EQUIVALENCE OF TWO SPIN OPERATOR APPROACHES TO A HEISENBERG FERROMAGNET WITH SPIN 1/2

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Different diagram expansions proposed by Izyumov and Kassan-Ogly and Kühnel are compared. A one-to-one correspondence of the diagrams holds up to second order of perturbation theory but different ways of diagram summation are used.

1. Introduction

In recent years several papers on a perturbation theoretical treatment of a many body system described by spin operators have been published. The commutation relations of spin operators prevent the application of Wick's theorem. Therefore, the perturbational approach to the calculation of thermodynamic Green functions (GF) is difficult. In the papers of Wang, Shtrikman and Callen [1], Lewis and Stinchcombe [2], Vaks, Larkin and Pikin (to be referred to as VLP) [3] and Kühnel [4] spin systems (Heisenberg model of ferromagnetism or antiferromagnetism) are treated in different ways with the help of perturbation theory without transformation of spin operators to Bose or Fermi operators. In particular, there exist several later papers based on VLP contributing to a better insight to the VLP method [5], [6]. On the other hand, the VLP method has been applied to the investigation of antiferromagnetic properties [7] and the treatment of kinetic equations and dynamical scaling [8]. Furthermore Stasyuk and Levizkii [9] have treated a model of ferroelectrics with hydrogen bonds by the VLP method.

With respect to further investigations and applications it seems to be interesting to compare the various theoretical perturbation methods and to show the equivalence or the distinction between them. In spite of identical starting points there are obtained different results when one calculates physically interesting quantities such as the low-temperature magnetization of the Heisenberg ferromagnet. These different results arise from the different ways of summing certain classes of diagrams or unmotivated neglection of diagrams.

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In the present paper we want to investigate the mentioned problems by comparing the perturbational approach introduced by Izyumov and Kassan-Ogly [5] (referred to as IKO) and the Pauli operator approach (POA) proposed by Kühnel [4]. For this purpose we write down the perturbation series for the thermodynamic Green function and the main idea of Wick's theorem (Section 2). Section 3 is devoted to the free GF and the contributions up to the first order. We give the diagrams of IKO in detail to correct abominable misprints in the original paper which make it unintelligible and which were pointed out to us by Kassan-Ogly [12]. Then the diagrammatic representations are introduced and the linked diagrams representing second order terms. Section 5 is devoted to the summation of some simple classes of diagrams. A summary and some concluding remarks are made in the last section. We are concerned with the case of spin 1/2 only.

2. *Perturbation series for the GF*

We consider the ideal isotropic Heisenberg ferromagnet with spin 1/2 at each lattice site. The Heisenberg Hamiltonian is $H = -\mu_B \mathscr{H} \sum_f S_f^z - \sum_{f,g} J_{fg} \vec{S}_f \vec{S}_g$. J_{fg} is the exchange integral; $J_{ff} = 0$, since no intra-atomic exchange is considered. $\mathscr{H}$ is an external magnetic field, and μ_B is Bohr's magneton. There are two possible ways of splitting the Hamiltonian into an unperturbed part H_0 and an interaction part H_1 in the case $S = 1/2$. One is to use the relation

$$S_f^z = \tfrac{1}{2} - b_f^+ b_f, \tag{2.1}$$

where b an b^+ are Pauli operators ($S_f^+ = b_f; S_f^- = b_f^+$) by which we obtain

$$H_0 = (\mu_B \mathscr{H} + J(0)) \sum_f b_f^+ b_f, \quad J(0) = \sum_f J_{fg},$$

$$H_1 = -\sum_{f,g} J_{fg}(b_f^+ b_g + b_f^+ b_f b_g^+ b_g). \tag{2.2}$$

This Hamiltonian is the starting point of the Pauli operator approach proposed by Jäger and Kühnel [11].

If we do not apply relation (2.1), we have the other possibility of choosing

$$H_0 = -\mu_B \mathscr{H} \sum_f S_f^z$$

$$H_1 = -\sum_{f,g} J_{fg}(S_f^- S_g^+ + S_f^z S_g^z). \tag{2.3}$$

Equation (2.3) is the outset of the investigation proposed by IKO [5]. Comparing IKO and POA we have to rise the question of which Hamiltonian is more appropriate to calculate the GF.

