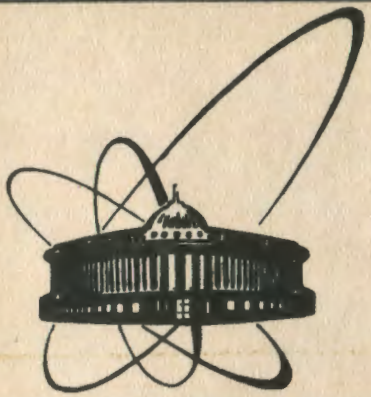

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SOME REMARKS ABOUT THE EQUATION OF MOTION OF GREEN FUNCTION´S METHOD

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1. INTRODUCTION

The Hubbard Hamiltonian[1]

$$H = \sum_{ij\sigma} t_{ij} a^{+}_{i\sigma} a_{j\sigma} + \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}$$

is surely one of the simplest to incorporate the electron-electron on-site repulsion U. The creation (annihilation) operators for electrons with spin σ in Wannier states centered around the i-th site of the crystal lattice are given by $a^{+}_{i\sigma}$ ($a_{i\sigma}$), $n_{i\sigma}$ is the corresponding number operator and t_{ij} is a corresponding hopping integral. In spite of its simplicity, very few exact results exist in the literature. One of the powerful tools for the investigation of the systems described by this Hamiltonian is the double-time retarded Green Function (GF) introduced by Bogolubov and Tyablikov[2] and by Zubarev[3] combined with the equation of motion for this function. But it is well recognized that relatively easy usage of the Green Functions is partly spoiled due to some shortcomings inherent in the equation of motion method. This method leads to a whole hierarchy of functions of higher order, and it is necessary to terminate this hierarchy at a certain stage. It means, one is forced to use some decoupling procedures or terminating the infinite set of equations. Very often "the branches" of "a tree" of equations have next "branches" and it is very difficult to use some definite decoupling procedure common for all higher-order Green Functions present at the ends of those "branches".

In literature there exist some methods for evaluation of the mentioned above GF and autocorrelation functions which base on a projection operator method of Zwanzig[4] and Mori[5] (see, e.g.[6-14]). In this case the construction of the higher-order GF (or autocorrelation functions) is highly putted in order.

In this paper, we demonstrate by the Hubbard Hamiltonian that all these "different" methods lead to the infinite continued fraction expansion for GF, and moreover, with the same successive steps of this expansion.

The paper is organized as follows. In the next section, in the subsection (2.1) we present the generalization of the Ichiyonagi's method[6] constructing the Dyson-type equations for higher-order GF and using the procedure of time differentiating over both time arguments. In the subsection (2.2) we have obtained the same equations using a projection operator method applied to the operators being functions of the left-hand side time argument, only. In the subsection (2.3), the general form of GF is obtained using a tridiagonal form of the corresponding basis operator set. The subsections (2.4) and (2.5) are devoted to some considerations concerning the known methods for calculations of the Green Functions. The last section contains concluding remarks.

2. THE EQUATION OF MOTION METHOD AND THE GREEN FUNCTION CALCULATIONS

In this section we are going to obtain formally exact expressions for the Green Functions. All methods to be discussed are founded on the equation of motion (for some operators) approach and the projection operator method. In subsections (2.4)and (2.5) we placed also a short discussion about methods known in literature and discussed their relation to the methods presented in former subsections.

2.1.

Using the method of differentiating the Green Function over both time arguments, Ichiyonagi was able to obtain the Dyson equation for this function with the explicit expression for the self-energy (mass) operator. Here, we generalize this approach to obtain a sequence of equations for the mass operators appearing in the corresponding Dyson-type equations.

Let us consider the double-time Green Function defined by Zubarev as follows[3]:

$$G(t-t') = -i\Theta(t-t')\langle\{f_0(t), f_0^+(t')\}\rangle \equiv \ll f_0(t) | f_0^+(t') \gg \qquad (1)$$

where $\langle \ldots \rangle$ denotes an average with respect to the canonical density matrix of the system described by the time-

independent Hamiltonian and temperature T

$$\langle A\rangle = Z^{-1}\,\mathrm{Tr}\,e^{-\beta H}A\,,\quad Z=\mathrm{Tr}\,e^{-\beta H},\quad \beta=(k_BT)^{-1},\quad A(t)=e^{iHt}Ae^{-iHt}$$

and $\theta(t)$ is the step function, unity for positive and zero for negative value of time.

