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REAL SPIN WAVE THEORY OF FERROMAGNETISM

By J. Szaniecki

Institute of Physics of the Polish Academy of Sciences, Ferromagnetics Laboratory, Poznań*

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The fundamentals of a theory of real spin waves are proposed. As a first step, a selected class of diagrams is calculated and the free energy and magnetization of a cubic ferromagnet are derived. These preliminary results are valid for temperatures between absolute zero and the Curie point.

1. *Introduction*

In the present decade, many authors have successfully applied the methods of time-dependent and causal Green functions to the problem of the Heisenberg ferromagnet. An interesting, critical survey of the relevant papers was given by Katsura and Horiguchi (1968). Besides its unquestionable advantages, the Green function theory of ferromagnetism has drawbacks. Thus, in order to be solved, the Green function equation of motion has to be broken off and the higher order Green functions have to be decoupled, involving inassessable error. As to the causal Green fuction method, (see Kuehnel (1969)), it resorts to Pauli operators and thus necessitates a modification of Wick's (1950) theorem. For this reason, only the lowest orders of the Green function can be derived. In short, use of the Green function formalism enables to obtain quite simply and easily results which, otherwise, would require very tedious procedures. Nevertheless, the Green function is not the sole mathematical tool for dealing with ferromagnetism. Spin wave theory is also an adequate method, provided it allows rigorously for both dynamical and kinematical interactions of magnons. An example of such a theory for large spin quantum numbers *i.e.* for weak kinematic interaction was given by Bloch (1962). Another approach to real spin wave theory is due to Praveczki (1969).

This investigation is based on ideas developed in recent papers by the present author (1962a), (1962b), (1963c). Since the problem of contributions to the sum-over-states from dynamical and kinematical interactions is highly involved, we can solve it only step by step.

* Address: Instytut Fizyki Polskiej Akademii Nauk, Zakład Ferromagnetyków, Poznań, Fredry 10, Polska.

Therefore, we shall derive here a selected class of diagrams without energy denominators. In a subsequent paper, graphs with energy denominators as well as lowest order kinematic corrections will be established.

2. *The Hamiltonian*

We assume the ferromagnet to be of cubic structure and to consist of N lattice points. To every site f, a spin operator S_f is attached. Including into Hamiltonian only Zeeman and Heisenberg terms, we have

$$\mathscr{H} = L\sum_f S_f^z - \frac{1}{2}\sum_{f,g} J_{f,g}(S_f^+ S_g^- + S_f^z S_g^z), \tag{2.1}$$

where $J_{f,g}$ is the exchange integral between points f and g, and

$$L = g\mu_B H, \tag{2.2}$$

with g being Landè's factor, μ_B — Bohr's magneton and H the magnetic field strength.

Let us relate the spin operators to new operators a_f^*, a_f by the substitutions (Maleyev (1957)):

$$S_f^+ \to \sqrt{2S}\, a_f^* \tag{2.3a}$$

$$S_f^- \to \sqrt{2S}\left(1 - \frac{1}{2S}\, a_f^* a_f\right) a_f, \tag{2.3b}$$

$$S_f^z \to -S + a_f^* a_f, \tag{2.3c}$$

wherein S is the spin quantum number.

As yet, we shall not consider the question of what commutation rules the operators a_f^*, a_f have to obey. On performing the Fourier transformations

$$a_f^* = N^{-1/2} \sum_\lambda a_\lambda^* e^{-i\lambda\cdot f}, \tag{2.4a}$$

$$a_f = N^{-1/2} \sum_\lambda a_\lambda e^{i\lambda\cdot f}, \tag{2.4b}$$

$$J_{f,g} = N^{-1} \sum_\lambda J_\lambda e^{i\lambda\cdot(f-g)} \tag{2.5}$$

where λ is the vector spanning the reciprocal lattice, and on recurring to Eqs (2.3), (2.4), (2.5), the Hamiltonian (2.1) can be recast as

$$\mathscr{H} = E_0 + \mathscr{H}_0 + \mathscr{H}_I, \tag{2.6}$$

$$E_0 = -LSN - \frac{1}{2} NJ_0 S^2, \tag{2.7}$$

$$\mathscr{H}_0 = \sum_\lambda (L + \varepsilon_\lambda) a_\lambda^* a_\lambda, \tag{2.8}$$

$$\varepsilon_\lambda = S(J_0 - J_\lambda), \tag{2.9}$$

$$\mathscr{H}_I = -\frac{1}{4} N^{-1} \sum_{\lambda\varrho\sigma} \Gamma^\lambda_{\varrho,\sigma} a^*_{\sigma+\lambda} a^*_{\varrho-\lambda} a_\varrho a_\sigma , \tag{2.10}$$

$$\Gamma^\lambda_{\varrho,\sigma} = J_\lambda + J_{\lambda+\sigma-\varrho} - J_{\lambda+\sigma} - J_{\lambda-\varrho}. \tag{2.11}$$

On account of the symmetry in ϱ and σ, $\Gamma^\lambda_{\varrho,\sigma}$ can moreover be expressed as

$$\Gamma^\lambda_{\varrho,\sigma} = 2J_\lambda - J_{\lambda+\sigma} - J_{\lambda-\varrho}. \tag{2.12}$$

On deriving (2.6), we invoked only the fact that

$$[a_f, a^*_g] = 0, \; f \neq g.$$

In the approximation of nearest neighbours,

$$J_\lambda \to J\gamma_\lambda, \tag{2.13}$$

$$\gamma_\lambda = \sum_\delta \exp i\lambda \cdot \delta, \tag{2.14}$$

where δ are vectors pointing to all nearest neighbours. The quantities (2.7)–(2.11) can be readjusted as

$$E_0 = -LSN - \frac{1}{2} JNS^2\gamma_0 , \tag{2.15}$$

$$\varepsilon_\lambda = JS(\gamma_0 - \gamma_\lambda), \tag{2.16}$$

$$\Gamma^\lambda_{\varrho,\sigma} = J(\gamma_\lambda + \gamma_{\lambda+\sigma-\varrho} - \gamma_{\lambda+\sigma} - \gamma_{\lambda-\varrho}), \tag{2.17}$$

or

$$\Gamma^\lambda_{\varrho,\sigma} = J(2\gamma_\lambda - \gamma_{\lambda+\sigma} - \gamma_{\lambda-\varrho}), \tag{2.18}$$

where γ_0 is the first coordination number. The a^*_f, a_f can now be identified either as the Yzyumov (1959) operators

$$[a_f, a^*_g] = \delta_{f,g} \left[1 - \frac{2S+1}{(2S)\,!} (a^*_f)^{2S} a_f^{2S}\right], \tag{2.19}$$

$$(a^*_f)^{2S+1} = 0, \; a_f^{2S+1} = 0, \tag{2.20}$$

which represent generalized Pauli operators, or as

$$[a_f, a^*_g] = \delta_{f,g}, \tag{2.21}$$

i.e. Bose operators.

