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HARTREE-FOCK-BOGOLUBOV APPROXIMATION IN THE MODELS WITH GENERAL FOUR-FERMION INTERACTION

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ABSTRACT

The foundation of this work was established by the lectures of Prof. N.N. Bogolubov (senior) written in the beginning of 1990. We should like to develop some of his ideas connected with Hartree-Fock-Bogolubov method and to show how this approximation works in connection with general equations for Green's functions with source terms for sufficiently general model Hamiltonian of four-fermion interaction type and how, for example, to get some results of superconductivity theory by means of this method.

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In this article the following Hamiltonian is considered:

$$H = \sum_{(ff')} \Omega_0(f,f')a_f^+a_{f'} + \frac{1}{2}\sum_{(f_1f_2f_2'f_1')} U(f_1f_2;f_2'f_1')a_{f_1}^+a_{f_2}^+a_{f_2'}a_{f_1'} \; , \tag{1}$$

where a_f^+, a_f are Fermi operators of creation and annihilation obeying anticommutative relations

$$[a_f, a_{f'}^+]_+ = a_f a_{f'}^+ + a_{f'}^+ a_f = \delta(f-f') \; ,$$
$$[a_f, a_{f'}]_+ = a_f a_{f'} + a_{f'} a_f = 0$$

and

$$\delta(f-f') = \delta(\vec{p}-\vec{p}\,')\delta(s-s')$$

is interpreted as a Kronecker delta for discrete arguments or as a Dirac delta function for continuous arguments. $f = (\vec{p}, s)$ is the set of four quantum numbers (i.e. momentum components and spin projection) determining the state of free fermion:

$$\vec{p} = \left(\frac{2\pi n_1}{L}, \frac{2\pi n_2}{L}, \frac{2\pi n_3}{L}\right), \quad s = \pm\frac{1}{2} \; ,$$

where n_1, n_2, n_3 are integers and $L^3 = V$ where V is the volume of the system. It is supposed that functions $\Omega_0(f,f')$ and $U(f_1f_2;\ f_2'f_1')$ are chosen to guarantee the fulfillment of laws of conservation for the number of particles

$$[H, \mathcal{N}] = 0 \; , \tag{2}$$

total momentum

$$[H, \mathcal{P}] = 0 \; , \tag{3}$$

and total spin projection

$$[H, S_z] = 0 \; , \tag{4}$$

where $\mathcal{N}$, $\mathcal{P}$, S_z are operators of correspondent dynamical variables. It is assumed that

$$U(f_1f_2;\ f_2'f_1') = U(f_2f_1;\ f_1'f_2') \; .$$

Because of technical reasons we consider also more general Hamiltonian with sources:

$$H_t = \sum_{(f'f)} \Omega(f',f,t)a_f^+a_{f'} + \frac{1}{2}\sum_{f_1f_2f_1'f_2'} U(f_1f_2;f_2'f_1')a_{f_1}^+a_{f_2}^+a_{f_2'}a_{f_1'} +$$
$$+\frac{1}{2}\sum_{(ff')}(j_+(f',f,t)a_fa_{f'} + j_-(f',f,t)a_f^+a_{f'}^+) +$$
$$\frac{1}{2}\sum_{(ff')}(j_+^{(0)}(f',f)a_fa_{f'} + j_-^{(0)}(f',f)a_f^+a_{f'}^+) +$$
$$\sum_{(f)}(\eta_+(f,t)a_f + \eta_-(f,t)a_f^+) \; ,$$

where

$$\Omega(f',f,t) = \Omega_0(f,f') + j(f',f,t) \; .$$

Sources $j_{\pm}^{(0)}(f', f)$ are independent on time t. It is assumed that the following sources are antisymmetric:

$$j_+(f', f, t) = -j_+(f, f', t);\ j_-(f', f, t) = -j_-(f, f', t),$$

$$j_+^{(0)}(f', f) = -j_+^{(0)}(f, f');\ j_-^{(0)}(f', f) = -j_-^{(0)}(f, f')\ . \tag{5}$$

In general, sources violate symmetries of the model (1) induced by conservation laws (2-4). The most important role will be played by the sources (5) which violate symmetries in the case of thermodynamic equilibrium implementing the concept of quasiaverages for the model (1).

Particular example of the model (1) is the generalized BCS-model investigated in [1]:

$$H_{BCS} = \sum_{(ff')} \Omega(f', f) a_f^+ a_{f'} - \frac{1}{2V} \sum_{(ff')} \lambda(f)\lambda(f') a_f^+ a_{-f}^{\pm} a_{-f'} a_{f'} \tag{6}$$

where $\Omega(f', f) = \delta(f - f')T(p)$; $T(p) = \frac{p^2}{2m} - \mu$; $p = |\vec{p}|$ and μ is chemical potential, $\mu > 0$. It is assumed that

$$\lambda(f) = \mathrm{sign}(s) I(p)\ , \tag{7}$$

where

$$\mathrm{sign}(s) = \begin{cases} 1 & \text{if } s = \frac{1}{2} \\ -1 & \text{if } s = -\frac{1}{2} \end{cases}$$

It was shown in [1,3,4] that the model (6) allows asymptotically exact solution (under the limit $V \to \infty$) and all important thermodynamic properties of the model (6) coincide under this limit with those of the reduced exactly solvable model that is called the approximating Hamiltonian. This Hamiltonian is constructed in accordance with some special rules outlined in [3,4].

