A COMPARISON OF TWO APPROACHES TO THE DIAGRAM TECHNIQUE FOR GREEN FUNCTIONS CONTAINING SPIN OPERATORS

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The construction of a diagram technique for Green functions containing spin operators is difficult due to the complicated commutation relations of spin operators. At present, there is no commonly accepted diagram technique for the problem in question. After giving a short review of several approaches, we show that the diagram technique of Izyumov, Kassan-Ogly, and Skryabin is not free of inconsistencies.

1. *Introduction*

The application of Green functions (GF) to spin problems is more difficult than to boson or fermion problems because of the commutation relations of the spin operators:

$$[S_f^+, S_g^-] = \delta_{fg} 2S_f^z, \quad [S_f^\pm, S_g^z] = \mp\delta_{fg} S_f^\pm. \tag{1}$$

The commutator of two spin operators is not a *c*-number but again an operator. Further, one has to take into account that the repeated application of a ladder operator S^+ or S^- yields zero at a certain step:

$$(S_f^+)^{2S+1} = (S_f^-)^{2S+1} = 0. \tag{2}$$

It is difficult to deal with this last property of the spin operators, too. There have been many attempts to the approximate calculation of the spin operator GF, the first of them was done by Bogolubov and Tyablikov [1], where the equation of motion for the one--particle GF of a Heisenberg ferromagnet was decoupled. The peculiarities of spin operators as expressed in Eqs. (1) and (2) do not allow one to go, using the equation of motion method, essentially beyond the Bogolubov-Tyablikov approximation without unavoidable ambiguities.

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On the other hand, a diagram technique allows an estimate of the accuracy of any approximation. Therefore, it would be quite useful to develop a diagram technique for the spin operator GF. The algebraic properties (1) and (2) of the spin operators are the main difficulty to overcome. Due to the fact that the commutator of two spin operators is again an operator, Wick's theorem does not apply to spin operators.

An analogue to Wick's theorem, valid for spin operators, was proposed first by Jäger and Kühnel [2] for $S = 1/2$, and by Izyumov and Kassan-Ogly [3] and by Haberlandt and Kühnel [4] for arbitrary S. In the case of arbitrary spin S, the analogue to Wick's theorem is [4]

$$\langle T(S_1^{\alpha_1} S_2^{\alpha_2} \ldots)\rangle_0 = \frac{1}{2\langle S^z\rangle_0} \{G_{12}^0(\tau_1-\tau_2) \langle T([S_1^{\alpha_1}, S_2^{\alpha_2}] S_3^{\alpha_3} \ldots)\rangle_0$$

$$+ G_{13}^0(\tau_1-\tau_3) \langle T(S_2^{\alpha_2}[S_1^{\alpha_1}, S_3^{\alpha_3}] \ldots)\rangle_0 + \ldots\}, \quad (3)$$

where

$$G_{lm}^0(\tau_l-\tau_m) = -\langle T\{S_l^+(\tau_l) S_m^-(\tau_m)\}\rangle_0$$

$$= \begin{cases} (1-e^{-\omega_0/T})^{-1} \delta_{lm} 2\langle S^z\rangle_0 e^{-(\tau_l-\tau_m)} & \text{if } \tau_l-\tau_m > 0, \\ -(1-e^{\omega_0/T})^{-1} \delta_{lm} 2\langle S^z\rangle_0 e^{-(\tau_l-\tau_m)} & \text{if } \tau_l-\tau_m < 0, \end{cases} \quad (4)$$

is the zeroth order GF. Relation (3) is written down for the case where $S_1^{\alpha_1}$ is S_1^+. Only an obvious change in the arguments of the zeroth order GF is necessary for the case $S_1^{\alpha_1} = S_1^-$.

