

THE CONTRIBUTION OF BUBBLE GRAPHS DUE TO DYNAMIC AND KINEMATIC SPIN WAVE INTERACTIONS TO THE GREEN FUNCTION OF THE NONCONDUCTING FERROMAGNET

BY K. ORLEWICZ

Institute of Molecular Physics of the Polish Academy of Sciences, Poznań*

(Received April 9, 1976)

Bloch's self-consistently renormalized spin wave approximation is extended to a kinematic interaction introduced by a kinematic operator. A uniform theory of dynamic and kinematic interactions in the bubble graph approximation is given. The resulting formula for the one-particle Green function is more general than those of previous works of this kind. Renormalization factors are obtained as the solutions of a set of three self-consistent integral equations which have to be dealt with numerically.

1. Introduction

The approximation of self-consistently renormalized spin waves (SCR) is generally considered to suffice for the correct description of the low temperature behaviour of Heisenberg ferromagnets and to account for their behaviour at higher temperatures excluding the critical region. This approximation, originally derived by Bloch [1], was subsequently improved and extended by Szaniecki [2] and by Loly [3]; The latter, using the diagrammatic perturbation theory obtained SCR as the result of summation over all possible bubble diagrams, his analysis being carried out for an arbitrary range of interactions between neighbours and nonzero uniaxial anisotropy.

Since SCR takes as a starting point the ideal Dyson spin wave model of a ferromagnet, kinematic effects, regarded as negligible, have not been taken into account. As long as we restrict ourselves to relatively low temperatures it is justified (Dyson [4], Wortis [5]) and SCR is well founded. The problem arises, however, of how to improve this approximation so that it should hold in the vicinity of the Curie point, where the kinematic effects can no longer be neglected and conventional SCR fails to describe correctly the experimental magnetization temperature dependence. We have to keep in mind that in order to transform the Heisenberg exchange Hamiltonian to its Dyson form, one replaces \hat{S}_j^z operating in $2S+1$ dimensional space by $-S+a_j^+a_j$ operating in the standard Hilbert space of all

* Address: Instytut Fizyki Molekularnej, PAN, Smoluchowskiego 17/19, 60-179 Poznań, Poland.

boson states. Therefore, in the ideal spin wave model, one evaluates traces over all boson states rather than over the lowest $(2S+1)^N$ states corresponding to the real physical deviations of the spins.

Several attempts have been made to include this effect into the theory. Szaniecki [6] (see also [16]), following Dyson [4], constructed a "kinematic" operator, i.e., a projection operator which cuts off all nonphysical spin deviations while the trace is taken. The kinematic operator, in principle, makes it possible to evaluate quantitatively the contribution of this so-called kinematic interaction to the Green function and partition function within the framework of Matsubara formalism (see [7, 8]). From the work based on the equation of motion method, we mention here that of Rudoi and Tserkovnikov [9, 10] (see also [11]). The authors expressed the Hamiltonian in terms of Pauli operators ($S = 1/2$) and basing on a formal solution of the equation of motion for the respective Green function (Tserkovnikov [12]) they were able to include the kinematic effects in their theory via non-boson commutation relations satisfied by the Pauli operators. The exact commutators were subsequently replaced by their mean values.

Our present aim is to include the kinematic interaction into the simple Loly scheme (via the method of Szaniecki), however, as opposed to [7, 8], without favouring either the dynamic or kinematic interaction. We propose a consistent theory (in the framework of the Hartree-Fock approximation) of spin waves, "dressing" the free spin wave propagator in all bubble diagrams of the dynamic and kinematic type, both types being treated on an equal footing. We shall show that Szaniecki's approach given in [7, 8] is a particular case of our approximation.

2. Formulation of the problem

We shall be dealing with the Dyson ideal Hamiltonian [3]:

$$H = H_0 + H_1, \quad (2.1)$$

$$H_0 = \sum_{\kappa} \omega_{\kappa} a_{\kappa}^{\dagger} a_{\kappa}, \quad (2.2)$$

$$\omega_{\kappa} = \varepsilon_{\kappa} + L + (2S+1)K, \quad \varepsilon_{\kappa} = \sum_i S J_i (\gamma_0^i - \gamma_{\kappa}^i), \quad (2.3)$$

$$H_1 = \sum_{\substack{\kappa\lambda \\ \kappa'\lambda'}} V_{\kappa\lambda\kappa'\lambda'} a_{\kappa}^{\dagger} a_{\lambda}^{\dagger} a_{\kappa'} a_{\lambda'}, \quad (2.4)$$

$$V_{\kappa\lambda\kappa'\lambda'} = \delta_{\kappa+\lambda, \kappa'+\lambda'} \left\{ \frac{1}{N} \sum_i \frac{1}{2} J_i (\gamma_{\kappa}^i - \gamma_{\lambda-\lambda'}^i) - \frac{K}{N} \right\}, \quad (2.5)$$

where a_{κ}^{\dagger} and a_{κ} represent the creation and annihilation operators of magnons, $\kappa, \kappa', \lambda, \lambda'$ are the reciprocal lattice vectors, i labels different coordination spheres, J_i is the exchange integral between i -th neighbours, and

$$\gamma_{\kappa}^i = \sum_{\varrho_i} \exp(i\kappa\varrho_i), \quad (2.6)$$

where ϱ_i denotes a site vector defining the position of each site in the i -th sphere — if there are Z_i sites in the i -th sphere, then $\gamma_0^i = Z_i$. In the above formulae S stands for the resultant spin quantum number of a single atom, N for the number of lattice sites in a crystalline specimen under consideration, K is the constant of the uniaxial anisotropy, and $L = g\mu_B H$, where H is the external magnetic field. For clarity, and to point out the connections between the present paper and [7, 8], we henceforth put the constant of the uniaxial anisotropy equal to zero ($K = 0$) and restrict summation over the coordination spheres to the sphere of the nearest neighbours ($i = 1$); nevertheless, our calculations can be performed throughout free of restrictions like those imposed above.

In order to permit a standard diagrammatic perturbation theory, it is useful to symmetrize the interaction vertex by replacing $V_{\kappa\lambda\kappa'\lambda'}$ by

$$\tilde{V}_{\kappa\lambda\kappa'\lambda'} = \frac{1}{4} (V_{\kappa\lambda\kappa'\lambda'} + V_{\kappa\lambda\lambda'\kappa'} + V_{\lambda\kappa\kappa'\lambda'} + V_{\lambda\kappa\lambda'\kappa'}). \quad (2.7)$$

It will enable us to express the perturbation theory expansions comprising H_1 in terms of compact boson diagrams [3].

