

Use of Green Functions in the Theory of Ferromagnetism. II. Dyson Spin Waves

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(Received February 13, 1962)

We treat Dyson's ideal-spin-wave Hamiltonian by Green's function methods. In the second section we consider only noninteracting Dyson spin waves. In the third section we consider interacting spin waves, using the simplest possible decoupling assumption. Our results lead then to the same expressions for the magnetization and the spin-wave specific heats as Dyson in the limit as $S \rightarrow \infty$ up to terms of order T^4 . The difference is of order T^4/S^2 . If we introduce a higher-order decoupling, we obtain results identical with those of Oguchi, which in turn agree fairly closely with those of Dyson. We also obtain a spin-wave dispersion law which is a slight improvement of the one obtained by Brout and Englert, especially for small values of S . In three appendices we discuss, respectively, the decoupling process, the shifts in the spin-wave energies, and their "damping."

1. INTRODUCTION

IN Paper I of the present series of papers¹ we discussed an extension of the Bogolyubov-Tyablikov theory of ferromagnetism² to the case of general spin. We considered there Green's functions of the S^+ and S^- operators [see Eq. (I 2.1)] and introduced a simple, Tyablikov-like decoupling. In the present paper we shall use the Dyson spin-wave operators³ and study higher-order decoupling.

In Sec. 2 we introduce Dyson's (non-Hermitian) Hamiltonian which when operating on the idealized spin-wave states gives the same results as the original Hamiltonian operating on the physical spin-wave states. This Hamiltonian is used in the equations of motion for the spin-wave Green's functions. We first of all neglect the interaction term in the Hamiltonian, and solve the equations of motion and obtain the low-temperature magnetization, and the spin-system specific heat. In Sec. 3 we take the interactions into account and consider the changes in the spin-wave dispersion law due to the simplest decoupling, in the magnetization, and in the spin specific heat. In Sec. 4 we look into the question of higher-order decoupling, and we discuss the consequences of this procedure. Details of the often tedious mathematical arguments are given in the appendices.

2. NONINTERACTING DYSON SPIN WAVES

We start from Dyson's Hamiltonian [compare Eq. (I 3.1)]

$$H = (g\mu_B B/\hbar) \sum_i S_i^z - \frac{1}{2} \sum_{i,m} I(1-m)(S_i \cdot S_m), \quad (2.1)$$

where μ_B is the Bohr magneton, g the Landé g factor, B the applied field which is assumed to be along the $-z$ direction, and where S_i is the spin on the lattice

¹ R. A. Tahir-Kheli and D. ter Haar, preceding paper [Phys. Rev. **127**, 88 (1962)]. This paper is referred to as I and its equations are quoted as (I 3.5) and so on.

² N. N. Bogolyubov and S. V. Tyablikov, Doklady Akad. Nauk S.S.S.R. **126**, 53 (1959) [translation: Soviet Phys.-Doklady **4**, 604 (1959)]; S. V. Tyablikov, Ukrain Mat. Zhur. **11**, 287 (1959); V. L. Bonch-Bruевич and S. V. Tyablikov, *Green Function Methods in Statistical Mechanics*; (Moscow, 1961) [English translation: North-Holland Publishing Company, Amsterdam, 1962], Chap. VII.

³ F. J. Dyson, Phys. Rev. **102**, 1217, 1230 (1956).

site 1. We now introduce the following transformation⁴

$$\begin{aligned} S_1^- &= (2S\hbar)^{\frac{1}{2}} [b_1 - (b_1^\dagger b_1 / 2S\hbar)], \\ S_1^+ &= (2S\hbar)^{\frac{1}{2}} b_1^\dagger, \quad S_1^z = b_1^\dagger b_1 - S\hbar, \end{aligned} \quad (2.2)$$

where the b_1^\dagger and b_1 are the harmonic oscillator creation and annihilation operators referring to the lattice site 1. They satisfy the boson commutation relations

$$[b_1, b_m^\dagger]_- = \hbar \delta_{1m}, \quad [b_1^\dagger, b_m^\dagger]_- = [b_1, b_m]_- = 0. \quad (2.3)$$

Combining (2.1) and (2.2) we get Dyson's ideal spin-wave Hamiltonian H_{id} :

$$\begin{aligned} H_{id} &= -g\mu_B B S N - \frac{1}{2} \hbar^2 S^2 N J(0) \\ &\quad + [(g\mu_B B/\hbar) + S\hbar J(0)] \sum_i b_i^\dagger b_i \\ &\quad - S\hbar \sum_{i,m} I(1-m) b_i^\dagger b_m \\ &\quad + \frac{1}{2} \sum_{i,m} I(1-m) [b_i^\dagger b_m^\dagger b_m b_m - b_i^\dagger b_1 b_m^\dagger b_m], \end{aligned} \quad (2.4)$$

where $J(0)$ is defined by Eq. (I 3.9).

We now introduce the spin-wave creation and annihilation operators by the Fourier transformation

$$\begin{aligned} b_1^\dagger &= (\hbar/N)^{\frac{1}{2}} \sum_{\lambda} e^{-i(\lambda \cdot 1)} a_{\lambda}^\dagger, \\ b_1 &= (\hbar/N)^{\frac{1}{2}} \sum_{\lambda} e^{i(\lambda \cdot 1)} a_{\lambda}, \end{aligned} \quad (2.5)$$

where N is the total number of spins in the lattice and where the sums over λ are over the first Brillouin zone. The commutation relations for the a_{λ}^\dagger and a_{λ} follow from (2.3) and are again of the boson type:

$$[a_{\lambda}, a_{\mu}^\dagger]_- = \delta_{\lambda, \mu}, \quad [a_{\lambda}^\dagger, a_{\mu}^\dagger]_- = [a_{\lambda}, a_{\mu}]_- = 0. \quad (2.6)$$