Accordingly, with the idea of the equation of motion method for the operator $f_0(t)$ and with the projection operator method of Zwanzig[4] and Mori[5] one can obtain [6]

$$\dot{f}_0(t)=\frac{\langle\{\dot{f}_0,f_0^+\}\rangle}{\langle\{f_0,f_0^+\}\rangle}f_0(t)+(1-P_0)\dot{f}_0(t)\equiv i\omega_0 f_0(t)+e^{iLt}i(1-P_0)Lf_0 \tag{2}$$

where P_0 is a projection operator on operator subspace spanned by f_0. Performing the differentiation of the Green Function (1) over the left-hand side time argument, we obtain

$$\frac{d}{dt}G(t-t')=-i\delta(t-t')\langle\{f_0,f_0^+\}\rangle+i\omega_0G(t-t')+F_0(t-t'), \tag{3}$$

where $F_0(t-t')$ is a new, higher-order Green Function defined as follows[6]:

$$F_0(t-t')=-i\Theta(t-t')\langle\{e^{iLt}i(1-P_0)Lf_0,f_0^+(t')\}\rangle. \tag{4}$$

For this new GF one has (after the differentiation over the right-hand side time argument)

$$\frac{d}{dt'}F_0(t-t')=i\delta(t-t')\langle\{i(1-P_0)Lf_0,f_0^+\}\rangle-i\omega_0F_0(t-t')+\Pi_0(t-t') \tag{5}$$

$$\Pi_0(t-t')=-i\Theta(t-t')\langle\{e^{iLt}i(1-P_0)Lf_0,(e^{iLt'}i(1-P_0)Lf_0)^+\}\rangle. \tag{6}$$

Now let us calculate GF $\Pi_0(t-t')$. Using the operator identity

$$e^{iLt}=e^{i(1-P_0)Lt}+\int_0^t e^{iL(t-t')}iP_0Le^{i(1-P_0)Lt'}dt' \tag{7}$$

one can obtain

$$e^{iLt}\, i(1-P_0)Lf_0 = f_1(t) + \int_0^t e^{iL(t-t')}\, iP_0 L f_1(t')\, dt' \tag{8}$$

where

$$f_1(t) = e^{i(1-P_0)Lt}\, i(1-P_0)Lf_0 \tag{9}$$

Introducing the new higher-order GF

$$M_1(t-t') = -i\Theta(t-t')\left\langle \left\{ f_1(t), f_1^+(t') \right\} \right\rangle \tag{10}$$

one can transform Eq.(8) as follows [7]:

$$e^{iLt}\, i(1-P_0)Lf_0 = f_1(t) + i\int_0^t e^{iL(t-t')}\, \frac{\langle\{Lf_1(t'), f_0^+\}\rangle}{\langle\{f_0, f_0^+\}\rangle} f_0\, dt' =$$

$$= f_1(t) - \int_0^t \frac{\langle\{f_1(t'), (iP_0Lf_0)^+\}\rangle}{\langle\{f_0, f_0^+\}\rangle} f_0(t-t')\, dt' - \tag{11}$$

$$- \int_0^t \frac{\langle\{f_1(t'), f_1^+\}\rangle}{\langle\{f_0, f_0^+\}\rangle} f_0(t-t')\, dt' = f_1(t) - i\int_0^t M_1(t') f_0(t-t') \Big/ \langle\{f_0, f_0^+\}\rangle\, dt'$$

and similarly

$$e^{-iLt}\, i(1-P_0)Lf_0 = f_1(-t) - i\int_0^t \frac{M_1(-t')\, f_0(t'-t)}{\langle\{f_0, f_0^+\}\rangle}\, dt' \tag{12}$$

where we have used the relation $\langle\{f_1(t), f_0^+\}\rangle = 0$ [5]. Having in hands this formula we can, as a next step, represent GF $\Pi_0(t)$, Eq.(6), as follows [6]:

$$\Pi_0(t) = -i\Theta(t)\left\langle \left\{ i(1-P_0)Lf_0, (e^{-iLt}\, i(1-P_0)Lf_0)^+ \right\} \right\rangle =$$

$$= -i\Theta(t)\left\langle \left\{ f_1, f_1^+(-t) \right\} \right\rangle - i\Theta(t)\int_0^t \left\langle \left\{ f_1, f_1^+(t'-t) \right\} \right\rangle M_1^*(-t')\, i \Big/ \left\langle \left\{ f_0, f_0^+ \right\} \right\rangle$$

$$= M_1(t) + i\int_{-\infty}^{+\infty} M_1(t') F_0(t-t') \Big/ \left\langle \left\{ f_0, f_0^+ \right\} \right\rangle dt', \quad t > 0. \tag{13}$$

Taking the time-Fourier transforms of Eqs.(3,5,13) Ichiyonagi get for GF (1) the following equations [6]:

$$G(E) = G_0(E) + G_0(E)\, \Pi_0(E) G_0(E) \Big/ \left\langle \left\{ f_0, f_0^+ \right\} \right\rangle^2 \tag{14}$$

$$\Pi_0(E) = M_1(E) + M_1(E)\, G_0(E)\, \Pi_0(E) / \langle\{f_0, f_0^+\}\rangle^2 \qquad (15)$$

from which the Dyson equation can be easily obtained

$$G(E) = G_0(E) + G_0(E)\, M_1(E)\, G(E) / \langle\{f_0, f_0^+\}\rangle^2 \qquad (16)$$

$$G_{f_0}(E) = \langle\{f_0, f_0^+\}\rangle / (E + \omega_0) \qquad (17)$$

and $G(E)$, $\Pi_0(E)$ and $M_1(E)$ are the Fourier transforms of the corresponding Green Functions (4), (6) and (10). The result (16) is exact but the evaluation of the self-energy requires considerable efforts. Approximations are possible, of course, but here we want to obtain formally exact representation for the self-energy. We proceed formally following the method described above, Eqs.(2-17).

