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Abstract

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ON THE GREEN' S FUNCTION METHOD IN THE ISING MODEL

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The statistical variational principle of N. N. Bogolyubov (see, for example, ([1])) establishes the following estimate for the upper bound of the free energy F of a system described by the Hamiltonian $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$, $\beta = 1/kT$:

$$F \leqslant \min\{F_0 + \langle \mathcal{H}_1 \rangle_0\}, \qquad -\beta F_0 = \ln \operatorname{Sp} e^{-\beta \mathcal{H}_0},$$
$$\langle ... \rangle_0 = \operatorname{Sp} ... e^{-\beta(F_0 - \mathcal{H}_0)}, \tag{1}$$

where the partitioning of $\mathcal{H}$ need only ensure the possibility of an exact calculation of $\langle ... \rangle_0$. Kvasnikov ([2]), applying (1) to the calculation of the statistical sum and the spontaneous magnetization σ of an Ising ferromagnet, obtained and studied a transcendental equation for the magnetic state of Weiss type, approximately valid for all temperatures and exhibiting a phase transition at the temperature $[k\beta_c^*]^{-1}$

$$\sigma = \frac{1}{2} \operatorname{th} \left[\frac{1}{2} \beta (\mu H + I_0 \sigma) \right], \qquad (\beta_c^*)^{-1} = \frac{1}{4} I_0 \quad (I_0 = Iz). \tag{2}$$

In the present note it will, in particular, be shown that the variational principle is equivalent to the summation of a certain class of diagrams of temperature perturbation theory.*

Let a spin system of a homogeneous isotropic ferromagnet in a constant external magnetic field H be described by the model Heisenberg Hamiltonian, which in the Pauli operators b_f, b_f^+ has the form ([1])

$$\mathcal{H} = E_J + \mathcal{H}_0 + \mathcal{H}_1^{(tr)} + \mathcal{H}_1^{(l)},$$

$$E_J = -\frac{1}{2} \mu H N - \frac{1}{8} N I_0, \qquad \mathcal{H}_0 = \varepsilon \sum_f n_f, \qquad \varepsilon = \mu H + \frac{1}{2} I_0, \tag{3}$$

$$\mathcal{H}_1^{(tr)} = -\frac{1}{2} I \sum_{\langle f_1 f_2 \rangle} b_{f_1}^+ b_{f_2}, \qquad \mathcal{H}_1^{(b)} = -\frac{1}{2} I \sum_{\langle f_1 f_2 \rangle} n_{f_1} n_{f_2},$$

(the indices tr and l refer to the interaction of the transverse and longitudinal components of the spins, respectively); here $\{f\}$ is the set of N lattice sites, $I > 0$ is the exchange integral, $\langle f_1 f_2 \rangle$ denotes summation over nearest neighbors (whose number is z), and μ is the magnetic moment.

Introduce the full one-particle Green' s function

$$G(f - f'|\tau - \tau') = \langle T(b_f(\tau) b_{f'}^+(\tau'))\rangle = \theta(\tau - \tau')\langle b_f(\tau) b_{f'}^+(\tau')\rangle + \eta_{ff'}\theta(\tau' - \tau)\langle b_{f'}^+(\tau') b_f(\tau)\rangle,$$

where $b_f(\tau) = e^{\tau\mathcal{H}} b_{fe}^{-\tau\mathcal{H}}$; $\langle ...\rangle \equiv \mathrm{Sp} \ldots e^{-\beta\mathcal{H}} / \mathrm{Sp}\, e^{-\beta\mathcal{H}}$; $\theta(\tau - \tau')$ is the step function, discontinuous at $\tau = \tau'$; the T-ordering operation is defined at $\tau = \tau'$ so that $G(f - f'|0) \equiv G(f - f'|0\_)$; the function $G(0|\tau - \tau')$ has a unit jump at $\tau = \tau'$; $G^+ - G^- = 1$; $G^\pm \equiv G(0|0\pm)$. We note that the magnetization (in units of μ) is given by the expression**:

$$\langle s^z \rangle = \frac{1}{2} + G^-. \tag{4}$$

* Apparently, this fact was first noted by V. V. Tolmachev ([3]) using the example of a nonideal Bose-Einstein system.

