lambda_1+\lambda_2}(\rho_1+\rho_2)J_{0+}(\lambda_1+\lambda_2,\lambda_1)] -\Theta_{\lambda_1+\lambda_2}(\rho_1+\rho_2)\}, \quad \text{(E4)}$$

where $g_\lambda(\rho)$ and $g^{(1)}{}_{\lambda,\mathbf{k}}(\rho,\nu)$ are the Fourier transforms, respectively, of the Green's functions $g[11']$ and $\delta g/\delta u$ in the limit that $u=0$, and where

$$[\partial\Theta(1)/\partial u(3)]_{u=0}=(-i\beta N)^{-1}\sum_\lambda{}'\sum_\rho\Theta_\lambda(\rho) \times\exp[i\lambda(1-3)-iZ_\rho(\tau_1-\tau_3)]. \quad \text{(E5)}$$

As before, let us use the mod RPA, obtained by approximating $g_\lambda(\rho)$ by the 1st RPA result following from Eqs. (E2a) and (E2b) introducing it into the right-hand side of Eq. (E4).

The kinematic sum rule is

$$\lim_{u=0;1=1';\tau_1=\tau_{1'}\pm\epsilon;\epsilon=(-i\beta)0}\left[\frac{\delta g[11']}{\delta u(3)}\right]=-i\left[\frac{\delta\Psi^{(\pm)}(1)}{\delta u(3)}\right], \quad \text{(E6a)}$$

where

$$\psi^{(+)}{}_{(1)}=\langle\langle\exp[xS^z{}_{(1)}]S^-{}_{(1)}S^+{}_{(1)}\rangle\rangle;$$

$$\psi^{(-)}{}_{(1)}=\langle\langle S^+{}_{(1)}\exp[xS^z{}_{(1)}]S^-{}_{(1)}\rangle\rangle. \quad \text{(E6b)}$$

Fourier transforming both sides of Eq. (E6a), we get

$$\lim_{\epsilon\to(-i\beta)0}(1/-i\beta N)\sum_\lambda{}'\sum_\rho g^{(1)}{}_{\mathbf{k}-\lambda,\lambda}(\nu-\rho,\rho) \times\exp(\pm iZ_\rho\epsilon)=-i\psi_{\mathbf{k}}{}^{(\pm)}(\nu), \quad \text{(E7)}$$

where the Fourier transforms $\psi_{\mathbf{k}}{}^{(\pm)}(\nu)$ are taken analogously to Eq. (E5).

Inserting the mod RPA result for $g^{(1)}{}_{\lambda_1,\lambda_2}(\rho_1,\rho_2)$ following from Eq. (E4) into Eq. (E7), we are led to the following differential equation in the variable x:

$$\left[\left(\frac{d^2}{dx^2}\right)+\frac{(1+\bar{n})\exp(x)+\bar{n}}{(1+\bar{n})\exp(x)-\bar{n}}\left(\frac{d}{dx}\right)-S(S+1)\right]M(x;\mathbf{k};\nu) =[A-M_{\mathbf{k}}{}^{(1)}(\nu)B]\Theta[1-\bar{n}(\exp(-x)-1)]^{-1}, \quad \text{(E8)}$$

where $\bar{n}$ and $M_{\mathbf{k}}{}^{(1)}(\nu)$ are defined as in the text and where

$$\Theta=[\Theta(1)]_{u=0};$$

$$A=(2/N)\sum_\lambda{}'[n(E_{\mathbf{k}-\lambda})-n(E_\lambda)][E_{\mathbf{k}-\lambda}-E_\lambda+Z_\nu]^{-1},$$

$$B=(1/N)\sum_\lambda{}'[n(E_{\mathbf{k}-\lambda})-n(E_\lambda)]\cdot[E_{\mathbf{k}-\lambda}-E_\lambda+Z_\nu]^{-1} \times[J_{0+}(\mathbf{k},\lambda)+J_{0+}(\mathbf{k},\mathbf{k}-\lambda)], \quad \text{(E9)}$$

$$\left[\frac{\partial\langle\langle\exp[xS^z{}_{(1)}]\rangle\rangle}{\partial u(3)}\right]_{u=0}=(-i\beta N)^{-1}\sum_\lambda{}'\sum_\rho M(x;\mathbf{k};\rho) \times\exp[i\lambda(1-3)-iZ_\rho(\tau_1-\tau_3)]. \quad \text{(E10)}$$