A real spin wave theory with Hamiltonian (2.6) and operators (2.19), (2.20) has been formulated by Praveczki (1969).

3. *Interpolation theories*

As mentioned in the Introduction, the past decade has witnessed the evolution of methods enabling to determine thermodynamic quantities of a ferromagnet at all temperatures. Here belongs the time-dependent Green function formalism (see Bogolyubov and Tyablikov (1959), Tyablikov (1959), Szaniecki (1962 d, f, g), Tahir Kheli and ter Haar (1962), Callen (1963)). Its basic formulas are the so-called spectral relations, of the form:

$$\langle \hat{A}\hat{B}(t)\rangle = \int_{-\infty}^{\infty} dE I(E) e^{\beta E} e^{iEt/\hbar}, \qquad \beta = (kT)^{-1}, \tag{3.1}$$

$$\langle \hat{B}(t)\hat{A}\rangle = \int_{-\infty}^{\infty} dE I(E) e^{iEt/\hbar}, \tag{3.2}$$

with

$$\langle \hat{C}\rangle = \frac{\mathrm{Tr}\,(e^{-\beta\mathscr{H}}\hat{C})}{\mathrm{Tr}\,(e^{-\beta\mathscr{H}})}. \tag{3.3}$$

$I(E)$ is the spectral intensity, $\hat{A}$ and $\hat{B}$ are spin operators, thus $\hat{A} \to S_f^+$, $\hat{B} \to S_g^-$, and

$$\hat{B}(t) = e^{i\mathscr{H}t/\hbar}\hat{B}e^{-i\mathscr{H}t/\hbar}. \tag{3.4}$$

The formulas (3.1), (3.2) derived by Lehman (1954) for pure fermions and bosons were subsequently adapted to magnons, which are neither Fermi nor Bose particles. Let us now try to verify whether they hold for magnons. Obviously, in order to check the validity of Eqs (3.1) and (3.2), we have to resort to the Hamiltonian (2.1). Unfortunately, we are unable to say anything about a complete orthonormal set of eigen-states of this Hamiltonian — an indispensable element in proving the applicability or otherwise of the spectral formulas. To circumvent this dilemma, we recur to the Hamiltonian (2.6) with the oscillatory operators a_λ^*, a_λ. As a matter of course, solving the Schroedinger equation

$$\mathscr{H}|m) = E_m|m) \tag{3.5}$$

for the energy operator from (2.6) is incomparably easier than for $\mathscr{H}$ from (2.1). There remains the question of how to compute (3.3) satisfying the condition that S_f^z, Eq. (2.3c), shall have only $2S+1$ projections, *i.e.* that the quantum numbers of $a_f^*a_f$ shall be $0, 1, 2, \ldots, 2S$. This problem is solved in Appendix *A*. By Eqs (3.1), (3,4), (3.5) and (A.10), (A. 13), (A.16), we get

$$\begin{aligned}\langle \hat{A}\hat{B}\,(t)\rangle &= Q^{-1}\,\mathrm{Tr}\,[e^{-\beta\mathscr{H}}\hat{A}\hat{B}(t)\hat{K}_S] \\ &= Q^{-1}\sum_{m,\,n} e^{-\beta E_m} e^{i(E_n-E_m)t/\hbar}\hat{A}_{m,n}\hat{B}_{n,m}(\hat{K}_S)_{m,m}\end{aligned} \tag{3.6}$$

where

$$Q = \mathrm{Tr}\,(e^{-\beta\mathscr{H}}\hat{K}_S). \tag{3.7}$$

The kinematic operators $\hat{K}_S$, Eqs (A.11), (A.14) and (A.17), consist of symmetric products of $a_f^*a_f$ and consequently contain diagonal matrix elements only.

On the other hand,

$$\langle\hat{B}(t)\hat{A}\rangle = \sum_{m,n} e^{-\beta E_n} e^{i(E_n-E_m)t/\hbar} \hat{A}_{m,n} \hat{B}_{n,m} (\hat{K}_S)_{n,n}. \tag{3.8}$$

Now,

$$(\hat{K}_S)_{m,m} = (\hat{K}_S)_{n,n},$$

$$= \begin{cases} 1 \ \textit{if} \ |m\rangle \text{ and } |n\rangle \text{ belong to the physical states,} \\ 0 \text{ otherwise,} \end{cases} \tag{3.9}$$

whence $I(E)$ can be represented in the form

$$I(E) = Q^{-1} \sum_{m,n} e^{-\beta E_m} \hat{B}_{m,n} \hat{A}_{n,m} \delta(E_m - E_n - E), \tag{3.10}$$

as usually done.

We thus see that the spectral formulas (3.1), (3.2) are well suited to for a Hamiltonian of the type (2.1).

4. *Sum-over-states*

For further calculations, we choose the theory recurring to Bose operators, *i.e.* we use the Hamiltonian (2.6) with relations (2.15)–(2.17) and commutation rule (2.21). Such a theory enables us to apply Wick's (1950) and Thouless' (1957) theorems and dispenses with spectral formulas. Computation of the relevant contributions to the sum-over-states from dynamical and kinematical interactions will provide correct results for the thermodynamical quantities of a ferromagnet. In this meaning, the present theory is a real spin wave theory. However, because of mathematical difficulties, many diagrams entering the sum-over-states will have to be neglected; they represent so highly intricate expressions as to be practically inaccessible to evaluation.