Let us explain briefly the scheme of the approximating Hamiltonian method on the basis of the model (6). Let us fulfill *the identity transformation of the Hamiltonian* (6):

$$H_{BCS} = H_a(c^*, c) + H_{int}(c^*, c)\ ,$$

where

$$H_a(c^*, c) = \sum_{(f)} \Omega(f, f) a_f^+ a_f - \frac{1}{2} \sum_{(f)} \lambda(f) \left(c^* a_{-f} a_f + c a_f^+ a_{-f}^{\pm} \right) + \frac{|c|^2}{2} V\ , \tag{8}$$

$$H_{int}(c^*, c) = -\frac{V}{2} \sum_{(ff')} \left(\frac{\lambda(f) a_f^+ a_{-f}^+}{V} - c^* \right) \left(\frac{\lambda(f') a_{-f'} a_{f'}}{V} - c \right) \tag{9}$$

and c is an arbitrary complex parameter for the present. Later the parameter c is determined by the extreme condition (absolute minimum) for the density of the free energy

$$\frac{\partial F(H_a(c^*, c))}{\partial c} = 0\ , \tag{10}$$

$$\frac{\partial F(H_a(c^*, c))}{\partial c^*} = 0\ , \tag{11}$$

where

$$F(H_a) = -\frac{1}{\beta V} \ln Sp(e^{-\beta H_a})$$

is finite as was shown in [3,4]. Eqs. (10-11) lead to the equation of self-consistency for the parameter c:

$$c = \frac{1}{V} \sum_{(f)} \lambda(f) \langle a_{-f} a_f \rangle\ , \tag{12}$$

where $\langle \ldots \rangle$ are calculated with respect to the approximating Hamiltonian (8). The modified interaction (9) does not influence on the thermodynamic properties of the model (6) under the limit $V \to \infty$ if parameters c^*, c are chosen in a proper way (10-11). This circumstance confirms the assumption that under the limit $V \to \infty$ operator

$$\sum_{(f)} \frac{\lambda(f)}{V} a_{-f} a_f$$

can be interpreted rather as c-number then as an operator. So one neglects interaction (9) in the model (6) and substitutes successfully (8) instead of the initial Hamiltonian (6) to calculate all thermodynamic properties and equilibrium two-time temperature Green functions of all orders for the model (6).

The procedure outlined above of the approximating Hamiltonian derivation is valid only for the models with separable interaction of the type (6). The aim of this study is to construct effective reasonable method of approximation for general model (1). As a whole this new method might suffer a lack of mathematical rigor especially in comparison with the standard approximating Hamiltonian method [3,4]. So the following consideration is marked with necessarily formal character sometimes. At the same time it is natural to demand the coincidence of the results (at least under the limit $V \to \infty$) obtained by the two methods for models with separable interaction.

The first step of approximation for the model (1) comprises in the following formal substitution for the product of four Fermi operators in the interaction term in the Hamiltonian (1):

$$\begin{aligned} a_{f_1}^+ a_{f_2}^+ a_{f'_2} a_{f'_1} \to & \langle a_{f_1}^+ a_{f'_1} \rangle a_{f_2}^+ a_{f'_2} - \\ & - \langle a_{f_1}^+ a_{f'_2} \rangle a_{f_2}^+ a_{f'_1} + \langle a_{f_2}^+ a_{f'_2} \rangle a_{f_1}^+ a_{f'_1} - \\ & - \langle a_{f_2}^+ a_{f'_1} \rangle a_{f_1}^+ a_{f'_2} + \langle a_{f_1}^+ a_{f_2}^+ \rangle a_{f'_2} a_{f'_1} + \\ & + \langle a_{f'_2} a_{f'_1} \rangle a_{f_1}^+ a_{f_2}^+ - R\ , \end{aligned} \tag{13}$$

where

$$R = \langle a_{f_1}^+ a_{f'_1} \rangle \langle a_{f_2}^+ a_{f'_2} \rangle + \langle a_{f_1}^+ a_{f_2}^+ \rangle \langle a_{f'_2} a_{f'_1} \rangle - \langle a_{f_1}^+ a_{f'_2} \rangle \langle a_{f_2}^+ a_{f'_1} \rangle\ .$$

The approximation (13) yields quadratic in Fermi operators Hamiltonian

$$H_a = \sum_{(ff')} \widetilde{K}(f', f) a_f^+ a_{f'} + \frac{1}{2} \sum_{(ff')} \widetilde{K}_-(f', f) a_f^+ a_{f'}^+ +$$

$$+ \frac{1}{2} \sum_{(ff')} \widetilde{K}_+(f', f) a_f a_{f'} - \frac{1}{2} \sum_{f_1 f_2 f'_1 f'_2} U(f_1 f_2; f'_2 f'_1) R(f_1 f_2; f'_2 f'_1)\ , \tag{14}$$

where

$$\widetilde{K}(f',f) = \Omega_0(f',f) + \sum_{(f_1 f_2)} W(f_1 f; f' f_2)\langle a^+_{f_1} a_{f_2}\rangle$$

$$\widetilde{K}_+(f',f) = \frac{1}{2}\sum_{(f_1 f_2)} W(f_1 f_2; f f')\langle a^+_{f_1} a^+_{f_2}\rangle$$

$$\widetilde{K}_-(f',f) = \frac{1}{2}\sum_{(f_1 f_2)} W(f f'; f_1 f_2)\langle a_{f_1} a_{f_2}\rangle$$

and function

$$W(f_1 f_2; f'_2 f'_1) = U(f_1 f_2; f'_2 f'_1) - U(f_1 f_2; f'_1 f'_2)$$

possesses properties of antisymmetry:

$$W(f_1 f_2; f'_2 f'_1) = -W(f_2 f_1; f'_2 f'_1) \tag{15}$$

$$W(f_1 f_2; f'_2 f'_1) = -W(f_1 f_2; f'_1 f'_2)\ . \tag{16}$$

c-numbers $\langle a^+_f a_{f'}\rangle$, $\langle a^+_f a^+_{f'}\rangle$, $\langle a_f a_{f'}\rangle$ can be fixed by the conditions of self-consistency by analogy with condition (12). These conditions are consequence of extreme conditions for the function of free energy for the Hamiltonian (14). Note that the approximation (13) looks like a procedure of partial calculation of equilibrium averages for the product of Fermi operators by means of the Wick theorem. The approximation (13) can be named Hartree-Fock-Bogolubov approximation because it joins ideas ascending equally to the Bogolubov's approximating Hamiltonian approach and to the principle of self-consistency inherited from the Hartree-Fock way of approximation [5].

In principle the Hamiltonian (14) can be diagonalized by the canonical Bogolubov's $u - v$ transformation for Fermi operators but in general this approach may encounter significant technical difficulties. So it seems reasonable to reformulate the problem in terms of more flexible formalism of two-time temperature dependent Green functions having in mind later possible approximate calculations. One could derive equations for the Green functions directly for the approximating Hamiltonian (14). But it seems more useful to choose more general approach and to try to construct dynamical approximation of Hartree-Fock-Bogolubov type which allows to investigate not only equilibrium but also nonequilibrium properties of the model (1).