Let us consider the equation of motion for the higher-order GF $M_1(t-t')$, Eq.(10). One obtains

$$\frac{d}{dt} M_1(t-t') = -i\delta(t-t')\langle\{f_1, f_1^+\}\rangle + F_1(t-t') + i\omega_1 M_1(t-t'), \qquad (18)$$

where we have introduced the higher-order GF $F_1(t-t')$ defined as follows:

$$F_1(t-t') = -i\Theta(t-t')\langle\{e^{i(1-P_0)Lt} f_2, f_1^+(t')\}\rangle, \qquad (19)$$

$$\dot{f}_1(t) = \frac{\langle\{\dot{f}_1, f_1^+\}\rangle}{\langle\{f_1, f_1^+\}\rangle} f_1(t) + (1-P_1)\dot{f}_1(t) \equiv i\omega_1 f_1(t) + e^{i(1-P_0)Lt} f_2, \qquad (20)$$

$$f_2 = i(1-P_0)(1-P_1)Lf_1 . \qquad (21)$$

Here, we have used the projection operator P_1 which projects onto the operator subspace spanned by f_1 /5/. Performing the differentiation of $F_1(t-t')$ over the second time argument, we get

$$\frac{d}{dt'}F_1(t-t') = i\delta(t-t')\langle\{f_2, f_1^+\}\rangle - i\omega_1 F_1(t-t') + \Pi_1(t-t'), \qquad (22)$$

where

$$\Pi_1(t-t') = -i\Theta(t-t')\langle\{e^{i(1-P_0)Lt} f_2, (e^{i(1-P_0)Lt'} f_2)^+\}\rangle . \qquad (23)$$

Using the operator identity similar to (7) but for the operator $(1-P_0)L$ rather than for L one obtains analogously to (8)

$$e^{i(1-P_0)Lt} f_2 = f_2(t) + \int_0^t e^{i(1-P_0)L(t-t')} i P_1 (1-P_0) L f_2(t')\, dt' \qquad (24)$$

where

$$f_2(t) = e^{i(1-P_0)(1-P_1)Lt} f_2 . \qquad (25)$$

Introducing the Green Function $M_2(t-t')$

$$M_2(t-t') = -i\Theta(t-t')\langle\{f_2(t), f_2^+(t')\}\rangle \qquad (26)$$

and performing similar calculations as in Eqs.(12-16) one obtains the Dyson-type equation for the Fourier transform of $M_1(t)$

$$M_1(E) = M_1^0(E) + M_1^0(E) M_2(E) M_1(E) / \langle\{f_1, f_1^+\}\rangle^2 , \qquad (27)$$

$$M_1^0(E) = \langle\{f_1, f_1^+\}\rangle / (E + \omega_1) . \qquad (28)$$

Continuing the procedure described above one can obtain in the i-th step the Dyson-type equation for GF

$$M_i(t-t') = -i\Theta(t-t')\langle\{f_i(t), f_i^+(t')\}\rangle \qquad (29)$$

with a "free-like" GF $M_i^0(E)$ in the form

$$M_i^{\circ}(E)=\langle\{f_i,f_i^{+}\}\rangle/(E-i\langle\{\dot{f}_i,f_i^{+}\}\rangle/\langle\langle\{f_i,f_i^{+}\}\rangle\rangle). \quad (30)$$

The operators f_i are constructed according to Mori algorithm /5/. Taking into account Eqs. (16),(27) and the next corresponding to greater values of index "i" one obtains the Green Function G(E) in the form of the finite continued fraction

$$G(E)=\frac{\langle\{f_0,f_0^{+}\}\rangle}{E+\omega_0-}\,\frac{\langle\{f_1,f_1^{+}\}\rangle/\langle\langle\{f_0,f_0^{+}\}\rangle\rangle}{E+\omega_1-}\cdots\frac{\langle\{f_m,f_m^{+}\}\rangle/\langle\langle\{f_{m-1},f_{m-1}^{+}\}\rangle\rangle}{E+\omega_m-M_{m+1}/\langle\langle\{f_m,f_m^{+}\}\rangle\rangle} \quad (31)$$

or infinite continued fraction

$$G(E)=\frac{1}{G_0^{-1}(E)-}\,\frac{\langle\{f_0,f_0^{+}\}\rangle^{-2}}{M_1^{\circ}(E)^{-1}-}\cdots\frac{\langle\{f_m,f_m^{+}\}\rangle^{-2}}{M_{m+1}^{\circ}(E)^{-1}-}\cdots \quad (32)$$

2.2.

