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ON THE DIAGRAM TECHNIQUE FOR GREEN FUNCTIONS OF THE HEISENBERG FERROMAGNET

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1. Introduction

Green functions (GF) have been applied very successfully in statistical physics. However, the application of GF to spin models is confronted with the difficulties due to the commutation relation of spin operators and the vanishing of the (2S + 1)-th power of the ladder operators. A diagram technique for GF containing spin operators is needed not only for the direct calculation of thermodynamic or dynamic quantities for spin systems but also for the representation of the partition function in terms of functional integrals /1/. In this connection it is necassary for a microscopic foundation of the application of the 3-component φ^4 model for the Heisenberg ferromagnet in the framework of renormalization group in the theory of critical phenomena.

Recently, a paper by van Hemmen et al. /2/ indicated that an energy gap between the physical ground state and the improper (unphysical) states does not exist in the Dyson formalism /3/. This statement again raises the question about the actual temperature dependence of the low temperature magnetization of a Heisenberg ferromagnet. On the other hand a book by Baryakhtar, Krivoruchko, and Yablonski (BKY) /4/ appeared recently proposing a new diagram technique for GF containing spin operators based an the diagram technique by Izyumov and Kassan-Ogly /5/. The results for the GF obtained for a Heisenberg ferromagnet by BKY applying their diagram technique do not agree with those of earlier papers on that problem using different diagram techniques /6,7,8/, decoupling the equations of motion for the GF /9,10,11/ or using a formal solution of the equations of motion /12,13/. In this paper, we answer the question about the origin of the just mentioned discrepancy in the resulting GF for a Heisenberg ferromagnet.

There is now no doubt, how the analytic expressions for the perturbation expansion of the GF for a Heisenberg ferromagnet do look like up to second order. In some earlier papers /14,15,16/, we could show that the perturbation series up to second order agree with each other as they were calculated by Lewis and Stinchcombe /17/, by Spencer using the drone-fermion representation /18/, by Izyumov and Kassan-Ogly /5/ (IKO) and by the present author et al. /6,8/. However, each of the mentioned authors obtains different results for the GF by summing certain classes of diagrams. Therefore, the main problem is to find a proper diagrammatic representation allowing to recognize how one has to sum suitable partial series of the perturbation series. We could show /19/ that IKO /5/ were not able to find a summation of their diagrams free from internal contradictions.

The diagram technique of BKY /4/ is a further development of the one proposed by IKO avoiding the unusual ovals for indicating coinciding lattice sites. BKY apply Dyson's equation for the summation of diagrams, and therefore, a direct comparison with our approach is possible.

The paper is organized as follows. In 2 we shortly explain the difficulties of a diagrammatic representation for GF containing spin operators and present the diagram technique by Kühnel and Haberlandt. Then, we introduce the diagram technique by BKY and compare different diagrams. It turns out that some diagrams are not drawn appropriately, and, as a consequence, BKY are not able to distinguish which diagrams must be included into the self-energy part of Dyson's equation and which must not. In Sec.4 we show explicitly the origin of the discrepancy between the result of BKY and the commonly accepted result for the GF by calculating one of the crucial terms. The conclusions in Sec. 5 are devoted to the problem of the low temperature magnetization and contain some remarks about the representation of spin operators in terms of boson operators.

2. Diagram technique proposed by Haberlandt and Kühnel

Spin operators obey the commutation rules

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

The commutator of two spin operators is again an operator. Therefore, Wick's theorem is not valid in the usual form as for boson or fermion operators. An analogue to Wick's theorem for spin operators has been formulated by Jäger and Kühnel /6/ in the case of spin 1/2 and by Izyumov and Kassan-Ogly /5/ and by Haberlandt and Kühnel /8/ in the case of arbitrary spin:

$$\langle T(S_1^{\alpha_1} S_2^{\alpha_2} \dots)\rangle_0 = \frac{1}{2\langle S^z\rangle_0}\Big\{ G^0_{12}(\tau_1-\tau_2)\langle T([S_1^{\alpha_1}, S_2^{\alpha_2}]\, S_3^{\alpha_3} \dots)\rangle_0 + G^0_{13}(\tau_1-\tau_3)\langle T(S_2^{\alpha_2}[S_1^{\alpha_1}, S_3^{\alpha_3}]\dots)\rangle_0 + \dots \Big\} . \qquad (2)$$