Consider equation of motion for some dynamical vairable A independent on time explicitly providing its evolution is determined by the Hamiltonian H_t with time-dependent sources (we put later $\hbar = 1$):

$$i\frac{d}{dt}A(t) = [A(t), H_t(t)]\ . \tag{17}$$

Then average both sides of Eq. (17) with some time-independent density operator $\mathcal{D}$: $\langle A(t)\rangle = \mathrm{Sp}(A(t)\mathcal{D})$,

$$i\frac{d}{dt}\langle A(t)\rangle = \langle [A(t), H_t(t)]\rangle\ . \tag{18}$$

The right side of Eq.(18) contains commutator term

$$\langle [A(t),\ \frac{1}{2}\sum_{(f_1 f_2 f'_1 f'_2)} U(f_1 f_2; f'_2 f'_1) a^+_{f_1}(t) a^+_{f_2}(t) a_{f'_2}(t) a_{f'_1}(t)]\rangle \tag{19}$$

where time dependence of all operators $a^+_f(t)$, $a_f(t)$ is determined by the Hamiltonian H_t with sources. Usually dynamical variable A is a product of finite number of Fermi operators a^+_f, a_f. So under the commutation (19) correlation functions of higher orders than the initial correlation function $\langle A(t)\rangle$ with respect to these operators would arise in the right side of Eq.(18). To unlink the chain of evolution equations for these functions and to derive closed system of equations for some set of correlation functions one has to split correlation functions of higher orders and to express them in terms of the lower ones. We elaborate here a different approach. Instead of writing down a chain of equations for correlation functions starting from some function $\langle A(t)\rangle$ and inventing each time unique procedure of splitting to unlink the chain we introduce once and forever some universal global approximation already in commutator term (19). The approximation ensures implicit splitting of correlation functions in each chain of equations built for a given dynamical variable A under the condition that A is a product or a sum of products of finite number of Fermi operators a^+_f, a_f. The proposed approximation results in formal substitution:

$$\begin{aligned}
&a^+_{f_1}(t)a^+_{f_2}(t)a_{f'_2}(t)a_{f'_1}(t) \longrightarrow \\
&\langle a^+_{f_1}(t)a_{f'_1}(t)\rangle a^+_{f_2}(t)a_{f'_2}(t) - \langle a^+_{f_1}(t)a_{f'_2}(t)\rangle a^+_{f_2}(t)a_{f'_1}(t) + \\
&+\langle a^+_{f_2}(t)a_{f'_2}(t)\rangle a^+_{f_1}(t)a_{f'_1}(t) - \langle a^+_{f_2}(t)a_{f'_1}(t)\rangle a^+_{f_1}(t)a_{f'_2}(t) + \\
&+\langle a^+_{f_1}(t)a^+_{f_2}(t)\rangle a_{f'_2}(t)a_{f'_1}(t) + \langle a_{f'_2}(t)a_{f'_1}(t)\rangle a^+_{f_1}(t)a^+_{f_2}(t)\ .
\end{aligned} \tag{20}$$

The approximation (20) is similar to the one (13) in the equilibrium case. All operators $a^+_{f(t)}$, $a_f(t)$ in Eq. (20) are interpreted to be operators in the Heisenberg representation with the Hamiltonian H_t:

$$a^+_f(t) = U^+(t)a^+_f U(t)\ ,$$

$$a_f(t) = U^+(t)a_f U(t)\ ,$$

$\langle a_f(t)a_g(t)\rangle = \mathrm{Sp}(U^+(t)a_f a_g U(t)\mathcal{D})$ and so on, where the evolution operator $U(t)$ satisfies the equation

$$i\frac{d}{dt}U(t) = H_t U(t)\ .$$

So all averages in Eq.(20) are interpreted as exact averages and the evolution of them is determined by the Hamiltonian H_t. Taking into account symmetry properties (15-16) the approximate evolution equation resulting after substitution of (20) to exact Eq. (18) can be written as

$$i\frac{d}{dt}\langle A(t)\rangle = \langle [A(t),\ Q_{eff}(t)]\rangle\ , \tag{21}$$

where the operator form $Q_{eff}(t)$ is defined as

$$\begin{aligned}
Q_{eff}(t) = &\sum_{(ff')} K(f',f,t)a^+_f(t)a_{f'}(t) + \\
&+\frac{1}{2}\sum_{(ff')}(K_+(f',f,t)a_f(t)a_{f'}(t) + K_-(f',f,t)a^+_f(t)a^+_{f'}(t)) + \\
&+\sum_{(f)}(\eta_+(f,t)a_f(t) + \eta_-(f,t)a^+_f(t))\ ,
\end{aligned} \tag{22}$$

where

$$K(f',f,t)=\Omega_0(f,f')+j(f',f,t)+\sum_{(f_1f_2)}W(f_1f;f'f_2)\langle a^+_{f_1}(t)a_{f_2}(t)\rangle$$

$$K_+(f',f,t)=j_+(f',f,t)+j^{(0)}_+(f',f)+\sum_{(f_1f_2)}U(f_1f_2;ff')\langle a^+_{f_1}(t)a^+_{f_2}(t)\rangle$$

$$K_-(f',f,t)=j_-(f',f,t)+j^{(0)}_-(f',f)+\sum_{(f_1f_2)}U(ff';f_1f_2)\langle a_{f_1}(t)a_{f_2}(t)\rangle\ .$$

Let us stress especially that the form $Q_{eff}(t)$ can be considered as neither approximating Hamiltonian nor, generally speaking, some effective Hamiltonian at all. This form is introduced only to make derivation of approximate equations of the type (21) for various dynamical variables A more compact and clear. It follows from Eq.(21) that starting from some dynamical variable A which is a product of finite number of Fermi operators one can derive a chain of equations closed with respect to some set of correlation functions including the initial function $\langle A(t)\rangle$. It is guaranteed because the form (22) contains only linear and quadratic dependence on Fermi operators.