In this subsection, we present the evaluation of the Green Function (1) within similar method as in a previous subsection but using the differentiation over the left-hand side time argument, only. This method was used in /7/ in considerations concerning the moment relaxation and related problems. Here, we adopt this technique for the calculation of the retarded double-time GF defined in Eq.(1).

Firstly, let us calculate the time derivative of the operator $f_0(t)$ /5,7/ using the operator identity (7)

$$\frac{df_0(t)}{dt}=i\omega_0 f_0(t)+f_1(t)+\int_0^t e^{iL(t-\tau)}\frac{\langle\{iLf_1(\tau),f_0^{+}\}\rangle}{\langle\{f_0,f_0^{+}\}\rangle}f_0\,d\tau \quad (33)$$

where $f_1(t)$ is given in Eq.(9).
Using this formula in the equation for the time derivative of the Green Function G(t) , we get

$$\frac{dG(t)}{dt} = -i\delta(t)\langle\{f_0, f_0^+\}\rangle + i\omega_0 G(t) + \int_{-\infty}^{\infty} \frac{\langle\{iLf_1(\tau), f_0^+\}\rangle}{\langle\{f_0, f_0^+\}\rangle}\Theta(\tau)G(t-\tau)d\tau. \qquad (34)$$

Taking into account the equality

$$\langle\{iLf_1(\tau), f_0^+\}\rangle = -\langle\{f_1(\tau), f_1^+\}\rangle \qquad (35)$$

one obtains

$$\frac{dG(t)}{dt} = -i\delta(t)\langle\{f_0, f_0^+\}\rangle + i\omega_0 G(t) - i\int_{-\infty}^{\infty} M_1(\tau)G(t-\tau)/\langle\{f_0, f_0^+\}\rangle d\tau \qquad (36)$$

where $M_1(\tau)$ is given by Eq.(10).

The Fourier transform of Eq.(36) leads to the result

$$G(E) = \langle\{f_0, f_0^+\}\rangle/(E + \omega_0 - M_1(E)/\langle\{f_0, f_0^+\}\rangle) \qquad (37)$$

which is equivalent to formula (16).

In comparison with the method presented in the previous subsection, here we use the operator identity (8) in the equation for G(t) (right in the function corresponding to $F_0(t)$ and not in the function $\Pi_0(t)$ which can be obtained writing down a next equation of motion for $F_0(t)$, only. The method presented now can be extended and, for example, in the n-th step one obtains

$$\frac{df_n(t)}{dt} = i\omega_n f_n(t) + e^{i(1-P_n)L_n t} f_{n+1} + \int_0^t e^{iL_n(t-\tau)} iP_n L_n e^{i(1-P_n)L_n\tau} f_{n+1} d\tau \qquad (38)$$

where L_n is defined as in /5/.

Transforming the last term in Eq.(38) in a similar way as in Eq.(33), we get

$$\frac{dM_n(t)}{dt} = -i\delta(t)\langle\{f_n, f_n^+\}\rangle - i\int_{-\infty}^{\infty} \frac{M_{n+1}(\tau)M_n(t-\tau)}{\langle\{f_n, f_n^+\}\rangle} d\tau + i\omega_n M_n(t) \qquad (39)$$

where $M_n(t)$ is defined by Eq.(29). Finally, for the Fourier transform of GF (1) one obtains the identical equation with Eq.(31). Thus, the Green Function G(E) obtained within the methods described in this and previous subsections are equivalent to one another even at each step of the continued fraction expansion.

Let us apply formula (31) for the calculation of the one-particle Green Function

$$\ll a_{i\sigma}(t) | a_{j\sigma}^+(t') \gg \qquad (40)$$

for the Hubbard Hamiltonian (1). Using the following form for the general expression for the space- and time-Fourier transforms of GF (40)

$$G(E) = \frac{\langle\{f_0, f_0^+\}\rangle}{E + \omega_0 - \dfrac{\langle\{f_1, f_1^+\}\rangle / \langle\{f_0, f_0^+\}\rangle}{E + \omega_1 - M_2(E)/\langle\{f_1, f_1^+\}\rangle}} \qquad (41)$$

one obtains

$$\ll a_{\vec{k}\sigma} | a_{\vec{k}\sigma}^+ \gg = \frac{1}{E - \epsilon_{\vec{k}} - U\langle n_{-\sigma}\rangle - \dfrac{U^2\langle n_{-\sigma}\rangle(1-\langle n_{-\sigma}\rangle)}{E - U(1-\langle n_{-\sigma}\rangle) - B_{\vec{k},-\sigma} - \dfrac{M_2(\vec{k},\sigma;E)}{U^2\langle n_{-\sigma}\rangle(1-\langle n_{-\sigma}\rangle)}}} \qquad (42)$$

The higher-order GF $M_2(\vec{k},\sigma;E)$ represents all the remaining terms of the infinite continued fraction expansion (32). If we reject M_2, i.e. we keep only two first steps of the continued fraction expansion, then the resulting GF $\langle\langle a_{\vec{k}\sigma} | a_{\vec{k}\sigma}^+ \rangle\rangle$ is equivalent to the solution obtained by Roth [15]. The function $B_{\vec{k},-\sigma}$ contains the higher-order

equal-time correlation functions (see, for example[15]) and $\varepsilon_{\vec{k}}$ is a Fourier transform of the hopping integral.