We use the usual Matsubara technique /20/. The operators have to be taken in the interaction representation:

$$O(\tau) = e^{H_0\tau}\, O\, e^{-H_0\tau} , \qquad (3)$$

where H_0 is the free part of the Hamiltonian. The index o at the bracket indicates that the trace has to be performed with the help of $\varrho_0 = \exp(-\beta H_0)$. In equation (2) $G^0_{lm}(\tau_l - \tau_m)$ is the zeroth order GF

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

$$= \begin{cases} (1-e^{-\varepsilon_0/T})^{-1}\,\delta_{lm}\, 2\langle S^z\rangle_0\, e^{-\varepsilon_0(\tau_l-\tau_m)} & \text{if } \tau_l > \tau_m , \\ -(1-e^{\varepsilon_0/T})^{-1}\,\delta_{lm}\, 2\langle S^z\rangle_0\, e^{-\varepsilon_0(\tau_l-\tau_m)} & \text{if } \tau_l < \tau_m . \end{cases} \qquad (4)$$

Equation (2) is written down for the case $S_1^{\alpha_1} = S_1^+$; the case $S_1^{\alpha_1} = S_1^-$ comes out simply by an immediately evident change in the argument of the zeroth order GF. The model we are dealing with is the isotropic Heisenberg ferromagnet.

This model encounters all the difficulties appearing in the diagram technique for a spin model. The Hamiltonian is

$$H = H_0 + H_1 , \qquad (5)$$

where

$$H_0 = -\varepsilon_0 \sum_f S_f^z , \quad \varepsilon_0 = \mu\mathcal{H},$$
$$H_1 = -\sum_{f,g} J_{fg}(S_f^- S_g^+ + S_f^z S_g^z). \qquad (6)$$

No intra-atomic exchange shall be present: $J_{ff} = 0$.

The GF to be calculated is defined as

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

where $\sigma(1/T)$ is the usual S operator the Taylor expansion of which results in the perturbation series; the single terms of that series have to be represented properly by diagrams.

We do not repeat all the details of diagrammatic rules - which are the standard ones- but indicate only the peculiarities resulting from the commutation relations (1) of the spin operators. The transverse interaction (first term in H_1) will be denoted by a dot; and the longitudinal interaction (second term in H_1), by a wavy line.

Besides these two dynamic vertex parts and the zeroth order GF, which we represent by a solid line, there appear further elements in the diagrams coming from the commutation relations (1), from the so-called kinematic interaction. An open circle stands for $\langle S^z\rangle_0$. A broken line corresponds to $K^{zz(o)}_{lm} = \langle S^z_l S^z_m\rangle_0 - \langle S^z\rangle_0^2$,

a broken double line means the connected part $K^{zzz(o)}_{lmn}$ of $\langle S^z_l S^z_m S^z_n\rangle_0$.

The end of a wavy line may be connected with two solid lines getting an additional factor $1/(2\langle S^z\rangle_0)$, with an open circle or with a broken line. The connection of a broken line with a solid line gets a factor $1/\langle S^z\rangle_0$. The triangle stands for a factor $1/(2\langle S^z\rangle_0)$ and it gets an additional factor $1/\langle S^z\rangle_0$ if one edge is parallel to a solid line; all three angles belong to the same lattice site. Two parts of a diagram (including disconnected diagrams) may be connected by means of triangles or broken lines if they do not belong a priori to the same lattice site and if $J_{ff} = 0$ does not rule out the connected term. Three parts of a diagram may be connected by a broken double line.