Now let us write successively the approximate equation (21) for the following combinations of Fermi operators:

$$i\frac{d}{dt}\langle a^+_f(t)\rangle=-\sum_{(f')}\left\{K(f,f',t)\langle a^+_{f'}(t)\rangle+K_+(f,f',t)\langle a_{f'}(t)\rangle\right\}+$$
$$+2\sum_{(f')}\left\{\eta_+(f',t)\langle a^+_f(t)a_{f'}(t)\rangle+\eta_-(f',t)\langle a^+_f(t)a^+_{f'}(t)\rangle\right\}-\eta_+(f,t) \qquad (23)$$

$$i\frac{d}{dt}\langle a_f(t)\rangle=\sum_{(f')}\left\{K(f',f,t)\langle a_{f'}(t)\rangle+K_-(f',f,t)\langle a^+_{f'}(t)\rangle\right\}-$$
$$-2\sum_{(f')}\left\{\eta_-(f',t)\langle a^+_{f'}(t)a_f(t)\rangle-\eta_+(f',t)\langle a_f(t)a_{f'}(t)\rangle\right\}+\eta_-(f,t) \qquad (24)$$

$$i\frac{d}{dt}\langle a_f(t)a_g(t)\rangle=\sum_{(f')}\left\{K(f',f,t)\langle a_{f'}(t)a_g(t)\rangle+K_-(f',f,t)\langle a^+_{f'}(t)a_f(t)\rangle\right\}+$$
$$+\sum_{(f')}\left\{K(f',g,t)\langle a_f(t)a_{f'}(t)\rangle+[\delta(f-f')-\langle a^+_{f'}(t)a_f(t)\rangle]K_-(f',g,t)\right\}+$$
$$+\eta_-(g,t)\langle a_f(t)\rangle-\eta_-(f,t)\langle a_g(t)\rangle \qquad (25)$$

$$i\frac{d}{dt}\langle a^+_f(t)a_g(t)\rangle=-\sum_{(f')}\left\{K(f,f',t)\langle a^+_{f'}(t)a_g(t)\rangle+\right.$$
$$\left.+K_+(f,f',t)\langle a_{f'}(t)a_g(t)\rangle\right\}+$$
$$+\sum_{(f')}\left\{K(f',g,t)\langle a^+_f(t)a_{f'}(t)\rangle+K_-(f',g,t)\langle a^+_f(t)a^+_{f'}(t)\rangle\right\}+$$
$$+\eta_-(g,t)\langle a^+_f(t)\rangle-\eta_+(f,t)\langle a_g(t)\rangle \qquad (26)$$

$$i\frac{d}{dt}\langle a^+_f(t)a^+_g(t)\rangle=-\sum_{(f')}\left\{K(f,f',t)\langle a^+_{f'}(t)a^+_g(t)\rangle+\right.$$

$$+[\delta(g-f')-\langle a^+_g(t)a_{f'}(t)\rangle]K_+(f,f',t)\Big\}-$$
$$-\sum_{(f')}\left\{K(g,f',t)\langle a^+_f(t)a^+_{f'}(t)\rangle+K_+(g,f',t)\langle a^+_f(t)a_{f'}(t)\rangle\right\}+$$
$$+\eta_+(g,t)\langle a^+_f(t)\rangle-\eta_+(f,t)\langle a^+_g(t)\rangle \qquad (27)$$

The system of nonlinear Eqs. (23-27) closed with respect to the set of functions

$$\langle a^+_f(t)\rangle,\ \langle a_f(t)\rangle,\ \langle a_f(t)a_g(t)\rangle,\ \langle a^+_f(t)a_g(t)\rangle,\ \langle a^+_f(t)a^+_g(t)\rangle$$

will be referred to later as the system of Hartree-Fock-Bogolubov equations with sources. It turns out to be that if one is interested only in investigation of equilibrium correlation functions of the model (1) then the system (23-27) can be linearized in some meaning if to pass from Eqs. (23-27) to linear equations for correspondent retarded or advanced two-time temperature Green functions. Here only those equations are outlined which are necessary for later investigation. Let us take statistical operator $\mathcal{D}$ in a particular form

$$\mathcal{D}=\exp(-\beta H(j^{(0)}_+,j^{(0)}_-)/\mathrm{Sp}(\exp(-\beta H(j^{(0)}_+,j^{(0)}_-)))\ ,$$

where

$$H(j^{(0)}_+,j^{(0)}_-)=H+\frac{1}{2}\sum_{(ff')}(j^{(0)}_+(f',f)a_fa_{f'}+j^{(0)}_-(f',f)a^+_fa^+_{f'}) \qquad (28)$$

is the Hamiltonian of four-fermion interaction (1) with time-independent sources (5). We linearize Eqs. (23-24) with respect to Green functions by means of Bogolubov's theorem on the variation of an average with respect to a time-dependent source (see App. 1). Varying Eq.(23) with respect to the source $\eta_+(g,\tau)$ and Eq. (24) with respect to the source $\eta_+(g,\tau)$ one gets two equations

$$i\frac{d}{dt}\langle\langle a^+_f(t)|a_g(\tau)\rangle\rangle=-\sum_{(f')}\left\{\langle a^+_{f'}\rangle\sum_{(f_1f_2)}W(f_1,f';ff_2)\langle\langle a^+_{f_1}(t)a_{f_2}(t)|a_g(\tau)\rangle\rangle+\right.$$
$$+K(f,f',0)\langle\langle a^+_{f'}(t)|a_g(\tau)\rangle\rangle+K_+(f,f',0)\langle\langle a_{f'}(t)|a_g(\tau)\rangle\rangle+$$
$$\left.+\langle a_{f'}\rangle\sum_{(f_1f_2)}U(f_1f_2;f'f)\langle\langle a^+_{f_1}(t)a^+_{f_2}(t)|a_g(\tau)\rangle\rangle\right\}+$$
$$i\delta(t-\tau)(2\langle a^+_fa_g\rangle-1) \qquad (29)$$