There is no doubt in the validity of the analogue to Wick's theorem (3). However, drawing the diagrams for a certain problem, different representations are used by Izyumov, Kassan-Ogly, and Skryabin (IKS) [5] and by Kühnel [6], Trimper [7], and Haberlandt and Kühnel (HK) [4]. In spite of the fact that it is a laborious and not very profitable task to compare different diagrammatic approaches, we feel it necessary to have a common view on competing approaches. It is our aim to find out whether the diagram techniques proposed by IKS and HK for the Heisenberg ferromagnet are identical, equivalent or contradictory. Our result will be that the analytic expressions for the single terms in the perturbation series are identical in both approaches and the diagrams of IKS and HK are equivalent to each other; however, the graphical representation and the way of summation of diagrams lead to inconsistent results in the IKS approach.

In Section 2 we present our approach and in Section 3 we present the IKS approach for the Heisenberg ferromagnet to that extent necessary for finding the essential differences. In Section 4 we show some internal difficulties of the IKS approach and compare the ways of summation of diagrams in both approaches.

We do not give the full history of numerous different diagram techniques for the spin operator GF, but refer to the literature [5, 6]. In earlier papers [8, 9] we could show that the expressions for the perturbation series obtained in the drone-fermion representation by Spencer [10] and by Izyumov and Kassan-Ogly [3] are identical with those of the Pauli operator approach [2, 6] we proposed for the case of spin 1/2. However, the summation of the terms in the perturbation series (summation of the diagrams) is carried out in different ways. A review of the comparison of different diagram techniques has been given recently [11].

2. *The diagrams introduced by Haberlandt and Kühnel*

In this paper we shall deal with the Heisenberg ferromagnet, the Hamiltonian of which is

$$H = H_0 + H_1, \tag{5}$$

where

$$H_0 = -\omega_0 \sum_f S_f^z, \quad \omega_0 = \mu\mathscr{H},$$

$$H_1 = -\sum_{f,g} J_{fg}(S_f^- S_g^+ + S_f^z S_g^z). \tag{6}$$

No intra-atomic exchange shall be present: $J_{ff} = 0$. The first term in H_1 represents the transverse interaction; the corresponding vertex connects two GF's and will be denoted by a point. The second term in H_1 gives the longitudinal interaction and will be denoted by a wavy line; one end of a wavy line is linked to one incoming GF line and to one outgoing GF line, to one broken line representing $K_0^{zz} = \langle S^z S^z \rangle_0 - \langle S^z \rangle_0^2$ or to a circle standing for $\langle S^z \rangle_0$. A zeroth order GF (4) is represented by a solid line. Additionally, we have a triangle: from one angle an outgoing line starts, at the second angle an incoming line ends, and the third angle is put onto another line without affecting it; all three angles belong to the same lattice site. A broken line or a triangle may be introduced between