Our main task is to determine the Green function (see, e. g., [13, 14]), since the Green function approach offers a direct route to the magnetization. According to [8], the one-particle kinematically improved Green function is given by the formula:

$$G_{\kappa_1\kappa_2}(\beta_1, \beta_2) = \frac{\text{Tr} \{ e^{-\beta H} \hat{T} [(e^{\beta_1 H} a_{\kappa_1}^+ e^{-\beta_1 H}) (e^{\beta_2 H} a_{\kappa_2} e^{-\beta_2 H}) \hat{K}_S] \}}{\text{Tr} (e^{-\beta H} \hat{K}_S)}, \quad (2.8)$$

where $\beta = 1/k_B T$, \hat{T} is Wick's ordering symbol, and \hat{K}_S the kinematic operator [6], mapping the standard space of all boson states onto the subspace of the lowest $(2S+1)^N$ physical states (in the coordinate representation), when the operation of taking the trace is being performed:

for $S = 1/2$

$$\begin{aligned} \hat{K}_{1/2} = & 1 - \frac{1}{2} \sum_f (a_f^+)^2 a_f^2 + \frac{1}{3} \sum_f (a_f^+)^3 a_f^3 + \frac{1}{2!} (-\frac{1}{2})^2 \sum_{f_1 f_2} (a_{f_1}^+)^2 (a_{f_2}^+)^2 a_{f_1}^2 a_{f_2}^2 \\ & - \frac{1}{4} \sum_f (a_f^+)^4 a_f^4 + (-\frac{1}{2}) (\frac{1}{3}) \sum_{f_1 f_2} (a_{f_1}^+)^2 (a_{f_2}^+)^3 a_{f_1}^2 a_{f_2}^3 + \frac{1}{5} \sum_f (a_f^+)^5 a_f^5 - \dots, \end{aligned} \quad (2.9a)$$

for $S = 1$

$$\begin{aligned} \hat{K}_1 = & 1 - \frac{1}{6} \sum_f (a_f^+)^3 a_f^3 + \frac{1}{8} \sum_f (a_f^+)^4 a_f^4 - \frac{1}{2 \cdot 6} \sum_f (a_f^+)^5 a_f^5 \\ & + \frac{1}{2!} (-\frac{1}{6})^2 \sum_{f_1 f_2} (a_{f_1}^+)^3 (a_{f_2}^+)^3 a_{f_1}^3 a_{f_2}^3 + \dots, \end{aligned} \quad (2.9b)$$

for $S = 3/2$

$$\hat{K}_{3/2} = 1 - \frac{1}{24} \sum_f (a_f^+)^4 a_f^4 + \frac{1}{30} \sum_f (a_f^+)^5 a_f^5 - \frac{1}{72} \sum_f (a_f^+)^6 a_f^6 + \dots \quad (2.9c)$$

Since the Green function (2.8) is written in momentum representation, all operators in (2.9a) (2.9b) (2.9c) should be expressed in terms of their Fourier transforms:

$$a_f^+ = N^{-1/2} \sum_{\lambda} a_{\lambda}^+ e^{i\lambda f}, \tag{2.10}$$

$$a_f = N^{-1/2} \sum_{\lambda} a_{\lambda} e^{-i\lambda f}. \tag{2.11}$$

Then, on carrying out the summation over all site vectors

$$\begin{aligned} \hat{K}_{1/2} = & 1 - \frac{1}{2} N^{-1} \sum_{\substack{\kappa\lambda \\ \kappa'\lambda'}} \delta_{\kappa+\lambda, \kappa'+\lambda'} a_{\kappa}^+ a_{\lambda}^+ a_{\kappa'} a_{\lambda'} \\ & + \frac{1}{3} N^{-2} \sum_{\substack{\kappa\lambda\varrho \\ \kappa'\lambda'\varrho'}} \delta_{\kappa+\lambda+\varrho, \kappa'+\lambda'+\varrho} a_{\kappa}^+ a_{\lambda}^+ a_{\varrho}^+ a_{\kappa'} a_{\lambda'} a_{\varrho'} \\ & + \frac{1}{2!} \left(-\frac{1}{2}\right)^2 N^{-2} \sum_{\substack{\kappa\lambda \\ \kappa'\lambda'}} \sum_{\substack{\mu\nu \\ \mu'\nu'}} \delta_{\kappa+\lambda, \kappa'+\lambda'} \delta_{\mu+\nu, \mu'+\nu'} a_{\kappa}^+ a_{\lambda}^+ a_{\mu}^+ a_{\nu}^+ a_{\kappa'} a_{\lambda'} a_{\mu'} a_{\nu'} \\ & - \frac{1}{4} N^{-3} \sum_{\substack{\kappa\lambda\varrho\sigma \\ \kappa'\lambda'\varrho'\sigma'}} \delta_{\kappa+\lambda+\varrho+\sigma, \kappa'+\lambda'+\varrho'+\sigma'} a_{\kappa}^+ a_{\lambda}^+ a_{\varrho}^+ a_{\sigma}^+ a_{\kappa'} a_{\lambda'} a_{\varrho'} a_{\sigma'} + \dots, \end{aligned} \tag{2.12a}$$

$$\begin{aligned} \hat{K}_1 = & 1 - \frac{1}{6} N^{-2} \sum_{\substack{\kappa\lambda\varrho \\ \kappa'\lambda'\varrho'}} \delta_{\kappa+\lambda+\varrho, \kappa'+\lambda'+\varrho} a_{\kappa}^+ a_{\lambda}^+ a_{\varrho}^+ a_{\kappa'} a_{\lambda'} a_{\varrho'} \\ & + \frac{1}{8} N^{-3} \sum_{\substack{\kappa\lambda\varrho\sigma \\ \kappa'\lambda'\varrho'\sigma'}} \delta_{\kappa+\lambda+\varrho+\sigma, \kappa'+\lambda'+\varrho'+\sigma'} a_{\kappa}^+ a_{\lambda}^+ a_{\varrho}^+ a_{\sigma}^+ a_{\kappa'} a_{\lambda'} a_{\varrho'} a_{\sigma'} + \dots, \end{aligned} \tag{2.12b}$$

$$\hat{K}_{3/2} = 1 - \frac{1}{24} N^{-3} \sum_{\substack{\kappa\lambda\varrho\sigma \\ \kappa'\lambda'\varrho'\sigma'}} \delta_{\kappa+\lambda+\varrho+\sigma, \kappa'+\lambda'+\varrho'+\sigma'} a_{\kappa}^+ a_{\lambda}^+ a_{\varrho}^+ a_{\sigma}^+ a_{\kappa'} a_{\lambda'} a_{\varrho'} a_{\sigma'} + \dots \tag{2.12c}$$

The kinematic operator consists of terms of the following structure:

$$\begin{aligned} & \frac{1}{h!} (B_r/N^{(r-1)})^h \sum_{\substack{\kappa_1, \lambda_1, \dots, \kappa'_1, \lambda'_1, \dots \\ \kappa_h, \lambda_h, \dots, \kappa'_h, \lambda'_h, \dots}} (\delta_{\kappa_1+\lambda_1+\dots, \kappa'_1+\lambda'_1+\dots}) \dots (\delta_{\kappa_h+\lambda_h+\dots, \kappa'_h+\lambda'_h+\dots}) \\ & \times \frac{1}{l!} (B_s/N^{(s-1)})^l \sum_{\substack{\mu_1, \nu_1, \dots, \mu'_1, \nu'_1, \dots \\ \mu_l, \nu_l, \dots, \mu'_l, \nu'_l, \dots}} (\delta_{\mu_1+\nu_1+\dots, \mu'_1+\nu'_1+\dots}) \dots (\delta_{\mu_l+\nu_l+\dots, \mu'_l+\nu'_l+\dots}) \dots \\ & \times \underbrace{(a_{\kappa_1}^+ a_{\lambda_1}^+ \dots) \dots (a_{\kappa_h}^+ a_{\lambda_h}^+ \dots)}_{\text{group of } r \text{ } a^+ \text{ operators recurring } h \text{ times}} \underbrace{(a_{\mu_1}^+ a_{\nu_1}^+ \dots) \dots (a_{\mu_l}^+ a_{\nu_l}^+ \dots)}_{\text{group of } s \text{ } a^+ \text{ operators recurring } l \text{ times}} \dots \\ & \times \underbrace{(a_{\kappa'_1} a_{\lambda'_1} \dots) \dots (a_{\kappa'_h} a_{\lambda'_h} \dots)}_{\text{group of } r \text{ } a \text{ operators recurring } h \text{ times}} \underbrace{(a_{\mu'_1} a_{\nu'_1} \dots) \dots (a_{\mu'_l} a_{\nu'_l} \dots)}_{\text{group of } s \text{ } a \text{ operators recurring } l \text{ times}} \dots \end{aligned} \tag{2.13}$$

Herein, $B_k(k = \dots r, \dots s, \dots)$ is a numerical factor depending on S ; for $S = 1/2$ $B_2 = 1/2$, $B_3 = -1/3$ etc.

