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Abstract

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THERMODYNAMIC GREEN' S FUNCTIONS OF AN ISOTROPIC FERROMAGNET WITH ARBITRARY SPIN

(Presented by Academician N. N. Bogolyubov, May 28, 1962)

Let us consider a system of spins with exchange interaction, assuming that the exchange integral is a nonnegative function of the distance between the points at which the spins are localized. The thermodynamic Green' s functions of such systems were investigated by N. N. Bogolyubov and S. V. Tyablikov ([1]), and also by Pu Fu-cho, S. V. Tyablikov, and T. Shiklosh ([2]-[4]) for spin 1/2.

In the present note we develop methods for solving the problem for higher spins. For this purpose we transform the exchange Hamiltonian, introducing the notation: $S_f = S_f^x - iS_f^y$, $S_f^+ = S_f^x + iS_f^y$, $\sigma_f = S_f^z$, where S_f^x, S_f^y, S_f^z are the components of the spin operator of the atom localized at the point f. In these operators the exchange Hamiltonian has the form

$$H = -h\sum_f \sigma_f - \frac{1}{2}\sum_f \sum_{f\neq g} I(|f-g|)(\sigma_f\sigma_g + S_f^+ S_g), \qquad \sum_f 1 = N. \quad (1)$$

Here h is the product of the external magnetic field by the Bohr magneton; summation is over the whole lattice with the additional condition $I(0) = 0$.

We shall show that the one-particle density matrix will be diagonal if all σ_f are taken in diagonal form. This follows from the following propositions:

1) If $\sigma_f|j\rangle = j|j\rangle$, the only nonvanishing elements of the operators S_f and S_f^+ are the elements $\langle j-1|S_f|j\rangle$ and $\langle j|S_f^+|j-1\rangle$.

2) It follows from 1) that an arbitrary product of S_f, S_f^+, σ_f will be diagonal in the $|j\rangle$-representation when it contains as many operators S_f^+ as S_f. Only in this case can this product be diagonal and different from zero.

3) Only those terms of the expansion in a series of $\exp(-H/\vartheta)$ in which the same number of S_f^+ and S_f operators occurs will contribute to the one-particle density matrix. Here f denotes the coordinates of atoms over whose states the trace is taken. It follows from the form of Hamiltonian (1) that in all terms contributing to the one-particle density matrix, the

operators S^+, S (associated with the atom over whose states the trace is not evaluated) enter in equal numbers—this is what ensures the diagonality of the one-particle density matrix. On the other hand, this indicates that for an isotropic ferromagnet with spin l there can exist only $2l$ linearly independent one-particle moments. In a similar way one can prove that the mean value of an arbitrary product of S_f^+, S_f, σ_f, where f runs through several values, will be nonzero only when in the product the numbers of S-operators "with a cross" and "without a cross" are equal. The same conclusions can be drawn for all mean values calculated with the aid of the density matrix $\exp(-H/\vartheta)$, where the Hamiltonian H is a sum of terms in which there are as many S^+ operators as S operators.

Following paper ([1]), we introduce the retarded and advanced Green functions:

$$\langle\langle A(t) \mid B\rangle\rangle_{\rm ret} = \theta(t)\langle[A(t), B]\rangle, \qquad \langle\langle A(t) \mid B\rangle\rangle_{\rm adv} = -\theta(-t)\langle[A(t), B]\rangle, \qquad \theta(t) = \begin{cases} 1, & t > 0, \\ 0, & t < 0, \end{cases}$$

where $\langle ... \rangle$ denotes averaging over the canonical ensemble; $A(t), B(t)$ are operators in the Heisenberg representation; $[\dots, \dots]$ denotes the commutator. The equations for the Green functions $C^1_{fg}(t) \equiv \langle\langle S_f(t) \mid S_g^+\rangle\rangle$ and $C^2_{fg}(t) \equiv \langle\langle S_f^+(t) \mid S_g\rangle\rangle$ do not depend on the spin of the ferromagnet and will be the same as in ([1]), if one takes into account the difference of units (we have $\hbar = 1$). Eliminating the higher Green functions by the device used in ([1]), namely $\langle\langle S_f(t)\sigma_d(t) \mid S_g^+\rangle\rangle = \langle\sigma_d\rangle C^1_{fg}(t)$, etc., we obtain the solution