From (2.4) and (2.5) we now get

$$H_{id} = H_{id}^{(0)} + H_{id}^{(1)}, \quad (2.7)$$

where

$$\begin{aligned} H_{id}^{(0)} &= \text{const} \\ &\quad + \sum_{\lambda} \{g\mu_B B + S\hbar^2 [J(0) - J(\lambda)]\} a_{\lambda}^\dagger a_{\lambda}, \end{aligned} \quad (2.8)$$

$$\begin{aligned} H_{id}^{(1)} &= (\hbar^2/2N) \\ &\quad \times \sum_{\lambda, \mu, \nu} [J(\lambda) - J(\lambda - \nu)] a_{\lambda}^\dagger a_{\mu}^\dagger a_{\nu} a_{\lambda + \mu - \nu}, \end{aligned} \quad (2.9)$$

⁴ S. V. Maleev, J. Exptl. Theoret. Phys. (U.S.S.R.) **33**, 1010 (1957) [translation: Soviet Phys.—JETP **6**, 776 (1958)]. We should like to point out here that Maleev's transformation enables us to obtain Dyson's result in a much simpler way than the original one.

with $J(\lambda)$ defined by [see Eq. (I 3.9)]

$$J(\lambda) = \sum_l I(l) e^{i(\lambda \cdot l)}. \quad (2.10)$$

We shall in the following again introduce the simplifying assumption [see (I 3.2)]

$$\begin{aligned} I(1-\mathbf{m}) &= I, \quad \text{if } l \text{ and } \mathbf{m} \text{ are nearest neighbors,} \\ I(1-\mathbf{m}) &= 0, \quad \text{otherwise.} \end{aligned} \quad (2.11)$$

For our discussions we need the equation of motion for the Fourier transform $\langle\langle a_k; a_{k'}^\dagger \rangle\rangle$ of the single spin-wave Green function. This is given by Eq. (2.9) which in the present case will be of the form

$$E \langle\langle a_k; a_{k'}^\dagger \rangle\rangle = (1/2\pi) \delta_{k,k'} + \langle\langle [a_k, H_{\text{id}}]_-; a_{k'}^\dagger \rangle\rangle. \quad (2.12)$$

We shall first of all neglect the interaction term $H_{\text{id}}^{(1)}$ and (2.12) then becomes of the form

$$\langle\langle a_k; a_{k'}^\dagger \rangle\rangle = \delta_{k,k'} / 2\pi (E - \epsilon_k^{(0)}), \quad (2.13)$$

where

$$\epsilon_k^{(0)} = g\mu_B B + \hbar^2 S [J(0) - J(\kappa)]. \quad (2.14)$$

From the general theory⁵ of the properties of the single-particle Green functions when there are no interactions, it follows that $\epsilon_k^{(0)}$ is the energy of a non-interacting spin wave with wave vector κ .

We now use the general relation (I 2.11) between the correlation functions $\langle B(t') A(t) \rangle$ and $\langle\langle A; B \rangle\rangle$ and the operator identity

$$\lim_{\epsilon \rightarrow +0} \frac{1}{E - E_0 \pm i\epsilon} = \frac{P}{E - E_0} \mp i\pi \delta(E - E_0), \quad (2.15)$$

where P indicates that whenever these expressions occur under an integral (or summation) sign, the principal part of the integral must be taken. We then get ($\beta = 1/k_B T$; k_B = Boltzmann's constant; T = absolute temperature)

$$\begin{aligned} \langle a_{k'}^\dagger(t') a_k(t) \rangle \\ = \delta_{k,k'} \exp[-i\epsilon_k^{(0)}(t-t')/\hbar] / [\exp(\beta\epsilon_k^{(0)}) - 1], \end{aligned} \quad (2.16)$$

and from (2.16), (2.5), (2.2), and the relation between the magnetization $M(\beta)$ at temperature $T = (\beta k_B)^{-1}$ and the average value of S^z , we then get

$$\begin{aligned} M(\beta) &= [M(\infty)/S] [S - N^{-1} \sum_k \langle a_k^\dagger a_k \rangle] \\ &= [M(\infty)/S] [S - a_0 \theta^{3/2} - a_1 \theta^{5/2} \\ &\quad - a_2 \theta^{7/2} + O(\theta^{9/2})], \end{aligned} \quad (2.17)$$

where $M(\infty)$ denotes the saturation magnetization, reached at $T=0$, where [compare the expansion (I 4.10) and Eqs. (I 4.1)]

$$\theta^{-1} = \frac{2}{3} \pi \beta S \hbar^2 J(0) \nu, \quad (2.18)$$

where ν is the numerical factor given by (I 4.12) which differs from one lattice to another, and where the a_i are

⁵ For instance, D. N. Zubarev, Uspekhi Fiz. Nauk **71**, 71 (1960) [translation: Soviet Phys.—Uspekhi **3**, 320 (1960)].

given by the equations

$$a_0 = Z(3/2), \quad a_1 = \frac{3}{4} \pi \nu Z(5/2), \quad a_2 = \pi^2 \omega \nu^2 Z(7/2) \quad (2.19)$$

with ω given by (I 4.13) and

$$Z(n) = \sum_{r=1}^{\infty} (e^{-r\beta g \mu_B B} / r^n). \quad (2.20)$$

Note that if $B=0$, $Z(n)$ is the Riemann zeta function $\zeta(n)$, and (2.19) reduces to (I 4.11) and (2.17) to (I 5.3 and 4), if we neglect in those last equations the terms in θ^3 and θ^4 .

The average magnetic energy per lattice site for the case where $B=0$ is in the present approximation ($H_{\text{id}}^{(1)}=0$) given by the expression

$$\begin{aligned} E_{\text{mag}} &= -(2N)^{-1} \sum_{l,m} I(1-\mathbf{m}) \langle (\mathbf{S}_l \cdot \mathbf{S}_m) \rangle \\ &= \text{const} + (\hbar^2/N) \sum_{\lambda} \mathbf{S} [J(0) - J(\lambda)] \langle a_{\lambda}^\dagger a_{\lambda} \rangle. \end{aligned} \quad (2.21)$$