The expression (2.8) can be put in the form (see [8] for details):

$$G_{\kappa_1 \kappa_2}(\beta_1, \beta_2) = \frac{\text{Tr} \{ e^{-\beta H_0} \hat{T} [a_{\kappa_1}^*(\beta_1) a_{\kappa_2}(\beta_2) \hat{S}(\beta) \hat{K}_S(0)] \}}{\text{Tr} [e^{-\beta H_0} \hat{S}(\beta) \hat{K}_S(0)]}, \quad (2.14)$$

where

$$\hat{S}(\beta) = e^{\beta H_0} e^{-\beta H} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^{\beta} d\tau_1 \dots \int_0^{\beta} d\tau_n \hat{T} [H_1(\tau_1) \dots H_1(\tau_n)], \quad (2.15)$$

$$a_{\kappa_1}^*(\beta_1) = e^{\beta_1 H_0} a_{\kappa_1}^+ e^{-\beta_1 H_0}, \quad (2.16)$$

$$a_{\kappa_2}(\beta_2) = e^{\beta_2 H_0} a_{\kappa_2} e^{-\beta_2 H_0}, \quad (2.17)$$

$$H_1(\tau_i) = e^{iH_0 \tau_i} H_1 e^{-iH_0 \tau_i}. \quad (2.18)$$

We can have recourse to Wick's theorem to calculate the thermodynamic mean value of formula (2.14) provided that, considering the arrangement of creation and annihilation operators in \hat{K}_S , we define

$$G_{\kappa_1 \kappa_2}^0(0, 0) = \delta_{\kappa_1 \kappa_2} n_{\kappa_1} \quad (n_{\kappa} = [\exp \beta \omega_{\kappa} - 1]^{-1}). \quad (2.19)$$

Similarly

$$G_{\kappa_1 \kappa_2}^0(\tau_i, \tau_i) = \delta_{\kappa_1 \kappa_2} n_{\kappa_1}. \quad (2.20)$$

Thus, following [8] again, we can write our Green function hereafter referred to as the modified Green function in terms of diagrams:

$$G_{\kappa_1 \kappa_2}(\beta_1, \beta_2) = \langle \hat{T} [a_{\kappa_1}^*(\beta_1) a_{\kappa_2}(\beta_2) \hat{S}(\beta) \hat{K}_S(0)] \rangle_c, \quad (2.21)$$

where c signifies that only connected diagrams should be taken into account (disconnected diagrams cancel out with the denominator in (2.14)). We have

$$G_{\kappa_1 \kappa_2}(\beta_1, \beta_2) = \sum_{n=0}^{\infty} G_{\kappa_1 \kappa_2}^{(n)}(\beta_1, \beta_2), \quad (2.22)$$

where

$$G_{\kappa_1 \kappa_2}^{(n)}(\beta_1, \beta_2) = \frac{(-1)^n}{n!} \int_0^{\beta} d\tau_1 \dots \int_0^{\beta} d\tau_n \langle \hat{T} [a_{\kappa_1}^*(\beta_1) a_{\kappa_2}(\beta_2) H_1(\tau_1) \dots H_1(\tau_n) \hat{K}_S(0)] \rangle_c. \quad (2.23)$$

3. The modified Green function in the bubble graph approximation

It proves convenient to represent each group of creation and annihilation operators in \hat{K}_S that correspond to one δ -function by an independent vertex, other rules of the graphical representation of the Green function being unchanged. Momentum is then pre-

served in every vertex. With the situation defined as above, we draw representative "bare" bubble graphs contributing to the modified Green function (Eqs (2.22) and (2.23)). For lack of space, we restrict ourselves to the case $S = 1/2$ (Fig. 1).

Two kinds of vertices occur in Fig. 1 — void circles and shaded circles — representing respectively groups of creation and annihilation operators from the kinematic and dynamic

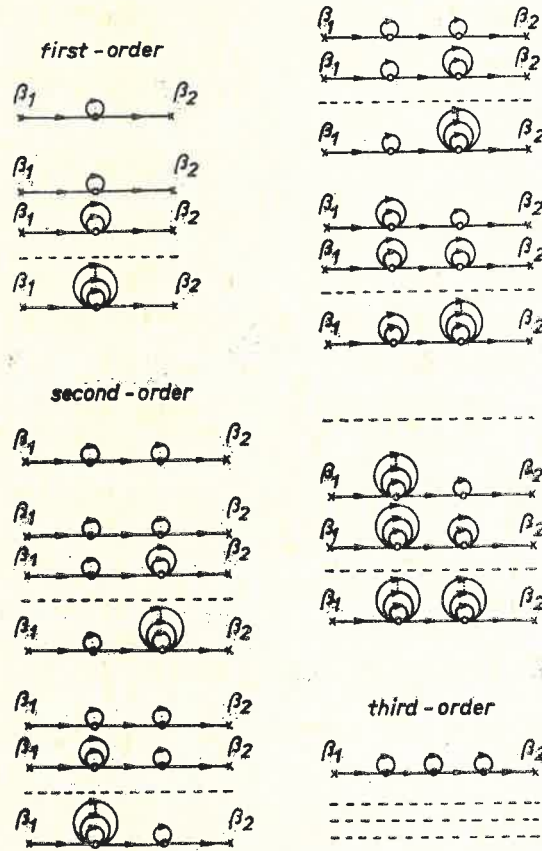


Fig. 1. Representative bare bubble graphs contributing to the modified Green function ($S = 1/2$)

parts of the Green function, the respective "times" being 0 and τ_i (i labels the dynamic vertices). Owing to the low symmetry of the diagrams with one line entering and one leaving, each diagram of $n+(h+l+\dots)$ -th order should be repeated $n!h!l!\dots$ -fold with n vertices corresponding to the dynamic and h, l, \dots to the kinematic part of the Green function permuted within either type. As each of the $n!h!l!\dots$ diagrams contributes equally to the Green function, the number of equivalent diagrams cancels out with the highly inconvenient factor $\frac{1}{n!} \frac{1}{h!} \frac{1}{l!} \dots$ (Cf(2.13) and (2.23)). In other words, we can regard our diagrams as unlabelled, all shaded circles, as well as all void circles with the same number of entering and leaving lines, being indistinguishable. It is worth empha-

sizing that these remarks refer to all diagrams of the kinematic-dynamic type, not only to the "bare" bubble graphs drawn in Fig. 1.