** By translational invariance, one-time averages do not depend on the lattice-site index.

Passing to the interaction representation, we apply to the calculation of G the diagram technique for Pauli operators developed in (4) in terms of the bare Green function $G^{(0)}$ on the basis of the generalized Wick theorem–K. Bloch–Dominicis (5). Since $\langle \mathcal{H}_1^{(tr)} \rangle_0 = 0$, the Heisenberg and Ising models are equivalent in the sense of the variational principle (1), and we need consider only diagrams arising from $\mathcal{H}_1^l$, in which the Pauli operators can be replaced by Fermi operators * ($\eta_{ff'} = -1$). The function G satisfies Dyson' s equation

$$G^{-1} = [G^{(0)}]^{-1} - M\{G\}, \tag{5}$$

where the mass operator $M\{G\}$ for the Ising system with two-particle interaction is represented in the form **

$$M = IG + IGG\Delta G \tag{6}$$

Fig. 1

(the corresponding skeleton diagrams are shown in Fig. 1a, b; the exchange diagram (Fig. 1c) gives no contribution because of the condition $I(0) = 0$);

Fig. 1

Figure 1: Fig. 1

for the vertex part Δ there is no general equation, and therefore the system of equations (5) and (6) is not closed. In the usual procedure of iterative solution of the nonlinear integral equation (5) one is restricted to the approximation $M\{G^{(0)}\}$, which clearly cannot yield a phase transition, since it contains no restrictions on the region of existence of a nontrivial solution. We shall show that application of the variational principle (1) is equivalent to solving equation (5) with the "cut-off" mass operator $M^*\{G\}$, corresponding to the diagram in Fig. 1a. Introducing the Fourier representation $G(0|\tau-\tau')$ (6), we obtain for the Fourier components $G_m \equiv G(0|\omega_m)$ the algebraic analogue of equation (5)

$$G_m^{-1} = [G_m^{(0)}]^{-1} - M_m\{G\}, \qquad G_m^{(0)} = (i\omega_m - \varepsilon)^{-1}, \qquad \omega_m = \beta^{-1}\pi(2m+1),$$
$$m = 0,\ \pm 1, ... \tag{7}$$

Taking into account in (7) only M^* leads to the equation

$$[G_m^{(1)}]^{-1} = [G_m^{(0)}]^{-1} + I_0\beta^{-1}\sum_n G_n^{(1)}\exp(i\omega_n 0^-). \tag{8}$$

The Fourier transform $M^*\{G\} = -I_0 G^-$ does not depend on ω_n, and therefore the action of the mass operator in (8) reduces merely to a renormalization of the spin-deviation energy $\varepsilon \to {}^*\varepsilon = \varepsilon - M^*$, i.e. (with (4) taken into account) $\varepsilon^* = \mu H + I_0\langle s^z\rangle$; summing (8) over all m, we obtain

$$\frac{1}{\beta}\sum_m G_m^{(1)} = \frac{1}{\beta}\sum_{m\geqslant 0}\frac{2\varepsilon^*}{\omega_m^2 + (\varepsilon^*)^2} = \frac{1}{2}\,\mathrm{th}\,\frac{\beta\varepsilon^*}{2}. \tag{9}$$

On the other hand, from the general theory of Fourier series it is known that if the function $G(0|\tau-\tau')$ is discontinuous at $\tau=\tau'$, then

$$\frac{1}{\beta}\sum_m G_m = -\frac{1}{2}[G^+ + G^-]. \tag{10}$$

Expressing G^+ in (10) through G^- and combining (4), (9) and (10), we obtain for $\langle s^z\rangle$ exactly equation (2). Let us note that at the same time there occurs a summation of the most branched "Mayer graphs" (4) on the lattice–Cayley trees, having in the k-th order $k+1$ vertices and k bonds.

*

- Taking into account $\mathcal{H}_1^{(tr)}$ in the quasiboson approximation ($\eta_{ff'} = 1$) leads at low temperatures ($\beta \gg \beta_c$) to the appearance of spin waves, substantially distinguishing the Heisenberg model from the Ising one.