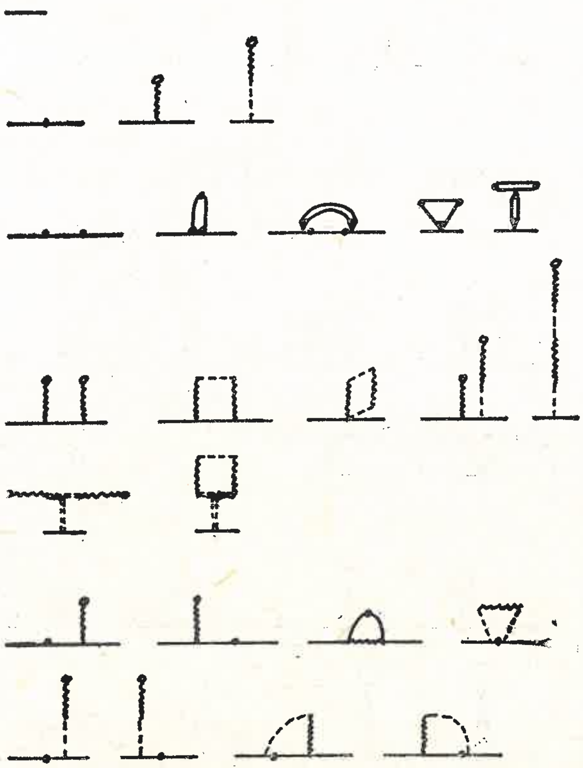

Fig. 1. Diagrams up to the second order according to Haberlandt and Kühnel

two parts of diagrams not belonging to the same lattice site, if it is not ruled out by the relation $J_{ff} = 0$. For further details, we refer to [4]. Three parts of diagrams not belonging to the same lattice site may be connected by a broken double line representing the joint part K_0^{zzz} of $\langle S^zS^zS^z\rangle_0$ etc.

The GF to be calculated is defined as

$$G_{lm}(\tau_l - \tau_m) = -\langle T\{S_l^+(\tau_l)S_m^-(\tau_m)\sigma(1/T)\}\rangle_0 / \langle\sigma(1/T)\rangle_0, \tag{7}$$

where $\sigma(1/T)$ is the usual S operator the expansion of which gives the perturbation series. Up to the second order one gets the diagrams of Fig. 1.

In the case of spin 1/2, the diagrammatic representation simplifies due to the relation

$$S_f^z = \tfrac{1}{2}(1 - 2S_f^- S_f^+) \quad \text{if } S = \tfrac{1}{2}. \tag{8}$$

As a consequence, the higher correlation functions K_0^{zz}, K_0^{zzz} etc. may be expressed in terms of GF lines, vertex parts and triangles; e. g. one has

$$\langle S_l^z S_m^z\rangle_0 = \langle S^z\rangle_0^2 + \bar{n}_0(1 - \bar{n}_0)\delta_{lm}, \tag{9}$$

where $\bar{n}_0 = -G_{ll}(-0) = \langle S_l^- S_l^+\rangle_0$. The diagrams for $S = 1/2$ are shown in Fig. 2 in the same sequence as in Fig. 1 for arbitrary spin. In the case of spin 1/2, in addition to the

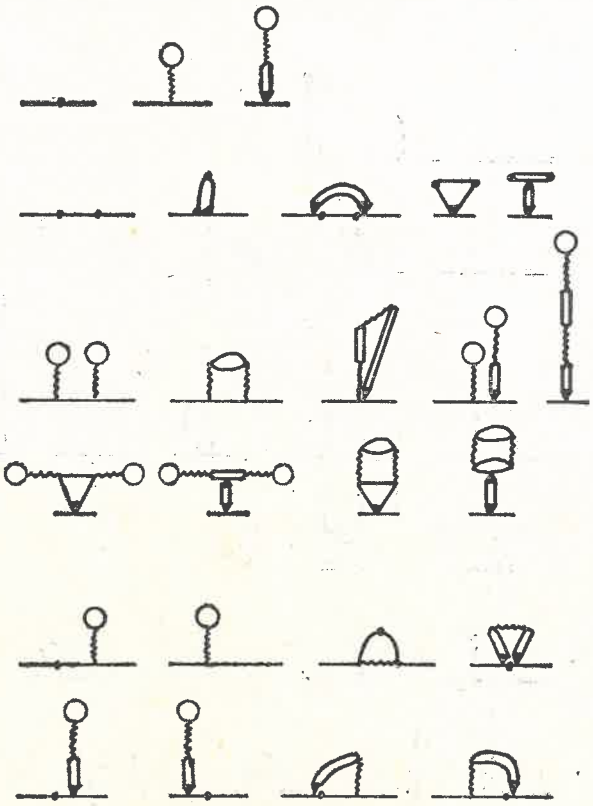

Fig. 2. Diagrams up to the second order according to the Pauli operator approach for spin 1/2

boson case we have only the triangle and the prescription to connect all parts of diagrams which do not belong to the same lattice site with the help of triangles. In this way additional diagrams appear in comparison with the boson case.