We now proceed to derive explicitly the contribution of the bubble graphs drawn in Fig. 1 to the modified Green function. Let us denote by \mathcal{K}_S the contribution from all irreducible diagrams comprising only kinematic operator elements

$$\mathcal{K}_{1/2} = \text{[diagram 1]} + \text{[diagram 2]} + \dots + \text{[diagram 3]} \quad \text{for } S = 1/2, \quad (3.1a)$$

$$\mathcal{K}_1 = \text{[diagram 4]} + \text{[diagram 5]} + \dots + \text{[diagram 6]} \quad \text{for } S = 1, \quad (3.1b)$$

$$\mathcal{K}_{3/2} = \text{[diagram 7]} + \text{[diagram 8]} + \dots + \text{[diagram 9]} \quad \text{for } S = 3/2, \quad (3.1c)$$

(in- and out-going lines are not included into \mathcal{K}_S). We refer to \mathcal{K}_S as the kinematic irreducible part, by analogy to the proper (dynamic) irreducible part \mathcal{D}_κ containing the interaction Hamiltonian:

$$\mathcal{D}_\kappa = \text{[diagram 10]} \quad (3.2)$$

Grouping together diagrams differing only in the number of in- and out-going lines at "kinematic" vertices, we write the Green function contributions of all orders in terms of \mathcal{K}_S , \mathcal{D}_κ and G_κ^0 . Then, having integrated over τ_i s, we sum up the contributions due to each class of bubble graphs and, after straightforward calculations (the reader is referred to Appendix A for details), we obtain

$$G_\kappa^S(\beta_1, \beta_2) = e^{(\beta_1 - \beta_2)(\omega_\kappa - \mathcal{D}_\kappa)} [\theta(\beta_2 - \beta_1) + \bar{n}_\kappa + \mathcal{K}_S \bar{n}_\kappa (\bar{n}_\kappa + 1) + \mathcal{K}_S^2 \bar{n}_\kappa^2 (\bar{n}_\kappa + 1) + \dots], \quad (3.3)$$

where

$$\bar{n}_\kappa = \frac{1}{\exp \beta(\omega_\kappa - \mathcal{D}_\kappa) - 1}. \quad (3.4)$$

The geometrical series is accessible to summation provided that $\mathcal{K}_S < 1$. Finally, we obtain the following expression for the modified Green function in the "bare bubble" approximation:

$$G_\kappa^S(\beta_1, \beta_2) = e^{(\beta_1 - \beta_2)(\omega_\kappa - \mathcal{D}_\kappa)} \left[\theta(\beta_2 - \beta_1) + \frac{1 + \mathcal{K}_S}{\exp \beta(\omega_\kappa - \mathcal{D}_\kappa) - (1 + \mathcal{K}_S)} \right]. \quad (3.5)$$

Herein, by definition,

$$\mathcal{K}_{1/2} = -\frac{2}{2} 2! \left[\frac{1}{N} \sum_{\kappa'} G_{\kappa'}^0(0, 0) \right] + \frac{3}{3} 3! \left[\frac{1}{N} \sum_{\kappa'} G_{\kappa'}^0(0, 0) \right]^2 - \dots, \quad (3.6a)$$

$$\mathcal{K}_1 = -\frac{3}{6} 3! \left[\frac{1}{N} \sum_{\kappa'} G_{\kappa'}^0(0, 0) \right]^2 + \frac{4}{8} 4! \left[\frac{1}{N} \sum_{\kappa'} G_{\kappa'}^0(0, 0) \right]^3 - \dots, \quad (3.6b)$$

$$\mathcal{K}_{3/2} = -\frac{4}{24} 4! \left[\frac{1}{N} \sum_{\kappa'} G_{\kappa'}^0(0, 0) \right]^3 + \frac{5}{30} 5! \left[\frac{1}{N} \sum_{\kappa'} G_{\kappa'}^0(0, 0) \right]^4 - \dots \quad (3.6c)$$

and

$$\mathcal{D}_\kappa = -4 \sum_{\kappa'} \tilde{V}_{\kappa'\kappa\kappa'\kappa} G_{\kappa'}^0(\tau_i, \tau_i), \tag{3.7}$$

where, according to (2.19) and (2.20), $G_\kappa^0(0, 0) = G_\kappa^0(\tau_i, \tau_i) = n_{\kappa'}$. The numbers of possible connections at various vertices, responsible for the numbers of equivalent diagrams, are correctly included by the numerical factors preceding the respective terms. The fractions in (3.6) arise from the definition of \tilde{K}_S (see (2.9)).

The next step consists in the replacement of "bare" bubbles in (3.1) and (3.2) by "dressed" bubbles (Fig. 2), $G_\kappa^0(0, 0)$ and $G_\kappa^0(\tau_i, \tau_i)$ in (3.6) and (3.7) being replaced by $G_\kappa^S(0, 0)$ and $G_\kappa^S(\tau_i, \tau_i)$, respectively. To find the form of $G_\kappa^S(0, 0)$ explicitly, we have to

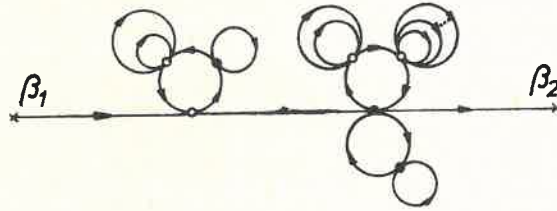


Fig. 2. Representative diagram under summation in the "once-dressed bubble" approximation

reiterate the derivation procedure of formula (3.5) albeit with β_1 and β_2 put equal to zero from the start. As might be expected, instead of (3.5) we get

$$G_\kappa^S(0, 0) = \bar{n}_\kappa + \mathcal{H}_S \bar{n}_\kappa^2 + \mathcal{H}_S^2 \bar{n}_\kappa^3 + \dots = \frac{1}{\exp \beta(\omega_\kappa - \mathcal{D}_\kappa) - (1 + \mathcal{H}_S)}. \tag{3.8}$$

From (3.5) we get immediately

$$G_\kappa^S(\tau_i, \tau_i) = \frac{1 + \mathcal{H}_S}{\exp \beta(\omega_\kappa - \mathcal{D}_\kappa) - (1 + \mathcal{H}_S)} = \frac{1}{(1 + \mathcal{H}_S)^{-1} \exp \beta(\omega_\kappa - \mathcal{D}_\kappa) - 1}. \tag{3.9}$$