** Multiplication denotes convolution over imaginary time and over the indices of lattice sites.

According to the Luttinger–Ward variational theorem (7), the free energy F is expressed in terms of M^* and $G^{(1)}$ from (8),

$$\frac{1}{N}F = E - \frac{1}{\beta}\ln 2 + \frac{1}{\beta}\sum_m \exp(i\omega_m 0^-)\{\ln[G_m^{(1)}]^{-1} - M^* G_m^{(1)}\} - \frac{1}{2}I_1|G^{(1)}|^2,$$

which, taking (4) into account, finally gives

$$\frac{1}{N}F = -\frac{1}{2}\mu H - \frac{1}{\beta}\ln 2 - \frac{1}{\beta}\ln Z(\varepsilon^*) - \frac{1}{2}I_1\langle s^z\rangle + \frac{1}{2}I_0\langle s^z\rangle^2. \tag{11}$$

It is easy to see that the value $\langle s^z\rangle$ satisfying (2) minimizes F from (11); this fact is a consequence of theorem (7) on the stationarity of the functional F with respect to variations of M (or G).

Finally, of interest is the expression for the specific susceptibility

$$\chi = N^{-1}\mu^2\beta\sum_{f_1 f_2}\{\langle s_{f_1}^z s_{f_2}^z\rangle - \langle s_{f_1}^z\rangle\langle s_{f_2}^z\rangle\} = N^{-1}\mu^2\beta\sum_{f_1 f_2}\{\mathfrak{G}(f_1 - f_2, 0^-) - |G|^2\},$$

where

$$\mathfrak{G}(f_1 - f_2|\tau_1 - \tau_2) = \langle T(b_{f_1}(\tau_1)b_{f_2}(\tau_2)b_{f_1}^+(\tau_1)b_{f_2}^+(\tau_2))\rangle$$

is the two-particle Green' s function, expressed through G from (5) and Δ; $\mathfrak{G} = G^2 + GG\Delta GG$. If one restricts oneself to taking into account the simplest compact vertex part $\Delta_c^* = I$ (Fig. 2a), corresponding to a narrowing of M^*, then Δ^* can be represented in the form of a modified interaction (Fig. 2b)

$$J(f-g) = N^{-1}\sum_q J_q \times \exp i(f-g, q)$$

(characteristic of strongly compressed systems), for whose Fourier transforms an equation analogous to (7) is valid,

$$J_q^{-1} = I_q^{-1} - P^*, \tag{12}$$

Fig. 2

Figure 2: Fig. 2

here $P^* = GG$ is the analogue of the polarization operator (Fig. 2c). In the present approximation

$$P^* = \beta^{-1}\sum_m |G_m^{(1)}|^2 = \frac{\partial}{\partial\varepsilon^*}\left\{\beta^{-1}\sum_m G_m^{(1)}\right\} = \frac{1}{4}\beta\left(1 - \mathrm{th}^2\,\frac{\beta\varepsilon^*}{2}\right);$$

then

$$\chi^{-1} \sim 1 - I_0 P^* = 1 - 4(\beta/\beta_c^*)(1/4 - \langle s^z\rangle^2) \tag{13}$$

with $\langle s^z\rangle$ from (2). At the phase-transition point ($\beta = \beta_c^*$)$\langle s^z\rangle$, by definition, vanishes at $H = 0$, while χ, as is seen from (13), has a simple-pole singularity.*

Fig. 2

Let us examine what results from including in the mass operator the term $\widetilde{M}\{G\}$, corresponding to the diagram in Fig. 2c and obtained by replacing Δ by Δ^* in (6). The corresponding Dyson equation has the form

$$[G_m^{(2)}]^{-1} = [G_m^{(0)}]^{-1} + I\beta^{-1}\sum_n G_n^{(2)}\exp(i\omega_n 0^-) - \widetilde{J}(0)G_m^{(2)}, \tag{14}$$

where $\widetilde{J}(0) = N^{-1}\sum_q \widetilde{J}_q > 0$, $\widetilde{J}_q$ satisfies an equation of type (12), in which, however, the polarization operator is constructed on the functions $G^{(2)}$. Solving the equation (14), quadratic with respect to $G_m^{(2)}$, we obtain for the analytic continuation of the Fourier transform $G^{(2)}$ in the complex domain the expression

$$G^{(2)}(\zeta) = 2[\zeta - \varepsilon^* + \sqrt{(\zeta-\varepsilon^*)^2 - 4\widetilde{J}(0)}]^{-1};$$

$G^{(2)}(\zeta)$ has a cut along the segment of the real axis joining the branch points $\zeta = \tilde{\varepsilon}^+$ and $\zeta = \tilde{\varepsilon}^-$, $\tilde{\varepsilon}^{\pm} = \varepsilon^* \pm 2\sqrt{\widetilde{J}(0)}$, and coincides with $G^{(1)}(\zeta)$ in the formal limiting transition $\widetilde{J}(0) \to 0$. In view of the complexity of comput–

* Of course, the same result for χ can be obtained by differentiating $\langle s^z\rangle$ in (2) as an implicit function of H.