One sees at once that some of the diagrams cannot be summed with the help of Dyson's equation. Such diagrams are found to yield just the expansion of $\langle S^z\rangle$, and the factor $\langle S^z\rangle_0$ in the numerator of the zeroth order GF will be replaced by $\langle S^z\rangle$ as the result of the summation of those diagrams [6].

Let us demonstrate the just mentioned situation by considering the trace $\langle T\{S_l^+S_m^-\sigma(1/T)\}\rangle_0$. According to our relation (3) we obtain

$$\langle T\{S_l^+S_m^-\sigma(1/T)\}\rangle_0 = \frac{1}{2\langle S^z\rangle_0}\,[2G^0_{lm}\langle T\{S_m^z\sigma(1/T)\}\rangle_0 + \ldots]. \tag{10}$$

The trace explicitly written down in equation (10) is the expression for the full $\langle S^z\rangle$ (except for the denominator $\langle\sigma\rangle_0$ left out in Eq. (10)). One finds out that the higher order correlation functions of zeroth order appearing in several diagrams become full functions, too [4].

The remaining diagrams may be summed with the help of Dyson's equation. If we take into account the diagrams of Fig. 3 in the self-energy part, we get the following GF:

$$G(\omega_n, k) = \frac{2\langle S^z\rangle}{i\omega_n - \varepsilon_1(k)}, \tag{11}$$

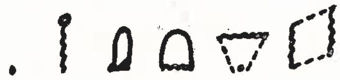

Fig. 3. Diagrams included in the self-energy part in the first order theory

where

$$\varepsilon_1(k) = \mu\mathscr{H} + 2\langle S^z\rangle\,[J(0)-J(k)]$$
$$+\frac{1}{N\langle S^z\rangle}\sum_q [J(q)-J(q-k)]\,[\bar{n}(q)+2K(q)]. \tag{12}$$

In Eq. (12) $K(q)$ is the Fourier transform of K^{zz}_{lm}; $\bar{n}(q) = 2\langle S^z\rangle\phi(q)$, where $\phi(q) = \exp[-\varepsilon(q)/T-1]^{-1}$. The spin wave energy $\varepsilon_1(q)$ is now the commonly accepted expression for the spin wave energy of a first order theory in the sense of Rudoy and Tserkovnikov [12], i. e. by neglection of the damping of the spin waves. This result was derived by Plakida [13] and corresponds to the results of Mubayi and Lange [14] and Kenan [15]. In the case of spin 1/2 the calculation of $\langle S^z\rangle$ is based on the relation (8)

$$\langle S^z\rangle = \tfrac{1}{2}(1-2\langle S^-S^+\rangle) = \tfrac{1}{2}(1+2G_{ll}(-0)) = \tfrac{1}{2}(1-4\langle S^z\rangle\phi),$$

where $\phi = (1/N)\sum_q \phi(q)$, and we get

$$\langle S^z\rangle = \frac{1}{2}\,\frac{1}{1+2\phi} = \tfrac{1}{2}(1-2\phi+4\phi^2+\ldots). \tag{13}$$

The term $4\phi^2$ yields a term proportional to T^3 in the low temperature magnetization, and one does not get agreement with Dyson's result [16]. Rudoy and Tserkovnikov [12] pointed out that only in a second order theory, taking into account the damping of the spin waves, one may get agreement with Dyson's low temperature magnetization in the framework of a spin operator approach.

In the case of higher spins we use the relation [17]

$$\langle S^z \rangle = S - \phi + (2S+1)\phi^{2S+1} + O(\phi^{2S+2}).$$

For $S \geqslant 1$, there is no additional term T^3 since ϕ^{2S+1} is at least of the order $T^{9/2}$ and does not affect either the term T^3 or the term T^4. As a consequence, the case $S = 1/2$ is the most interesting one at low temperatures, and we shall see that the difficulties in the approach of IKS are most evident even for spin 1/2.