The resulting terms up to second order of perturbation theory are represented by the diagrams in Fig.1.

In the course of disentangling the traces of several operators $S_1^{\alpha_l}$, there result traces of more and more operators S_1^z. Those traces are calculated as follows:

$$\langle S^z_l S^z_m\rangle_0 = K^{zz(0)}_{lm} + \langle S^z\rangle_0^2$$

$$\langle S^z_l S^z_m S^z_n\rangle_0 = K^{zzz(0)}_{lmn} + \langle S^z\rangle_0\left(K^{zz(0)}_{lm} + K^{zz(0)}_{ln} + K^{zz(0)}_{mn}\right) + \langle S^z\rangle_0^3$$

$$\cdots\cdots\cdots\cdots\cdots\cdots \tag{8}$$

The connected longitudinal correlation functions are defined as

$$K^{zz(0)}_{lm} = \langle\left(S^z_l - \langle S^z\rangle_0\right)\left(S^z_m - \langle S^z\rangle_0\right)\rangle_0 . \tag{9}$$

We are now concerned with the summation of the diagrams shown in Fig. 1. Some diagrams may be summed immediately with the help of Dyson's equation (1, 2, 3, 5, 6, 7, 10, 11, 12, 13, 18, 19, 20, 21, 24, 25). Other diagrams contain only one single zeroth order GF and cannot be summed by means of Dyson's equation. Those diagrams are 4, 8, 9, 15, 16, 17 in Fig. 1. We have established earlier

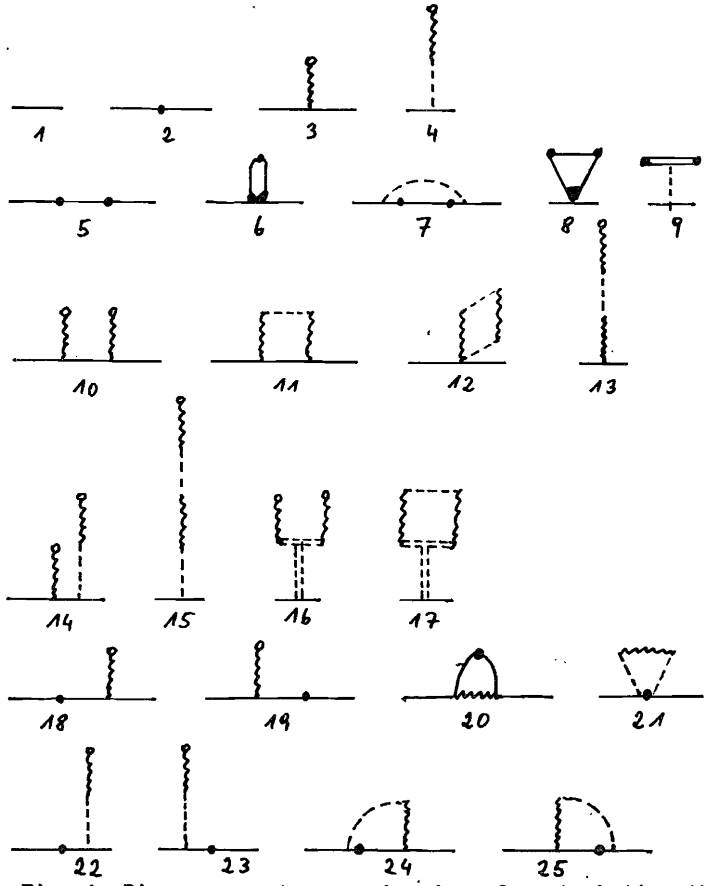


Fig. 1. Diagrams up to second order of perturbation theory

/6,8/ that those diagrams correspond just to the expansion of $\langle S^z\rangle$ (Fig.2). One can see this fact very simply if one calculates the trace in the numerator of (7) by means of relation (2)

$$\langle T\{S^+_l S^-_m \sigma(1/T)\}\rangle_0 = \frac{1}{2\langle S^z\rangle_0}\left(2G^0_{lm}\langle T\{S^z_l\sigma(1/T\}\rangle_0 + \cdots\right). \tag{10}$$

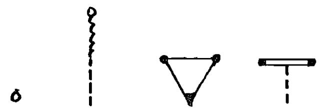


Fig. 2. First diagrams in the expansion of $\langle S^z\rangle$.