The sum over λ can be changed into an integral over the first Brillouin zone in the manner discussed in I, and we find

$$\begin{aligned} E_{\text{mag}} &= \text{const} + \hbar^2 S J(0) [\pi \nu \zeta(\frac{5}{2}) \theta^{5/2} + (5\pi^2/4) \nu^2 \zeta(\frac{7}{2}) \theta^{7/2} \\ &\quad + (7\pi^2/3) \omega \nu^3 \zeta(\frac{9}{2}) \theta^{9/2} + O(\theta^{11/2})], \end{aligned} \quad (2.22)$$

and for the spin-wave specific heat we have

$$\begin{aligned} C_{\text{mag}} &= k \partial E_{\text{mag}} / \partial (1/\beta) \\ &= k [(15/4) \zeta(\frac{5}{2}) \theta^{3/2} + (105/16) \pi \nu \zeta(\frac{7}{2}) \theta^{5/2} \\ &\quad + (63\pi^2/4) \omega^2 \nu^2 \zeta(\frac{9}{2}) \theta^{7/2} + O(\theta^{9/2})]. \end{aligned} \quad (2.23)$$

The results for $M(\beta)$ and C_{mag} are identical with Dyson's results and give corrections to Bloch's results.⁶

3. INTERACTING DYSON SPIN WAVES

If we take $H_{\text{id}}^{(1)}$ into account we have instead of (2.12) or (2.13) the following equation for $\langle\langle a_k; a_{k'}^\dagger \rangle\rangle$:

$$\begin{aligned} [E - \epsilon_k^{(0)}] \langle\langle a_k; a_{k'}^\dagger \rangle\rangle \\ = \delta_{k,k'} / 2\pi + (\hbar^2/2N) \sum_{\lambda_1, \mu_1} [J(\lambda_1) + J(\kappa) - J(\lambda_1 - \mathbf{u}_1) \\ - J(\kappa - \mathbf{u}_1)] \langle\langle a_{\lambda_1}^\dagger a_{\mu_1} a_{k+\lambda_1-\mu_1}; a_{k'}^\dagger \rangle\rangle. \end{aligned} \quad (3.1)$$

We notice here the well-known appearance of higher order Green functions which make it necessary to introduce some kind of decoupling. We expect that to a first approximation only those Green functions will appreciably contribute to the sum on the right-hand side of (3.1) for which at least one of the two indices \mathbf{u}_1 , and $\kappa + \lambda_1 - \mathbf{u}_1$ is equal to λ_1 . We therefore write

$$\begin{aligned} \langle\langle a_{\lambda_1}^\dagger a_{\mu_1} a_{k+\lambda_1-\mu_1}; a_{k'}^\dagger \rangle\rangle &= \{ [\delta_{\lambda_1, \mu_1} + \delta_{\mu_1, \kappa} \\ &\quad - \delta_{\lambda_1, \kappa} \delta_{\mu_1, \kappa} + [1 - \delta_{\lambda_1, \mu_1} - \delta_{\mu_1, \kappa} + \delta_{\lambda_1, \kappa} \delta_{\mu_1, \kappa}] \} \\ &\quad \times \langle\langle a_{\lambda_1}^\dagger a_{\mu_1} a_{k+\lambda_1-\mu_1}; a_{k'}^\dagger \rangle\rangle, \end{aligned} \quad (3.2)$$

⁶ F. Bloch, Z. Physik **61**, 206 (1930); **74**, 295 (1932).

and introduce the decoupling assumptions

$$\langle\langle a_{\lambda_1}^\dagger a_{\lambda_1} a_{\kappa}; a_{\kappa'}^\dagger \rangle\rangle \cong \langle a_{\lambda_1}^\dagger a_{\lambda_1} \rangle \langle\langle a_{\kappa}; a_{\kappa'}^\dagger \rangle\rangle \cong \bar{n}_{\lambda_1} \langle\langle a_{\kappa}; a_{\kappa'}^\dagger \rangle\rangle, \quad (3.3)$$

$$(1 - \delta_{\lambda_1 \mu_1} - \delta_{\mu_1 \kappa} + \delta_{\lambda_1 \kappa} \delta_{\mu_1 \kappa}) \langle\langle a_{\lambda_1}^\dagger a_{\mu_1} a_{\lambda_1 + \kappa - \mu_1}; a_{\kappa'}^\dagger \rangle\rangle \\ \cong (1 - \delta_{\lambda_1 \mu_1} - \delta_{\mu_1 \kappa} + \delta_{\lambda_1 \kappa} \delta_{\mu_1 \kappa}) \langle a_{\lambda_1}^\dagger a_{\mu_1} \rangle \\ \times \langle\langle a_{\kappa}; a_{\kappa'}^\dagger \rangle\rangle = 0, \quad (3.4)$$

where \bar{n}_λ is the average number of spin waves ($\langle a_\lambda^\dagger a_\lambda \rangle$) with wave vector λ . The term $\delta_{\lambda_1 \kappa} \delta_{\mu_1 \kappa} \langle\langle a_{\kappa}^\dagger a_{\kappa} a_{\kappa'}; a_{\kappa'}^\dagger \rangle\rangle$ occurs only when all these indices are equal and has thus a weight in the sum on the right-hand side of (3.1) which is smaller by a factor N^{-1} as compared to the weight of terms such as $\langle\langle a_{\lambda_1}^\dagger a_{\lambda_1} a_{\kappa}; a_{\kappa'}^\dagger \rangle\rangle$. In the limit as $N \rightarrow \infty$ we can thus ignore that term. This means that we write

$$\langle\langle a_{\lambda_1}^\dagger a_{\mu_1} a_{\lambda_1 + \mu_1 - \mu_1}; a_{\kappa'}^\dagger \rangle\rangle \\ \cong (\delta_{\lambda_1, \mu_1} + \delta_{\mu_1, \kappa}) \bar{n}_{\lambda_1} \langle\langle a_{\kappa}; a_{\kappa'}^\dagger \rangle\rangle. \quad (3.5)$$

Substituting this into (3.1) we get finally for $\langle\langle a_{\kappa}; a_{\kappa'}^\dagger \rangle\rangle$ instead of (2.13) the equation

$$\langle\langle a_{\kappa}; a_{\kappa'}^\dagger \rangle\rangle = (1/2\pi) \delta_{\kappa \kappa'} / (E - \epsilon_{\kappa}^{(0)} - \Delta \epsilon_{\kappa}), \quad (3.6)$$

where

$$\Delta \epsilon_{\kappa} = (\hbar/N) \sum_{\lambda} [J(\lambda) + J(\kappa) - J(\lambda - \kappa) - J(0)] \bar{n}_{\lambda}. \quad (3.7)$$