We define the thermodynamic GF for both Hamiltonians as [10]

$$G_{lm}(\tau_l - \tau_m) = -\frac{\langle T_\tau [S_l^+(\tau_l) S_m^-(\tau_m) S(\beta)]\rangle_0}{\langle S(\beta)\rangle_0} \tag{2.4}$$

with the usual notation. Because of the commutation relations of spin operators

$$[S_f^{\pm}, S_g^z] = \pm S_f^{\pm}\delta_{fg}; \quad [S_f^-, S_g^+] = 2S_f^z\delta_{fg} \tag{2.5}$$

a perturbation theory is more difficult than in the case of Fermi or Bose operators. The reason for this is the lack of Wick's theorem in a closed form [4].

We apply the analogue of Wick's theorem proposed by Jäger and Kühnel [11]. This analogue is used by IKO, too. It holds for any operators $a, b, c, d, \ldots$ satisfying the relation [4]

$$\langle abcd\ldots\rangle_0 = \frac{1}{1-e^{\pm\frac{\omega_0}{T}}}\{\langle[a, b]cd\ldots\rangle_0+\langle b[a, c]d\ldots\rangle_0+\ldots\}. \tag{2.6}$$

Now we choose $a, b, c, d, \ldots$ as operators obeying the commutation relations of spin operators.

We remark that equation (2.6) does not hold for trace of the T_τ-product operators, but we have to disentangle the traces for different orders seperately. This complication is caused by the algebraic properties of spin operators, especially by

$$(S_f^-)^2 = (S_f^+)^2 = 0 \tag{2.7}$$

in the case $S = 1/2$. In the POA all algebraic properties of spin operators are taken into account exactly.

3. *The free Green function and the first order of the perturbation series*

The free GF is calculated easily using (2.6)

$$G_{lm}(\tau) = \begin{cases} -\dfrac{\sigma_0}{1-\exp(-\beta\omega_0)} e^{-\omega_0\tau}\delta_{lm} \text{ for } \tau_l > \tau_m, \\ -\dfrac{\sigma_0}{\exp(\beta\omega_0)-1} e^{-\omega_0\tau}\delta_{lm} \text{ for } \tau_l < \tau_m, \end{cases} \tag{3.1}$$

where $\sigma_0 = 2\langle S^z\rangle_0$ is the relative magnetization per lattice site. IKO choose the free GF without the factor σ_0. Moreover, in the general case of arbitrary spin one must use $\omega_0 = \mu_B\mathscr{H}$ instead of $\omega_0 = \mu_B\mathscr{H}+J(0)$ in POA. The magnetization calculated with the help of the GF (3.1) yields $\sigma_0 = \tanh(\omega_0/2T)$. Thus, the GF G^0 in IKO yields a zero magnetization for $\mathscr{H} = 0$. By summing diagrams with the help of Dyson's equation we can change the GF and obtain a nonzero magnetization (Section 5).

We have to disentangle two first-order terms

$$\langle T_\tau\{S_l^+(\tau_l)S_m^-(\tau_m)S_f^-(\tau_1)S_g^+(\tau_1)\}\rangle_0 \text{ and } \langle T_\tau\{S_l^+(\tau_l)S_m^-(\tau_m)S_f^z(\tau_1)S_g^z(\tau_1)\}\rangle_0. \tag{3.2}$$

In the following we drop the arguments τ for brevity. Because of the absence of intra-atomic exchange ($J_{ff} = 0$) the first term of expression (3.2) is very easily calculated,

$$\langle T_\tau(S_l^+S_m^-S_f^-S_g^+)\rangle_0 = \langle T_\tau(S_l^+S_f^-)\rangle_0\langle T_\tau(S_g^+S_m^-)\rangle_0.$$

Calculating the second term of (3.2) according to IKO we obtain

$$\langle T_\tau(S_l^+ S_m^- S_f^z S_g^z)\rangle_0 = \frac{1}{\langle S^z\rangle_0}\langle T_\tau(S_l^+ S_m^-)\rangle_0[\langle S^z\rangle_0^3 + \langle S^z\rangle_0\langle S^z\rangle_0'(\delta_{lf}+\delta_{lg})] -$$

$$-\tfrac{1}{2}\langle T_\tau(S_l^+ S_f^-)\rangle_0\langle T_\tau(S_f^+ S_m^-)\rangle_0 - \tfrac{1}{2}\langle T_\tau(S_l^+ S_g^-)\rangle_0\langle T_\tau(S_g^+ S_m^-)\rangle_0, \qquad (3.3)$$

with $\langle S^z\rangle_0' = \langle (S^z)^2\rangle_0 - \langle S^z\rangle_0^2$ [5].