The trace explicitly written down is just the expression for $\langle S^z \rangle$ (except for the omitted denominator). Therefore, the summation of the diagrams 4, 8, 9, 15, 16, 17 and similar diagrams result in a factor $\langle S^z \rangle$ in the numerator of the GF instead of $\langle S^z \rangle_0$. After performing this summation the remaining diagrams 14, 22, 23 in Fig. 1 may be summed with the help of Dyson's equation.
The resulting GF is after Fourier transformation

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

where $\langle S^z \rangle$ and $\varepsilon(\omega_n, \underline{k})$ are to be taken in the corresponding approximations. Taking into account the vertex parts shown in Fig.3 in the self-energy part of Dyson's equation the standard spin wave energy /10, 11, 12, 13, 8/ results (first order theory neglecting the damping of the spin waves).

$$\varepsilon_1(\underline{k}) = \mu\mathcal{H} + 2\langle S^z \rangle [J(0) - J(\underline{k})] + \frac{1}{N\langle S^z \rangle} \sum_{\underline{q}} [J(\underline{q}) - J(\underline{q}-\underline{k})][\bar{m}(\underline{q}) + 2K(\underline{q})]. \qquad (12)$$

$K(\underline{q})$ is the Fourier transform of K^{zz}_{lm} in the correspondig approximation; $\bar{m}(\underline{q}) = 2\langle S^z \rangle \phi(\underline{q})$, where $\phi(\underline{q}) = \{\exp[-\beta\varepsilon_1(\underline{q})] - 1\}^{-1}$.

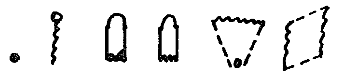


Fig. 3. Diagrams in the self-energy-part in the first order theory

In the case of spin 1/2, $\langle S^z \rangle$ can be calculated according to

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

$$\langle S^z \rangle = \frac{1}{2}\,\frac{1}{1+2\phi}, \qquad (13)$$

where $\phi = (1/N)\sum_{\underline{q}} \phi(\underline{q})$. In the case of arbitrary spin, one uses the relation given by Callen /9/ to calculate $\langle S^z \rangle$:

$$\langle S^z \rangle = S - \phi + (2S+1)\phi^{2S+1} + O(\phi^{2S+2}). \qquad (14)$$

3. The diagram technique proposed by BKY

The diagram technique proposed by BKY is based on that developed by IKO. BKY do not use the ovals introduced by IKO for indicating the same lattice site. Fig. 4 shows the diagrams of BKY in the same sequence as in Fig.1. The zeroth order GF is represented by a solid line, a wavy line with one open circle stands for the transverse interaction and a wavy line with two open circles means the longitudinal interaction. A dotted line has different meaning depending on the number of different symbols, which it connects with each other: If it connects n otherwise unconnected symbols it means the n-th derivative $b^{(n)}$ of the Brillouin function $b = \langle S^z \rangle_0$. The open circle does not have a unique meaning. The additional kinematic diagrams containing the transverse interaction, in which we introduced the triangle, are represented by diagrams the number of incoming solid lines in which is not equal to the number of outgoing solid lines (diagrams 6 and 8 in Fig. 4).
There is a one-to-one correspondence between the diagrams introduced by HK (in the case of spin 1/2 already introduced in /6/) and by BKY (after correction of some misprints: in Fig. 1, 2, 3, in /19/ the diagram 13 is missing, in Fig. 26.1 in /4/ the diagram 14 is absent, in Fig. 4 in /8/ the second line with diagrams 15, 16, 17 was omitted).