This "renormalization" of the spin-wave energies is identical with the result given (without proof) by Brout and Englert.⁷ These renormalized spin-wave energies can now be used to evaluate the magnetization and spin-wave specific heat. Before doing this, however, we shall briefly discuss (3.7) which can be written in the form

$$\Delta \epsilon_{\kappa} = -(\hbar^2 J(0)/N) \sum_{\lambda} \bar{n}_{\lambda} [\eta(\kappa) + \eta(\lambda) - \eta(\lambda - \kappa)], \quad (3.8)$$

where $\eta(\kappa)$ is defined by (I 4.3). We note here that the spin-wave energies are temperature dependent through \bar{n}_{λ} . The question of temperature-dependent energy levels is usually a difficult one,⁸ but they fit rather naturally into the Green's function formalism. If we use the expression obtained in the previous section for the \bar{n}_{λ} we find for the renormalized spin-wave energies

$$\epsilon_{\kappa}^{(1)} = \epsilon_{\kappa}^{(0)} + \Delta \epsilon_{\kappa} = g \mu_B B + \hbar^2 S [J(0) - J(\kappa)] \\ \times [1 - (\pi \nu / S) Z(\frac{5}{2}) \theta^{5/2} + O(\theta^{7/2})]. \quad (3.9)$$

The terms neglected by taking for \bar{n}_{λ} the expression from Sec. 2 are of higher order in θ than the ones retained in (3.9).

Using the renormalized spin-wave energies, we obtain for the magnetization instead of (2.17)

$$M(\beta) = [M(\infty)/S] [S - a_0 \theta^{3/2} - a_1 \theta^{5/2} - a_2 \theta^{7/2} \\ - (a_3/S) \theta^4 + O(\theta^{9/2})], \quad (3.10)$$

where

$$a_3 = \frac{3}{2} \pi \nu Z(\frac{3}{2}) Z(\frac{5}{2}). \quad (3.11)$$

⁷ R. Brout and F. Englert, Bull. Am. Phys. Soc. **6**, 55 (1961).
⁸ G. S. Rushbrooke, Trans. Faraday Soc. **36**, 1055 (1940); see also the book by Bonch-Bruyevich and Tyablikov (reference 2).

It should be emphasized here that in evaluating the averages, we have followed Dyson and assumed that all kinematical interactions may be neglected.⁹ We should also mention here that the coefficient of θ^4 for which we find here a_3/S agrees only in the limit as $S \rightarrow \infty$ with the results of Dyson and of Oguchi⁹ who found, respectively (for the simple-cubic lattice), $(a_3/S)[1 + (0.31/S) + O(S^{-2})]$ and $(a_3/S)[1 + (0.2/S)]$. The magnetic energy is no longer given by (2.21), but by the equation

$$E_{\text{mag}} = \text{const} + N^{-1} \sum_{\lambda} S \hbar^2 [J(0) - J(\lambda)] \langle a_{\lambda}^\dagger a_{\lambda} \rangle \\ + (\hbar^2/2N^2) \sum_{\lambda, \mu, \nu} [J(\lambda) - J(\lambda - \nu)] \\ \times \langle a_{\lambda}^\dagger a_{\mu}^\dagger a_{\nu} a_{\lambda + \mu - \nu} \rangle. \quad (3.12)$$

If we evaluate $\langle a_{\lambda}^\dagger a_{\mu}^\dagger a_{\nu} a_{\lambda + \mu - \nu} \rangle$ using the decoupling (3.5) and the relation (I 2.11), we find

$$E_{\text{mag}} = \text{const} + (S \hbar^2/N) \sum_{\lambda} [J(0) - J(\lambda)] \langle a_{\lambda}^\dagger a_{\lambda} \rangle \\ + (\hbar^2/2N^2) \sum_{\lambda, \mu} \langle a_{\lambda}^\dagger a_{\lambda} \rangle \langle a_{\mu}^\dagger a_{\mu} \rangle \\ \times [2J(\lambda) - J(\lambda - \mu) - J(0)]. \quad (3.13)$$

The integrations involved in the evaluation of the last double sum are tedious, but straightforward and for the case $B=0$, we get instead of (2.22) the equation

$$E_{\text{mag}} = \text{const} + \hbar^2 S J(0) \left[\pi \nu \zeta(5/2) \theta^{5/2} \right. \\ \left. + \frac{5\pi^2}{4} \nu^2 \zeta(7/2) \theta^{7/2} + \frac{7\pi^3}{3} \nu^3 \omega \zeta(9/2) \theta^{9/2} \right. \\ \left. + (2\pi^2 \nu^2/S) \zeta(5/2) \zeta(5/2) \theta^5 + O(\theta^{11/2}) \right], \quad (3.14)$$

and for the spin-wave specific heat per lattice site we get instead of (2.23)

$$C_{\text{mag}} = k [(15/4) \zeta(5/2) \theta^{3/2} + (105\pi/16) \nu \zeta(7/2) \theta^{5/2} \\ + (63\pi^2/4) \nu^2 \omega \zeta(9/2) \theta^{7/2} \\ + (15\pi \nu/S) \zeta(5/2) \zeta(5/2) \theta^4 + O(\theta^{9/2})]. \quad (3.15)$$

This last result differs from Dyson's result in the coefficient of θ^4 for which Dyson finds our coefficient multiplied by $1 + (0.31/S) + O(S^{-2})$. This difference arises because our simple decoupling (3.5) does not properly take the dynamic interactions between the spin waves into account. It is, however, surprising how well this simple decoupling works. We also note that, as was already mentioned in I, the first-order decoupling is the better, the larger S .