Hence, in the "once-dressed bubble" approximation we obtain

$$\mathcal{H}_{1/2}^{(1)} = -\frac{2}{2} 2! \left[\frac{1}{N} \sum_{\kappa'} (1 + \mathcal{H}_{1/2})^{-1} \bar{n}_{\kappa'}^{(1/2)} \right] + \frac{3}{3} 3! \left[\frac{1}{N} \sum_{\kappa'} (1 + \mathcal{H}_{1/2})^{-1} \bar{n}_{\kappa'}^{(1/2)} \right]^2 - \dots, \tag{3.10a}$$

$$\mathcal{H}_1^{(1)} = -\frac{3}{6} 3! \left[\frac{1}{N} \sum_{\kappa'} (1 + \mathcal{H}_1)^{-1} \bar{n}_{\kappa'}^{(1)} \right]^2 + \frac{4}{8} 4! \left[\frac{1}{N} \sum_{\kappa'} (1 + \mathcal{H}_1)^{-1} \bar{n}_{\kappa'}^{(1)} \right]^3 - \dots, \tag{3.10b}$$

$$\mathcal{H}_{3/2}^{(1)} = -\frac{4}{24} 4! \left[\frac{1}{N} \sum_{\kappa'} (1 + \mathcal{H}_{3/2})^{-1} \bar{n}_{\kappa'}^{(3/2)} \right]^3 + \frac{5}{30} 5! \left[\frac{1}{N} \sum_{\kappa'} (1 + \mathcal{H}_{3/2})^{-1} \bar{n}_{\kappa'}^{(3/2)} \right]^4 - \dots \tag{3.10c}$$

and

$$\mathcal{D}_\kappa^{S(1)} = -4 \sum_{\kappa'} \tilde{V}_{\kappa'\kappa\kappa'\kappa} \bar{n}_{\kappa'}^S, \quad (3.11)$$

where, by definition (see 3.9),

$$\bar{n}_{\kappa'}^S = \frac{1}{(1 + \mathcal{H}_S)^{-1} \exp \beta(\omega_{\kappa'} - \mathcal{D}_{\kappa'}) - 1}. \quad (3.12)$$

Subsequently, we can substitute

$$G_\kappa^{S(1)}(0, 0) = \frac{1}{\exp \beta(\omega_{\kappa'} - \mathcal{D}_{\kappa'}^{S(1)}) - (1 + \mathcal{H}_S^{(1)})} \quad (3.13)$$

for $G_\kappa^0(0, 0)$ in (3.6) and

$$G_\kappa^{S(1)}(\tau_i, \tau_i) = \frac{1}{(1 + \mathcal{H}_S^{(1)})^{-1} \exp \beta(\omega_{\kappa'} - \mathcal{D}_{\kappa'}^{S(1)}) - 1} \quad (3.14)$$

for $G_\kappa^0(\tau_i, \tau_i)$ in (3.7), obtaining as a result $\mathcal{H}_S^{(2)}$ and $\mathcal{D}_\kappa^{S(2)}$ in the "twice-dressed bubble" approximation. Repeating the procedure again and again on the assumption that, for $n \rightarrow \infty$,

$$\mathcal{H}_S^{(n+1)} \approx \mathcal{H}_S^{(n)} \rightarrow \tilde{\mathcal{H}}_S \quad (3.15)$$

and

$$\mathcal{D}_\kappa^{S(n+1)} \approx \mathcal{D}_\kappa^{S(n)} \rightarrow \tilde{\mathcal{D}}_\kappa^S \quad (3.16)$$

we finally obtain the following self-consistent sets of equations:

$$\tilde{\mathcal{H}}_{1/2} = -\frac{2}{2} 2! \left[\frac{1}{N} \sum_{\kappa'} (1 + \tilde{\mathcal{H}}_{1/2})^{-1} \tilde{n}_{\kappa'}^{(1/2)} \right] + \frac{3}{3} 3! \left[\frac{1}{N} \sum_{\kappa'} (1 + \tilde{\mathcal{H}}_{1/2})^{-1} \tilde{n}_{\kappa'}^{(1/2)} \right]^2 - \dots, \quad (3.17a)$$

$$\tilde{\mathcal{H}}_1 = -\frac{3}{6} 3! \left[\frac{1}{N} \sum_{\kappa'} (1 + \tilde{\mathcal{H}}_1)^{-1} \tilde{n}_{\kappa'}^{(1)} \right]^2 + \frac{4}{8} 4! \left[\frac{1}{N} \sum_{\kappa'} (1 + \tilde{\mathcal{H}}_1)^{-1} \tilde{n}_{\kappa'}^{(1)} \right]^3 - \dots \quad (3.17b)$$

$$\tilde{\mathcal{H}}_{3/2} = -\frac{4}{24} 4! \left[\frac{1}{N} \sum_{\kappa'} (1 + \tilde{\mathcal{H}}_{3/2})^{-1} \tilde{n}_{\kappa'}^{(3/2)} \right]^3 + \frac{5}{36} 5! \left[\frac{1}{N} \sum_{\kappa'} (1 + \tilde{\mathcal{H}}_{3/2})^{-1} \tilde{n}_{\kappa'}^{(3/2)} \right]^4 - \dots, \quad (3.17c)$$

and

$$\tilde{\mathcal{D}}_\kappa^S = -4 \sum_{\kappa'} \tilde{V}_{\kappa'\kappa\kappa'\kappa} \tilde{n}_{\kappa'}^S, \quad (3.18)$$

where

$$\tilde{n}_{\kappa'}^S = \frac{1}{(1 + \tilde{\mathcal{H}}_S)^{-1} \exp \beta(\omega_{\kappa'} - \tilde{\mathcal{D}}_\kappa^S) - 1}. \quad (3.19)$$

For the cubic ferromagnet, and keeping in mind our basic restriction to nearest neighbours ($i = 1$) and to zero uniaxial anisotropy ($K = 0$), formula (3.18) transforms to:

$$\tilde{\mathcal{D}}_{\kappa}^S = \varepsilon_{\kappa} \frac{1}{SN} \sum_{\kappa'} (1 - \gamma_{\kappa'}/\gamma_0) \tilde{n}_{\kappa'}^S \quad (3.20)$$

(for details, see [3]). We can now rewrite the sets of equations (3.17)–(3.19) in more compact form by introducing the new quantities

$$Y_S = \frac{1}{N} \sum_{\kappa} (1 - \gamma_{\kappa}/\gamma_0) \tilde{n}_{\kappa}^S, \quad (3.21)$$

$$X_S = \frac{1}{N} \sum_{\kappa} (1 + \tilde{\mathcal{K}}_S)^{-1} \tilde{n}_{\kappa}^S. \quad (3.22)$$

We thus have
for $S = 1/2$

$$\tilde{n}_{\kappa} = \frac{1}{(1 - 2!X + 3!X^2 - \dots)^{-1} \exp \beta[\varepsilon_{\kappa}(1 - Y/S) + L] - 1}, \quad (3.23a)$$

$$Y = \frac{1}{N} \sum_{\kappa} (1 - \gamma_{\kappa}/\gamma_0) \tilde{n}_{\kappa}, \quad (3.24a)$$

$$X = (1 - 2!X + 3!X^2 - \dots)^{-1} \frac{1}{N} \sum_{\kappa} \tilde{n}_{\kappa}. \quad (3.25a)$$

for $S = 1$

$$\tilde{n}_{\kappa} = \frac{1}{(1 - \frac{1}{2} 3!X^2 + \frac{1}{2} 4!X^3 - \dots)^{-1} \exp \beta[\varepsilon_{\kappa}(1 - Y/S) + L] - 1}, \quad (3.23b)$$

$$Y = \frac{1}{N} \sum_{\kappa} (1 - \gamma_{\kappa}/\gamma_0) \tilde{n}_{\kappa}, \quad (3.24b)$$

$$X = (1 - \frac{1}{2} 3!X^2 + \frac{1}{2} 4!X^3 - \dots)^{-1} \frac{1}{N} \sum_{\kappa} \tilde{n}_{\kappa}, \quad (3.25b)$$

for $S = 3/2$

$$\tilde{n}_{\kappa} = \frac{1}{(1 - \frac{1}{6} 4!X^3 + \frac{1}{6} 5!X^4 - \dots)^{-1} \exp \beta[\varepsilon_{\kappa}(1 - Y/S) + L] - 1}, \quad (3.23c)$$

$$Y = \frac{1}{N} \sum_{\kappa} (1 - \gamma_{\kappa}/\gamma_0) \tilde{n}_{\kappa}, \quad (3.24c)$$

$$X = (1 - \frac{1}{6} 4!X^3 + \frac{1}{6} 5!X^4 - \dots)^{-1} \frac{1}{N} \sum_{\kappa} \tilde{n}_{\kappa}. \quad (3.25c)$$

