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Abstract. The equation of motion for nonequilibrium Green functions is derived within the framework of the Schwinger and Keldysh formalism of perturbation expansion. For nonequilibrium distribution Green functions, the equation of motion derived from quantum mechanics contains undefined singularities, whose explicit form depends on the specific initial or boundary condition. In the present work, the exact expression of singular terms is found in the equation of motion from the time-looped perturbation theory in which the adiabatic initial condition is implied. Unlike the usual Dyson perturbation formalism or the well known Kadanoff–Baym equation of motion, our resulting equation can be adopted directly for calculations without the graphical analysis, which depends on the specific form of the Hamiltonian. On the basis of this equation of motion, the procedure of a nonperturbative solution is outlined and potential applications are briefly discussed.

1. Introduction

The Green function (GF) technique has long been regarded as a powerful tool for the treatment of many-body systems in equilibrium. At finite temperatures, the initial state is no longer the ground state, and the final state is not well defined due to possible transitions to various excited states [1, 2]. If the initial state is $\phi_0(t = -\infty)$, then the eigenstate becomes $\psi = S(0, -\infty)\phi_0$ by switching on the interaction adiabatically for a long time. It is therefore difficult to define the state at a later time $t = \tau$ at finite temperatures. In dealing with such complications, Schwinger [3] introduced the time-loop technique to handle the S-matrix $S(-\infty, +\infty)$ by breaking up the time integration to two stages, namely, from $-\infty$ to τ and from τ to $-\infty$, and then letting $\tau \to +\infty$. Thus, Schwinger's time loop technique allows one to start and end the S-matrix expansion with a well defined state ϕ_0.

Because the time-loop technique does not depend on the statistical ensemble, it should be useful in dealing with nonequilibrium systems. This was carried out by Keldysh [4] who developed the GF formalism to treat nonequilibrium problems on the basis of Schwinger's method. The Green functions developed in this theory are known as either the nonequilibrium GF [5–8] or the time-looped GF [1]. The purpose of this paper is to derive an equation of motion (EOM) which determines directly the nonequilibrium distribution GF. We remark that the physical quantity can be calculated from the retarded GF alone in equilibrium case.

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In general the transport phenomena occur only in nonequilibrium systems and hence, strictly speaking, cannot be handled by the ordinary equilibrium GF. The equilibrium GF may be applied to systems involving only linear responses. To treat quantum transport problems with strong interactions in mesoscopic systems, on the other hand, the nonequilibrium formalism of Keldysh [4] is perhaps one of the most general approaches [9–18]. In fact, the nonequilibrium GF has been employed in recent years to study a variety of problems beyond the linear response regime. Furthermore, the theory is also applied to discuss the dynamic behaviour of systems, for example, the nonequilibrium screening in a three-dimensional electron gas [6, 7], and photoabsorption in a two-dimensional electron gas under time-dependent electric fields [19].

The perturbation expansion and graph technique has been well developed for the nonequilibrium GF [4, 20]. The equation of motion (EOM) for the nonequilibrium GF has also been developed by analytic continuation from the imaginary to the real time domain [21]. However, it has been recognized that the two approaches are equivalent and lead to the same nonequilibrium Dyson equation [20]. More recently, the nonequilibrium GF has been generalized to include an arbitrary initial density matrix [22], and a general rule of graphic expansion has been given for nonequilibrium processes by the path-integral technique [23]. It may be of some interest just to mention in passing that the method of Legendre transformation can reduce a huge number of degrees of freedom to a small number of coordinates and is therefore able to handle macroscopic nonequilibrium systems [24].

On the other hand, the EOM for the nonequilibrium GF can be derived from the Heisenberg equation although the singular terms remain undefined. In the Kadanoff–Baym EOM, a specific self-energy term must be constructed for a given Hamiltonian so that the singular behaviour can be handled. In fact, the quantum Boltzmann equation is derived this way [20]. For practical calculations, however, the singular term may be avoided by introducing phenomenologically a decay rate and allowing the system to interact with an external reservoir. The procedure is similar to the quasi-equilibrium approximation in calculations of semiconductor quantum well lasers [25]. To our knowledge, there does not exist a *general* expression for this singular term in the literature.