$$C^1(E, k) = \frac{i\sigma}{\pi}\{E + h + \sigma[I'(0) - I'(k)]\}^{-1} = C^2(-E, k), \tag{2}$$

in which $I'(k) = \sum_g I(|g|) \exp i(g, k)$; $\sigma = \langle\sigma_d\rangle$; $C^\nu(E, k)$ is defined by means of $C^\nu_{fg}(t)$, $\nu = 1, 2$:

$$C^\nu(E, k) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dt \sum_g \exp[i(k, g) + itE]\, C^\nu_{f+g,f}(t). \tag{3}$$

Calculating the spectral functions and the mean values of the operators by the method developed in ([1]), we obtain equations for σ:

$$\langle S_g^+ S_g + S_{gS} g^+\rangle = 2\sigma\,\frac{v}{(2\pi)^3}\int d^3k \;\mathrm{cth}\,\frac{L + \sigma\varepsilon(k)}{\tau}, \tag{4}$$

where $\varepsilon(k) = 1 - I'(k)/I'(0)$, $L = h/I'(0)$, $\tau = 2\vartheta/I'(0)$, $v = V/N$, and V is the volume of the system. For a ferromagnet with spin 1/2 the operator under the averaging sign is equal to unity, and we obtain the result of paper ([1]) for $\hbar = 1$.

It is useful to note that from equation (4) one can obtain the critical temperature for arbitrary spin. This is connected with the fact that for $L = 0$ at the Curie point the one-particle density matrix possesses spherical symmetry, i.e. all spin projections are equiprobable. Since $(S_g^+ S_g + S_{gS} g^+)|j\rangle = 2[l(l+1) - j^2]|j\rangle$, where $\sigma_g|j\rangle = j|j\rangle$ and l is the maximal value of j, calculation of the mean value reduces to simple summation. Hence, taking (4) into account, we have

$$\tau_c^{-1} = \frac{3}{2l(l+1)} \frac{v}{(2\pi)^3} \int \frac{d^3k}{\varepsilon(k)}. \tag{5}$$

To consider higher spins we take the Green functions

$$\langle\langle P_f(t) \mid S_g^+ \rangle\rangle \equiv Q_{fg}^1(t), \qquad \langle\langle P_f^+(t) \mid S_g \rangle\rangle \equiv Q_{fg}^2(t),$$

where $P_f = S_f \sigma_f + \sigma_{fS} f$ and $\langle P_f \rangle = 0$, which follows from the diagonality of the one-particle density matrix. The equation for Q^1 will be

$$i\dot{Q}_{fg}^1(t) = i\varphi\, \Delta(f-g)\, \delta(t) - hQ_{fg}^1(t) - \tag{6}$$

$$-\sum_d I(|f-d|) \left\{ \langle\langle P_f(t)\sigma_d(t) \mid S_g^+ \rangle\rangle + \frac{1}{2} \langle\langle \varphi_f(t) S_d(t) \mid S_g^+ \rangle\rangle - \langle\langle S_f^2(t) S_d^+(t) \mid S_g^+ \rangle\rangle \right\},$$

and the equation for Q^2 can be obtained from the equation for Q^1 by changing the sign in one of the parts of the equation, replacing at the same time the operators standing in the Green functions by their Hermitian conjugates. In equation (6) $\varphi = \langle \varphi_f \rangle$; $\varphi_f = -4\sigma_f^2 + S_f^+ S_f + S_{fS} f^+$; $\Delta(f-g)$ is the Kronecker δ-function, and $\delta(t)$ is the Dirac δ-function. Decoupling the equations for Q^1 and Q^2 by means of the approximation given by the formulas

$$\langle\langle P_f(t)\sigma_d(t) \mid S_g^+ \rangle\rangle = \sigma Q_{fg}^1(t), \qquad \langle\langle \varphi_f(t) S_d(t) \mid S_g^+ \rangle\rangle = \varphi C_{dg}^1(t),$$

$$\langle\langle S_f^2(t) S_d^+(t) \mid S_g^+ \rangle\rangle = 0$$

and by analogous formulas for the Green function of the conjugate operators, using transformation (3) and solution (2), we obtain

$$Q^1(E,k) = \frac{i\varphi}{2\pi} \{E + h + \sigma[I'(0) - I'(k)]\}^{-1} = Q^2(-E,k). \tag{7}$$