The modified Green function has the form

$$G_{\kappa}^S(\beta_1, \beta_2) = e^{(\beta_1 - \beta_2) [\epsilon_{\kappa}(1 - Y/S) + L]} [\theta(\beta_1 - \beta_2) \tilde{n}_{\kappa}^S + \theta(\beta_2 - \beta_1) (\tilde{n}_{\kappa}^S + 1)] \quad (3.26)$$

whence the magnetization becomes

$$\mu(T) = 1 - \frac{1}{SN} \sum_{\kappa} G_{\kappa}^S(\beta + 0, \beta) = 1 - \frac{1}{SN} \sum_{\kappa} \tilde{n}_{\kappa}^S. \quad (3.27)$$

The above formulae contain the series

$$f_{1/2}(X) = 1 - 2!X + 3!X^2 - \dots, \quad (3.28a)$$

$$f_1(X) = 1 - \frac{1}{2} 3!X^2 + \frac{1}{2} 4!X^3 - \dots, \quad (3.28b)$$

$$f_{3/2}(X) = 1 - \frac{1}{6} 4!X^3 + \frac{1}{6} 5!X^4 - \dots, \quad (3.28c)$$

usually referred to as being semiconvergent (see, e. g., [11]). Hitherto, we took into account the kinematic operator terms (2.13) with $k \leq n$, the structural terms in the series (2.9) being cut off at some term, for instance at the one with $k = n$, where n is a small number. This implies that the series (3.28) are truncated at X^{n+1} ; moreover, because $X \ll 1$, the contribution of higher power terms in these series is negligible as long as n is a small number, and we are justified in retaining the first terms only.

$$f_{1/2}(X) = 1 - 2X, \quad (3.29a)$$

$$f_1(X) = 1 - 3X^2, \quad (3.29b)$$

$$f_{3/2}(X) = 1 - 4X^3. \quad (3.29c)$$

The inequality $X \ll 1$ may be seen to be true by iterating each set of equations (3.23) - (3.25) with the initial conditions $X = 0$, $Y = 0$ and

$$\frac{1}{N} \sum_{\kappa} n_{\kappa} \ll 1. \quad (3.30)$$

The condition $\mathcal{K}_S < 1$ is a direct consequence of the inequality (3.30), valid in a fairly wide range of temperatures, all the iteration procedure that leads to Eqs (3.23) - (3.25) being therefore justified. When lower temperatures are taken into account, the inequality (3.30) is fulfilled more strictly and the value of n for which the condition $\mathcal{K}_S < 1$ can still be presumed to be satisfied is larger.

4. Nature of the approximation

Were we to allow for terms of all orders from \hat{K}_S , the series (3.28) would become divergent. Consequently, we are always restricted to a finite number of kinematic "structural" terms. The omission of higher order terms in (2.9) is, however, far from being obvious,

for n (cf. Sect. 3) was chosen quite arbitrarily. Our objections are founded on the following considerations:

Let us write the kinematic operator in the form given by Yuin [16]:

$$\hat{K}_S = \prod_f \vartheta_S(a_f^+, a_f), \quad (4.1)$$

where

$$\begin{aligned} \vartheta_S(a_f^+, a_f) &= 1 + b_0(2S)a_f^{+2S+1}a_f^{2S+1} + b_1(2S)a_f^{+(2S+1)+1}a_f^{(2S+1)+1} \\ &\dots + b_l(2S)a_f^{+(2S+1)+l}a_f^{(2S+1)+l} + \dots, \quad b_l(2S) = -\frac{(-1)^l}{(2S)!!(l+2S+1)}. \end{aligned} \quad (4.2)$$

This form of \hat{K}_S is equivalent to that given by Szaniecki in [6]. One can show [17] that the following relations hold:

$$\begin{aligned} &1 + b_0(2S)a_f^+a_f(a_f^+a_f - 1) \dots (a_f^+a_f - 2S) + b_1(2S)a_f^+a_f(a_f^+a_f - 1) \dots (a_f^+a_f - 2S - 1) \\ &\dots + b_{(n-1)-2S}(2S)a_f^+a_f(a_f^+a_f - 1) \dots (a_f^+a_f - (n-1)) \\ &= 1 + b_0(2S)a_f^{+2S+1}a_f^{2S+1} + b_1(2S)a_f^{+(2S+1)+1}a_f^{(2S+1)+1} + \dots + b_{(n-1)-2S}(2S)a_f^{+n}a_f \end{aligned} \quad (4.3)$$

and

$$\begin{aligned} &1 + b_0(2S)n(n-1) \dots (n-2S) + b_1(2S)n(n-1) \dots (n-2S-1) + \dots + b_{(n-1)-2S}(2S)n! \\ &= \theta(2S-n). \end{aligned} \quad (4.4)$$

Suppose we now replace the full Yuin series (4.2) by the series containing the first $n-2S+1$ terms only. Since $a_f^{+n}a_f^n|m_f\rangle = 0$ for $n > m_f$, in view of (4.3) and (4.4) this would imply that the statistical sum over the states up to n -fold excited ones would be calculated correctly and we would be liable to errors only when calculating a part of the sum comprising the higher excited states, the contribution of which is comparatively smaller. This sounds logical; still, such a procedure is by no means equivalent to neglecting the higher order structural terms of \hat{K}_S . In fact, on performing the multiplication in (4.1), we again get an infinite series of the form (2.9), with coefficients B_k (see (2.13)) modified from $k = n+1$ upwards.

In other words, if every vertex is to be repeated an infinite number of times ($N \rightarrow \infty$) and if we want the approximation to be consistent mathematically, we cannot avoid dealing with an infinite number of structural terms of $\hat{K}_S(n \rightarrow \infty)$. Therefore, if one intends to construct a theory valid for the whole temperature range, one cannot restrict oneself to the bubble graph approximation. This approximation, although fully satisfactory as far as only dynamic interaction is concerned, seems to be hardly sufficient with regard to the kinematic interaction. Our approach should be extended so as to include a wider class of graphs than the mere bubbles and it is not until we sum them up that we shall be able to get rid of the divergences arising now for $n \rightarrow \infty$. Fortunately, formula (3.5) is quite general and should hold in other approximations as well, so long as mixed dynamic-

-kinematic terms are neglected. Only the forms of \mathcal{H}_S and \mathcal{D}_κ depend on the particular approximation used here. We intend to deal with this problem in our next paper. So far, we regard our results as a first step in this direction.

At low temperatures, in common with other first order theories based on the Hartree-Fock approximation, we get a spurious T^3 term in the magnetization. The occurrence of such a term due to the kinematic interaction appears to be a common feature of all Hartree-Fock-like approximations allowing for kinematic effects (cf. [9]).

5. Comments on related work

The set of simultaneous integral equations derived by us for each S reduces to a set of two equations if we neglect either kinematic or dynamic interaction.