Mathematically, the undefined singular terms have their origin in the undefined initial conditions. Thus, the general EOM for the nonequilibrium GF cannot be determined by quantum mechanics alone. This is because different nonequilibrium statistical ensembles may imply different initial conditions [22] and hence correspond to different expressions of the singular term, which behaves like a δ-function inhomogeneity. We derive, in the present work, the EOM for the nonequilibrium GF from the Schwinger–Keldysh perturbation formalism. The singular term is expressed in a well defined general form, and is consistent with the initial condition that the interaction is switched on adiabatically as implied in the time-looped perturbation theory. However, it is not impossible that the form of the singular function may change when different initial conditions are assumed.

This paper is organized as follows. In section 2, the time-looped Green function is very briefly reviewed. The EOM for the nonequilibrium GF is derived from the Heisenberg equation of motion in section 3. It is shown that the singular term introduced in the distribution GF is still undefined. In section 4, we derive the EOM for nonequilibrium GFs with the singular term expressed explicitly in a well defined general form. This is in contrast to the nonequilibrium Dyson equation, in which the self-energy terms are treated by graphic methods, depending on the specific Hamiltonian. The EOM can then be solved self-consistently with the decoupling procedure similar to what is known in the equilibrium cases. It is emphasized that all interactions are treated dynamically in this approach without introducing other parameters phenomenologically. In conclusion, we discuss a few remarks in section 5.

2. Nonequilibrium Green functions

The Green function is defined in the Heisenberg picture by

$$i\langle\langle A(t_a), B(t_b)\rangle\rangle = \text{tr}\{\rho T[A(t_a)B(t_b)]\} \tag{1}$$

where ρ is the density matrix and T denotes the time-ordering operator. The explicit form of the density operator ρ may not be specified but we assume that it will be evolved at $t = -\infty$ from the ρ_0 which involves only single particle operators. With the help of a time-loop procedure, we can express at finite temperatures the Green function as

$$i\langle\langle A(t_a), B(t_b)\rangle\rangle = \text{tr}\{\rho_0 T[A(t_a)B(t_b)S_c]\} \tag{2a}$$

where ρ_0 stands for the density matrix of the initially noninteracting system, the subscript c indicates the time loop and the time-loop S-matrix is defined by

$$S_c = T_c\left\{\exp\left[-i\int_c H_I(t)\,dt\right]\right\}. \tag{2b}$$

Since the one-direction time axis is changed to a loop with two branches, we define four Green functions depending on the relative positions of t_a and t_b in the loop. These are the time-ordered, anti-time-ordered and two distribution Green functions

$$i\langle\langle A(t_a), B(t_b)\rangle\rangle^{++} = \text{tr}\{\rho T[A(t_a)B(t_b)]\} \tag{3a}$$

$$i\langle\langle A(t_a), B(t_b)\rangle\rangle^{+-} = \mp\text{tr}\{\rho[B(t_b)A(t_a)]\} \tag{3b}$$

$$i\langle\langle A(t_a), B(t_b)\rangle\rangle^{-+} = \text{tr}\{\rho[A(t_a)B(t_b)]\} \tag{3c}$$

$$i\langle\langle A(t_a), B(t_b)\rangle\rangle^{--} = \text{tr}\{\rho\tilde{T}[A(t_a)B(t_b)]\}. \tag{3d}$$

The functions in equations (3b, c) are related to the conventional distribution GF by

$$\langle\langle A(t_a), B(t_b)\rangle\rangle^< = \langle\langle A(t_a), B(t_b)\rangle\rangle^{+-} \tag{4a}$$

$$\langle\langle A(t_a), B(t_b)\rangle\rangle^> = \langle\langle A(t_a), B(t_b)\rangle\rangle^{-+}. \tag{4b}$$