We now proceed to compute the sum-over-states. For this purpose, we introduce the set of orthonormal states

$$|n) = \prod_{\lambda} [(n_\lambda!)^{-1/2} (a_\lambda^*)^{n_\lambda}] |0), \tag{4.1}$$

where $|0)$ is the magnon vacuum state. Thus,

$$Z = \mathrm{Tr}\,(e^{-\beta\mathscr{H}} \hat{K}_S) = \sum_n (n|e^{-\beta\mathscr{H}} \hat{K}_S|n)$$

$$= e^{-\beta E_0} \sum_n (n|e^{-\beta\mathscr{H}_0}|n) \frac{\sum_n (n|e^{-\beta\mathscr{H}_0} \hat{S}(\beta) \hat{K}_S|n)}{\sum_n (n|e^{-\beta\mathscr{H}_0}|n)} = e^{-\beta E_0} \sum_n (n|e^{-\beta\mathscr{H}_0}|n) \langle \hat{S}(\beta) \hat{K}_S \rangle, \tag{4.2}$$

and

$$\hat{S}(\beta) = e^{\beta\mathscr{H}_0} e^{-\beta(\mathscr{H}_0 + \mathscr{H}_I)} = \exp\,[-\int_0^\beta d\tau \mathscr{H}_I(\tau)], \tag{4.3}$$

$$\mathscr{H}_I(\tau) = e^{\tau\mathscr{H}_0} \mathscr{H}_I e^{-\tau\mathscr{H}_0}. \tag{4.4}$$

Applying Matsubara's (1955) formalism, we get by Eqs (2.6)–(2.17);

$$Z = \exp\left[-\beta E_0 + \sum_{\lambda}\sum_{n=1}^{\infty} n^{-1}e^{-\beta n(L+\varepsilon_\lambda)} + \sum_{n=1}^{\infty} D_n + \sum_{n=0}^{\infty} C_n(S)\right], \tag{4.5}$$

with

$$D_n = \frac{(-1)^n}{n!}\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \ldots \int_0^\beta d\tau_n \langle \hat{T}[\mathscr{H}_I(\tau_1)\mathscr{H}_I(\tau_2)\ldots\mathscr{H}_I(\tau_n)]\rangle_c, \tag{4.6}$$

$$C_n(S) = \frac{(-1)^n}{n!}\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \ldots \int_0^\beta d\tau_n \langle \hat{T}[\mathscr{H}_I(\tau_1)\mathscr{H}_I(\tau_2)\ldots\mathscr{H}_I(\tau_n)]\,(\hat{K}_S-1)\rangle_c. \tag{4.7}$$

The lower index c in (4.6) and (4.7) denotes that only connected graphs have to be taken, as the disconnected ones result by expanding the exponent $\exp\left[\sum_n D_n + \sum_n C_n(S)\right]$ in a series. $\hat{T}$ is Wick's ordering symbol.

The diagrams D_n arise due to the dynamic interaction, C_0 is the contribution to the sum-over-states from kinematic interaction, and the diagrams $C_n(S)$, $n \neq 0$, are mixed terms.

To derive explicitely the diagrams (4.6) and (4.7), we introduce the following contractions:

$$a_\varrho^*(\tau_1)^\bullet a_\sigma(\tau_2)^\bullet = \delta_{\varrho,\sigma} e^{(L+\varepsilon_\varrho)(\tau_1-\tau_2)}[\theta_{1,2}\bar{n}_\varrho + \theta_{2,1}(\bar{n}_\varrho+1)], \tag{4.8}$$

$$a_\varrho(\tau_1)^\bullet a_\sigma^*(\tau_2)^\bullet = \delta_{\varrho,\sigma} e^{-(L+\varepsilon_\varrho)(\tau_1-\tau_2)}[\theta_{1,2}(\bar{n}_\varrho+1) + \theta_{2,1}\bar{n}_\varrho], \tag{4.9}$$

$$a_\varrho^*(\tau_1)^\bullet a_\sigma^*(\tau_2)^\bullet = 0, \quad a_\varrho(\tau_1)^\bullet a_\sigma(\tau_2)^\bullet = 0, \tag{4.10}$$

$$a_\varrho^*(\tau)^\bullet a_\sigma(\tau)^\bullet = \delta_{\varrho,\sigma}\bar{n}_\varrho, \tag{4.11}$$

$$a_\varrho(\tau)^\bullet a_\sigma^*(\tau)^\bullet = \delta_{\varrho,\sigma}(\bar{n}_\varrho+1), \tag{4.12}$$

$$\theta_{i,k} \equiv \theta(\tau_i-\tau_k) = \begin{cases} 1, & \tau_i > \tau_k, \\ 0, & \tau_i < \tau_k, \end{cases} \tag{4.13}$$

$$\bar{n}_\varrho = [\exp\beta(L+\varepsilon_\varrho)-1]^{-1}. \tag{4.14}$$

Let us derive the first order diagram D_1. By Eqs (2.10), (2.17), (4.6), (4.11) and applying Wick's (1950) and Thouless' (1957) theorems, we obtain

$$D_1 = -\int_0^\beta d\tau \langle \hat{T}[\mathscr{H}_I(\tau)]\rangle$$

$$= \frac{1}{4} N^{-1} \sum_{\lambda\varrho\sigma} \Gamma^\lambda_{\varrho,\sigma} \int_0^\beta d\tau\; 2a^*_{\sigma+\lambda}(\tau)^\bullet a^*_{\varrho-\lambda}(\tau)^{\bullet\bullet} a_\varrho(\tau)^{\bullet\bullet} a_\sigma(\tau)^\bullet$$

$$= \frac{1}{2}\beta N^{-1} \sum_{\varrho\sigma} \Gamma^0_{\varrho,\sigma}\bar{n}_\varrho\bar{n}_\sigma = \frac{1}{2}\beta J N^{-1} \sum_{\lambda\varrho\sigma} (\gamma_0+\gamma_{\varrho-\sigma}-\gamma_\varrho-\gamma_\sigma)\bar{n}_\varrho\bar{n}_\sigma. \tag{4.15}$$

For all three types of cubic lattices

$$\sum_{\varrho\sigma} \gamma_{\varrho-\sigma}\bar{n}_\varrho\bar{n}_\sigma = \sum_{\varrho\sigma} \frac{\gamma_\varrho\gamma_\sigma}{\gamma_0}\,\bar{n}_\varrho\bar{n}_\sigma, \tag{4.16}$$

whence

$$D_1 = \frac{1}{2}\,\beta J\gamma_0 N\left[N^{-1}\sum_{\varrho}(1-x_\varrho)\bar{n}_\varrho\right]^2, \tag{4.17}$$

where

$$x_\varrho = \gamma_\varrho/\gamma_\sigma. \tag{4.18}$$

In the second order,

$$D_2 = \frac{1}{2!}\int_0^\beta d\tau_1\int_0^\beta d\tau_2\langle\hat{T}[\mathscr{H}_I(\tau_1)\mathscr{H}_I(\tau_2)]\rangle_c$$

$$= \frac{1}{32}\,N^{-2}\sum_{\substack{\varkappa\mu\nu\\ \lambda\varrho\sigma}} \Gamma^{\varkappa}_{\mu,\nu}\Gamma^{\lambda}_{\varrho,\sigma}\int_0^\beta d\tau_1\int_0^\beta d\tau_2\langle\hat{T}[a^*_{\nu+\varkappa}(\tau_1)a^*_{\mu-\varkappa}(\tau_1)\times$$

$$\times a_\mu(\tau_1)a_\nu(\tau_1)a^*_{\sigma+\lambda}(\tau_2)a^*_{\varrho-\lambda}(\tau_2)a_\varrho(\tau_2)a_\sigma(\tau_2)]\rangle_c.$$