4. Summation of diagrams

BKY try to sum their diagrams with the help of Dyson's equation and, therefore, a direct comparison of BKY approach of our summation of diagrams /6,8/ is possible. BKY divide the diagrams into two classes: one class may be summed by introducing them into the self-energy part of Dyson's equation, the other class does not fit into Dyson's equation and is summed to give a new numerator of the GF. However, the division of diagrams into those two classes is not correctly done by BKY. The diagrams introduced by BKY have the following drawback: the dotted lines are connected always with the end of a solid line, not with the solid line as a whole. This erroneous prescription results from the fact that BKY allways give an argument τ to any S^z, while S^z is independent of τ in the interaction representation to be used in the perturbation series. This inadequate diagrammatic representation provides BKY from recognizing that, e.g., their diagrams 7, 12, 21, 25 (diagrams 15, 16, 20, 22 in Fig. 26.1 in /4/) must be introduced into the self-energy part of Dyson's equation and do not contribute to the so-called force part.

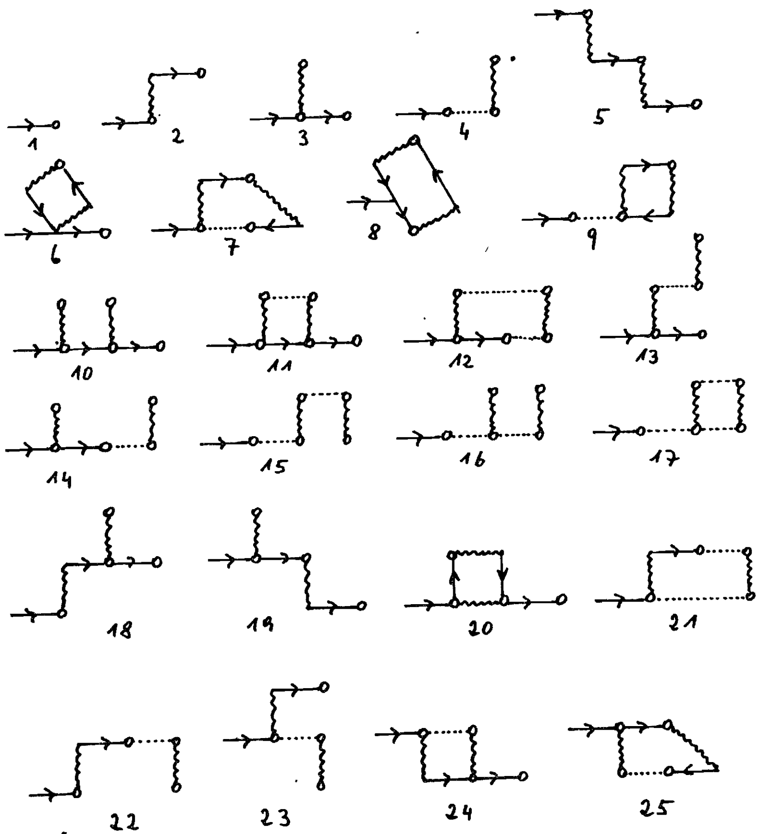


Fig.4. Diagrams introduced by BKY

On the other hand, BKY notice that some of the diagrams which cannot be summed with the help of Dyson's equation yield a full $\langle S^z \rangle$ in the numerator of the GF. However, BKY get the GF in the form

$$G_{lm}(\omega_m, \underline{k}) = \frac{2\langle S^z \rangle + A(\omega_m, \underline{k})}{i\omega_m - \varepsilon(\omega_m, \underline{k})} , \qquad (15)$$

where just those four diagrams 7, 12, 21, 25 contribute to $A(\omega_m, \underline{k})$ which are not erroneously included by BKY into the self-energy part of Dyson's equation according to their unfavourable diagrammatic representation. We now give a simple argument for our point of view. With this aim we calculate explicitly the trace

