ON THE QUESTION OF POINTS OF NONANALYTICITY OF THE GREEN FUNCTIONS OF A SYSTEM OF INTERACTING PARTICLES

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Abstract

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L. Ya. KOBELEV

ON THE QUESTION OF POINTS OF NONANALYTICITY OF THE GREEN FUNCTIONS OF A SYSTEM OF INTERACTING PARTICLES

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1. Phase transitions (including those of the second kind) in nonrelativistic systems of interacting particles (see, for example, ($^{1-5}$)) testify to a nonanalytic dependence of the specific heat and the thermodynamic potential of the indicated systems on the temperature difference $\Delta T = T_0 - T$ (T_0 is the temperature of the phase transition). The nonanalytic dependence on ΔT may be a consequence of the nonanalyticity of the exact one-particle (two-particle, etc.) thermodynamic Green functions of the system, defined by the corresponding equations with variational derivatives (Schwinger equations). It is shown below that such a dependence does indeed exist and can be extracted from the exact Green functions of the system, written with the aid of functional integrals over "external fields" (^{6}) and "classical" trajectories (^{7}), using a variant of perturbation theory consisting in expanding the functional integrals (without restrictions on the interaction parameter or the density of the number of particles) in a series in their deviation from Gaussian integrals over "external fields." It is also shown that near the points of nonanalyticity, i.e., as $\Delta T \to 0$, the "non-Gaussian" corrections to the Green function are small.

2. Consider a system of N interacting nonrelativistic particles (Bose or Fermi particles), described by the creation and annihilation operators from the ground state of particles and field quanta of the interaction $\Psi(x)$, $\Psi^*(x)$, and $A(x)$, respectively, and by the Hamiltonian $H = \Delta/2m + A(x)$ ($\hbar = c = 1$). We define the interaction energy of two particles of the system by the relation (g is the interaction constant)

$$D_0(x) = g^2 \sum_n \int dp \, \frac{e^{ipx}}{L(p, w_n)},$$

where $L(p, w_n)$ characterizes the type of interaction and satisfies the condition $L(0) < \infty$. Following (^{6,8,9}), it is not difficult to show that the exact solution of the thermodynamic Schwinger equation ($t = -i\beta;\ \beta = 1/kT;\ x = \mathbf{x}, t$)

$$\left[-i\frac{\partial}{\partial t} - \frac{\Delta}{2m} - \langle A(x)\rangle + ig\frac{\delta}{\delta I_0(x)}\right] G(x, x') = \delta(x - x'),$$

$$L(\Delta, \partial/\partial t)\langle A(x)\rangle = I_0(x) + igG(x, x) \tag{1}$$

for the thermodynamic one-particle causal Green function $G(x, x') = \langle T(\Psi(x)\Psi^*(x'))\rangle$ ($\langle ...\rangle$ denotes averaging over the statistical ensemble), which describes the behavior of the system under consideration, has the form

$$G(x, x) = \frac{1}{\langle S\rangle}\int dA(x)\ \exp\left\{-\frac{i}{2}\int A(x)D_0^{-1}(x - y)A(y)\, dx\, dy - \int_0^1 d\lambda \int G(x, x \mid \lambda A)A(x)\, dx\right\} G(x, x' \mid A); \tag{2}$$

$$\langle S\rangle = \int dA(x)\ \exp\left\{-\frac{i}{2}\int A(x)D_0^{-1}(x - y)A(y)\, dx\, dy - \int_0^1 d\lambda \int G(x, x \mid \lambda A)A(x)\, dx\right\}; \tag{3}$$

$$[-i\partial/\partial t - \Delta/2m - \lambda A(x)]G(x, x'|\lambda A) = \delta(x - x'); \tag{4}$$

$$[-i\partial/\partial t - (\Delta - \Delta')/2m - \lambda(A(x) - A^*(x'))]G(x, x') = 0, \quad x' \to x. \tag{5}$$

In (2)–(3) the continual integral over $A(x)$ of the functional $\varphi(x|A)$ (the functional dependence is separated by a vertical bar) is defined as the limit of an n-fold integral of a function of n variables $\varphi(x; A_1, \ldots, A_n)$ as $n \to \infty$, $A_{i+1} - A_i \to 0$, $\Delta x_i \to 0$.