4. HIGHER ORDER DECOUPLING

If we wish to improve our approximations, we need the equation of motion for the Green function $\langle\langle a_{\lambda_1}^\dagger a_{\mu_1} a_{\kappa + \lambda_1 - \mu_1}; a_{\kappa'}^\dagger \rangle\rangle$ occurring on the right-hand side of (3.1). This equation is obtained from (I 2.9) and is

⁹ See also T. Oguchi, Phys. Rev. **117**, 117 (1960); F. Keffer and R. Loudon, Suppl. J. Appl. Phys. **32**, 2 (1961).

of the form

$$\begin{aligned} & \langle\langle a_{\lambda_1}^\dagger a_{\mu_1} a_{\kappa+\lambda_1-\mu_1}; a_{\kappa'}^\dagger \rangle\rangle [E - \epsilon_{\mu_1}^{(0)} - \epsilon_{\kappa+\lambda_1-\mu_1}^{(0)} + \epsilon_{\lambda_1}^{(0)}] \\ &= [\bar{n}_{\lambda_1} \delta_{\kappa, \kappa'} / 2\pi] [\delta_{\lambda_1, \mu_1} + \delta_{\kappa, \mu_1}] + (\hbar^2/2N) \sum_{\nu} D(\kappa + \lambda_1 - \mathbf{u}_1, \mathbf{u}_1, \kappa + \lambda_1 - \mathbf{u}_1 - \mathbf{v}, \mathbf{u}_1 - \mathbf{v}) \langle\langle a_{\lambda_1}^\dagger a_{\nu} a_{\kappa+\lambda_1-\nu}; a_{\kappa'}^\dagger \rangle\rangle \\ &+ (\hbar^2/2N) \sum_{\lambda, \nu} D(\lambda, \kappa + \lambda_1 - \mathbf{u}_1, \lambda - \mathbf{v}, \kappa + \lambda_1 - \mathbf{u}_1 - \mathbf{v}) \langle\langle a_{\lambda_1}^\dagger a_{\lambda}^\dagger a_{\mu_1} a_{\nu} a_{\kappa+\lambda_1+\lambda-\mu_1-\nu}; a_{\kappa'}^\dagger \rangle\rangle \\ &+ (\hbar^2/2N) \sum_{\lambda, \nu} D(\lambda, \mathbf{u}_1, \lambda - \mathbf{v}, \mathbf{u}_1 - \mathbf{v}) \langle\langle a_{\lambda_1}^\dagger a_{\lambda}^\dagger a_{\nu} a_{\kappa+\lambda_1-\mu_1} a_{\lambda+\mu_1-\nu}; a_{\kappa'}^\dagger \rangle\rangle - (\hbar^2/2N) \sum_{\lambda, \nu} D(\lambda, \lambda, \lambda - \lambda_1, \lambda - \lambda_1) \\ &\quad \times \langle\langle a_{\lambda}^\dagger a_{\nu}^\dagger a_{\lambda+\nu-\lambda_1} a_{\mu_1} a_{\kappa+\lambda_1-\mu_1}; a_{\kappa'}^\dagger \rangle\rangle, \quad (4.1) \end{aligned}$$

where

$$D(\alpha, \beta, \gamma, \delta) = J(\alpha) + J(\beta) - J(\gamma) - J(\delta). \quad (4.2)$$

This is clearly a formidable equation, and we discuss in Appendix A the way in which we can introduce a decoupling into this equation of motion. The final result is the following equation for $\langle\langle a_{\kappa}; a_{\kappa'}^\dagger \rangle\rangle$:

$$\begin{aligned} \langle\langle a_{\kappa}; a_{\kappa'}^\dagger \rangle\rangle [E - \epsilon_{\kappa}^{(0)}] &= \frac{\delta_{\kappa, \kappa'}}{2\pi} + \frac{\delta_{\kappa, \kappa'}}{2\pi} \frac{\Delta \epsilon_{\kappa}}{E - \epsilon_{\kappa}^{(1)}} \\ &+ \sum_{\lambda_1, \mu_1} \frac{A(\kappa, \lambda_1, \mathbf{u}_1) \langle\langle a_{\kappa}; a_{\kappa'}^\dagger \rangle\rangle}{E - \epsilon_{\mu_1}^{(1)} - \epsilon_{\kappa+\lambda_1-\mu_1}^{(1)} + \epsilon_{\lambda_1}^{(1)}}, \quad (4.3) \end{aligned}$$

where

$$\begin{aligned} A(\kappa, \lambda_1, \mathbf{u}_1) &= (\hbar^2/2N^2) D(\lambda_1, \kappa, \lambda_1 - \mathbf{u}_1, \kappa - \mathbf{u}_1) \\ &\times D(\mathbf{u}_1, \kappa + \lambda_1 - \mathbf{u}_1, \mathbf{u}_1 - \lambda_1, \kappa - \mathbf{u}_1) \\ &\times [(1 + \bar{n}_{\mu_1} + \bar{n}_{\kappa+\lambda_1-\mu_1}) \bar{n}_{\lambda_1} - \bar{n}_{\mu_1} \bar{n}_{\kappa+\lambda_1-\mu_1}]. \quad (4.4) \end{aligned}$$

We note that, if we neglect the last sum in (4.3) we get again (3.6) for $\langle\langle a_{\kappa}; a_{\kappa'}^\dagger \rangle\rangle$; this sum is thus the term due to the higher-order decoupling.

Solving (4.3) for $\langle\langle a_{\kappa}; a_{\kappa'}^\dagger \rangle\rangle$, we get

$$\langle\langle a_{\kappa}; a_{\kappa'}^\dagger \rangle\rangle_{\pm} = (\delta_{\kappa, \kappa'} / 2\pi) [E_{\pm} - \epsilon_{\kappa}^{(2)}(E_{\pm})]^{-1}, \quad (4.5)$$

where

$$\epsilon_{\kappa}^{(2)}(E_{\pm}) = \epsilon_{\kappa}^{(1)} + R_{\kappa}(E) \mp i\gamma_{\kappa}(E), \quad (4.6)$$

$$R_{\kappa}(E) = P \sum_{\lambda_1, \mu_1} \frac{A(\kappa, \lambda_1, \mathbf{u}_1)}{E - \epsilon_{\mu_1}^{(1)} - \epsilon_{\kappa+\lambda_1-\mu_1}^{(1)} + \epsilon_{\lambda_1}^{(1)}}, \quad (4.7)$$

$$\begin{aligned} \gamma_{\kappa}(E) &= \pi \sum_{\lambda_1, \mu_1} A(\kappa, \lambda_1, \mathbf{u}_1) \\ &\times \delta(E - \epsilon_{\mu_1}^{(1)} - \epsilon_{\kappa+\lambda_1-\mu_1}^{(1)} + \epsilon_{\lambda_1}^{(1)}). \quad (4.8) \end{aligned}$$

Equation (4.5) is derived by replacing under the summation sign $(E - \epsilon_{\kappa}^{(1)})/(E - \epsilon_{\kappa}^{(0)})$ by 1, bearing in mind that ultimately we need (I 2.11) and thus the Fourier transform for energy values $E \pm i\epsilon$ ($\epsilon \rightarrow +0$), as indicated by the subscript \pm , and using (2.15).