$$i\frac{d}{dt}\langle\langle a_f(t)|a_g(\tau)\rangle\rangle=\sum_{(f')}\left\{\langle a_{f'}\rangle\sum_{(f_1f_2)}W(f_1f;f'f_2)\langle\langle a^+_{f_1}(t)a_{f_2}(t)|a_g(\tau)\rangle\rangle+\right.$$
$$+K(f',f,0)\langle\langle a_{f'}(t)|a_g(\tau)\rangle\rangle+K_-(f',f,0)\langle\langle a^+_{f'}(t)|a_g(\tau)\rangle\rangle+$$
$$\left.+\langle a^+_{f'}\rangle\sum_{(f_1f_2)}U(ff';f_1f_2)\langle\langle a_{f_1}(t)a_{f_2}(t)|a_g(\tau)\rangle\rangle\right\}+$$
$$+2i\delta(t-\tau)\langle a_fa_g\rangle\ , \qquad (30)$$

where

$$K(f',f,0)=\Omega_0(f,f')+\sum_{(f_1f_2)}W(f_1f;f'f_2)\langle a^+_{f_1}a_{f_2}\rangle$$

$$K_+(f',f,0) = j_+^{(0)}(f',f) + \sum_{(f_1f_2)} U(f_1f_2;ff')\langle a_{f_1}^+ a_{f_2}^+ \rangle$$

$$K_-(f',f,0) = j_-^{(0)}(f',f) + \sum_{(f_1f_2)} U(ff';f_1f_2)\langle a_{f_1} a_{f_2} \rangle$$

and $\langle\langle a_f(t)|a_g(\tau)\rangle\rangle$, $\langle\langle a_f^+(t)|a_g(\tau)\rangle\rangle$ are commutative retarded or advanced two-time temperature Green functions defined as

$$\langle\langle A(t)|B(\tau)\rangle\rangle^{(ret)} = \theta(t-\tau)\langle[A(t),B(\tau)]\rangle \tag{31}$$

$$\langle\langle A(t)|B(\tau)\rangle\rangle^{(adv)} = -\theta(\tau-t)\langle[A(t),B(\tau)]\rangle \tag{32}$$

$$\theta(x) = \begin{cases} 1 & \text{if} \quad x>0 \\ 0 & \text{if} \quad x<0 \end{cases} .$$

The system of Eqs. (29-30) can be simplified if we take into account selecting rules for the correlation functions and Green functions. The Hamiltonian (28) is invariant under canonical transformation

$$a_f^+ \to -a_f^+ \; ; \quad a_f \to -a_f \; .$$

So only those Green and correlation functions differ from zero which contain even number of Fermi operators. Then sources $j_+^{(0)}(f',f)$, $j_-^{(0)}(f',f)$ can be chosen in such a manner that only the law of particle number conservation (2) and correspondent symmetry are violated but other symmetries connected with laws of momentum and spin projection conservation (3-4) take place. It can be guaranteed if to put

$$j_+^{(0)}(f',f) = \nu\lambda(f)\delta(f+f'); \quad j_-^{(0)}(f',f) = -\nu\lambda(f)\delta(f+f') \; , \tag{33}$$

where ν is a formal small parameter and $\lambda(f)$ is, for example, antisymmetric function (7). Sources (33) have been used traditionally to introduce quasiaverages in order to investigate the phenomenon of superconductivity in fermion system [1,2]. Conservation laws (3-4) induce the following selecting rules for correlation functions

$$\langle a_f(t)\rangle = \langle a_f^+(t)\rangle = 0 \tag{34}$$

$$\langle a_f^+(t)a_{f'}^+(t')\rangle = \langle a_f^+(t)a_{-f}^+(t')\rangle\delta(f+f') \tag{35}$$

$$\langle a_{-f}(t)a_{-f'}(t')\rangle = \langle a_{-f}(t)a_f(t')\rangle\delta(f+f') \tag{36}$$

$$\langle a_f^+(t)a_{f'}(t')\rangle = \delta(f-f')\langle a_f^+(t)a_f(t')\rangle \; . \tag{37}$$

The same rules take place for pair Green functions. Rules (34-37) lead to the system of equations:

$$i\frac{d}{dt}\langle\langle a_f^+(t)|a_f(\tau)\rangle\rangle = -\left\{K^{(0)}(f,f)\langle\langle a_f^+(t)|a_f(\tau)\rangle\rangle + \right.$$
$$\left. + K_+^{(0)}(f,-f)\langle\langle a_{-f}(t)|a_f(\tau)\rangle\rangle\right\} + i\delta(t-\tau)(2\langle a_f^+a_f\rangle - 1) \tag{38}$$

$$i\frac{d}{dt}\langle\langle a_{-f}(t)|a_f(\tau)\rangle\rangle = \left\{K^{(0)}(-f,-f)\langle\langle a_{-f}(t)|a_f(\tau)\rangle\rangle + \right.$$
$$\left. + K_-^{(0)}(f,-f)\langle\langle a_f^+(t)|a_f(\tau)\rangle\rangle\right\} + 2i\delta(t-\tau)\langle a_{-f}a_f\rangle \; , \tag{39}$$

where

$$K_+^{(0)}(f',f) = j_+^{(0)}(f',f) + \sum_{(f_1)} U(f_1,-f_1;ff')\langle a_{f_1}^+ a_{-f_1}^+\rangle$$

$$K_-^{(0)}(f',f) = j_-^{(0)}(f',f) + \sum_{(f_1)} U(ff';-f_1f_1)\langle a_{-f_1} a_{f_1}\rangle$$

$$K^{(0)}(f',f) = \Omega_0(f,f') + \sum_{(f_1)} W(f_1f;f'f_1)\langle a_{f_1}^+ a_{f_1}\rangle \; .$$

Equilibrium Green functions depend only on the difference of time arguments $t-\tau$ so it is possible to implement energetic E-representation for them:

$$\langle\langle A|B\rangle\rangle_E^{(ret,adv)} = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\langle\langle A(t)|B\rangle\rangle^{(ret,adv)} e^{iEt}dt \tag{40}$$