Straightforward computation yields

$$D_2 = D_2^{(1)}+D_2^{(2)}, \tag{4.19}$$

$$D_2^{(1)} = \frac{1}{2}\,\beta^2N^{-2}\sum_{\lambda\varrho\sigma}\Gamma^0_{\varrho,\sigma}\Gamma^0_{\lambda,\sigma}\bar{n}_\lambda\bar{n}_\varrho\bar{n}_\sigma(\bar{n}_\sigma+1), \tag{4.20}$$

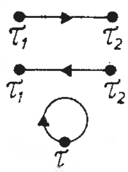
$$D_2^{(2)} = \frac{1}{8}\,\beta N^{-2}\sum_{\lambda\varrho\sigma}\Gamma^{\lambda}_{\varrho,\sigma}\Gamma^{\lambda}_{\sigma+\lambda,\varrho-\lambda}(\varepsilon_{\sigma+\lambda}+\varepsilon_{\varrho-\lambda}-\varepsilon_\varrho-\varepsilon_\sigma)^{-1}\times$$

$$\times[\bar{n}_\varrho\bar{n}_\sigma(\bar{n}_{\sigma+\lambda}+1)\,(\bar{n}_{\varrho-\lambda}+1)-(\bar{n}_\varrho+1)\,(\bar{n}_\sigma+1)\bar{n}_{\sigma+\lambda}\bar{n}_{\varrho-\lambda}]. \tag{4.21}$$

In this paper, we refrain from considering diagrams with energy denominators, since their intricacy for temperatures near the Curie point is obvious, as exemplified by the graph $D_2^{(2)}$. Indeed, at low temperatures only magnons with small wave vectors are excited, whence the summations in (4.21) and, consequently, the integrations are easily feasible, contrary to the high temperature region where all magnon wave vectors are admissible and the sums (and integrals resulting from them) become complicated. We shall also be neglecting the graphs (4.7). This is not to say that they are unimportant. Simply, the problem of how they affect the sum-over-states is extremely involved and has to be carefully investigated, as will be done in a separate paper. Postponing the evaluation of the class with energy denominators and the problem of kinematic interaction to our future papers, we now proceed to figure out diagrams in higher orders.

With the help of following scheme of mathematical symbols and their graphical equivalents:

$$a_\varrho^*(\tau_1)^\bullet a_\sigma(\tau_2)^\bullet$$
$$a_\varrho(\tau_1)^\bullet a_\sigma^*(\tau_2)^\bullet$$
$$\begin{cases} a_\varrho^*(\tau)^\bullet a_\sigma(\tau)^\bullet \\ a_\varrho(\tau)^\bullet a_\sigma^*(\tau)^\bullet \end{cases}$$



the diagrams D_n can be plotted in the form represented in Fig. 1. The numbers above the graphs are multiplicity factors. They result by topological equivalence of diagram parts. Let us also hint that many graphs, thus $D_5^{(2)}$, $D_5^{(3)}$ or $D_6^{(2)}$, $D_6^{(3)}$, $D_6^{(4)}$, have the same mathematical form, though they are not topologically equivalent.

Referring the reader to Appendix B for details, we quote here the final results. According to (4.5), the free energy

$$F = -\beta^{-1} \ln Z \tag{4.22}$$

is

$$F = E_0 - \beta^{-1} \sum_\lambda \ln (1+\bar{n}_\lambda) - \beta^{-1} \sum_{n=1}^{\infty} D_n. \tag{4.23}$$

It can be easily verified that

$$F = E_0 + \sum_\lambda (L+\varepsilon_\lambda)\tilde{n}_\lambda - \frac{1}{2JS^2\gamma_0} N^{-1} \sum_{\varrho\sigma} \varepsilon_\varrho \varepsilon_\sigma \bar{n}_\varrho \bar{n}_\sigma +$$
$$+\beta^{-1} \sum_\lambda [\tilde{n}_\lambda \ln \tilde{n}_\lambda - (1+\tilde{n}_\lambda) \ln (1+\tilde{n}_\lambda)], \tag{4.24}$$

where

$$\tilde{n}_\lambda = \left\{\exp \beta \left[L+\varepsilon_\lambda \left(1-\frac{1}{S} Y\right)\right] -1\right\}^{-1} \tag{4.25}$$

and

$$Y = N^{-1} \sum_\lambda (1-x_\lambda)\tilde{n}_\lambda = \frac{1}{JSN\gamma_0} \sum_\lambda \varepsilon_\lambda \tilde{n}_\lambda. \tag{4.26}$$

Indeed, by Eqs (4.25), (4.26) and (B.15), the free energy (4.23) can be transformed to the form (4.24).