In the first case, we get a set of equations identical with that of self-consistently renormalized spin wave theory [2, 3]

$$\tilde{n}_\kappa = \frac{1}{\exp \beta[\epsilon_\kappa(1 - Y/S) + L] - 1}, \quad (5.1)$$

$$Y = \frac{1}{N} \sum_\kappa (1 - \gamma_\kappa/\gamma_0) \tilde{n}_\kappa. \quad (5.2)$$

In the latter case, if kinematic effects only are taken into account, one gets the following sets of equations:

for $S = 1/2$

$$\tilde{n}_\kappa = \frac{1}{(1 - 2!X + 3!X^2 - \dots)^{-1} \exp \beta(\epsilon_\kappa + L) - 1}, \quad (5.3a)$$

$$X = (1 - 2!X + 3!X^2 - \dots)^{-1} \frac{1}{N} \sum_\kappa \tilde{n}_\kappa, \quad (5.4a)$$

for $S = 1$

$$\tilde{n}_\kappa = \frac{1}{(1 - \frac{1}{2} 3!X^2 + \frac{1}{2} 4!X^3 - \dots)^{-1} \exp \beta(\epsilon_\kappa + L) - 1}, \quad (5.3b)$$

$$X = (1 - \frac{1}{2} 3!X^2 + \frac{1}{2} 4!X^3 - \dots)^{-1} \frac{1}{N} \sum_\kappa \tilde{n}_\kappa, \quad (5.4b)$$

for $S = 3/2$

$$\tilde{n}_\kappa = \frac{1}{(1 - \frac{1}{6} 4!X^3 + \frac{1}{6} 5!X^4 - \dots)^{-1} \exp \beta(\epsilon_\kappa + L) - 1}, \quad (5.3c)$$

$$X = (1 - \frac{1}{6} 4!X^3 + \frac{1}{6} 5!X^4 - \dots)^{-1} \frac{1}{N} \sum_\kappa \tilde{n}_\kappa. \quad (5.4c)$$

The value of \tilde{n}_κ for $S = 1/2$ obtained by successive iterations from equations (5.3a)-(5.4a) ($X^{(0)} = 0$) was compared by us with the expression $\langle a_\kappa^+ a_\kappa \hat{K}_S \rangle_0$,

calculated in the bubble graph approximation directly from Wick's theorem (including the terms: $1 - \frac{1}{2} \sum_f a_f^{+2} a_f^2 + \frac{1}{3} \sum_f a_f^{+3} a_f^3 - \frac{1}{4} \sum_f a_f^{+4} a_f^4 + \frac{1}{2!} (-\frac{1}{2})^2 \sum_{f_1 f_2} a_{f_1}^{+2} a_{f_2}^{+2} a_{f_1}^2 a_{f_2}^2 + (-\frac{1}{2}) (\frac{1}{3}) \sum_{f_1 f_2} a_{f_1}^{+2} a_{f_2}^{+3} a_{f_1}^2 a_{f_2}^3 + \frac{1}{3!} (-\frac{1}{2})^3 \sum_{f_1 f_2 f_3} a_{f_1}^{+2} a_{f_2}^{+2} a_{f_3}^{+2} a_{f_1}^2 a_{f_2}^2 a_{f_3}^2$), proving without doubt the validity of equations (5.3) and (5.4). A similar renormalization on the basis of the partition function approach was carried out in [7]. The results are strictly equivalent since the same class of diagrams is taken into account in both cases, though this equivalence is hardly obvious in a direct way since the two results are expressed in different terms, the functions \tilde{n}_κ of our paper and $\tilde{\tilde{n}}_\kappa$ of [7] being only apparently identical. Concerning the renormalization due to kinematic effects within the Green function approach, however, our renormalization given by Eqs (5.3)–(5.4) is in our opinion the only possible one.

Throughout this investigation, dynamic and kinematic interactions are regarded as equivalent from the mathematical point of view, neither being favoured in any way. In [7] the kinematic interaction is “dressed” in dynamic interaction, so that diagrams corresponding in the “language” of Green functions to those like (a) of Fig. 3 are absent, whereas in



Fig. 3. Representative diagrams not taken into account in Szaniecki's approach

[8], inversely, the dynamic interaction is “dressed” in the kinematic one and hence diagrams like (b) of Fig. 3 are absent. Both (a) and (b) have been included in our approximation; in this respect, our approach is more general.

The author is strongly indebted to Dr J. Szaniecki for his interest and thoughtful help throughout this investigation.

APPENDIX A

Referring the reader to Fig. 1, we have in the zeroth order

$$G_\kappa^0(\beta_1, \beta_2) = e^{(\beta_1 - \beta_2)\omega_\kappa} [\theta(\beta_1 - \beta_2)n_\kappa + \theta(\beta_2 - \beta_1)(n_\kappa + 1)]; \quad (\text{A.1})$$

in the first order

$$\int_0^\beta d\tau_1 G_\kappa^0(\beta_1, \tau_1) \mathcal{D}_\kappa G_\kappa^0(\tau_1, \beta_2) = e^{(\beta_1 - \beta_2)\omega_\kappa} \mathcal{D}_\kappa \left\{ \frac{1}{1!} \beta n_\kappa (n_\kappa + 1) - \frac{1}{1!} (\beta_1 - \beta_2) [\theta(\beta_1 - \beta_2)n_\kappa + \theta(\beta_2 - \beta_1)(n_\kappa + 1)] \right\}, \quad (\text{A.2})$$

$$G_\kappa^0(\beta_1, 0) \mathcal{H}_S G_\kappa^0(0, \beta_2) = e^{(\beta_1 - \beta_2)\omega_\kappa} \mathcal{H}_S n_\kappa (n_\kappa + 1); \quad (\text{A.3})$$

in the second order

$$\begin{aligned} & \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 G_\kappa^0(\beta_1, \tau_1) \mathcal{D}_\kappa G_\kappa^0(\tau_1, \tau_2) \mathcal{D}_\kappa(\tau_2, \beta_2) \\ &= e^{(\beta_1 - \beta_2)\omega_\kappa} \mathcal{D}_\kappa^2 \left\{ \frac{1}{2!} \beta^2 [n_\kappa^2(n_\kappa + 1) + n_\kappa(n_\kappa + 1)^2] - \frac{1}{1!} \beta \frac{1}{1!} (\beta_1 - \beta_2) n_\kappa(n_\kappa + 1) \right. \\ & \quad \left. + \frac{1}{2!} (\beta_1 - \beta_2)^2 [\theta(\beta_1 - \beta_2) n_\kappa + \theta(\beta_2 - \beta_1) (n_\kappa + 1)] \right\}, \end{aligned} \quad (\text{A.4})$$

$$\begin{aligned} & \int_0^\beta d\tau_1 G_\kappa^0(\beta_1, \tau_1) \mathcal{D}_\kappa G_\kappa^0(\tau_1, 0) \mathcal{K}_S G_\kappa^0(0, \beta_2) \\ &= e^{(\beta_1 - \beta_2)\omega_\kappa} \mathcal{D}_\kappa \mathcal{K}_S \left[\frac{1}{1!} \beta n_\kappa(n_\kappa + 1)^2 - \frac{1}{1!} \beta_1 n_\kappa(n_\kappa + 1) \right], \end{aligned} \quad (\text{A.5})$$

$$\begin{aligned} & \int_0^\beta d\tau_1 G_\kappa^0(\beta_1, 0) \mathcal{K}_S G_\kappa^0(0, \tau_1) \mathcal{D}_\kappa G_\kappa^0(\tau_1, \beta_2) \\ &= e^{(\beta_1 - \beta_2)\omega_\kappa} \mathcal{K}_S \mathcal{D}_\kappa \left[\frac{1}{1!} \beta n_\kappa^2(n_\kappa + 1) - \frac{1}{1!} (-\beta_2) n_\kappa(n_\kappa + 1) \right], \end{aligned} \quad (\text{A.6})$$

$$G_\kappa^0(\beta_1, 0) \mathcal{K}_S G_\kappa^0(0, 0) \mathcal{K}_S G_\kappa^0(0, \beta_2) = e^{(\beta_1 - \beta_2)\omega_\kappa} \mathcal{K}_S^2 n_\kappa^2(n_\kappa + 1); \quad (\text{A.7})$$

etc.