Then

$$E\langle\langle a_f^+|a_f\rangle\rangle_E = -\left\{K^{(0)}(f,f)\langle\langle a_f^+|a_f\rangle\rangle_E + \right.$$
$$\left. + K_+^{(0)}(f,-f)\langle\langle a_{-f}|a_f\rangle\rangle_E\right\} + \frac{i}{2\pi}(2\langle a_f^+a_f\rangle - 1) \tag{41}$$

$$E\langle\langle a_{-f}|a_f\rangle\rangle_E = \left\{K^{(0)}(-f,-f)\langle\langle a_{-f}|a_f\rangle\rangle_E + \right.$$
$$\left. + K_-^{(0)}(f,-f)\langle\langle a_f^+|a_f\rangle\rangle_E\right\} + \frac{i}{\pi}\langle a_{-f}a_f\rangle \; . \tag{42}$$

Note that only one approximation (20) was involved to derive Eqs. (41-42). These equations contain anomalous averages $\langle a_{-f}a_f\rangle$ and anomalous Green functions $\langle\langle a_{-f}|a_f\rangle\rangle_E$ because the Hamiltonian (28) contains sources (33) violating the conservation law (2). These anomalous averages must be interpreted as quasiaverages with usual rules of handling with them [1,2]. Eqs (41-42) contain following coefficients in the right side:

$$\sum_{(f_1)} W(f_1f;ff_1)\langle a_{f_1}^+a_{f_1}\rangle \; , \tag{43}$$

$$\sum_{(f_1)} U(f_1,-f_1;-ff)\langle a_{f_1}^+a_{-f_1}^+\rangle \; , \tag{44}$$

$$\sum_{(f_1)} W(f_1,-f;-ff_1)\langle a_{f_1}^+a_{f_1}\rangle \; , \tag{45}$$

$$\sum_{(f_1)} U(-ff;-f_1f_1)\langle a_{-f_1}a_{f_1}\rangle \; , \tag{46}$$

where the dependence on f is not factorable in general. So although the spectral theorem for the Green functions allows to derive formally closed system of integral equations with respect to averages

$$\langle a_f^+a_f\rangle, \; \langle a_{-f}a_f\rangle, \; \langle a_f^+a_{-f}^+\rangle$$

it is impossible to solve these equations as a rule. At the same time the system (41-42) gives a possibility of further approximations in coefficients (43-46) to obtain approximate solutions for the Green functions, correlation functions and spectrum of quasiparticle excitations. To understand what the character of these approximations ought to be let us analyze traditional BCS model (6) within frames of the proposed method. For the BCS model

$$U(f_1f_2;f_2'f_1') = -\frac{1}{V}\lambda(f_1)\lambda(f_2)\delta(f_1+f_2)\delta(f_1'+f_2'),$$

$$W(f_1f_2;f_2'f_1') = -\frac{2}{V}\lambda(f_1)\lambda(f_2)\delta(f_1+f_2)\delta(f_1'+f_2'),$$

$$K^{(0)}(f',f) = T(p)\delta(f-f') \text{ if } V\to\infty,$$

$$K_+^{(0)}(f',f) = -\delta(f+f')\lambda(f')\left[\frac{1}{V}\sum_{(f_1)}\lambda(f_1)\langle a_{f_1}^+a_{-f_1}^+\rangle + \nu\right] \equiv$$

$$\equiv -\delta(f+f')\lambda(f')[c^*+\nu],$$

$$K_-^{(0)}(f',f) = -\delta(f+f')\lambda(f)\left[\frac{1}{V}\sum_{(f_1)}\langle a_{-f_1}a_{f_1}\rangle + \nu\right] \equiv$$

$$\equiv -\delta(f+f')\lambda(f)[c+\nu].$$

So Eqs. (41-42) take the form:

$$(E+T(p))\langle\langle a_f^+|a_f\rangle\rangle_E - (c^*+\nu)\lambda(f)\langle\langle a_{-f}|a_f\rangle\rangle_E = \frac{i}{2\pi}(2\langle a_f^+a_f\rangle - 1) \quad (47)$$

$$(E-T(p))\langle\langle a_{-f}|a_f\rangle\rangle_E - (c+\nu)\lambda(f)\langle\langle a_f^+|a_f\rangle\rangle_E = \frac{i}{\pi}\langle a_{-f}a_f\rangle \quad (48)$$

Eqs. (47-48) are similar in structure to the equations for the commutative retarded or advanced Green functions written for the approximating Hamiltonian (8). So results of approximation (20) coincide with the ones obtained previously by the approximating Hamiltonian method [1,3,4]. So here we outline only final results derived from Eqs. (47-48).

$$\langle a_f^+a_f\rangle = \frac{1}{2}\left(1 - \frac{T(p)}{E(p)}th\left(\frac{\beta E(p)}{2}\right)\right)$$

$$\langle a_{-f}a_f\rangle = \frac{c\lambda(f)}{2E(p)}th\left(\frac{\beta E(p)}{2}\right),$$

where $E(p)$ is a spectrum of quasiparticle excitations

$$E(p) = [T^2(p) + |c|^2\lambda^2(f)]^{1/2}$$

and the parameter c is defined by the solution of the following transcendent equation:

$$c\left(1 - \frac{1}{(2\pi)^3}\int d\vec{p}\,\frac{|I(p)|^2}{E(p)}th\left(\frac{\beta E(p)}{2}\right)\right) = 0 \quad (49)$$

which always has trivial solution $c=0$. Nontrivial solution is eligible only if $\beta > \beta_c$ where the critical value β_c is determined by the relation

$$1 = \frac{1}{(2\pi)^3}\int d\vec{p}\,\frac{|I(p)|^2}{T(p)}th\left(\frac{\beta T(p)}{2}\right)$$

So the condition

$$\frac{1}{(2\pi)^3}\int d\vec{p}\,\frac{|I(p)|^2}{T(p)}th\left(\frac{\beta T(p)}{2}\right) > 1 \quad (50)$$

is a condition of existence for nontrivial solution of Eq. (49). When solving Eqs. (47-48) the following formulation of the spectral theorem was used:

$$(1-e^{-\beta\omega})\mathcal{J}_{AB}(\omega) = \langle\langle A|B\rangle\rangle_{\omega+i\epsilon} - \langle\langle A|B\rangle\rangle_{\omega-i\epsilon}$$

$$\langle A(t)B(\tau)\rangle = \langle A(t-\tau)B\rangle = \int_{-\infty}^{+\infty} d\omega\,\mathcal{J}_{AB}(\omega)e^{-i\omega(t-\tau)} \quad (51)$$

$$\langle B(\tau)A(t)\rangle = \langle B(\tau-t)A\rangle = \int_{-\infty}^{+\infty} d\omega\,\mathcal{J}_{AB}(\omega)e^{\beta\omega}e^{-i\omega(t-\tau)} \quad (52)$$