Differentiation of (4.24) with respect to L yields the magnetization

$$\mu(T) = 1 - \frac{1}{NS} \sum_\lambda \tilde{n}_\lambda. \tag{4.27}$$

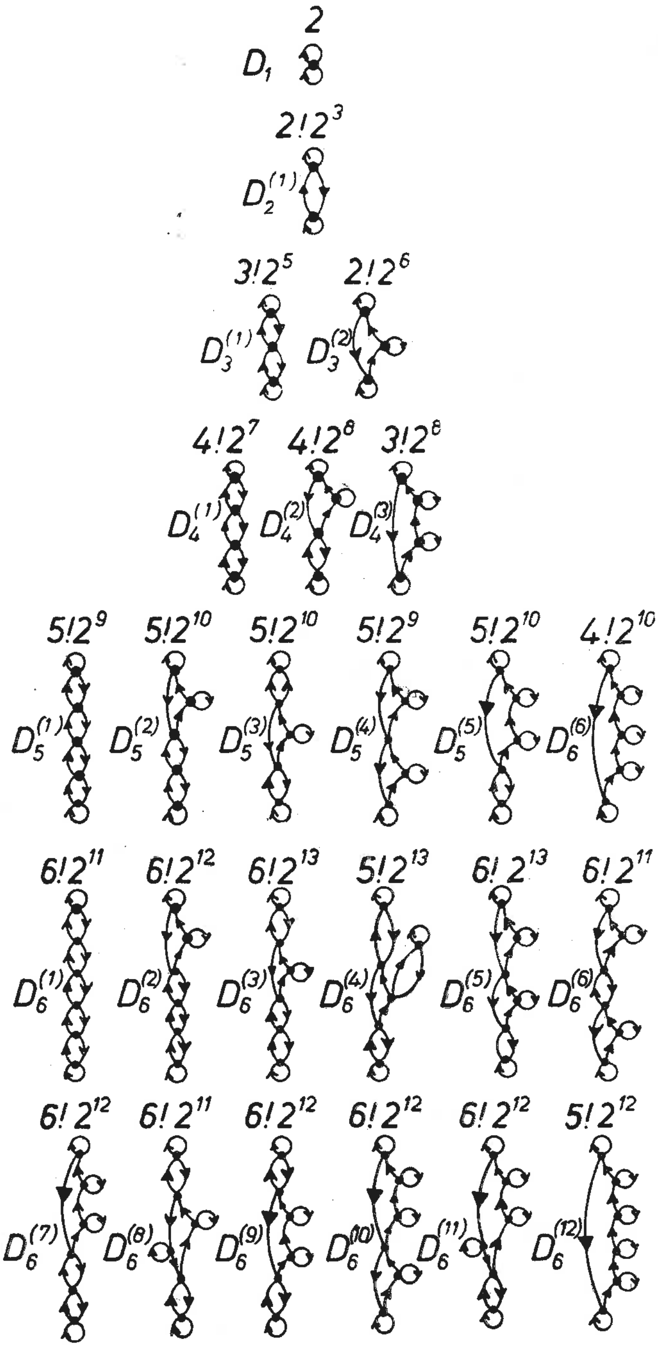


Fig. 1. Graphical representation of one class of dynamical diagrams

Along different lines, Eqs (4.24)–(4.27) have been computed by Bloch (1962), who assumed that the dynamical interaction of spin waves was small throughout the entire range of temperatures and, neglecting interfering terms in Eq. (2.17) *i.e.* putting $\lambda = 0$, succeeded in obtaining Eqs (4.24) and (4.27) by variation of the free energy. She determined the magnetization (4.27) numerically with the help of computer. As she did not consider kinematical interaction, the magnetization for $S = 1/2$, 1 probably turned out to be too large. In connection with this question, let us figure out the graph C_0, Eq. (4.7). By Eqs (2.4), (4.11), (4.12) and (A.11), we have for $S = 1/2$

$$C_0(1/2) = -N^{-1} \sum_{\varrho\sigma} \bar{n}_\varrho \bar{n}_\sigma + 2N^{-2} \sum_{\lambda\varrho\sigma} \bar{n}_\lambda \bar{n}_\varrho \bar{n}_\sigma (\bar{n}_\sigma + 1) +$$

$$+ \frac{1}{2} N^{-2} \sum_{\lambda\varrho\sigma} \bar{n}_\lambda \bar{n}_\varrho \bar{n}_\sigma \bar{n}_{\varrho+\sigma-\lambda} - 6 N^{-3} \sum_{\varkappa\lambda\varrho\sigma} \bar{n}_\varkappa \bar{n}_\lambda \bar{n}_\varrho \bar{n}_\sigma + \dots . \tag{4.28}$$

The above expression corrects the average spin wave population number, *i. e.*

$$\sum_\lambda (\bar{n}_\lambda + \Delta \bar{n}_\lambda) = \sum_\lambda \bar{n}_\lambda - \beta^{-1} \frac{\partial}{\partial L} C_0(1/2)$$

$$= \sum_\lambda \bar{n}_\lambda [1 - 2(\bar{n}_\lambda + 1) N^{-1} \sum_\varrho \bar{n}_\varrho + 6 (\bar{n}_\lambda + 1) (N^{-1} \sum_\varrho \bar{n}_\varrho)^2 -$$

$$-24(\bar{n}_\lambda + 1)(N^{-1} \sum_\varrho \bar{n}_\varrho)^3 + 4\bar{n}_\lambda (\bar{n}_\lambda + 1)(N^{-1} \sum_\varrho \bar{n}_\varrho)^2 +$$

$$+4(\bar{n}_\lambda + 1) (N^{-1} \sum_\varrho \bar{n}_\varrho) (N^{-1} \sum_\sigma \bar{n}_\sigma^2) + 2(\bar{n}_\lambda + 1) N^{-1} \sum_{\varrho\sigma} \bar{n}_\varrho \bar{n}_\sigma \bar{n}_{\varrho+\sigma-\lambda} + \dots]. \tag{4.29}$$

Thus we see that, for small spins, omission of kinematic interaction entails some error, which seems to be by no means insignificant. We shall deal with this problem more closely in our next paper. Finally, we mention that the formula (4.29) does not coincide with a similar one derived by Praveczki (1969).

APPENDIX A

Let us derive the formulas (3.6) and (3.8). It is reasonable to start with states

$$|n) = \prod_f [(n_f!)^{-1/2} (a_f^*)^{n_f}] \, |0), \quad n_f = 0, 1, 2, \dots, 2S. \tag{A.1}$$

For $S = 1/2$ and $N \to \infty$, we have

$$\mathrm{Tr}\, (e^{-\beta \mathscr{H}} \hat{C})_{\text{cut-off}} = (0|e^{-\beta \mathscr{H}} \hat{C}|0) + \sum_f (0|a_f e^{-\beta \mathscr{H}} \hat{C} a_f^*|0) +$$

$$+ \sum_{f_1 < f_2} (0|a_{f_1} a_{f_2} e^{-\beta \mathscr{H}} \hat{C} a_{f_1}^* a_{f_2}^*|0) + \sum_{f_1 < f_2 < f_3} (0|a_{f_1} a_{f_2} a_{f_3} e^{-\beta \mathscr{H}} \hat{C} a_{f_1}^* a_{f_2}^* a_{f_3}^*|0) +$$

$$+ \dots + \sum_{f_1 < f_2 < \dots < f_k} (0|a_{f_1} a_{f_2} \dots a_{f_k} e^{-\beta \mathscr{H}} \hat{C} a_{f_1}^* a_{f_2}^* \dots a_{f_k}^*|0) + \dots . \tag{A.2}$$