Similar approaches has been developed in papers[8-12]. For example, Fedro and Wilson[13] also obtained the Dyson equation for the one-particle GF. They considered the time differential equation for GF and also applied the projection operator P_o which projects out of the equation of motion of $f_o(t)$ the needed GF and relates the complementary part to GF at another time . After formal solving of the corresponding differential equation, they obtained exactly the same equation as was obtained above. Kishore[4] also studied the quasiparticle spectrum of the Hubbard model using the projection operator formalism. He used another form of the operator identity (9)

$$\frac{1}{E-L} = \frac{1}{E-(1-P)L} + \frac{1}{E-(1-P)L} PL \frac{1}{E-L} .$$

Chao et al.[10] derived also the same Dyson equation for GF (2) and proposed a differential equation approach for the calculation of the higher-order GF entering into the corresponding mass operator. Also, a perturbation scheme was developed for calculation of this mass operator[8,9,13].

It is not surprising that all these methods (and the one presented in the subsection (2.1)) give the same expression for the self-energy operator. All the methods are constructed, in fact, on the same operator identity (7), although this identity is used in different places of the theory or in various representations (in the Laplace or Fourier form, in the time-differential equation form).

Let us compare the self-energy $M_1(t)/\langle\{f_o, f_o^+\}\rangle^2$ calculated from Eq.(10) (for operators satisfying $\langle\{f_o, f_o^+\}\rangle=1$) with the self-energy expression given by Kishore[9]. We have in the successive steps

$$M(t) = -i\Theta(t)\left\langle\left\{e^{i(1-P_0)Lt} i(1-P_0)L f_0, (i(1-P_0)L f_0)^+\right\}\right\rangle \longrightarrow$$

$$-i\Theta(t)\langle\{Le^{i(1-P_0)Lt}(1-P_0)Lf_0, f_0^+\}\rangle \longrightarrow$$
$$-\langle\{L\frac{1}{E-(1-P_0)L}(1-P_0)Lf_0, f_0^+\}\rangle .$$

The last expression coincides with the results of Ref.[9].

2.3.

In this subsection, another method is suggested for calculations of the Green Function. We are going to obtain GF defined in Eq.(1) applying the algorithm of differentiation over the left-hand time argument of the corresponding higher- and higher-order GF which appear in successive equations for lower-order GF. But opposite to the usual scheme, see e.g.[1], where the higher-order GF are constructed simply from the operators which are obtained from the equation of motion of lower-order operators, here we will work with GF built from the operators forming a special operator basis. Using the projection operator technique developed by Mori[5] and a modified Lanczos algorighm of Sherman[16] one obtains the basis operator set $\{f_n\}$ as follows (cf.[7]):

$$\begin{aligned}
i\dot{f}_0 &= b_0^0 f_0 + f_1 ,\\
i\dot{f}_1 &= b_0^1 f_0 + b_1^1 f_1 + f_2 ,\\
i\dot{f}_2 &= b_1^2 f_1 + b_2^2 f_2 + f_3 ,\\
&\cdots\cdots\cdots\\
i\dot{f}_n &= b_{n-1}^n f_{n-1} + b_n^n f_n + f_{n+1} .
\end{aligned} \tag{43}$$

Here, f_0 is an operator which is used in the definition of the required GF, Eq.(2). The coefficients b_n^n, b_{n-1}^n are given by the formulas ([17,16])

$$b_n^n = \langle\{[f_n, H], f_n^+\}\rangle / \langle\{f_n, f_n^+\}\rangle , \quad b_{-1}^0 = 0,$$
$$b_{n-1}^n = \langle\{f_n, f_n^+\}\rangle / \langle f_{n-1}, f_{n-1}^+\}\rangle . \tag{44}$$