···values in the exact function $G^{(2)}$, it seems reasonable to resort to an iteration scheme, approximating $\widehat{M}_m\{G^{(2)}\}$ in (14) by the value $\widehat{M}_m\{G^{(1)}\}$, which is equivalent to restricting oneself to the pole approximation for $G^{(2)}(\zeta)$:

$$G^{(2)}_{\text{pole}}(\zeta) = \frac{1}{2}\left[(\zeta-\varepsilon^-)^{-1} + (\zeta-\varepsilon^+)^{-1}\right], \tag{15}$$

where

$$\varepsilon^{\pm} = \varepsilon^* \pm \sqrt{J(0)}, \qquad J(0) = N^{-1}\sum_q I_q\left[1-\beta I_q\cdot\frac{1}{4}\left(1-\text{th}^2\,\frac{\beta\varepsilon^*}{2}\right)\right]^{-1} > 0.$$

Putting $\zeta = i\omega_m$ in (15) and summing over all m, we obtain the following equation for the magnetization ($\varepsilon^* = \mu H + I_0\langle s^z\rangle$)

$$\langle s^z\rangle = \frac{1}{4}\,\frac{\text{sh}\,\beta\varepsilon^*}{\text{ch}(\beta\varepsilon^-/2)\,\text{ch}(\beta\varepsilon^+/2)} = \frac{1}{2}\,\frac{\text{sh}\,\beta\varepsilon^*}{\text{ch}\,\beta\varepsilon^* + \text{ch}\,\beta\sqrt{J(0)}}. \tag{16}$$

The equation for the Curie point β_c is found from the condition $\chi^{-1} = (\partial\langle s^z\rangle/\partial H)^{-1} = 0$ at $H = 0$ and $\beta = \beta_c$ ($\langle s^z\rangle = 0$ and $\varepsilon^* = 0$):

$$1 = \frac{\beta_c}{\beta_c^*}\left\{1-\text{th}^2\,\frac{\beta_c}{2}\left[\frac{1}{N}\sum_q I_q\left(1-\frac{\beta_c I_q}{4}\right)^{-1}\right]^{-1/2}\right\}. \tag{17}$$

The transcendental equation (17) indicates a lowering of the true Curie point in comparison with the Weiss value, $\beta_c > \beta_c^*$, which corresponds to the physical meaning of the theory. Introducing the function $F(x) = N^{-1}\sum_q (x-\gamma_q)^{-1}$, $\gamma_q = I_q/I_0$, we represent (17) in the form

$$\beta_c = \beta_c^*\left\{1-\text{th}^2\left[\alpha^2 F(\alpha)-\alpha\right]^{1/2}\right\}^{-1}, \qquad \alpha = \beta_c^*/\beta_c \le 1. \tag{18}$$

Putting $\alpha = 1$ in (18), we find as a result of the first iteration that

$$\beta_c = \beta_c^*\{1-\text{th}^2[F(1)-1]^{1/2}\}^{-1};$$

expanding further the right-hand side in powers of $F(1)-1$, we obtain (in the linear approximation) the result of the spherical Ising model* (8):

$$\beta_c/\beta_c^* = F(1),$$

reproduced by Brout (10) in the formalism of "high-density" expansions** to first order in $1/z$.

We note that exactly the same result for the Curie point is obtained in the Heisenberg model by the method of retarded Green' s functions in the random-phase approximation (1).

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* The values $F(1) = 1.34;\ 1.39;\ 1.52$ in the nearest-neighbor approximation for face-centered, body-centered, and simple cubic lattices, respectively ($z = 12, 8, 6$), were first calculated by Watson (9).

** In the "infinite-density" limit $z \to \infty$, $I \to 0$ ($I_0 = \text{const}$), $\gamma_q = z^{-1} \sum \exp(iq\delta) \to A(q)$, and $F(\alpha) \to 1/\alpha$ ($\alpha \geq 1$) in the statistical limiting transition $N \to \infty$; in this case, as is seen from (18), the value of the Curie point $\beta_c = \beta_c^*$ becomes exact.