Introducing the auxiliary function

$$f_{1/2}(\mu; x_1, x_2, \ldots, x_N) \equiv f_{1/2}(\mu) = \prod_{p=1}^{N} (1+\mu x_p), \tag{A.3}$$

where μ is a small parameter, we can expand it either as

$$f_{1/2}(\mu) = 1+\mu \sum_{p=1}^{N} x_p + \mu^2 \sum_{p_1<p_2} x_{p_1}x_{p_2} + \mu^3 \sum_{p_1<p_2<p_3} x_{p_1}x_{p_2}x_{p_3} + \\ + \ldots + \mu^k \sum_{p_1<p_2<\ldots<p_k} x_{p_1}x_{p_2}\ldots x_{p_k} + \ldots \tag{A.4}$$

or as

$$f_{1/2}(\mu) = \exp \ln \prod_{p=1}^{N} (1+\mu x_p) = \exp \sum_{p=1}^{N} \ln (1+\mu x_p)$$

$$= \exp \sum_{l=0}^{\infty} \frac{(-1)^{l+1}}{(l+1)!} \mu^{l+1} y_{l-1}, \tag{A.5}$$

$$y_{l+1} = \sum_{p=1}^{N} x_p^{l+1}. \tag{A.6}$$

We now exponentiate (A.5) and equate equal powers of μ in (A.4) and (A.5), getting

$$\sum_{p_1<p_2<\ldots<p_k} x_{p_1}, x_{p_2} \ldots x_{p_k} = \frac{1}{k!} y_1^k + \frac{1}{(k-2)!} y_1^{k-2} \left(-\frac{1}{2} y_2\right) + \\ + \frac{1}{(k-3)!} y_1^{k-3} \left(\frac{1}{3} y_3\right) + \frac{1}{(k-4)!} y_1^{k-4} \left[\frac{1}{2!}\left(-\frac{1}{2} y_2\right)^2 - \frac{1}{4} y_4\right] + \\ + \frac{1}{(k-5)!} y_1^{k-5} \left[\left(-\frac{1}{2} y_2\right)\left(\frac{1}{3} y_3\right) + \frac{1}{5} y_5\right] + \frac{1}{(k-6)!} y_1^{k-6} \left[\frac{1}{3!}\left(-\frac{1}{2} y_2\right)^3 + \\ + \frac{1}{2!}\left(\frac{1}{3} y_3\right)^2 + \left(-\frac{1}{2} y_2\right)\left(-\frac{1}{4} y_4\right) - \frac{1}{6} y_6\right] + \frac{1}{(k-7)!} y_1^{k-7} \left[\frac{1}{2!}\left(-\frac{1}{2} y_2\right)^2 \times \\ \times \left(\frac{1}{3} y_3\right) + \left(-\frac{1}{2} y_2\right)\left(\frac{1}{5} y_5\right) + \left(\frac{1}{3} y_3\right)\left(-\frac{1}{4} y_4\right) + \frac{1}{7} y_7\right] + \ldots. \tag{A.7}$$

With regard to (A.6) and (A.7), we can transform (A.2) as follows:

$$\sum_{f_1<f_2<\ldots<f_k} (0|a_{f_1}a_{f_2} \ldots a_{f_k} e^{-\beta\mathscr{H}} \hat{C} a_{f_1}^* a_{f_2}^* \ldots a_{f_k}^*|0)$$

$$= \frac{1}{k!} \sum_{f_1, f_2, \ldots, f_k} (0|a_{f_1}a_{f_2} \ldots a_{f_k} e^{-\beta\mathscr{H}} \hat{C} a_{f_1}^* a_{f_2}^* \ldots a_{f_k}^*|0) -$$

$$- \frac{1}{2(k-2)!} \sum_{f_1, f_2, \ldots, f_{k-2}} \sum_{g} (0|a_{f_1}a_{f_2} \ldots a_{f_{k-2}} a_g^2 e^{-\beta\mathscr{H}} \hat{C} (a_g^*)^2 a_{f_1}^* a_{f_2}^* \ldots a_{f_{k-2}}^*|0) +$$

$$+\frac{1}{3(k-3)!}\sum_{f_1,f_2,\dots,f_{k-3}}\sum_{g}(0|a_{f_1}a_{f_2}\dots a_{f_{k-3}}a_g^3 e^{-\beta\mathscr{H}}\hat{C}(a_g^*)^3 a_{f_1}^* a_{f_2}^*\dots a_{f_{k-3}}^*|0)+$$

$$+\frac{1}{2!}\left(-\frac{1}{2}\right)^2\frac{1}{(k-4)!}\sum_{f_1,f_2,\dots,f_{k-4}}\sum_{g_1,g_2}(0|a_{f_1}a_{f_2}\dots a_{f_{k-4}}a_{g_1}^2 a_{g_2}^2 e^{-\beta\mathscr{H}}\hat{C}(a_{g_1}^*)^2(a_{g_2}^*)^2 a_{f_1}^* a_{f_2}^*\dots a_{f_{k-4}}^*|0)-$$

$$-\frac{1}{4(k-4)!}\sum_{f_1,f_2,\dots,f_{k-4}}\sum_{g}(0|a_{f_1}a_{f_2}\dots a_{f_{k-4}}a_g^4 e^{-\beta\mathscr{H}}\hat{C}(a_g^*)^4 a_{f_1}^* a_{f_2}^*\dots a_{f_{k-4}}^*|0)+\dots. \quad \text{(A.8)}$$

On carrying out summations over k to infinity, we get

$$\mathrm{Tr}\,(e^{-\beta\mathscr{H}}\hat{C})_{\text{cut-off}}=\mathrm{Tr}\,(e^{-\beta\mathscr{H}}\hat{C})-\frac{1}{2}\sum_{f}\mathrm{Tr}\,[a_f^2 e^{-\beta\mathscr{H}}\hat{C}(a_f^*)^2]+$$

$$+\frac{1}{3}\sum_{f}\mathrm{Tr}\,[a_f^3 e^{-\beta\mathscr{H}}\hat{C}(a_f^*)^3]+\frac{1}{2}\left(-\frac{1}{2}\right)^2\sum_{f_1,f_2}\mathrm{Tr}\,[a_{f_1}^2 a_{f_2}^2 e^{-\beta\mathscr{H}}\hat{C}(a_{f_1}^*)^2(a_{f_2}^{*2}]-$$

$$-\frac{1}{4}\sum_{f}\mathrm{Tr}\,[a_f^4 e^{-\beta\mathscr{H}}\hat{C}(a_f^*)]^4+\dots. \quad \text{(A.9)}$$