From (4.5), we can find the spectral intensity $f(E)$ defined by the relation

$$\langle a_{\kappa'}^\dagger(t') a_{\kappa}(t) \rangle = \int_{-\infty}^{+\infty} f(E) d(E/\hbar) e^{-iE(t-t')/\hbar}, \quad (4.9)$$

which satisfies the equation [compare (I 2.11)]

$$if(E)(e^{\beta E} - 1) = \langle\langle a_{\kappa}; a_{\kappa'}^\dagger \rangle\rangle_- - \langle\langle a_{\kappa}; a_{\kappa'}^\dagger \rangle\rangle_+. \quad (4.10)$$

Combining (4.5), (4.6), and (4.10), we find

$$f(E)(e^{\beta E} - 1) = \frac{(\delta_{\kappa, \kappa'} / \pi)}{(E - \epsilon_{\kappa}^{(1)} - R_{\kappa})^2 + \gamma_{\kappa}^2}. \quad (4.11)$$

In Appendices B and C we show that R_{κ} and γ_{κ} are small quantities which vanish as θ tends to zero. We know that if R_{κ} and γ_{κ} vanished rigorously, (4.10) will lead to a delta function on the right-hand side of (4.11). As long as R_{κ} and γ_{κ} are small and γ_{κ} is of a smaller order of magnitude than R_{κ} we may thus expect the right-hand side of (4.11) to be strongly peaked at an energy $\tilde{\epsilon}_{\kappa}$ satisfying the equation

$$\tilde{\epsilon}_{\kappa} - \epsilon_{\kappa}^{(1)} - R_{\kappa}(\tilde{\epsilon}_{\kappa}) = 0, \quad (4.12)$$

provided $\gamma_{\kappa}(E)$ is a slowly varying function of E . We note that $\gamma_{\kappa}(E)$ plays the role of a damping coefficient.¹⁰ If $R_{\kappa}(E)$ is also a slowly varying function of E , we get approximately

$$f(E)(e^{\beta E} - 1) \cong \frac{(\delta_{\kappa, \kappa'} / \pi)}{(E - \tilde{\epsilon}_{\kappa})^2 + \gamma_{\kappa}(\tilde{\epsilon}_{\kappa})^2} \cong \delta_{\kappa, \kappa'} \delta(E - \tilde{\epsilon}_{\kappa}). \quad (4.13)$$

From (4.12) and (4.8), we then get

$$\bar{n}_{\kappa} = [\exp \beta \tilde{\epsilon}_{\kappa} - 1]^{-1}, \quad (4.14)$$

that is, a boson-distribution for the spin-wave occupation numbers. The distribution is, however, smeared out over a width of the order of γ_{κ} . Inasmuch as the distribution is nearly the one produced by "undamped" energy-levels, we can still approximately talk about spin-wave energies; these satisfy (4.12), or

$$\tilde{\epsilon}_{\kappa} = \epsilon_{\kappa}^{(1)} + R_{\kappa}(\tilde{\epsilon}_{\kappa}), \quad (4.15)$$

and R_{κ} thus plays the role of an energy-shift.

In Appendix B, we evaluate this energy shift and find that our result is identical with the one obtained by Oguchi⁹; it is an improvement on the results obtained by Brout and Englert.⁷ We can use the improved spin-wave energies $\tilde{\epsilon}_{\kappa}$ to evaluate $M(\beta)$ and C_{mag} and we now find that for a simple cubic lattice the coefficients of θ^4 are changed from a_3/S for $M(\beta)$ and $k_B(15\pi\nu/S)\zeta^2(\frac{5}{2})$ for C_{mag} by a factor $1 + (0.2/S)$. Our results are, of course, general and can be applied to any lattice.

ACKNOWLEDGMENTS

We should like to express our gratitude to the Colombo Plan authorities, the Government of Pakistan,

¹⁰ Compare reference 5, Sec. 8.1.

and the British Council for a grant to one of us (R. A. T.-K.), to Oriel College, Oxford, for the award of a Bishop Fraser Scholarship to R. A. T.-K., and to Dr. R. J. Elliott, Dr. W. E. Parry, Dr. H. Stern, and Dr. R. E. Turner for helpful discussions.

APPENDIX A

To illustrate how (4.3) can be derived from (4.1) by suitable decoupling procedures, we shall first of all discuss the function $\langle\langle a_{\lambda_1}^\dagger a_{\lambda_1}^\dagger a_{\mu_1} a_{\mu_1} a_{\kappa+\lambda_1+\lambda-\mu_1-\nu}; a_{\kappa'}^\dagger \rangle\rangle$. For this function we write