On combining terms with equal powers of \mathcal{K}_S and \mathcal{D}_κ , we get

$$\begin{aligned} G_\kappa(\beta_1, \beta_2) &= e^{(\beta_1 - \beta_2)\omega_\kappa} \left([\theta(\beta_1 - \beta_2) n_\kappa + \theta(\beta_2 - \beta_1) (n_\kappa + 1)] \right. \\ &+ \mathcal{D}_\kappa \left\{ \frac{1}{1!} \beta n_\kappa(n_\kappa + 1) - \frac{1}{1!} (\beta_1 - \beta_2) [\theta(\beta_1 - \beta_2) n_\kappa + \theta(\beta_2 - \beta_1) (n_\kappa + 1)] \right\} + \mathcal{K}_S n_\kappa(n_\kappa + 1) \\ &+ \mathcal{D}_\kappa^2 \left\{ \frac{1}{2!} \beta^2 [n_\kappa^2(n_\kappa + 1) + n_\kappa(n_\kappa + 1)^2] - \frac{1}{1!} \beta \frac{1}{1!} (\beta_1 - \beta_2) n_\kappa(n_\kappa + 1) \right. \\ & \quad \left. + \frac{1}{2!} (\beta_1 - \beta_2)^2 [\theta(\beta_1 - \beta_2) n_\kappa + \theta(\beta_2 - \beta_1) (n_\kappa + 1)] \right\} \\ &+ \mathcal{K}_S \mathcal{D}_\kappa \left\{ \frac{1}{1!} \beta [n_\kappa^2(n_\kappa + 1) + n_\kappa(n_\kappa + 1)^2] - \frac{1}{1!} (\beta_1 - \beta_2) n_\kappa(n_\kappa + 1) \right\} + \mathcal{K}_S^2 n_\kappa^2(n_\kappa + 1) + \dots \Big). \end{aligned} \quad (\text{A.8})$$

We can rewrite the preceding expression in the form

$$\begin{aligned}
 G_{\kappa}(\beta_1, \beta_2) &= e^{(\beta_1 - \beta_2)\omega_{\kappa}} \left([\theta(\beta_2 - \beta_1) \right. \\
 &+ n_{\kappa}] \left[1 - \frac{1}{1!} (\beta_1 - \beta_2) \mathcal{D}_{\kappa} + \frac{1}{2!} (\beta_1 - \beta_2)^2 \mathcal{D}_{\kappa}^2 - \dots \right] \\
 &+ \frac{1}{1!} (\beta \mathcal{D}_{\kappa}) n_{\kappa} (n_{\kappa} + 1) \left[1 - \frac{1}{1!} (\beta_1 - \beta_2) \mathcal{D}_{\kappa} + \dots \right] \\
 &+ \frac{1}{2!} (\beta \mathcal{D}_{\kappa})^2 [n_{\kappa}^2 (n_{\kappa} + 1) + n_{\kappa} (n_{\kappa} + 1)^2] [1 - \dots] + \dots \\
 &+ \mathcal{K}_S \left\{ n_{\kappa} (n_{\kappa} + 1) \left[1 - \frac{1}{1!} (\beta_1 - \beta_2) \mathcal{D}_{\kappa} + \dots \right] \right. \\
 &+ \left. \frac{1}{1!} (\beta \mathcal{D}_{\kappa}) [n_{\kappa}^2 (n_{\kappa} + 1) + n_{\kappa} (n_{\kappa} + 1)^2] [1 - \dots] + \dots \right\} \\
 &+ \mathcal{K}_S^2 \{ n_{\kappa}^2 (n_{\kappa} + 1) [1 - \dots] + \dots \} + \dots \Big) = e^{(\beta_1 - \beta_2)(\omega_{\kappa} - \mathcal{D}_{\kappa})} \left(\theta(\beta_2 - \beta_1) \right. \\
 &+ n_{\kappa} + \frac{1}{1!} (\beta \mathcal{D}_{\kappa}) n_{\kappa} (n_{\kappa} + 1) + \frac{1}{2!} (\beta \mathcal{D}_{\kappa})^2 [n_{\kappa}^2 (n_{\kappa} + 1) + n_{\kappa} (n_{\kappa} + 1)^2] + \dots \\
 &+ \mathcal{K}_S \left\{ n_{\kappa} (n_{\kappa} + 1) + \frac{1}{1!} (\beta \mathcal{D}_{\kappa}) [n_{\kappa}^2 (n_{\kappa} + 1) + n_{\kappa} (n_{\kappa} + 1)^2] + \dots \right\} \\
 &+ \left. \mathcal{K}_S^2 \{ n_{\kappa}^2 (n_{\kappa} + 1) + \dots \} + \dots \right). \tag{A.9}
 \end{aligned}$$

It is easy to note that the expressions in brackets are Taylor expansions of the functions \bar{n}_{κ} , $\bar{n}_{\kappa}(\bar{n}_{\kappa} + 1)$, ... etc., respectively, where

$$\bar{n}_{\kappa} = \frac{1}{\exp \beta(\omega_{\kappa} - \mathcal{D}_{\kappa}) - 1}. \tag{A.10}$$

In fact, we have

$$\begin{aligned}
 \left[\frac{\partial}{\partial \beta \mathcal{D}_{\kappa}} \bar{n}_{\kappa} \right]_{\beta \mathcal{D}_{\kappa} = 0} &= n_{\kappa} (n_{\kappa} + 1), \\
 \left[\frac{\partial^2}{\partial (\beta \mathcal{D}_{\kappa})^2} \bar{n}_{\kappa} \right]_{\beta \mathcal{D}_{\kappa} = 0} &= n_{\kappa}^2 (n_{\kappa} + 1) + n_{\kappa} (n_{\kappa} + 1)^2, \\
 \dots \dots \dots
 \end{aligned} \tag{A.11}$$

Similarly

$$\left[\frac{\partial}{\partial \beta \mathcal{D}_k} \bar{n}_k (\bar{n}_k + 1) \right]_{\beta \mathcal{D}_k = 0} = n_k^2 (n_k + 1) + n_k (n_k + 1)^2, \quad (\text{A.12})$$

.....

etc.

Thus,

$$G_{\beta}^S(\beta_1, \beta_2) = e^{(\beta_1 - \beta_2)(\omega_k - \mathcal{D}_k)} [\theta(\beta_2 - \beta_1) + \bar{n}_k + \mathcal{H}_S \bar{n}_k (\bar{n}_k + 1) + \mathcal{H}_S^2 \bar{n}_k^2 (\bar{n}_k + 1) + \dots].$$

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