Comparing our equation (3.3) with formulae (3.3) in IKO we see that the last two terms are omitted, because of a misprint [12]. The complete set of diagrams is found

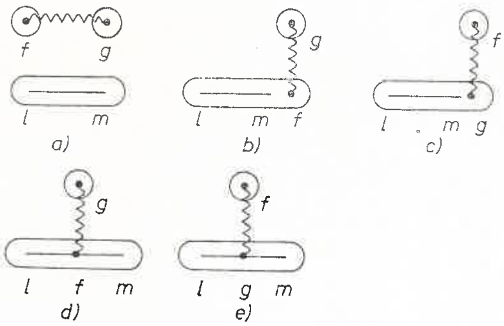

Fig. 1. First order diagrams of IKO

in Fig. 1 in the notation of IKO [12]. A line represents a GF G^0; a wavy line stands for the exchange interaction, and the oval surrounds points which belong to the same lattice site.

Equation (3.3) is valid for general spin. Now we turn to the case $S = 1/2$ and consider two different T_τ-orders using Pauli operators (2.1). First we consider $\tau_l > \tau_m > \tau_1$. Because of $\langle b_l b_f^+\rangle_0 = (1-\bar{n}_0)\,\delta_{lf} e^{-\omega_0(\tau_l-\tau_1)}$ and $\langle b_f^+ b_m\rangle_0 = \bar{n}_0 \delta_{fm} e^{-\omega_0(\tau_m-\tau_1)}$, $\bar{n}_0 = \langle b_f^+ b_f\rangle_0$ we can gather all terms with $l = f = m$ and $l = g = m$, respectively, and obtain

$$\tfrac{1}{2}\langle b_l b_f^+\rangle_0\langle b_m^+ b_f\rangle_0\sigma_0 + \tfrac{1}{2}\langle b_l b_g^+\rangle_0\langle b_m^+ b_g\rangle_0\sigma_0. \qquad (3.4a)$$

Thereby we have used $\langle S^z\rangle_0' = \bar{n}_0(1-\bar{n}_0)$ for $S = 1/2$. On the other hand, we get for $\tau_l > \tau_1 > \tau_m$

$$-\tfrac{1}{2}\langle b_l b_f^+\rangle_0\langle b_f b_m^+\rangle_0\sigma_0 - \tfrac{1}{2}\langle b_l b_g^+\rangle_0\langle b_g b_m^+\rangle_0\sigma_0. \qquad (3.4b)$$

This change of sign in different τ-orders (3.4) expresses the effect of the so-called "half-overlapping lines" [13].

The same difficulties are found in POA [4]. The way out of these difficulties is to keep the single terms as they arise during the calculations without summing all terms with $l = f = m$ and $l = g = m$, respectively. The result is

$$\langle T_\tau(b_l b_m^+ b_f^+ b_f b_g^+ b_g)\rangle_0 = \langle T_\tau(b_l b_m^+)\rangle_0 \bar{n}_0^2 + \frac{1}{\sigma_0}\langle T_\tau(b_l b_f^+)\rangle_0\langle T_\tau(b_f b_m^+)\rangle_0 \bar{n}_0 +$$

$$+\frac{1}{\sigma_0}\langle T_\tau(b_l b_g^+)\rangle_0\langle T_\tau(b_g b_m^+)\rangle_0 \bar{n}_0 -$$

$$-\frac{2}{\sigma_0}\langle T_\tau(b_l b_m^+)\rangle_0\langle T_\tau(b_l b_f^+)\rangle_0\langle T_\tau(b_f b_l^+)\rangle_0 \bar{n}_0 - \frac{2}{\sigma_0}\langle T_\tau(b_l b_m^+)\rangle_0\langle T_\tau(b_l b_g^+)\rangle_0\langle T_\tau(b_g b_l^+)\rangle_0 \bar{n}_0.$$

In Fig. 2 we present the corresponding diagrams using the diagram rules of POA [4]. A free GF is represented by a full line, a square means $2\sum_{f,g} J_{fg}\int d\tau$ and is the vertex part of the longitudinal interaction $(-\sum_{f,g} J_{fg}\, b_f^+\, b_f\, b_g^+\, b_g)$ and a triangle stands for a multiplier $2/\sigma_0$ and characterizes the correction diagrams (details can be found in [4]). In Fig. 2 we gathered the terms differing only by the exchange $f \leftrightarrow g$ (because of $J_{fg} = J_{gf}$) and get a factor 2.