$$\begin{aligned} \langle\langle a_{\lambda_1}^\dagger a_{\lambda_1}^\dagger a_{\mu_1} a_{\mu_1} a_{\kappa+\lambda_1+\lambda-\mu_1-\nu}; a_{\kappa'}^\dagger \rangle\rangle \\ \cong [(\delta_{\lambda,\nu} + \delta_{\kappa+\lambda_1,\mu_1+\nu} + \delta_{\lambda,\mu_1} + \delta_{\lambda_1,\nu} + \delta_{\kappa+\lambda,\mu_1+\nu} + \delta_{\lambda_1,\mu_1}) \\ - \delta_{\lambda,\nu}(\delta_{\kappa+\lambda_1,\mu_1+\nu} + \delta_{\lambda,\mu_1} + \delta_{\lambda_1,\nu} + \delta_{\kappa+\lambda,\mu_1+\nu} + \delta_{\lambda_1,\mu_1}) \\ - \delta_{\kappa+\lambda_1,\mu_1+\nu}(\delta_{\lambda,\mu_1} + \delta_{\lambda_1,\nu} + \delta_{\kappa+\lambda,\mu_1+\nu} + \delta_{\lambda_1,\mu_1}) \\ - \delta_{\lambda,\mu_1}(\delta_{\lambda_1,\nu} + \delta_{\kappa+\lambda,\mu_1+\nu} + \delta_{\lambda_1,\mu_1}) \\ - \delta_{\lambda_1,\nu}(\delta_{\kappa+\lambda,\mu_1+\nu} + \delta_{\lambda_1,\mu_1}) - \delta_{\kappa+\lambda,\mu_1+\nu} \delta_{\lambda_1,\mu_1}] \\ \langle\langle a_{\lambda_1}^\dagger a_{\lambda_1}^\dagger a_{\mu_1} a_{\mu_1} a_{\kappa+\lambda_1+\lambda-\mu_1-\nu}; a_{\kappa'}^\dagger \rangle\rangle. \quad (A1) \end{aligned}$$

This approximation consists in neglecting all terms where neither λ nor λ_1 is equal to at least one of \mathbf{u}_1, \mathbf{v} , or $\kappa+\lambda_1+\lambda-\mathbf{u}_1-\mathbf{v}$. It is a straightforward generalization of our earlier approximation and can be regarded as a higher-order random-phase approximation. We have not included in (A1) terms involving three or more Kronecker deltas, as their occurrence is smaller than that of the terms retained by a factor of at least N^{-1} which in the limit as $N \rightarrow \infty$ leads to their making a vanishing contribution (compare the discussion in Sec. III; the difference between the situations then and now is that now terms with two delta functions will make a nonvanishing contribution because of the occurrence of at least two annihilation and two creation operators).

If we now consider all the terms which are left in the sum on the right-hand side of (4.1), once (A1) has been substituted, we see that a representative term will be of the form

$$(\hbar^2/2N) \sum_{\lambda} D(\lambda, \kappa+\lambda_1-\mathbf{u}_1, 0, \kappa+\lambda_1-\mathbf{u}_1-\lambda) \langle\langle a_{\lambda_1}^\dagger a_{\lambda_1}^\dagger a_{\mu_1} a_{\mu_1} a_{\kappa+\lambda_1-\mu}; a_{\kappa'}^\dagger \rangle\rangle. \quad (A2)$$

In the Green function in (A2) we now decouple as follows

$$\begin{aligned} \langle\langle a_{\lambda_1}^\dagger a_{\lambda_1}^\dagger a_{\mu_1} a_{\mu_1} a_{\kappa+\lambda_1-\mu_1}; a_{\kappa'}^\dagger \rangle\rangle &= [\langle a_{\lambda_1}^\dagger a_{\lambda_1} \rangle - \delta_{\lambda,\lambda_1}] \\ &\quad [\delta_{\lambda_1,\mu_1} \langle a_{\lambda_1}^\dagger a_{\lambda_1} \rangle \langle a_{\kappa}; a_{\kappa'}^\dagger \rangle + (1 - \delta_{\lambda_1,\mu_1}) \\ &\quad \times \langle\langle a_{\lambda_1}^\dagger a_{\mu_1} a_{\kappa+\lambda_1-\mu_1}; a_{\kappa'}^\dagger \rangle\rangle]. \quad (A3) \end{aligned}$$

This leads to an equation for $\langle\langle a_{\lambda_1}^\dagger a_{\mu_1} a_{\kappa+\lambda_1-\mu_1}; a_{\kappa'}^\dagger \rangle\rangle$ where on the left-hand side we have the term $\langle\langle a_{\lambda_1}^\dagger a_{\mu_1} a_{\kappa+\lambda_1-\mu_1}; a_{\kappa'}^\dagger \rangle\rangle [E - \epsilon_{\mu_1}^{(1)} - \epsilon_{\kappa+\lambda_1-\mu_1}^{(1)} + \epsilon_{\lambda_1}^{(1)}]$ and on the right-hand side first of all a term $(\tilde{n}_{\lambda_1} \delta_{\kappa,\kappa'} / 2\pi) \times [\delta_{\lambda_1,\mu_1} + \delta_{\kappa,\mu_1}]$ which corresponds to the result of the first-order decoupling procedure of Sec. 2. The remaining terms on the right-hand side are a consequence of the improved decoupling and contain Green functions involving two creation and two annihilation operators. As the first-order decoupling led already to reasonable results, these extra terms will only contribute relatively small corrections and it thus seems reasonable to use the first-order decoupling approximation (3.5) for the higher-order Green functions occurring in the correction terms. If that is done we are led to the following equation for $\langle\langle a_{\lambda_1}^\dagger a_{\mu_1} a_{\kappa+\lambda_1-\mu_1}; a_{\kappa'}^\dagger \rangle\rangle$:

$$\begin{aligned} \langle\langle a_{\lambda_1}^\dagger a_{\mu_1} a_{\kappa+\lambda_1-\mu_1}; a_{\kappa'}^\dagger \rangle\rangle [E - \epsilon_{\mu_1}^{(1)} - \epsilon_{\kappa+\lambda_1-\mu_1}^{(1)} + \epsilon_{\lambda_1}^{(1)}] \\ = (\delta_{\kappa,\kappa'} \tilde{n}_{\lambda_1} / 2\pi) [\delta_{\lambda_1,\mu_1} + \delta_{\kappa,\mu_1}] \\ + (\hbar^2/N) D(\mathbf{u}_1, \kappa+\lambda_1-\mathbf{u}_1, \mathbf{u}_1-\lambda_1, \kappa-\mathbf{u}_1) \\ \times [\tilde{n}_{\lambda_1}(1 + \tilde{n}_{\mu_1} + \tilde{n}_{\kappa+\lambda_1-\mu_1}) - \tilde{n}_{\mu_1} \tilde{n}_{\kappa+\lambda_1-\mu_1}] \\ \times \langle\langle a_{\kappa}; a_{\kappa'}^\dagger \rangle\rangle, \quad (A4) \end{aligned}$$

where we have neglected terms which on substituting into (4.1) will lead to terms which vanish in the limit as $N \rightarrow \infty$. Substitution of (A4) into (4.1) leads to (4.3).