We also put $\nu = 0$ in final results according to the theory of quasiaverages. Now the criterion of selection between trivial and nontrivial solutions in the region $\beta > \beta_c$ must be worked out. Striving to stay within frames of the proposed formalism we avoid to involve auxiliary conditions such that the true solution must provide the absolute minimum for the free energy of the system and so on. Instead of that we show that if nontrivial solution exists, i.e. if condition (50) fulfills, the trivial solution has to be neglected because it contradicts to spectral properties of the dynamical system. To prove this statement let us consider equation for Green function $\langle\langle a_{-f}a_f|a_g^+a_{-g}^+\rangle\rangle_E$ in the case when $\beta > \beta_c$ and only trivial solution is chosen to be true solution. To derive the equation we vary Eq.(25) with respect to the source $j_-(-g,g,\tau)$ as it was done before when deriving Eqs.(29-30) and then take into account selecting rules induced by laws of conservation (3-4) and use E-representation (40). The result is:

$$(E-2T(p))\langle\langle a_{-f}a_f|a_g^+a_{-g}^+\rangle\rangle_E =$$

$$= \lambda(f)\left\{\langle a_f^+a_f\rangle - \langle a_{-f}a_{-f}^+\rangle\right\}\sum_{(f_1)}\frac{\lambda(f_1)}{V}\langle\langle a_{-f_1}a_{f_1}|a_g^+a_{-g}^+\rangle\rangle_E +$$

$$+\frac{i}{2\pi}\{\delta(f-g)-\delta(f+g)\}\left(\langle a_{-f}a_{-f}^+\rangle - \langle a_f^+a_f\rangle\right).$$

So

$$\langle\langle a_{-f}a_f|a_g^+a_{-g}^+\rangle\rangle_E =$$

$$= \left(\frac{\lambda(f)C_g(E)}{2T(p)-E} + \frac{i}{2\pi}\frac{\delta(f-g)-\delta(f+g)}{E-2T(p)}\right)th\left(\frac{\beta T(p)}{2}\right), \quad (53)$$

where it was denoted that

$$C_g(E) = \sum_{(f_1)}\frac{\lambda(f_1)}{V}\langle\langle a_{-f_1}a_{f_1}|a_g^+a_{-g}^+\rangle\rangle_E. \quad (54)$$

It follows from Eqs. (53-54) that

$$C_g(E)\left(1 - \sum_{(f)}\frac{|\lambda(f)|^2 th(\frac{\beta T(p)}{2})}{V(2T(p)-E)}\right) = \frac{i}{2\pi V}\frac{2\lambda(g)}{E-2T(p)}th\left(\frac{\beta T(p)}{2}\right). \quad (55)$$

Eqs. (53, 55) show that the deviation of the magnitude $\langle\langle a_{-f}a_f|a_g^+a_{-g}^+\rangle\rangle_E$ from its value in the absence of interaction $\lambda(f)\equiv 0$ tends to zero while $V\to\infty$ if we chose trivial solution $c=0$. Now let us introduce dynamical variable

$$A=\frac{1}{\sqrt{V}}\sum_{(f)}\lambda(f)a_{-f}a_f$$

It follows from Eq.(54) that

$$\langle\langle A|A^+\rangle\rangle_E=\sum_g\lambda(g)C_g(E)$$

and from Eq.(55) one has

$$\langle\langle A|A^+\rangle\rangle_E=-\frac{i}{2\pi}\frac{2F(E)}{1-F(E)}\,, \tag{56}$$

where

$$F(E)=\frac{2}{(2\pi)^3}\int|I(p)|^2\frac{th(\frac{\beta T(p)}{2})}{2T(p)-E}d\vec{p}\,.$$

Taking into account spectral representation (51-52) we have

$$\langle\langle A|A^+\rangle\rangle_E=\frac{i}{2\pi}\int_{-\infty}^{+\infty}d\omega\mathcal{J}_{AA^+}(\omega)\frac{1-e^{-\beta\omega}}{E-\omega}$$

$$\mathcal{J}_{AA^+}(\omega)\geq 0\,.$$

Because of Eq.(56)

$$\frac{1}{2}\int_{-\infty}^{+\infty}d\omega\mathcal{J}_{AA^+}(\omega)\frac{1-e^{-\beta\omega}}{E-\omega}=-\frac{F(E)}{1-F(E)}=1-\frac{1}{1-F(E)}\,,$$

where $\mathcal{J}_{AA^+}(\omega)$ is correspondent spectral density. Then

$$\frac{1}{1-F(E)}=1-\frac{1}{2}\int_{-\infty}^{+\infty}d\omega\mathcal{J}_{AA^+}(\omega)\frac{1-e^{-\beta\omega}}{E-\omega} \tag{57}$$

Variable E can take values on the imaginary axis

$$E=iz\,.$$

So

$$\frac{1}{E-\omega}=-\frac{iz+\omega}{z^2+\omega^2}$$

and

$$\omega(1-e^{-\beta\omega})\geq 0\,.$$

Therefore for the real part we have

$$\mathrm{Re}\left(-\frac{1}{2}\int_{-\infty}^{+\infty}d\omega\mathcal{J}_{AA^+}(\omega\frac{1-e^{-\beta\omega}}{E-\omega}\right)=\frac{1}{2}\int_{-\infty}^{+\infty}d\omega\mathcal{J}_{AA^+}(\omega)\frac{\omega(1-e^{-\beta\omega})}{\omega^2+z^2}\geq 0$$

and

$$\mathrm{Re}\left(\frac{1}{1-F(E)}\right)=\mathrm{Re}\left(\frac{1}{1-F(iz)}\right)\geq 1\,.$$

But because of Eq.(57)

$$1-F(iz)\neq 0$$

So

$$1-\mathrm{Re}F(iz)>0$$

i.e.

$$\mathrm{Re}F(iz)<1$$

But in this case

$$\mathrm{Re}F(iz)=\frac{1}{(2\pi)^3}\int|I(p)|^2\frac{T(p)th\left(\frac{\beta T(p)}{2}\right)}{T^2(p)+\frac{z^2}{2}}d\vec{p}<1\,.$$

If $z\to 0$ then this condition contradicts the condition for the existence of nontrivial solution (50). This circumstance leads to the necessity to choose nontrivial solution as true solution of Eq.(49) if condition (50) holds.