Changing cyclically the order of operators under the sign of trace, we finally obtain:

$$\mathrm{Tr}\,(e^{-\beta\mathscr{H}}\hat{C})_{\text{cut-off}}=\mathrm{Tr}\,(e^{-\beta\mathscr{H}}\hat{C}\hat{K}_{1/2}), \quad \text{(A.10)}$$

$$\hat{K}_{1/2}=1-\frac{1}{2}\sum_{f}(a_f^*)^2 a_f^2+\frac{1}{3}\sum_{f}(a_f^*)^3 a_f^3+\frac{1}{2!}\left(-\frac{1}{2}\right)^2\sum_{f_1,f_2}(a_{f_1}^*)^2(a_{f_2}^*)^2\times$$

$$\times a_{f_1}^2 a_{f_2}^2-\frac{1}{4}\sum_{f}(a_f^*)^4 a_f^4+\left(-\frac{1}{2}\right)\left(\frac{1}{3}\right)\sum_{f_1,f_2}(a_{f_1}^*)^2(a_{f_2}^*)^3 a_{f_1}^2 a_{f_2}^3+$$

$$+\frac{1}{5}\sum_{f}(a_f^*)^5 a_f^5+\frac{1}{3!}\left(-\frac{1}{2}\right)^3\sum_{f_1,f_2,f_3}(a_{f_1}^*)^2(a_{f_2}^*)^2(a_{f_3}^*)^2 a_{f_1}^2 a_{f_2}^2 a_{f_3}^2+$$

$$+\frac{1}{2!}\left(\frac{1}{3}\right)^2\sum_{f_1,f_2}(a_{f_1}^*)^3(a_{f_2}^*)^3 a_{f_1}^3 a_{f_2}^3+\left(-\frac{1}{2}\right)\left(-\frac{1}{4}\right)\sum_{f_1,f_2}(a_{f_1}^*)^2(a_{f_2}^*)^4 a_{f_1}^2 a_{f_2}^4-$$

$$-\frac{1}{6}\sum_{f}(a_f^*)^6 a_f^6+\dots, \quad \text{(A.11)}$$

where the traces on the right-hand sides of Eqs (A.9), (A.10) are taken over the states (A.1), without any restriction on n_f.

Quite similarly, with the auxiliary function

$$f_1(\mu;x_1,x_2,\dots,x_N)=\prod_{p=1}^{N}\left(1+\mu x_p+\frac{1}{2!}\mu^2 x_p^2\right), \quad \text{(A.12)}$$

one can obtain for $S=1$ and $N\to\infty$,

$$\mathrm{Tr}\,(e^{-\beta\mathscr{H}}\hat{C})_{\text{cut-off}}=\mathrm{Tr}\,(e^{-\beta\mathscr{H}}\hat{C}\hat{K}_1), \tag{A.13}$$

$$\hat{K}_1=1-\frac{1}{6}\sum_f (a_f^*)^3a_f^3+\frac{1}{8}\sum_f (a_f^*)^4a_f^4-\frac{1}{20}\sum_f (a_f^*)^5a_f^5+$$
$$+\frac{1}{2!}\left(-\frac{1}{6}\right)^2\sum_{f_1,f_2}(a_{f_1}^*)^3\,(a_{f_2}^*)^3a_{f_1}^3a_{f_2}^3+\dots \tag{A.14}$$

In the case of $S=3/2$, $N\to\infty$,

$$f_{3/2}(\mu;x_1,x_2,\dots,x_N)=\prod_{p=1}^{N}\left(1+\mu x_p+\frac{1}{2!}\mu^2x_p^2+\frac{1}{3!}\mu^3x_p^3\right), \tag{A.15}$$

$$\mathrm{Tr}\,(e^{-\beta\mathscr{H}}\hat{C})_{\text{cut-off}}=\mathrm{Tr}\,(e^{-\beta\mathscr{H}}\hat{C}\hat{K}_{3/2}), \tag{A.16}$$

$$\hat{K}_{3/2}=1-\frac{1}{24}\sum_f (a_f^*)^4a_f^4+\frac{1}{30}\sum_f (a_f^*)^5a_f^5-\frac{1}{72}\sum_f (a_f^*)^6a_f^6+\dots \tag{A.17}$$

etc. Resorting to the fact that the operation of trace is invariant with respect to replacing one orthonormal set of states by another, we get (3.6), (3.7) and (3.8).

APPENDIX B

To exemplify the procedure of obtaining the graphs D_n, let us compute $D_6^{(12)}$. By Eqs (2.10), (2.17), (4.8)–(4.14) and according to the graphical shape of $D_6^{(12)}$, we have

$$D_6^{(12)}=\frac{1}{6!}\,5!\,2^{12}\frac{1}{2^{12}}\,N^{-6}\sum_{\substack{\lambda_1\varrho_1\sigma_1\\ \lambda_2\varrho_2\sigma_2\\ \dots\dots\\ \lambda_6\varrho_6\sigma_6}}\Gamma^{\lambda_1}_{\varrho_1,\sigma_1}\Gamma^{\lambda_2}_{\varrho_2,\sigma_2}\dots\Gamma^{\lambda_6}_{\varrho_6,\sigma_6}\times$$
$$\times\int_0^\beta d\tau_1\int_0^\beta d\tau_2\dots\int_0^\beta d\tau_6[a^*_{\sigma_1+\lambda_1}(\tau_1)^\bullet a_{\sigma_1}(\tau_1)^\bullet][a^*_{\varrho_1-\lambda_1}(\tau_1)^\bullet a_{\varrho_2}(\tau_2)^\bullet]\times$$
$$\times[a^*_{\sigma_2+\lambda_2}(\tau_2)^\bullet a_{\sigma_2}(\tau_2)^\bullet][a^*_{\varrho_2-\lambda_2}(\tau_2)^\bullet a_{\varrho_3}(\tau_3)^\bullet][a^*_{\varrho_3+\lambda_3}(\tau_3)^\bullet a_{\sigma_3}(\tau_3)^\bullet]\times$$
$$\times[a^*_{\varrho_3-\lambda_3}(\tau_3)^\bullet a_{\varrho_4}(\tau_4)^\bullet][a^*_{\sigma_4+\lambda_4}(\tau_4)^\bullet a_{\sigma_4}(\tau_4)^\bullet][a^*_{\varrho_4-\lambda_4}(\tau_4)^\bullet a_{\varrho_5}(\tau_5)]\times$$
$$\times[a^*_{\sigma_5+\lambda_5}(\tau_5)^\bullet a_{\sigma_5}(\tau_5)^\bullet][a^*_{\varrho_5-\lambda_5}(\tau_5)^\bullet a_{\varrho_6}(\tau_6)^\bullet][a^*_{\sigma_6+\lambda_6}(\tau_6)^\bullet a_{\sigma_6}(\tau_6)^\bullet]\times$$
$$\times[a_{\varrho_1}(\tau_1)^\bullet a^*_{\varrho_6-\lambda_6}(\tau_6)^\bullet]$$
$$=\frac{1}{6}N^{-6}\sum_{\varrho}\sum_{\substack{\sigma_1\sigma_2\sigma_3\\ \sigma_4\sigma_5\sigma_6}}\Gamma^0_{\varrho,\sigma_1}\Gamma^0_{\varrho,\sigma_2}\Gamma^0_{\varrho,\sigma_3}\Gamma^0_{\varrho,\sigma_4}\Gamma^0_{\varrho,\sigma_5}\Gamma^0_{\varrho,\sigma_6}\times$$
$$\times\bar{n}_{\sigma_1}\bar{n}_{\sigma_2}\bar{n}_{\sigma_3}\bar{n}_{\sigma_4}\bar{n}_{\sigma_5}\bar{n}_{\sigma_6}I_6(\varrho), \tag{B.1}$$