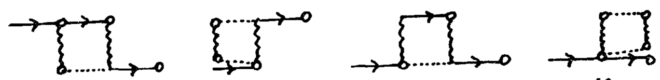
$$\langle T\,(S_l^+ S_f^z S_g^z S_r^- S_s^+ S_m^-)\rangle_0 \qquad (16)$$

which results in the mixed product of transverse and longitudinal interaction in the second order of perturbation theory. We apply the relation (2) three times and disentangle the traces containing 3 or 4 operators S^z using the algorithm (8). As a result, we get ($K^0_{lm} \equiv K^{zz(0)}_{lm}$).

$$\begin{aligned}\langle T(S_l^+ S_f^z S_g^z S_r^- S_s^+ S_m^-)\rangle_0 = \\ -\frac{1}{2\langle S^z\rangle_0^2}\Big(& G^0_{lr} G^0_{sf} G^0_{fm} K^0_{rg} + G^0_{lr} G^0_{sg} G^0_{gm} K^0_{rf} \\ &+ G^0_{lf} G^0_{fr} G^0_{sm} K^0_{gm} + G^0_{lg} G^0_{gr} G^0_{sm} K^0_{fm} \Big) \\ + \frac{1}{2\langle S^z\rangle_0^2}\, & G^0_{lr} G^0_{sm} \left(K^0_{rf} K^0_{gs} + K^0_{rg} K^0_{fs} \right) + \cdots \qquad (17)\end{aligned}$$

The terms omitted in equation (17) correspond to the diagrams 18, 19, 20, 22, 23 which are treated likewise according to the summation procedures of BKY and of HK, respectively. The terms in the first line on the right-hand side in (17) are represented by the diagram 24 in Fig. 1 and Fig. 4; they are included into the self-energy part. The terms in the second line have the same analytical shape like the terms in the first line. However, BKY represent those terms by a diagram (diagram 25 in Fig. 4) which apparently cannot be included into the self-energy part. Of course, the analytic expressions in the second line (17) have to be summed in the self-energy part of Dyson's equation, and our diagram 25 exhibits this property evidently. As concerns diagram 25, the statement that it contributes to the so-called force part of the GF is even wrong: in a diagram contributing to the force part it must be possible to isolate GF G^0_{lm}, what is impossible for diagram 25 (and also for diagram 21) since there is $l=f\neq g=m$. This discrepancy does not affect the spin wave energy (12) because the diagram 25 contributes only to a second order theory taking into account the damping of the spin waves.

The last two terms written down in equation (17) correspond to the diagram 21. It is immediately evident that they may be summed with the help of Dyson's equation since they are products of two GF connected by a vertex part. The product of the two correlation functions $K^{zz(o)}$ is contained in the first order of the expansion of K^{zz} /8/. Using the symbols of BKY one should represent the last four terms in equation (17) by the diagrams 21 and 25 in Fig.5 showing clearly that they are to be included into the self-energy part. Similarly, one can draw the diagrams 7 and 12, as it was done in Fig.5. Having drawn diagrams 7, 12, 21, 25, as it was done in Fig. 5, one never would think of a force part giving an additional term in the numerator of the GF.



25 21 7 12

Fig.5. Proper shape of diagrams contributing apperently to the force part using symbols of BKY

Further, BKY do not notice that the series expansion of the correlation function K^{zz} is contained in the perturbation series, too /8/. Due to that observation the expression b' coming from the molecular field approximation has to be substituted by K^{zz} in subsequent approximations. This is the reason why BKY are not able to reproduce the commonly accepted result (12) for the spin wave energy at low temperatures.