So we proved that the proposed method of approximation contains its own internal criterium of selection between trivial and nontrivial solutions of self-consistence equation (49).

The example of the BCS model shows that investigating models with arbitrary interaction $U(f_1f_2;f_2'f_1')$ one has to carry out approximations in Eqs.(41-42) in such a way that the structure of final equations would be similar to the one of Eqs.(47-48). These equations are eligible to be solved by the method of self-consistence as in the case of BCS model. But in contrast to the BCS model the final result would include two transcendent equations of self-consistence with respect to two unknown parameters, namely, one real parametre C_1 and one complex parameter C_2. It is so because in general case coefficients (43-46) include summation over three types of averages:

$$\langle a_f^+a_f\rangle,\ \langle a_f^+a_{-f}^+\rangle,\ \langle a_{-f}a_f\rangle$$

The spectrum of quasiparticle excitations will be the function of parameters C_1, C_2. An investigation of this kind for more involved realistic model than the BCS one will be an item of the next article.

Appendix A

Let us consider the following Hamiltonian with sources

$$H_t = H + \mathcal{J}_t \ ,$$

$$\mathcal{J}_t = (\Sigma \int) dx B(x) j(x,t)$$

where operators H and $B(x)$ are independent on time t and C-functions $j(x,t)$ contain time dependence. The symbol $(\Sigma \int)dx$ implies summation over discrete and integration over continuous indexes simultaneously. The complicated index x may denote a set of quantum numbers or (and) other ordinary indexes defining type of a particular source. It is assumed that each source $j(x,t)$ contains multiplier $e^{\varepsilon t}$, $(\varepsilon > 0)$, so

$$j(x,t) \to 0 \quad \text{if} \quad t \to -\infty \tag{A.1}$$

The equation for the evolution operator is ($\hbar = 1$):

$$i\frac{dU(t)}{dt} = H_t U(t) \tag{A.2}$$

$$U^+(t)U(t) = 1 \ ,$$

and the boundary condition follows from Eq.(A.1):

$$e^{iHt}U(t) \to \quad \text{if} \quad t \to -\infty \tag{A.3}$$

In the Heisenberg representation one has for any time independent dynamical variable

$$A(t) = U^+(t) A U(t)$$

$$\langle A(t) \rangle = \mathrm{Sp}(U^+(t) A U(t) \mathcal{D}) \ ,$$

where $\mathcal{D}$ is some statistical operator. Let us vary $\langle A(t) \rangle$ with respect to $j(x,t)$. So

$$\delta\langle A(t) \rangle = \langle (\delta U^+(t)) A U(t) \rangle + \langle U^+(t) A \delta U(t) \rangle \ . \tag{A.4}$$

Let us define

$$\delta U(t) = U(t)\delta V(t)$$

then the equation for $\delta V(t)$ is (if one varies Eq.(1.2)):

$$i\frac{d}{dt}\delta V(t) = U^+(t)(\delta \mathcal{J}_t)U(t) \tag{A.5}$$

But

$$U^+(t)B(x)U(t) = B(t,x)$$

$$U^+(t)(\delta\mathcal{J}_t)U(t) = \delta\mathcal{J}(t) = (\Sigma \int) dx B(t,x) \delta j(x,t)$$

and taking into account boundary condition (A.3) leads to the formal solution of Eq.(A.5)

$$\delta U(t) = -iU(t)\int_{-\infty}^{t} \delta\mathcal{J}(t_1)dt_1 = -iU(t)\int_{-\infty}^{+\infty} \theta(t-t_1)\delta\mathcal{J}(t_1)dt_1 \ . \tag{A.6}$$

In full analogy with above calculations one has

$$-i\frac{d}{dt}U^+(t) = U^+(t)H_t$$

with boundary condition

$$U^+(t)e^{-iHt} \to 1 \quad \text{if} \quad t \to -\infty$$

and

$$-i\frac{d}{dt}\delta U^+(t) = (\delta U^+(t))H_t + U^+(t)\delta\mathcal{J}_t \ .$$

So

$$\delta U^+(t) = i\int_{-\infty}^{+\infty} \theta(t-t_1)\delta\mathcal{J}(t_1)dt_1 U^+(t) \ . \tag{A.7}$$

From Eqs. (A.4, A.6, A.7) it follows that

$$\delta\langle A(t) \rangle = -i\int_{-\infty}^{+\infty} \theta(t-t_1)\langle [A(t),\ \delta\mathcal{J}(t_1)] \rangle \ .$$

Therefore

$$\left.\frac{\delta\langle A(t) \rangle}{\delta j(x_1,\tau)}\right|_{j(x,t)=0} = -i\theta(t-\tau)\langle [A(t), B(\tau,x_1)] \rangle \tag{A.8}$$

Let us note that we did not use any special form of density operator $\mathcal{D}$ deriving relation (A.8). For

$$\mathcal{D} = e^{-\beta H}/\mathrm{Sp}(e^{-\beta H})$$

the right side of (A.8) becomes proportional to usual two-time temperature retarded Green function (31). The result (A.9) for the advanced Green functions can be derived in the same manner. It is only necessary to assume that each source contains multiplier $e^{-\varepsilon t}$ $(\varepsilon > 0)$ and to impose correspondent boundary conditions for $t \to +\infty$:

$$e^{-iHt}U(t) \to 1 \quad \text{if} \quad t \to +\infty$$

$$U^+(t)e^{-iHt} \to 1 \quad \text{if} \quad t \to +\infty$$

The final result will be:

$$\left.\frac{\delta\langle A(t) \rangle}{\delta j(x_1,\tau)}\right|_{j(x,t)=0} = i\theta(\tau-t)\langle [A(t), B(\tau,x_1)] \rangle \ . \tag{A.9}$$

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