The required solution to the differential equation (E8) satisfying the kinematic boundary conditions

$$M(x;\mathbf{k};\nu)\,|_{x=0}=0, \quad \text{(E11a)}$$

$$\left[\prod_{p=-S}^{+S}[(d/dx)-p]M(x;\mathbf{k};\nu)\right]_{x=0}=0 \quad \text{(E11b)}$$

is found to be

$$M(x;\mathbf{k};\nu)=[A-BM_{\mathbf{k}}{}^{(1)}(\nu)][\bar{n}(1+\bar{n})]^{-1} \times\left[\frac{d\Omega(x)}{dx}-\sigma\Omega(x)\right], \quad \text{(E12a)}$$

where

$$\Omega(x)=[(\bar{n})^{2S+1}\exp(-Sx)-(1+\bar{n})^{2S+1}\times\exp[(S+1)x]]\cdot[(\bar{n})^{2S+1}-(1+\bar{n})^{2S+1}]^{-1}\times[(1+\bar{n})\exp(x)-\bar{n}]^{-1}. \quad \text{(E12b)}$$

[Note that $\Omega(x)$ is the solution of the homogeneous differential equation on the left-hand side of Eq. (E8), as first noted by Callen in Ref. 13.]

The Green's function $M_{\mathbf{k}}^{(1)}(\nu)$ is obtained simply from the function $M(x;\mathbf{k};\nu)$ by the relation

$$[(d/dx)M(x;\mathbf{k};\nu)]_{x=0}=M_{\mathbf{k}}^{(1)}(\nu); \quad \text{(E13)}$$

and we get

$$M_{\mathbf{k}}^{(1)}(\nu)\underset{\text{general spin}}{=}(2\sigma A)[\eta+2\sigma B]^{-1}, \quad \text{(E14)}$$

where

$$\eta=2\sigma\bar{n}(1+\bar{n})[S(S+1)-\sigma(\sigma+1+2\bar{n})]^{-1}, \quad \text{(E15)}$$

$$\sigma=[d\Omega(x)/dx]_{x=0}. \quad \text{(E16)}$$

For $S=\frac{1}{2}$, $\sigma=(2+4\bar{n})^{-1}$ and $\eta=(1+2\bar{n})$ in agreement with the results given in the text.

APPENDIX F

In this Appendix we shall give a brief discussion of the results of the various existing calculations for the longitudinal correlation function (see Refs. 14 and 15).

Tahir-Kheli and Callen's RPA treatment gave the following result for the equal-time longitudinal correlation function:

$$\langle\tilde{S}_1^z(t_1)\tilde{S}_{1'}^z(t_1)\rangle=[\bar{n}(1+\bar{n})]^{-1}[\langle[S^z(1)]^2\rangle-\sigma^2]\times\{\bar{n}\delta_{1,1'}+[\Phi(11')]^2\}, \quad \text{(F1)}$$

where

$$\Phi(11')=(1/N)\sum_{\mathbf{k}}{}'\,n(E_{\mathbf{k}})\exp[i\mathbf{k}(1-1')];$$

$$\bar{n}=\Phi(11). \quad \text{(F2)}$$

Whereas the expression (F1) is reasonably satisfactory at low temperatures, it fails completely near the Curie point—except for the trivial case of $1=1'$. In fact, it violates the fundamental requirement of spatial isotropy referred to in Appendix D and in the text, which should obtain at and beyond the Curie point.

Liu has calculated the time-dependent correlation function $\langle S_1^z(t_1)S_2^z(t_2)\rangle$ for the Heisenberg interaction. In the notation of the present paper, his result for the Green's function $M_{\mathbf{k}}^{(1)}(Z)$ is

$$M_{\mathbf{k}}^{(1)}(Z)=Q_{\mathbf{k}}^{(1)}(Z)[Q_{\mathbf{k}}^{(2)}(Z)]^{-1}, \quad \text{(F3a)}$$

where

$$Q_{\mathbf{k}}^{(1)}(Z)=(4\sigma^2/N)\sum_{\lambda}{}'[n(E_{\mathbf{k}-\lambda})-n(E_\lambda)]\times[E_{\mathbf{k}-\lambda}-E_\lambda+Z]^{-1}, \quad \text{(F3b)}$$

$$Q_{\mathbf{k}}^{(2)}(Z)=1+(4\sigma/N)\sum_{\lambda}{}'[E_{\mathbf{k}}-E_{\mathbf{k}-\lambda}][n(E_\lambda)-n(E_{\mathbf{k}-\lambda})]\times[E_{\mathbf{k}-\lambda}-E_\lambda+Z]^{-1}. \quad \text{(F3c)}$$

For simplicity, in Eq. (F3) we have considered $S=\frac{1}{2}$.