5. Conclusions

We have shown that the GF has the shape (11) and that no additional term (force part) does appear in the numerator of the GF if one does sum the terms in the perturbation series according to their analytical structure. It is important to state /8,6/ that the longitudinal correlation function $K^{zz(0)}$ will as well become a full K^{zz} by summation of partial series as $\langle S^z \rangle_0$ in the numerator of the GF becomes a full $\langle S^z \rangle$. This fact leads to the substitution of the input quantities b, b',... in molecular field approximation (MFA) by the quantities $\langle S^z \rangle$, K^{zz},... in the corresponding approximations. This fact was not recognized by BKY and IKO. As a consequence, quantities of MFA survive in the expressions for the GF. At low temperature we have $b = S$, $b' = b^{(n)} = 0$. Therefore, BKY are not able to obtain the commonly accepted expression (12) for the spin wave energy in a first order theory. Calculating the damping of the spin waves in a second order theory the result will be still poorer. We are now going to discuss the low temperature magnetization and confine ourselves to the case $S = 1/2$, since the essential features can be seen most transparently in that case. According to equation (13) the low temperature magnetization is calculated from

$$\langle S^z \rangle = \frac{1}{2(1+2\phi)} = \frac{1}{2}(1 - 2\phi + 4\phi^2 + \cdots). \tag{18}$$

This relation follows from the commutation relations of the spin operators and from the shape (11) of the GF. The term ϕ^2 produces a term T^3 in distinction to the low temperature magnetization obtained by Dyson /3/. The term T^3 was the subject of many investigations (see /21/ and references therein). If one uses the series expansion for $\langle S^z \rangle$ according to BKY, one gets at low temperatures

$$\langle S^z \rangle = \frac{1}{2}(1 - 2\phi) \tag{19}$$

in contradiction to equation (18), but avoiding the term T^3. This contradiction does not appear in our approach since the series for $\langle S^z \rangle$ contain $\langle S^z \rangle$ itself, and the resulting implicit equation corresponds approximately to (18).

We still add some remarks on a paper by BKY /22/ in which the statement was made that the calculation of the GF gives the same results using spin operators or performing first the Dyson-Maleyev transformation to boson operators. This statement is valid only in MFA. As soon as one passes beyond MFA, the quantities b, b',... become $\langle S^z \rangle$, K^{zz},... and do not differ only by an exponentially small amount from the corresponding quantities obtained after bosonization according to Dyson-Maleyev. However, even if the single terms in the perturbation series would differ only by exponentially small amounts the summation of infinite series may give strongly different results, as it is obviously the case according to the results given above.

There is now doubt in the fact that the GF for a Heisenberg ferromagnet has the shape (11) and the resulting mean occupation numbers of spin wave states obey a Bose distribution modified by the temperature dependent factor $\langle S^z \rangle$ in the numerator.

Acknowledgement

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Кюнель А. E17-86-275
О диаграммной технике для функций Грина гейзенберговского ферромагнетика

Развитие диаграммной техники для функций Грина, построенных из спиновых операторов, сложно из-за перестановочных соотношений этих операторов. Недавно Барьяхтар, Криворучко и Яблонский /БКЯ/ предложили новую диаграммную технику для функций Грина, содержащих спиновые операторы. Мы сравнили эту диаграммную технику с предложенной Хаберландтом и Кюнелем. Вычисляя главные члены, мы показали, что диаграммы БКЯ не определяют вклад при суммировании ряда возмущений. Обсуждены результаты для энергии спиновых волн и магнетизации при низких температурах.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Kühnel A. E17-86-275
On the Diagram Technique for Green Functions of the Heisenberg Ferromagnet

The Green function approach to the Heisenberg ferromagnet is confronted with the difficulties connected with the commutation relations of spin operators. Recently, Baryakhtar, Krivoruchko, and Yablonski (BKY) proposed a new diagram technique for Green functions containing spin operators based on the corresponding technique by Izyumov and Kassan-Ogly. We compared the new approach with that proposed earlier by Haberlandt and Kühnel. Calculating some crucial terms we could show why the diagrams of BKY do not represent the corresponding analytical terms properly if kinematic interaction due to the peculiar commutation relations is involved. The results for the low temperature spin wave energy and magnetization are discussed.

The Investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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