APPENDIX B

In this Appendix we shall briefly study the energy-shift R_κ for which we have Eq. (4.7). As we expect R_κ to be a small correction to $\epsilon_\kappa^{(1)}$, we may replace its argument E everywhere by $\epsilon_\kappa^{(1)}$. We also remind ourselves that as we are interested in the influence of the higher-order decoupling on the θ^4 term in the magnetization and spin-wave specific heat, we can neglect all terms which will lead to terms of higher order in θ . From (2.17) we note that the \tilde{n}_κ are of order $\theta^{3/2}$ so that to first-order we neglect in (4.4) all terms involving a product of two spin-wave occupation numbers. We thus write approximately

$$R_\kappa \cong (\hbar^2/2N^2) P \sum_{\lambda,\mu} \frac{D(\lambda, \kappa, \lambda-\mathbf{u}, \kappa-\mathbf{u}) D(\mathbf{u}, \kappa+\lambda-\mathbf{u}, \mathbf{u}-\lambda, \kappa-\mathbf{u}) \tilde{n}_\lambda}{\epsilon_\kappa^{(1)} - \epsilon_\mu^{(1)} - \epsilon_{\kappa+\lambda-\mu}^{(1)} + \epsilon_\lambda^{(1)}}, \quad (B1)$$

Moreover, we replace in the denominator on the right-hand side of (B1) the $\epsilon_\kappa^{(1)}$ by $\epsilon_\kappa^{(0)}$, as the difference between the two is of relative order $\theta^{5/2}$ [see Eq. (3.9)]. We then get

$$\begin{aligned} R_\kappa = (\hbar^2/2N^2) P \sum_{\lambda,\mu} \tilde{n}_\lambda D(\lambda, \kappa, \lambda-\mathbf{u}, \kappa-\mathbf{u}) \\ \times D(\mathbf{u}, \kappa+\lambda-\mathbf{u}, \mathbf{u}-\lambda, \kappa-\mathbf{u}) / \\ D(\mathbf{u}, \kappa+\lambda-\mathbf{u}, \kappa, \lambda). \quad (B2) \end{aligned}$$

Comparing (B2) with (3.7) we see that R_κ is of the same order in θ as $\Delta\epsilon_\kappa$, but of higher order in S^{-1} . It will thus contribute to the θ^4 terms in $M(\beta)$ and C_{mag} , and the neglect of the quadratic terms in the \tilde{n}_λ and of the difference between $\epsilon_\kappa^{(1)}$ and $\epsilon_\kappa^{(0)}$ is thus justified. If we rearrange the sums in (B2) for the case of a simple-cubic lattice, we obtain Oguchi's result.⁹

APPENDIX C

In this Appendix we consider the “damping coefficient” γ_{κ} . We shall indicate a proof which shows that it is related to the lifetime τ_{κ} of a spin-wave as calculated by second-order time-dependent perturbation theory through the equation^{11,12}

$$\gamma_{\kappa}\tau_{\kappa}=\hbar. \quad (C1)$$

Once this relation has been established, we can use the results obtained from perturbation theory¹³ which shows that the contribution from γ_{κ} to $M(\beta)$ and C_{mag} will not arise until the $\theta^{9/2}$ -term at the earliest, and that (except for very short wavelength spin waves which will not be excited in the temperature range in which we are interested) $\gamma_{\kappa}\ll R_{\kappa}$.

The terms in the sum on the right-hand side of ex-

¹¹ Morkowski [Acta Phys. Polon. **19**, 3 (1960)] has also calculated τ_{κ} , but his results are slightly different from ours, due to slight errors in his numerical factors.

¹² For a discussion of the relation between the results obtained from Green function techniques and perturbation theory see also D. ter Haar, Kgl. Norske Videnskab. Selskabs, Forh. Skrifter **34**, No. 14 (1961) and D. ter Haar and H. Wergerland, Kgl. Norske Videnskab. Selskabs, Forh. Skrifter **34**, No. 15 (1961).

¹³ For instance, R. J. Elliott and H. Stern, *Report to the International Atomic Energy Agency Vienna Symposium on Inelastic Scattering of Neutrons in Solids and Liquids, Vienna October, 1960* [International Atomic Energy Agency (to be published)] or P. Pincus, M. Sparks, and R. C. Lecraw, Phys. Rev. **124**, 1015 (1961).

pression (2.9) for $H_{\text{id}}^{(1)}$ represent scattering processes where two spin-waves of wave-vectors \mathbf{v} and $\mathbf{\lambda}+\mathbf{u}-\mathbf{v}$ are annihilated and two spin waves of wave vectors $\mathbf{\lambda}$ and \mathbf{u} are created. The transition probability for such a process follows in a straightforward fashion from ordinary perturbation theory, if we use the well-known relations for boson operators. The delta function in (4.8) corresponds—provided we put $E=\epsilon_{\kappa}^{(1)}$ as we may do in the approximation in which we have been working throughout (compare the discussion in Appendix B)—to the energy-conservation law, while $A(\kappa, \mathbf{\lambda}_1, \mathbf{u}_1)$ contains both the exchange integrals which occur in $H_{\text{id}}^{(1)}$ and the occupation numbers which arise from the matrix elements of the a_{κ} and a_{κ}^{\dagger} . We must emphasize, though, that we have the thermodynamic averages of the \bar{n}_{λ} in (4.8) which do not occur in the quantum-mechanical formula. One can, however, show that this does not lead to an appreciable error.^{11,14} One obtains finally (C1) by writing down the transport equation for \bar{n}_{κ} , using the transition probabilities obtained from perturbation theory, and writing this transport equation in the form

$$(d\bar{n}_{\kappa}/dt)_{\text{scattering}} = -\bar{n}_{\kappa}/\tau_{\kappa}. \quad (C2)$$

¹⁴ A. Akhiezer, J. Phys. (U.S.S.R.) **10**, 217 (1946); M. I. Kaganov and V. M. Tsukernik, J. Exptl. Theoret. Phys. (U.S.S.R.) **34**, 1610 (1958) [translation: Soviet Phys.—JETP **7**, 1107 (1958)].