Integration over x_4 and variational derivatives with respect to $I_0(x)$, $\langle A(x)\rangle$, etc., differ from zero only for $0 \le ix_4 \le 1/T$; the function $\delta(x_4)$ is defined at discrete "time" points $^{(10)}$. For retarded, advanced, commutator, etc., thermodynamic Green functions, the representation (2)–(4) remains valid when equation (4) for $G(x, x'|A)$ is replaced by the equation for the retarded, advanced, etc., function $G(x, x'|A)$. The "external source" $I_0(x)$ in (2)–(3) is equal to zero.

3. Let us now represent $G(x, x'|A)$ and $G(x, x|A)$ through continual integrals over all continuous trajectories $\mathbf{x}(\nu)$, beginning at "time" $\nu = t'$ at the point $\mathbf{x}'$ and ending at "time" t at the point $\mathbf{x}$ $^{(11,12)}$:

$$G(x, x'|A) = \int_{G_{x,x'}} d_G\mathbf{x}(\nu) \exp\left\{ i \int_{t'}^{t} A(x(\nu))\, d\nu \right\} \equiv$$

$$\equiv \lim_{\substack{\Delta\nu=\nu_{i+1}-\nu_i\to 0 \\ \Delta A = A(x_{i+1})-A(x_i)\to 0 \\ \Delta x = x_{i+1}-x_i \to 0 \\ n\to\infty}} \int dx_1 \ldots \int dx_n\, G_0(\mathbf{x}-\mathbf{x}_1; t-\nu_1) \ldots G_0(\mathbf{x}_n - \mathbf{x}'; \nu_n - t') \times$$

$$\times \exp\left\{ i \sum_{i=1}^{n} A(\mathbf{x}_i)(\nu_{i+1}-\nu_i) \right\}, \qquad it' < it, \quad t = -i\beta; \tag{6}$$

$$(-i\partial/\partial t - \Delta/2m) G_0(x, x') = \delta(x - x'); \tag{7}$$

$$G(x, x) = \lim_{x'\to x} \int_{G_{x,x'}} d_G\mathbf{x}(\nu) \exp\left\{ i \int_{x_4^0}^{x_4} [dA_1(x(\nu)) + 2iA_2(x(\nu))]\, d\nu \right\}. \tag{8}$$

Here x_4^0 is an arbitrary parameter, which in what follows, for convenience, is taken equal to x_4; $dA_1(x) = A_1(x+\Delta x) - A_1(x) + d_{A_1}A_1(x)$ ($d_{A_1}A_1(x)$ is the variation of $A_1(x)$ at the points x); $A = \operatorname{Re} A + i \operatorname{Im} A = A_1 + iA_2$. In the last integrals in (6)–(8) one should replace the solutions (7) $G_0(p)$ by $G_0(p)n(p)$. Taking (6) into account, $G(x, x')$ takes the form ($G(x, x') = 0$ for $ix_4' > ix_4$)

$$G(x, x') = \frac{1}{\langle S \rangle} \int dA(x) \int_{G_{x,x'}} d_G\mathbf{x}(\nu) \exp\left\{ -\frac{i}{2} \int A(x) D_0^{-1}(x-y) A(y)\, dx\, dy \right.$$
$$\left. - \int_0^1 d\lambda \int G(x, x|\lambda A) A(x)\, dx + i \int_{x_4^0}^{x_4} A(x(\nu))\, d\nu \right\}, \qquad ix_4' < ix_4. \tag{9}$$

4. Let us isolate in (9) the "Gaussian" part in $A(x)$ by means of a nonlinear transformation of $A(x)$ of the form

$$A(x) = A'(x) + \int D_0(x-y) \widetilde{F}(y)\, dy,$$

where

$$\widetilde{F}(y) = F(y) + \varepsilon(x(\nu)) = i \int_0^1 d\lambda\, G(yy|\lambda A) + \int_{x_4^0}^{x_4} d\nu\, \delta(x(\nu) - y)\delta(\nu - y^0).$$

This transformation eliminates from the exponent (9) the second and third terms and brings (9) to the form

$$G(x,x') = \frac{1}{\langle S\rangle}\int dA'(x)\int_{G_{x,x'}} d_G\mathbf{x}(\nu)\,D(|A)\exp\left\{-\frac{i}{2}\int A'(x)D_0^{-1}(x-y)\times\right.$$
$$\left.\times A'(y)\,dx\,dy + \frac{i}{2}\int \widetilde{F}(x)D_0(x-y)\widetilde{F}(y)\,dx\,dy\right\}, \tag{10}$$

where $D(|A)$ is the Jacobian of the transformation, coinciding with the Fredholm determinant of the integral equation (see (13)), $A(x) = A'(x) + \int K(x,y)A(y)\,dy$, for $K(x,y) = \int D_0(x-y_1)\dfrac{\delta F(y_1)}{\delta A(y)}\,dy_1$.