Using formulas (43) one can write the equation for GF

$$\ll f_n \mid f_0^+ \gg \equiv G_{n0}(E)$$

$$(E-b_n^m)G_{n0}(E)=\delta_{n0}\langle\{f_n,f_0^+\}\rangle+b_{n-1}^n G_{n-1,0}(E)+G_{n+1,0}(E) \tag{45}$$

or in the matrix form

$$\begin{pmatrix}G_{00}(E)\\G_{10}(E)\\\vdots\end{pmatrix}=\begin{pmatrix}1&-b_0&0&0&\dots\\-a_1&1&-b_1&0&\\0&-a_2&1&-b_2&\\\vdots&&&&\end{pmatrix}^{-1}\cdot\begin{pmatrix}(E-b_0^0)^{-1}\\0\\0\\\vdots\end{pmatrix}\equiv\bar{A}^{-1}\begin{pmatrix}(E-b_0^0)^{-1}\\0\\0\\\vdots\end{pmatrix} \tag{46}$$

where $\quad b_i=(E-b_i^i)^{-1},\ a_i=(E-b_i^i)^{-1}b_{i-1}^i\ .$

In order to obtain $G_{00}(E)$ is is sufficient to calculate only the (1,1) -element of the matrix A^{-1} . Defining

$$D_i=\det\begin{vmatrix}1&-b_i&0&0\dots\\-a_{i+1}&1&-b_{i+1}&0\\0&&&\\\vdots&&&\end{vmatrix} \tag{47}$$

one can obtain (cf.[7])

$$(A^{-1})_{11}=\left(1-b_0a_1\frac{D_2}{D_1}\right)^{-1},\quad \frac{D_{i+1}}{D_i}=\left(1-b_ia_{i+1}\frac{D_{i+2}}{D_{i+1}}\right)^{-1}. \tag{48}$$

Finally, for the Green Function $G_{00}(E)$ we obtain

$$\ll f_0\,|\,f_0^+\gg=\cfrac{1}{E-b_0^0-\cfrac{b_0^1}{E-b_1^1-\cfrac{b_1^2}{E-b_2^2-}}}\dots \tag{49}$$

Similar calculations have also been performed by Lado et al.[18] (see also [19]) for the Laplace transform of the time-autocorrelation function.

Taking as an example the Hubbard model and identifying the operators f_0 with $a_{i\sigma}$ (now the coefficients (44) will be matrices), we immediately obtain for $\vec{k}$-transform of the

Green Function (4.9) the expression given by Eq.(42) but in the form of the infinite continued fraction (without the "mass" operator present in (42)). The Fourier transforms of the coefficients $b_0^1(i,j)$ and $b_1^1(i,j)$ are as folows:

$$b_0^1(\vec{k}) = U^2 \langle n_{-\sigma} \rangle (1 - \langle n_{-\sigma} \rangle)$$

$$b_1^1(\vec{k}) = B_{\vec{k},-\sigma} + U(1 - \langle n_{-\sigma} \rangle).$$

Note that this variant of the method for calculations of GF can be comparable with the methods described in the previous subsections only in the limit of the infinite continued fraction expansion. In the case of finite number of levels of the corresponding continued fraction one cannot describe the effect of the omitted equations for higher-order GF in the form of the mass-like operator. In this case we have

$$\begin{pmatrix} G_{00}(E) \\ G_{10}(E) \\ \vdots \\ G_{m0}(E) \end{pmatrix} = (I - B)^{-1} \cdot \begin{pmatrix} (E - b_0^0)^{-1} \\ 0 \\ \vdots \\ (E - b_m^m)^{-1} G_{m+1,0}(E) \end{pmatrix} \qquad (50)$$

where

$$B \equiv \begin{pmatrix} 0 & (E-b_0^0)^{-1} & 0 & \cdots & \\ (E-b_1^1)^{-1} b_0^1 & 0 & (E-b_1^1)^{-1} & & \\ 0 & (E-b_2^2)^{-1} b_1^2 & 0 & & \\ \vdots & & \ddots & \ddots & \\ & & & 0 & (E-b_{m-1}^{m-1})^{-1} \\ & & & (E-b_m^m)^{-1} b_{m-1}^m & 0 \end{pmatrix}$$

and finally, for the Green Function $\langle\langle f_0 | f_0^+ \rangle\rangle$ we get

$$\ll f_0 | f_0^+ \gg = \prod_{i=0}^{n} \frac{b_{i-1}^{i}}{E - b_i^{i-}} + (-1)^n \prod_{i=0}^{n} (E - b_i^{i})^{-1} \frac{G_{n+1,0}(E)}{\det |\hat{1} - B|} \qquad (51)$$

Although, in principle, Eq.(49) is a complete solution, but in practice one must remember that only a few coefficients (for a many-body Hamiltonian) can be calculated. So, in some points approximations are inevitable. In this respect, expressions (31) or (41) are more useful for construction of approximations. In this case, after abrupting a corresponding continued fraction at some level, one can use various approximation for a mass-like operator. In this way, some information about the rejected higher-order GF can be saved. Expression (51) does not give such a possibility.

2.4.

Another way of constructing the infinite set of coupled Dyson-type equations for the Green Functions of increasing order has been given by Tsercovnikov[14]. For the sake of completeness we shall here briefly outline the main idea of this approach.