3. The diagrams introduced by Izyumov, Kassan-Ogly, and Skryabin

Izyumov, Kassan-Ogly, and Skryabin [5] obtained the same expressions for the single terms in the perturbation series as we did [4, 6]. We could show [9] that there is a one-to-one correspondence between the diagrams of IKS and ours. Fig. 4 shows the diagrams of IKS in the same sequence as the diagrams in Fig. 1 and 2.

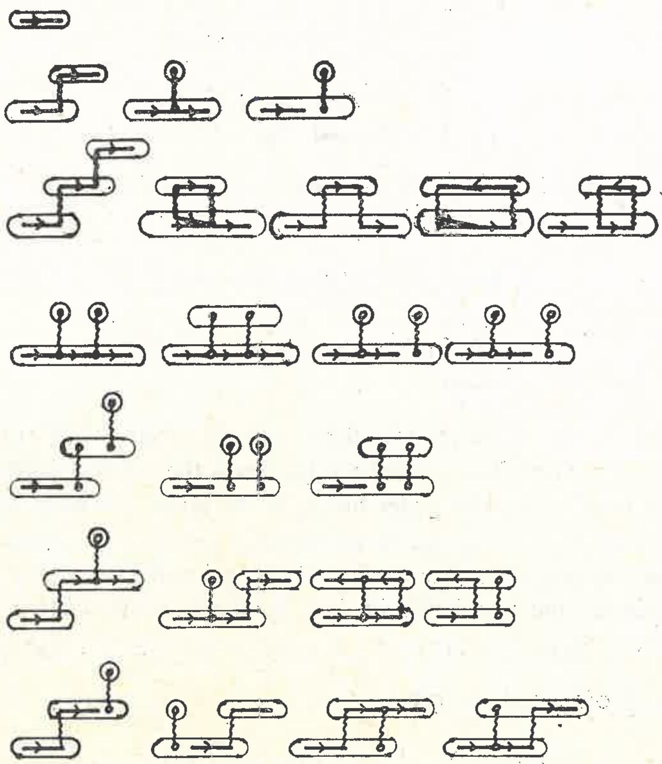

Fig. 4. Diagrams up to the second order according to Izyumov, Kassan-Ogly, and Skryabin

The diagrams in Fig. 4 have the following meaning: A solid line stands for a zeroth order GF, a wavy line represents the longitudinal or the transverse interaction. The additional symbol  comes from the unusual commutation relations. An oval indicates that all parts of a diagram enclosed in it belong to the same lattice site. If an oval encloses 1, 2, 3, ... disjoint symbols, then the corresponding expression is multiplied by $b = \langle S^z \rangle_{\text{MFA}}$, b', b'', ... and by the appropriate product of Kronecker δ's indicating the coinciding lattice sites. All the other diagrammatic rules are as usual.

As a first remark we mention that one free end has been lost in the fourth diagram in the third line in Fig. 4. This lack of one free end is very unusual and may raise difficulties in a consistent summation of the diagrams. In any case, the number of free ends — two for the one-particle GF — is a fixed number during any calculation, and so the graphical representation in the form of the mentioned diagram is very dubious.

The second remark is concerned with the unusual ovals around some parts of the diagrams. These ovals are an expression of the fact that IKS did not really overcome the difficulties with coinciding lattice sites in their graphical representation. In fact, the ovals stand for an infinite number of symbols representing the factors b, b', b'', ... and the corresponding product of Kronecker δ's. In our representation we used a broken line, a broken double line etc. to express the fact in question. In more complicated diagrams the IKS ovals produce an infinite number of new vertex parts. The use of the term "vertex part" is unusual in IKS. In the usual sense, they do not have five vertex parts — as they claim to have — but an infinite number, as it is clear from our representation.