We shall show that $D(|A)$ contains a nonanalytic factor due to the dependence of $G(x,x|A)$ on the real part A. Considering the transformation only for A_1 and using the relations $G(x,y) - G(y,x) = \delta_{x,y}$, $\delta F(x)/\delta A_1(y) = \delta_{y,x}\cdot\widetilde{\Pi}_\lambda(0) = \delta_{y,x}\cdot\Pi_\lambda(0)(1-\Pi_\lambda(0)D_0(0))^{-1}$, where

$$\Pi_\lambda(0) = -\frac{T}{(2\pi)^2}\sum_{w_n}\int dp\int_0^1 \lambda\,d\lambda\,G^2(p,w_n|\lambda A), \qquad D_0(0) = g^2L^{-1}(0) \tag{11}$$

and $G(p,w_n|A)$ satisfies (5), and restricting ourselves to the study of the case $F(x)$ independent of x (the analogue of a Bose-particle condensate), we find, separating from $\Pi_\lambda(0|A)$ the term with $d_{A_1}A_1(x)$ in the linear approximation ($\widetilde{D}_0(0) = D_0(0)(1-\Pi_\lambda(0)D_0(0))^{-1}$:

$$D(|A) = D(|A_2)(1-\Pi_\lambda(0)\widetilde{D}_0(0))^{-1}\exp\left\{\frac{\Pi_\lambda(0)D_0(0)}{1-2\Pi_\lambda(0)D_0(0)}\,d_{AA}1\,dv\,\eta\right\},$$

$$\eta = \pm 1. \tag{12}$$

The appearance of the nonanalytic term is due to the retention in $G(x,x|A)$ of first-order terms with respect to the variation of A_1. The ambiguity of the integral over A_1 is removed by the choice of the sign of $d_{AA}1$ (determined by η) from the normalization condition of $G(x,x')$.

5. To eliminate the remaining linear dependence on $dA_1(x)$ (and $A_2(x)$), we separate in $D(|A)$ and in one of the functionals $F(x)$ in the expression $\int\overline{F}(x)D_0F(y)\,dx\,dy$ the terms linear in A_1 and A_2, and eliminate them by means of the transformation

$$A'(x) = A''(x) + \int D_1(x-y)F_1(y)\,dy, \tag{*}$$

where $F_1(x)$ is a functional of A_1 (and A_2), chosen from the condition of compensation of the linear terms (F_1 has the form $F_1 = \int F D_0 \Pi_\lambda \,dx\,dy - \int_{x_4^0}^{x_4'} D_0(x(y)-y)\Pi_\lambda(y-x)\,dy\,dx\,dy$). In this case, in (10) there will appear the Jacobian $D_1'(|A'')$ and the factor $\exp\left\{\frac{i}{2}\int F_1(x)D_1(x-y)F_1(y)\,dx\,dy\right\}$. Omitting the intermediate calculations, we give the expression for $G(x,x')$ after application of an infinite number of transformations of the form (*) and complete elimination from the subintegral expression (10) of the terms linear in $A_1(x)$ (it is not difficult to show that elimination of the terms linear in $A_2(x)$ does not lead to the appearance of new nonanalyticities):

$$G(x,x') = \langle S\rangle^{-1}\int dA^\infty(x)\int_{G_{x,x'}} d_G\mathbf{x}(y)\,D(|A)\prod_{i\geqslant 1}^{\infty} D_i(|A^\infty)\times$$

$$\times\exp\left\{-\frac{i}{2}\int A^\infty D_\infty^{-1}(x-y)A^\infty\,dx\,dy + \frac{i}{2}\int\left[F(x)D_0(x-y)F(y) + \sum_{i=1}^{\infty}F_i(x)D_i(x-y)F_i(y)\right]dx\,dy\right\}, \tag{13}$$

where $A^\infty = A^i|_{i=\infty}$; $D_i(x)$ is the function $D_0(x)$ renormalized by the inclusion of terms $\sim AA$ at each of the transformations; F_i is a functional of A^i, eliminating the linear terms in the $(i+1)$-st transformation; $D_i(|A^i)$ are the Jacobians of the $(i+1)$-st transformation. For $i=\infty$ the quantities F and F_i, and also the variational derivatives of F and F_i with respect to A^i, do not contain terms linear and quadratic in $A(x)$. The parts $D_i(|A)$ that depend on A_1^i have the symbolic form