The difficulty with Liu's result is that the symmetry condition

$$M_{\mathbf{k}}^{(1)}(Z)=M_{-\mathbf{k}}^{(1)}(-Z)=M_{\mathbf{k}}^{(1)}(-Z) \quad \text{(F4a)}$$

is violated, and consequently the spectral function $F_{\mathbf{k}}(\omega)$ fails to obey the sum rule:

$$\int_{-\infty}^{+\infty}F_{\mathbf{k}}(\omega)\,d\omega=0. \quad \text{(F4b)}$$

It should be noted that if the sum rule (F4b) does not hold, there is, in general, no consistent way of calculating the longitudinal correlation function.

For the specific case of $Z=0$, the symmetry condition (F4a) is trivial and as such Liu's result for $M_{\mathbf{k}}^{(1)}(0)$ is valid. It turns out that his $M_{\mathbf{k}}^{(1)}(0)$ is the same as our modified RPA—kinematic sum rule result and is, moreover, in agreement with the Kawasaki and Mori[33] result for the wave-dependent longitudinal susceptibility.

Kaschev has also reported a solution of the time-dependent longitudinal correlation function for the Heisenberg model. He employs the Tanaka-Tomita[34] decoupling prescription and in the present notation his result is

$$M_{\mathbf{k}}^{(1)}(\nu)=Q_{\mathbf{k}}^{(3)}(\nu)[Q_{\mathbf{k}}^{(4)}(\nu)]^{-1}, \quad \text{(F5a)}$$

where

$$Q_{\mathbf{k}}^{(3)}(\nu)=(2\sigma/N)\sum_{\lambda}{}'J(\lambda,\mathbf{k}-\lambda)[Z_\nu+E_{\mathbf{k}-\lambda}-E_\lambda]^{-1}\times[n(E_\lambda)-n(E_{\mathbf{k}-\lambda})], \quad \text{(F5b)}$$

$$Q_{\mathbf{k}}^{(4)}(\nu)=Z_\nu+(4\sigma/N)\sum_{\lambda}{}'J(\lambda,\mathbf{k}-\lambda)\times[Z_\nu+E_{\mathbf{k}-\lambda}-E_\lambda]^{-1}\{[n(E_\lambda)+1]J(\mathbf{k},\lambda)-[n(E_{\mathbf{k}-\lambda})+1]J(\mathbf{k},\mathbf{k}-\lambda)\}^{-1}. \quad \text{(F5c)}$$

This result looks much like our mod RPA, dynamic sum rule result following from the 2nd RPA (II).

Near and beyond the critical point, the difference between Eq. (F5) and our result is of the order σ and is as such negligible. In the ferromagnetic region, however, the difference is likely to be appreciable.

Very recently Bennett has also reported a solution of the Green's function $M_{\mathbf{k}}^{(1)}(Z)$. He works with the Heisenberg interaction and his result is [see his Eq. (83)]

$$M_{\mathbf{k}}^{(1)}(Z)=Q_{\mathbf{k}}^{(3)}(Z)[Q_{\mathbf{k}}^{(5)}(Z)]^{-1}, \quad \text{(F6a)}$$

where

$$Q_{\mathbf{k}}^{(5)}(Z)=Z-(2/N)\sum_{\lambda}{}'J(\lambda,\mathbf{k}-\lambda)n(E_\lambda)+(4\sigma/N)\sum_{\lambda}{}'J(\mathbf{k}-\lambda,\lambda)J(\mathbf{k}-\lambda,\mathbf{k})[n(E_\lambda)-n(E_{\mathbf{k}-\lambda})]\times[Z+E_{\mathbf{k}-\lambda}-E_\lambda]^{-1}. \quad \text{(F6b)}$$

Once again, the above Green's function does not satisfy the symmetry condition (F4a) nor the sum rule (F4b).

[33] H. Mori and K. Kawasaki, Progr. Theoret. Phys. (Kyoto) **27**, 529 (1962); K. Kawasaki and H. Mori, *ibid.*, **28**, 690 (1962).

[34] M. Tanaka and K. Tomita, Progr. Theoret. Phys. (Kyoto) **29**, 651 (1963).