The graphic representation of IKS is not adequate for the summation of the diagrams with the help of Dyson's equation. One does not see which diagrams may be included in the self-energy part and which diagrams cannot be treated by means of Dyson's equation. In particular, this statement applies to the second and to the fourth diagram in the third line in Fig. 4; the second one contributes to the self-energy, the fourth one to $\langle S^z \rangle$. IKS do not use Dyson's equation for the summation of more complicated diagrams, but Larkin's equation [5]. Nevertheless, a clear distinction of the diagrams contributing to the expansion of $\langle S^z \rangle$ and to the self-energy part, respectively, would be useful.

4. Summation of diagrams by Izyumov, Kassan-Ogly, and Skryabin

IKS sum their diagrams step by step up to the consideration of the damping of the spin waves. We shall follow their summation procedure and indicate some errors in their second step, and we find a contradiction in the calculation of $\langle S^z \rangle$.

First, IKS noticed that one may sum diagrams such that $\langle S^z \rangle_0$ becomes a full $\langle S^z \rangle$ at the end of single tails, which is graphically represented by the substitution of the white

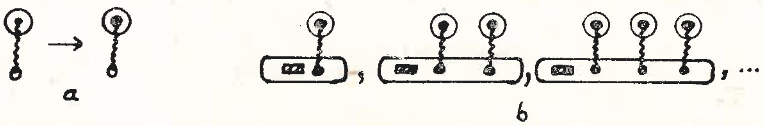

Fig. 5. Diagrams summed by IKS in the molecular field approximation

circle by a black one in all single tails (Fig. 5a). Then, in fact, IKS use Dyson's equation to sum all diagrams contributing a single tail to the self-energy part. Further, they sum all single-tail diagrams appearing as disjoint parts in a diagram (Fig. 5; Fig. 5b is Eq. (3.1) in IKS [5] with the misprints corrected). The resulting GF is in our notations ($J = J_{\mathrm{IKS}}/2$)

$$G_{\mathrm{MFA}}(\omega_n) = \frac{2b(y)}{i\omega_n - \varepsilon_{\mathrm{MFA}}}, \tag{14}$$

where

$$\varepsilon_{\mathrm{MFA}} = y = \mu\mathscr{H} + 2\langle S^z\rangle J(0). \tag{15}$$

This approximation is the molecular field approximation (MFA); in MFA, we have $\langle S^z\rangle_{\mathrm{MFA}} \equiv b(y)$.

The next approximation consists again in the use of Dyson's equation including the wavy line for the transverse interaction into the self-energy part (in the notation of Section 2: including the point). The resulting GF is

$$G_I(\omega_n, k) = \frac{2b(y)}{i\omega_n - \varepsilon_I(k)}, \tag{16}$$

where

$$\varepsilon_I(k) = \mu\mathscr{H} + 2b(y)\,[J(0) - J(k)]. \tag{17}$$

It should be noted that the expression for the spin wave energy (17) is not quite correct. As stated above, $J(0)$ has to be multiplied by $\langle S^z\rangle$ in the corresponding approximation. However, $J(k)$ has to be multiplied by the numerator of the GF, i. e. by $b(y)$. So one really does not obtain the spin wave energy (17) but

$$\tilde{\varepsilon}(k) = \mu\mathscr{H} + 2\langle S^z\rangle J(0) - 2b(y)J(k). \tag{18}$$

Fig. 6. The first diagram is neglected with respect to the second one

Expression (18) is not a reasonable spin wave energy, because $\tilde{\varepsilon}(0) \neq 0$ if $T \neq 0$, since $\langle S^z\rangle \neq b(y)$ in the approximation (16), (17). Deriving expression (16) for the GF, the first diagram in Fig. 6 was neglected as compared to the second one without any foundation. We remember that the neglected diagram is just the diagram in which one free end has been lost.

A consistent approximation would yield the GF

$$G_{\mathrm{BT}}(\omega_n, k) = \frac{2\langle S^z\rangle}{i\omega_n - \varepsilon_{\mathrm{BT}}(k)}, \tag{19}$$

where

$$\varepsilon_{\mathrm{BT}}(k) = \mu\mathscr{H} + 2\langle S^z\rangle\,[J(0) - J(k)]. \tag{20}$$

The GF (19) with the spin wave energy (20) is the result obtained by Bogolubov and Tyablikov [1].