$$D_i(|A_1^i) = \exp\left\{\ln\left[1 + D_i(0)\frac{\delta F_i}{\delta A^i}\left(1 + d_{A_1}A_1 dv\,\eta\right)\right]\right\}, \tag{14}$$

$$D_i(0)\frac{\delta F_i}{\delta A^i} = \frac{a_i}{1-b_i} = D_i(0)\frac{\delta A F_i}{\delta A^i}\left[1 - \int_{x_4^0}^{x_4} D_i(x(\nu)-y')\frac{\delta F_i(y')}{\delta F_i(y)}\,dy'\,dy\,d\nu\right]^{-1},$$

where $\delta F_i/\delta A^i$ and $\delta A F_i/\delta A^i$ are the total and "partial" (with respect to the explicit dependence on A) variational derivatives. In computing F_i and D_i one must take into account that $\delta_F F_i/\delta F_i$ no longer depends on A_1, and the dependence on A_1 remains only in $\int F_{iD_{iF}} i\,dx\,dy$ and in $\delta A F_i/\delta A^i$. Each of the Jacobians $D_i(|A_1^i)$ has a point of nonanalyticity determined by the relation $1 - b_{iT} = 0$.

6. The perturbation-theory method used below consists in separating out in (13) (when representing $\langle S\rangle$ by means of analytic transformations A', A'', (*) etc.) the Gaussian quadratic form in $A_1(x)$ (i.e., in separating out in the exponent the terms proportional to A_1^∞) and expanding the remaining terms in powers of A_1^∞. Taking account of the normalization

$$\lim_{j\to\infty,\ dA_1\to 0,\ \rho x\to 0} \sum d_{A_1} A_1(x_j)\, d\nu = 1,$$

we then obtain $(G(x,x') = G_\Gamma(x,x') + G_{\mathrm{nG}}(x,x'))$

$$G_\Gamma(x,x') = \prod_{i\geq 0}^{\infty} \left(\frac{D_\infty}{D_\infty^s}\right)^{1/2} \left(1+\frac{a_i}{1-b_i}\right)\left(1+\frac{a_i^s}{1-b_i^s}\right)^{-1} \times$$

$$\times \exp\left\{\frac{a_i}{1-b_i} - \frac{a_i^s}{1-b_i^s} + \frac{i}{2}\int (F_i^0 D_{iF} i^0 - F_i^{0s} D_i^s F_i^{0s})\, dx\, dy\right\} G_\Gamma^0(x,x'). \quad (15)$$

In (15), $a_0 = \widetilde{D}_0(0)\Pi_\lambda(0)$; F_i^0 does not depend on $x(\nu)$; $b_0 = \widetilde{D}_0(0)\Pi_\lambda(0)$; the index s means that the quantity was obtained under the transformation $\langle S\rangle$;

$$D_i^{-1} = \widetilde{D}_i^{-1}(0) + \sum_{n=0}^{i} \frac{\delta^2 a_n}{\delta A^i \delta A^i}(1-b_n)^{-1} \simeq D_0^{-1}(0) + \sum_{n=0}^{i} \frac{\tilde{a}_n}{1-b_n};$$

$$F_j \simeq \frac{i}{2}\int F_{j-1} D_j \frac{\delta F_{j-1}}{\delta A^j}\, dx\, dy - \frac{\delta a_j}{\delta A^j}(1-b_j)^{-1}; \qquad F_0 \equiv \widetilde{F} \quad (i,j = 1,2,\dots,\infty).$$

The function G_Γ^0 satisfies an approximate Dyson equation. The non-Gaussian part of the Green function G_{nG} near $1-b_i \simeq \Delta T_i/T \to 0$ has order $(1-b_i)^2\tilde{a}_i^{-2}G_\Gamma$, since $D_\infty^{-1} \sim \tilde{a}_{iT}/\Delta T_i$; therefore, near the points of nonanalyticity, $G \simeq G_\Gamma + O(G_\Gamma \Delta T_i^2/T^2)$. It can be shown that the presence of nonanalytic singularities in ΔT_i in the thermodynamic potential Ω of the particle system, continuous at the point T_i, leads to $\partial^2\Omega/\partial T^2 \sim \ln(T/\Delta T_i)$, which makes it possible to regard the smallest of the T_i as the temperature of a second-order phase transition. In this case the dependence of $\partial\Omega/\partial\mu$ (μ is the chemical potential) on ΔT contains both an analytic and a nonanalytic term.

Ural State University
named after A. M. Gorky

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