$$I_6(\varrho) = \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \dots \int_0^\beta d\tau_6 \, [\theta_{1,2}\bar{n}_\varrho + \theta_{2,1}(\bar{n}_\varrho + 1)] \times$$

$$\times [\theta_{2,3}\bar{n}_\varrho + \theta_{3,2}(\bar{n}_\varrho+1)] \, [\theta_{3,4}\bar{n}_\varrho + \theta_{4,3}(\bar{n}_\varrho+1)] \, [\theta_{4,5}\bar{n}_\varrho + \theta_{5,4}(\bar{n}_\varrho+1)] \times$$

$$\times [\theta_{5,6}\bar{n}_\varrho + \theta_{6,5}(\bar{n}_\varrho+1)] \, [\theta_{6,1}\bar{n}_\varrho + \theta_{1,6}(\bar{n}_\varrho+1)]. \tag{B.2}$$

The sixfold integral (B.2) is

$$I_6(\varrho) = \frac{1}{5!} \beta^6 \sum_{n=1}^{\infty} n^6 e^{-\beta n (L+\varepsilon_\varrho)} . \tag{B.3}$$

Introducing the quantities

$$m_i = N^{-1} \sum_\lambda \sum_{n=1}^{\infty} n^{i-1} (1-x_\lambda)^i \, e^{-\beta n (L+\varepsilon_\lambda)}, \quad i = 1, 2, 3, \dots, \infty, \tag{B.4}$$

and taking into consideration that, owing to the symmetry properties of the three cubic lattices,

$$\Gamma^0_{\varrho,\sigma i} \to \gamma_0 (1-x_\varrho)(1-x_{\sigma i}), \tag{B.5}$$

we finally get

$$D_6^{(12)} = \frac{1}{6!} (\beta J \gamma_0)^6 N m_1^6 m_6 . \tag{B.6}$$

Along similar lines one can derive the remaining diagrams. Putting

$$\beta J \gamma_0 = x, \tag{B.7}$$

we can represent them as

$$\mathrm{D}_1 = \frac{1}{2} N x m_1^2, \tag{B.8}$$

$$D_2^{(1)} = \frac{1}{2} N x^2 m_1^2 m_2, \tag{B.9}$$

$$D_3^{(1)} + D_3^{(2)} = N x^3 \left(\frac{1}{2} m_1^2 m_2^2 + \frac{1}{3!} m_1^3 m_3 \right), \tag{B.10}$$

$$D_4^{(1)} + {}_4^{(2)}D + D_4^{(3)} = N x^4 \left(\frac{1}{2} m_1^2 m_2^3 + \frac{1}{2} m_1^3 m_2 m_3 + \frac{1}{4!} m_1^4 m_4 \right), \tag{B.11}$$

$$\sum_{p=1}^{6} D_5^{(p)} = N x^5 \left(\frac{1}{2} m_1^2 m_2^4 + m_1^3 m_2^2 m_3 + \frac{1}{8} m_1^4 m_3^2 + \frac{1}{6} m_1^4 m_2 m_4 + \frac{1}{5!} m_1^5 m_5 \right), \tag{B.12}$$

$$\sum_{p=1}^{12} D_6^{(p)} = N x^6 \left(\frac{1}{2} m_1^2 m_2^5 + \frac{5}{3} m_1^3 m_2^3 m_3 + \frac{5}{12} m_1^4 m_2^2 m_4 + \right.$$

$$\left. + \frac{5}{8} m_1^4 m_2 m_3^2 + \frac{1}{24} m_1^5 m_2 m_5 + \frac{1}{12} m_1^5 m_3 m_4 + \frac{1}{6!} m_1^6 m_6 \right) . \tag{B.13}$$

Recurring to the quantity (4.26) and figuring it out by an iteration procedure in the form

$$Y = m_1 + x m_1 m_2 + x^2 \left(m_1 m_2^2 + \frac{1}{2!} m_1^2 m_3 \right) + x^3 \left(m_1 m_2^3 + \right.$$

$$\left. + \frac{3}{2} m_1^2 m_2 m_3 + \frac{1}{3!} m_1^3 m_4 \right) + x^4 \left(m_1 m_2^4 + 3 m_1^2 m_2^2 m_3 + \right.$$

$$\left. + \frac{2}{3} m_1^3 m_2 m_4 + \frac{1}{2} m_1^3 m_3^2 + \frac{1}{4!} m_1^4 m_5 \right) + \ldots , \tag{B.14}$$

we easily show that the sum of diagrams is

$$\sum_n D_n = N \left[x m_1 Y + \frac{1}{2!} (x^2 m_2 - x) Y^2 + \frac{1}{3!} x^3 m_3 Y^3 + \frac{1}{4!} x^4 m_4 Y^4 + \right.$$

$$\left. + \frac{1}{5!} x^5 m_5 Y^5 + \frac{1}{6!} x^6 m_6 Y^6 + \ldots \right]$$

$$= - \sum_\lambda \ln(1 + \bar{n}_\lambda) + \sum_\lambda \ln(1 + \tilde{n}_\lambda) - \frac{1}{2} x N^{-1} \sum_{\varrho\sigma} (1 - x_\varrho)(1 - x_\sigma) \tilde{n}_\varrho \tilde{n}_\sigma . \tag{B.15}$$

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