The third diagram in Fig. 2 is due the unusual commutation relations of spin operators.

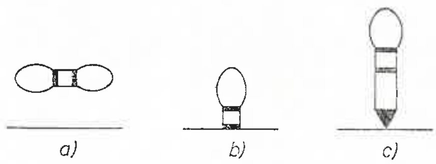

Fig. 2. First order diagrams resulting from $\langle T_\tau(b_l b_m^+ b_f^+ b_f b_g^+ b_g)\rangle_0$

A slight difference between IKO and POA lies in the fact that for the special case $S = 1/2$ there holds the identity $\langle S^z\rangle_0' = \bar{n}_0(1-\bar{n}_0)$ and we can interpret this expression in the diagrammatic representation as two lines running forth and back. (One can easily verify that there are no averages of the form $\langle S^z \ldots S^z\rangle_0$ as in IKO for $S = 1/2$, since $\langle (S^z)^{2k}\rangle_0 = (1/4)^k$ and $\langle (S^z)^{2k+1}\rangle_0' = (1/4)^k \langle S^z\rangle_0$ if $k = 1, 2, \ldots$).

We find a one-to-one correspondence between different diagrams (Figs 1 and 2) and the corresponding mathematical expressions. (Diagrams 1a, 1b and 1c, 1d and 1e correspond to 2a, 2c and 2b, respectively).

We remark that similar investigations as in this section were made to compare the perturbation theory with the help of the drone fermion representation of spin operators with POA and full coincidence is found to exist at the present stage [15].

4. *Second order of perturbation theory*

In the second order we have to calculate the expressions

$$\langle T_\tau(S_l^+ S_m^- S_f^- S_g^+ S_r^- S_S^+)\rangle_0, \quad \langle T_\tau(S_l^+ S_m^- S_f^z S_g^z S_r^z S_S^z)\rangle_0, \quad \langle T_\tau(S_l^+ S_m^- S_f^- S_g^+ S_r^z S_S^z)\rangle_0.$$

After somewhat tedious calculations the first term yields expressions which can be represented by the diagrams in Fig. 3. Comparing them with the expressions resulting from $\langle T_\tau(b_l b_m^+ b_f^+ b_g b_r^+ b_S)\rangle_0$ one finds the correspondence to be unambiguous. The corresponding diagrams are drawn in Fig. 3 [12, 4].

A point in Fig. 3b represents the vertex part of the transversal interaction $(-\sum_{f,g} J_{fg} b_f^+ b_g)$. In the third and fourth diagram of IKO one must keep the indices to distinguish them from each other, since they are topologically equivalent. In POA the two diagrams in question are treated quite differently during summation according to Dyson's equation.

Calculating the remaining second order terms according to IKO and POA one finds full agreement of the results.

5. Summation of diagrams

While we found full agreement of the perturbation series of IKO and POA up to second order terms there is no agreement as regards summation of diagrams. In POA the correction diagrams containing triangles are divided into two classes. One class consists

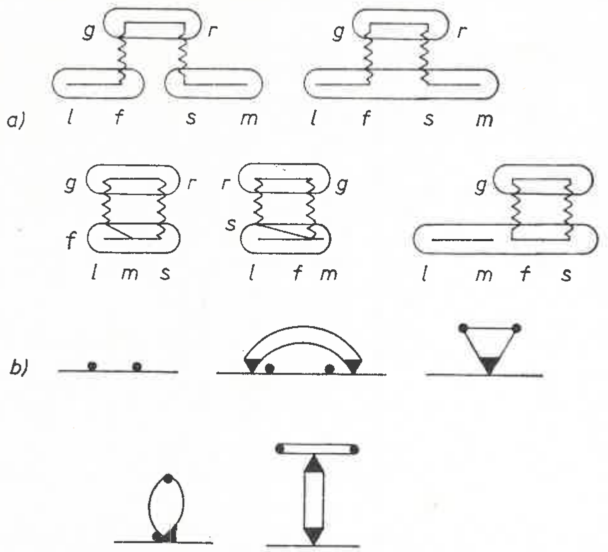

Fig. 3. Second order diagrams of IKO (a) and POA (b)