With the aid of the methods developed in (1), we have

$$\langle S_g^+ P_g \rangle = \frac{\varphi v}{(2\pi)^3} \int d^3k \, [e^{-\omega(k)/\vartheta} - 1]^{-1}, \qquad \langle S_{gP} g^+ \rangle = -\frac{\varphi v}{(2\pi)^3} \int d^3k \, [e^{-\omega(k)/\vartheta} - 1]^{-1},$$

$$\omega(k) = h + \sigma[I'(0) - I'(k)],$$

whence

$$\langle S_g^+ P_g + S_{gP} g^+ \rangle = -\frac{\varphi v}{(2\pi)^3} \int d^3k \ \mathrm{cth} \, \frac{L + \sigma\varepsilon(k)}{\tau}. \tag{8}$$

Equations (4) and (8) are suitable for arbitrary spin. For spin 1 they determine two independent one-particle moments. If, in addition to σ, one takes the mean number of atoms with zero spin projection in the z direction, referred to the number of atoms in the lattice—n, equations (4) and (8) can be reduced to the form

$$n = \frac{1}{3}\left[(4 - 3\sigma^2)^{1/2} - 1\right], \qquad 2 + [4 - 3\sigma^2]^{1/2} = \frac{3\sigma v}{(2\pi)^3} \int d^3k \ \mathrm{cth} \, \frac{L + \sigma\varepsilon(k)}{\tau}. \tag{9}$$

Let us now solve equations (9) in the case of low temperatures. Expanding $\mathrm{cth}\,\xi$ in a series in powers of $e^{-\xi}$, and evaluating the integrals by the saddle-point method, we find for a simple cubic lattice, as in work ([2]):

$$\sigma = 1 - \sum_{j \geq 3} A_j \tau^{j/2}, \qquad n = \sum_{j \geq 3} B_j \tau^{j/2},$$

where

$$A_3 = B_3 = \frac{1}{2}\left(\frac{3}{4\pi}\right)^{3/2} Z_{3/2}; \qquad A_4 = B_4 = 0;$$

$$A_5 = B_5 = \frac{3\pi}{4}\left(\frac{3}{4\pi}\right)^{5/2} Z_{5/2}; \qquad A_6 = \frac{3}{8}\left(\frac{3}{4\pi}\right)^{3} Z_{3/2}^2; \qquad B_6 = -\frac{1}{8}\left(\frac{3}{4\pi}\right)^{3} Z_{3/2}^2;$$

$$A_7 = B_7 = \frac{33\pi^2}{32}\left(\frac{3}{4\pi}\right)^{7/2} Z_{7/2}; \qquad A_8 = \frac{3\pi}{2}\left(\frac{3}{4\pi}\right)^{4} Z_{3/2} Z_{5/2}; \qquad B_8 = 0;$$

$$A_9 = B_9 = \frac{1}{64}\left(\frac{3}{4\pi}\right)^{1/2}\left[9 Z_{3/2}^3 + 281\pi^3 Z_{9/2}\right];$$

$$A_{10} = B_{10} = \frac{5\pi^2}{32}\left(\frac{3}{4\pi}\right)^5\left[\frac{33}{2}Z_{3/2}Z_{7/2} + 9Z_{5/2}^2\right].$$

The expression Z_p is given by the sum

$$\sum_{m=1}^{\infty} m^{-p}\exp\left(-\frac{Lm}{v}\right).$$

A comparison of these results with the results of Dyson ([5]) and S. V. Tyablikov ([2]) can be represented by the formulas (Tyablikov' s result is taken for $\hbar = 1$):

$$A_k = A_{k,T} = A_{k,D} \quad \text{for } k = 3, 5, 7;$$

$$A_6 = \frac{3}{8}A_{6,T}; \qquad A_{6,D} = 0; \qquad A_8 = 0.5\,A_{8,T} = 0.3\,A_{8,D} \quad \text{for } l = \frac{1}{2};$$

$$A_8 = 0.6\,A_{8,D} \quad \text{for } l = 1.$$

The terms A_9 and A_{10} were not calculated by Dyson or Tyablikov.