Let A_o be an operator or vector built up from operators depending on the problem under consideration. For example, for the Hubbard Hamiltonian we can identity the operator vector with the annihilation operators $a_{i\sigma}$ of the electron with spin σ described by a Wannier state centered on a site "i" of the crystal lattice. Next, one constructs the sequence of the vector operators according to the prescription

$$i\dot{A}_n = \omega(n) A_n + U(n, n+1) A_{n+1}, \quad n = 0, 1, 2, \ldots \qquad (52)$$

Note that such definition of the operator sequence is different from the definition used in the previous subsections and the set A_n does not create an orthogonal operator basis of the corresponding superoperator space. The Fourier tranform of the equation of motion for the Green

Function $\ll A_0(t) \mid A_0^+(t) \gg$ after the differentiation over the first and second time arguments) can be transformed so that as a final result we get the Dyson equation

$$\ll A_0 | A_0^+ \gg = \ll A_0 | A_0^+ \gg^{(0)} + \ll A_0 | A_0^+ \gg^{(0)} M(1) \ll A_0 | A_0^+ \gg \qquad (53)$$

where

$$E \ll A_0 | A_0^+ \gg^{(0)} = \langle \{A_0, A_0^+\} \rangle + \left[\omega(0) + W(0) \right] \ll A_0 | A_0^+ \gg^{(0)} \qquad (56)$$

$$W(0) = U(0,1) \langle \{A_1, A_0^+\} \rangle / \langle \{A_0, A_0^+\} \rangle$$

and

$$M(0) = \langle \{A_0, A_0^+\} \rangle^{-1} U(0,1) \ll A_1 | A_1^+ \gg_1 U(1,0) \langle \{A_0, A_0^+\} \rangle^{-1}. \qquad (57)$$

Such a construction of the Dyson equation was possible only because of introducing the so-called irreducible Green Function $\ll A_1 | A_1^+ \gg_1$ according to the formula

$$\ll A | B \gg_1 = \ll A | B \gg - \ll A | A_0^+ \gg \ll A_0 | A_0^+ \gg^{-1} \ll A_0 | B \gg .$$

The irreducible GF $\ll A | B \gg_1$ is defined so that any linear in A_0 operator part of A and B does not give any contribution to it. This procedure can be repeated and it results in an infinite set of the Dyson-type equations for still higher-order irreducible Green Functions[14]. This set of equations can be written in the form of the continued fraction expansion

$$\ll A_0 | A_0^+ \gg = \cfrac{1}{\left(\ll A_0 | A_0^+ \gg^{(0)} \right)^{-1} - \cfrac{\langle \{A_0, A_0^+\} \rangle^{-2}}{\left(\ll A_1 | A_1^+ \gg_1^{(0)} \right)^{-1} - \cfrac{\langle \{A_1, A_1^+\} \rangle^{-2}}{\left(\ll A_2 | A_2^+ \gg_2^{(0)} \right)^{-1} - \cdots}}} \qquad (58)$$

which is nearly the same as that in Eq.(32). Note howewer, that now the effect of the nonorthogonality of the basis operator set is recompensated by introduction of the irreducible GF approach. Taking into consideration only the

first two steps of the continued fraction (58) one immediately obtains the Roth result [15]. It should be stressed that this approach is very elastic with respect to the decomposition (52). It can be easy checked that it is a rather difficult task to obtain an operator A_2 and matrix U(1,2) for the Hubbard model using this formula. Fortunately, we can work within this approach taking simply

$$i\dot{A}_n = \omega(n) A_n + A_{n+1}$$

or even $$i\dot{A}_n = A_{n+1} .$$

In every case the general formula (58) remains the same and the subsequent steps of the continued fraction are unchanged.

2.5.

It shoudl be emphasized that such a choice of a basis operator set as in the previous subsections was performed is not in every case the best choice which can be found. In this context, we mention the work by Elk [17]. Performing similar operations as in the previous subsections, i.e. after the differentiation of the GF $\ll A(t) \mid A^{+}(t') \gg$ over both time arguments and using the decomposition

$$i\dot{A} = \omega \cdot A + B \tag{59}$$

one can obtain the Dyson equation with the self-energy defined as follows[17]:

$$\Sigma(E) = \langle\{A,A^{+}\}\rangle^{-1} \Pi(E) \langle\{A,A^{+}\}\rangle^{-1} \left[1 + G^{(\omega)}(E) \langle\{A,A^{+}\}\rangle^{-1} \Pi(E) \langle\{A,A^{+}\}\rangle^{-1}\right]^{-1} \tag{60}$$

where

$$G^{(\omega)}(E) = \langle\{A,A^{+}\}\rangle / (E-\omega)$$

$$\Pi(E) = \langle\{B,A^{+}\}\rangle + \ll B \mid B^{+} \gg . \tag{61}$$

The form of the decomposition (59) is still sufficiently arbitrary, although the term B contains operators which cannot be expressed by operators A. On the other hand, as was