of vertex parts which are included into the mass operator in Dyson's equation. An example of this kind of correction diagram is the forth diagram in Fig. 3b. The other class includes all correction diagrams which are connected to a full line only by a triangle (Fig. 2, last diagram; Fig. 3, third and fifth diagram). These diagrams cannot be introduced into the mass operator of Dyson's equation. However, we find them all appearing in the perturbation expansion of σ. Therefore, we add them up obtaining a full σ (instead of σ_0) in the numerator of the unperturbed GF. In this way any σ appearing in the GF is understood as a full σ at an equal stage of approximation. Because $\sigma = 1\text{–}2\bar{n}$ and $\bar{n} = -G_{ll}\,(-0)$, there is an unique prescription for the summation: sum the diagrams with the help of Dyson's equation and use the resulting $\bar{n}$ at any place in the GF where it appears.

In the paper of IKO the summation of diagrams is treated rather shortly because the authors could refer to the paper of Vaks, Larkin an Pikin, who calculated the free energy of a Heisenberg ferromagnet. Nevertheless, there are different ways of summing correction diagrams. In IKO correction diagrams are divided into "single tails", "double tails", *etc.* Examples of single tails are the second and the third diagram in Fig. 1, examples of double tails are all the diagrams in Fig. 3a, except the first. The corresponding correction diagrams of POA are found in Figs 2 and 3b, respectively. In IKO the series in Fig. 4a is summed (equation (4.4) in IKO). Below the diagrams of IKO Fig. 4b shows the simplest corresponding diagrams of POA.

According to IKO, in the last two diagrams of Fig. 4b all terms with $l = f = s = m$ are summed (other cases like $l = g = s = m$ merely give a factor 2). While the analytical expression corresponding to the last diagram in Fig. 4b is the same in all τ-orders, the

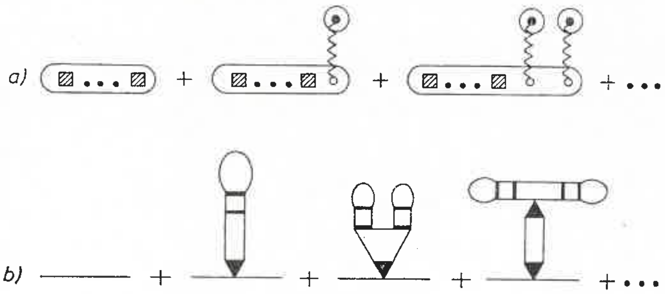

Fig. 4. Correction diagrams in IKO (a) and POA (b)

last but one diagram corresponds to different analytical expressions in different τ-orders. This difficulty is overcome by adding the terms corresponding to $\tau_1 > \tau_2$ and $\tau_2 > \tau_1$, *e. g.* $\tau_l > \tau_1 > \tau_2 > \tau_m$ and $\tau_l > \tau_2 > \tau_1 > \tau_m$. The summation is inconvenient in the GF method and prevents cancellation of the factor $n!$ in the denominator altering the usual geometric series into exponential series. From the point of view of POA this kind of summation is unusual and the question arises why one may neglect the third diagram in Fig. 3b in comparison with the last diagram in Fig. 2. In the language of IKO, one has to explain to what extent the division into single tails, double tails, *etc.*, obeys an order rule showing that they are of different orders of magnitude.

Looking at the result of the summation of IKO one can completely understand the procedure of summation: summing the single tails in basic and correction diagrams always yields the result of molecular field theory [2, 16, 4] and equation (4.6) of IKO is the equation for the magnetization in the molecular field approximation in the special case $S = 1/2$

$$\langle S^z \rangle_{MFA} = \tfrac{1}{2} \tanh \left[(\mu_B \mathscr{H} + J(0) \langle S^z \rangle_{MFA}) / T \right].$$

6. *Conclusions*

We have shown that a one-to-one correspondence holds between the diagrams of POA and IKO in the case $S = 1/2$ up to the second order of perturbation theory. Full equivalence of the two methods calculating the perturbation series is expected.

No agreement can be found in the summation of diagrams. Only the summation carried out in IKO giving molecular field approximation results can be understood within the framework of POA. However, solving the more difficult problem of summing correction diagrams resulting from the transversal interactions (including double tails) has not been attempted by IKO, since the authors could refer to the paper of Vaks, Larkin and Pikin, who calculated the free energy, but not the thermodynamic GF, whereby further direct comparison is impossible.

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