The diagrammatic representation of IKS is inadequate for the application of Dyson's equation and led IKS to the unreasonable spin wave energy (18). Unfortunately, IKS do not distinguish correctly between $b(y)$ and $\langle S^z \rangle$ in the approximation (16), (17). They claim that their result (16), (17) becomes Bloch's linear spin wave theory as well as that it agrees with the result of Bogolubov and Tyablikov. As we pointed out, the spin wave energy (18) results from the very rules of IKS, so neither of these statements is true. The expressions for the low temperature magnetization obtained by Bloch and by Bogolubov and Tyablikov differ from each other by a term T^3 and by higher terms, and one cannot get both results at the same level of approximation as IKS claim to do.

The spin wave energy (18) will be used by IKS in higher approximations in the form (20), without obtaining (20) really in their approach.

The next approximation of IKS results in

$$G_C(\omega_n, \boldsymbol{k}) = \frac{2\langle S^z \rangle}{i\omega_n - E(\boldsymbol{k})}, \tag{21}$$

where at low temperatures (in our notations)

$$E(\boldsymbol{k}) = \mu\mathscr{H} + 2\langle S^z \rangle [J(0) - J(\boldsymbol{k})] + \frac{2}{N} \sum_{\boldsymbol{q}} [J(\boldsymbol{q}) - J(\boldsymbol{q}-\boldsymbol{k})]\phi(\boldsymbol{q}). \tag{22}$$

The shape (21) for the GF was obtained after neglecting some terms in the numerator, but as it stands it is identical with our GF (11) with the spin wave energy (12) neglecting the longitudinal correlation function $K(\boldsymbol{q})$ in (12).

However, in the same approximation $\langle S^z \rangle$ is given as

$$\langle S^z \rangle = S - \phi. \tag{23}$$

In the case $S = 1/2$, expression (23) is in contradiction to the relation (13) which follows from the GF (21):

$$\langle S^z \rangle = \tfrac{1}{2}(1 - 2\phi + 4\phi^2 + \ldots).$$

The additional term $4\phi^2$ yields a term T^3 in the low temperature magnetization, and Dyson's result cannot be obtained from (13), but it comes out starting with (23). In expression (23) the term $(2S+1)\phi^{2S+1}$ is missing.

We do not follow IKS to higher approximations, but the inconsistent treatment of the lowest approximations must reflect in higher ones, too.

5. *Conclusions*

We have shown that the diagrammatic representation proposed by Izyumov, Kassan-Ogly, and Skryabin for the Heisenberg ferromagnet is not adequate for the summation of diagrams at low temperatures. On the contrary, those authors were led to inconsistent and even to contradictory results for the low temperature magnetization after summing their diagrams. Therefore, the diagrammatic method in the book of Izyumov, Kassan-Ogly, and Skryabin should be used very cautiously.

As far as it concerns the Heisenberg model for spin 1/2 at low temperatures, the summation of diagrams performed by IKS is wrong in the approximations (16) and (21)–(23). For a long time it has been unclear whether one could reach agreement with Dyson's low temperature magnetization in a spin operator approach using an approximation such as (21). There were some attempts to obtain this agreement (e. g. Lewis and Stinchcombe [18]), but we could show [19] that this agreement was achieved at the cost of unjustified neglections.

From the coinciding results obtained by several authors by using either the equation of motion method and a decoupling procedure [1, 14, 15, 17, 20] or a formal solution of the equations of motion [12], or perturbation theory [6, 13] it is now well established that a spin operator approach via GF yields a term T^3 in the low temperature magnetization in an approximation such as (21). Agreement with Dyson's low temperature magnetization may be found only in higher order approximations [12]. The results (21)–(23) of IKS are in contradiction to all other spin operator approaches to the Heisenberg model.

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