mentioned by Elk[17], this decomposition is essential because it influences the mean-field solution of the problem under consideration (61). From the general point of view (compare, for example, the coherent potential approximation in the theory of the electron propagation in alloys) this decomposition should be performed so that the expression

$$\langle\langle\{A,A^+\}\rangle\rangle^{-1}\left[\langle\langle\{B,A^+\}\rangle\rangle + \ll B|B^+\gg\right]\langle\langle\{A,A^+\}\rangle\rangle^{-1} \qquad (62)$$

could reach the smallest value as possible. Only in this case one can say that almost all information about the system which can be put in the zero-order (mean-field) Green Function is indeed contained in it. In other words, the self-energy contribution reaches the minimal values. It means that one should minimize expression (62) [17]. Generally, it is very difficult to say anything about the higher-order GF $\langle\langle B|B^+\rangle\rangle$ and usually one accepts the condition of vanishing value of the correlation function $\langle\{B,A^+\}\rangle$. Note that this is exactly the same condition which we met during the derivation of the Dyson equation in the previous subsections 2.1, 2.2 and 2.3. It is equivalent, speaking in the language of those methods, to the orthogonalization procedure of the operator elements of some superoperator space. As was mentioned by Elk, the spin systems may be examples of such systems for which a vanishing value of $\langle\{B,A^+\}\rangle$ does not denote the best choice of the mean-field Green Function.

3. CONCLUSIONS AND REMARKS

In this paper we have investigated one of the existing technique used in a solid state theory for calculations of the many-body effects, namely, a technique of the retarded, double-time Green Functions calculated within the equation of motion method. As the standard equation of motion method for Green Functions leads to a very complicated system of many equations for many higher-order Green Functions, we have considered another method within which the corresponding

equations for higher-order functions were obtained in rather a regular way, i.e. within the method constructed on the basis of the projection operator formalism of Zwanzig and Mori. It is well known that this formalism has been succesfully applied to a large variety of problems concerning relaxation phenomena in physical systems. Here, as has already been mentioned, we used the idea of this approach to the calculations of the retarded, double-time Green Functions. We have shown that "different" methods, e.g., 'the methods using a concept of differentiation over both (or one) time arguments or method using the operator basis set in a tridiagonal form, lead to the same, even at each stage of the calculations, continued fraction expansion for calculated GF. The continued fraction expansion for GF is, in fact, only a formal exact solution because only a few of the coefficients can be calculated. So at some place of the theory, the approximations are inevitable. In this respect the methods using the idea of the differentiation over both time arguments are more appropriate as in this case one can obtain GF in the form of the finite continued fraction with a mass-like operator (in the last stage of this fraction) in the form more useful for further approximations (see, e.g. /14,19/).

One can check in a relatively easy way that the successive parts of the continued fraction expansion of GF lead to known solutions. For example, for Hubbard model and the Green Function constructed from the annihilation and creation electron operators one obtains the Hartree-Fock solution taking only the first part of the infinite continued fraction (42), (49) or (58). Taking into consideration the first two parts of this fraction one obtains the Roth result. On the other hand, one can use a finite continued fraction representation of the GF, e.g. Eq.(31). In such a case, even after abrupting the fraction after the first step and using the simplest possible approximation for the self-energy term, i.e. approximating the corresponding correlation functions by the products of all possible two-point correlators with

different time arguments, one obtains results equivalent to the self-consistent second-order in U perturbation theory[14,20]. If one calculates the Green Function built from the so-called Hubbard operators $a_{i\sigma}(1-n_{i-\sigma})$ and $a_{i\sigma}n_{i-\sigma}$, the first step of the infined continued fraction gives the result of Roth. It is not surprising that now one obtains the same result as this in the two-step approximation of the corresponding infinite fraction in the former case. Now, the Hubbard operators contain also the second basis operator f_1 which was needed to construct the Roth's solution using the one-particle GF.

Although the projection operator methods discussed above allow us for more systematic, in comparison with a usually used version of the equation of motion method, construction of the successive equations for higher-order GF, they have also some shortcomings inherent in the equation of motion method independently of their modifications. Namely, the higher correlation functions appear in the successive steps of this approach. For example, the function $B_{\vec{k},-\sigma}$ in Eq.(42) contains the spin, double-hop and density correlation functions. The problem of this higher-order correlation function can be, to a certain extent, removed using the matrix GF $\langle\langle F \mid F^{+} \rangle\rangle$, where $F=(f_0,f_1,f_2,\ldots)$ rather than $\langle\langle f_i \mid f_i^{+} \rangle\rangle$. It is also worth noticing that the continued fraction expansion of GF can be identified with the results of Feenberg's perturbational approach[21].

In summary, we have calculated the retarded, double-time Green Function using the ideas of the projection operator and the equation of motion methods. Different modifications of these approaches, as well as the results known from the literature can be represented by the continued fraction expansion with exactly the same steps of the fraction.

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