A solution for temperatures $0 \le (t_c - t)t_c^{-1} \ll 1$ can be obtained by expanding $\operatorname{cth}\xi$ in a series in ξ. We find

$$\sigma = \sum_{m\ge 0} a_m v^{2m+1}, \qquad n = \frac{1}{3} + \sum_{m\ge 1} b_m v^{2m},$$

where

$$v = (1 - \tau/\tau_c)^{1/2}, \qquad a_0 = 2\left[\frac{3}{4} + \frac{1}{\tau_c}\right]^{-1/2},$$

$$a_1 = -\tau_c^{-1}\left(\frac{3}{4} + \frac{1}{\tau_c}\right)^{-3/2} - \left[\frac{9}{16} - \frac{4c}{15\tau_c^3}\right]\left(\frac{3}{4} + \frac{1}{\tau_c}\right)^{-5/2},$$

$$b_1 = -\frac{3}{4}a_1^2, \qquad b_2 = -\left[\frac{3}{2}a_1 a_2 + \frac{27}{32}a_1^4\right],$$

and c is equal to $3/2$, $11/8$, $11/9$ for the simple, body-centered, and face-centered cubic lattices, respectively. In contrast to the solution for spin 1/2, this solution cannot be represented in the form of an expansion in powers of $[\tau^{-1} - \tau_c^{-1}]^{1/2}$. It should be noted that the term a_0 for cubic lattices is very close to $4\sqrt{2}/3$, which corresponds to the result of the self-consistent-field theory for $l = 1$.

In the region above the Curie point, in the presence of an external field, we have

$$\sigma = \sum_{m\geq 0} C_m \tau^{-m}, \qquad n = \sum_{m\geq 0} D_m \tau^{-m},$$

where

$$C_0 = 4v\,(3+v^2)^{-1},$$

$$C_1 = 8(1-v^2)(3-v^2)(3+v^2)^{-1}(5-2v^2)^{-1};$$

$$D_0 = (1-v^2)(3+v^2)^{-1},$$

$$D_1 = 64v(1-v^2)(3-v^2)(3+v^2)^{-2}(5-2v^2)^{-1}$$

for $v = \mathrm{th}(L/\tau)$.

An analogous consideration of the problem of spins greater than unity presents no fundamental difficulties.

One should mention one attempt to study higher spins in the work of Kawasaki and Mori (^{6}). In addition to the functions C^1 and C^2, they also introduce the three-time Green function $\langle\langle S_f^+(t) S_d^+(t) \mid S_g^2 \rangle\rangle$. It can be shown that introducing the two-time function $\langle\langle [S_f^+(t)]^2 \mid S_g^2 \rangle\rangle$ instead of Q^2 leads, in the superposition approximation, to serious shortcomings of the solutions near absolute zero and the critical point, since in (^{6}) double integrations over k enter into the equation for σ; however, as is clear from this note, this is not a necessary condition for a satisfactory solution of the problem.

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REFERENCES

[1] N. N. Bogolyubov, S. V. Tyablikov, DAN, **126**, 53 (1959).
[2] S. V. Tyablikov, Ukr. Math. J., **11**, 287 (1959).
[3] Pu Fu-cho, S. V. Tyablikov, T. Shiklosh, Acta Phys. Acad. Sci. Hung., **11**, 323 (1960).
[4] Pu Fu-cho, Scientific Reports of Higher Schools, **2**, 141 (1959).

[5] F. Dyson, Phys. Rev., **102**, 1217, 1230 (1956).
[6] K. Kawasaki, H. Mori, Progr. Theor. Phys., **25**, 1045 (1961).

Note: Figure translations are in progress. See original paper for figures.