The well known retarded and advanced Green functions are related to the time-loop Green functions by

$$\langle\langle A(t_a), B(t_b)\rangle\rangle^r = \langle\langle A(t_a), B(t_b)\rangle\rangle^{++} - \langle\langle A(t_a), B(t_b)\rangle\rangle^{+-}$$
$$= \langle\langle A(t_a), B(t_b)\rangle\rangle^{-+} - \langle\langle A(t_a), B(t_b)\rangle\rangle^{--} \tag{5a}$$

$$\langle\langle A(t_a), B(t_b)\rangle\rangle^a = \langle\langle A(t_a), B(t_b)\rangle\rangle^{++} - \langle\langle A(t_a), B(t_b)\rangle\rangle^{-+}$$
$$= \langle\langle A(t_a), B(t_b)\rangle\rangle^{+-} - \langle\langle A(t_a), B(t_b)\rangle\rangle^{--}. \tag{5b}$$

It is important to note that the six Green functions are not independent. From the distribution and retarded Green functions, all the other four can be determined.

Since the Matsubara Green function [26] is able to treat the general equilibrium behaviour, it is not necessary to apply the time-loop technique even at finite temperatures. The time-loop Green functions are particularly useful in dealing with nonequilibrium problems which cannot be handled by other types of Green function. The idea that these time-loop Green functions can be applied to deal with the nonequilibrium quantum transport phenomena was first proposed by Keldysh [4].

Consider a system evolving under the Hamiltonian

$$H = H_0 + H_1 \tag{6}$$

where H_0 describes the noninteracting system, and H_1 represents interactions between all particles in the system. Let us suppose that $H_1 = 0$ initially ($t = -\infty$). This means that the system is initially described by H_0 only. Unlike the equilibrium case, this initial system

consists of several subsystems. Each subsystem may be characterized by a given temperature and chemical potential. Because these subsystems are not coupled to one another initially, such chemical potential or temperature differences do not produce any current in the system. When H_1 is switched on adiabatically, such differences begin to drive currents in the system. It is in this spirit, the tunnelling current through a metal–insulator–metal junction is calculated directly [27] We remark at this point that the procedure of adiabatic switching-on is usually sufficient in the calculation of steady state properties of the system. A more general formalism including arbitrary initial preparation of the system is discussed in [22].

Thus the nonequilibrium GF can be expressed as

$$i\langle\langle A(t_a), B(t_b)\rangle\rangle = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_c dt_1 \dots \int_c dt_n \text{tr}\{\rho_0 T_c[A_I(t_a)B_I(t_b)H_{1I}(t_1)\dots H_{1I}(t_n)]\} \quad (7)$$

where the subscript I indicates the interaction picture of the operator. Equation (7) forms the basis for theoretical calculations on which a well known graph technique of the perturbation method can be established. All characteristic properties of the transport phenomena can be calculated from first principles beyond the linear response theory, and similar perturbation procedures as in the equilibrium case can be developed to treat the many-body effects.

On the other hand, the EOM [28, 29] has not been developed for the nonequilibrium GF because the nonequilibrium GF cannot be completely determined by Heisenberg equations of motion alone. The EOM method for a properly selected retarded GF [29] has been widely used in the study of a variety of problems in equilibrium and linear response regime. By means of the usual procedure of decoupling, the retarded GF is obtained from a hierarchy of equations and the physical quantity under consideration can be related to the retarded GF by the spectrum theorem. In the case of nonequilibrium systems, however, the spectrum theorem is not valid, and it is necessary to calculate the physical quantity in question directly from the distribution GF.

The singular behaviour that appears in the EOM for the retarded GF is usually treated by the causality relation. The situation is, however, qualitatively different in the case of distribution GF. Generally speaking, the singularity in the EOM for distribution GF depends on details of the statistical behaviour of the system. Hence, different statistical ensembles may result in different expressions for the singularity. In this work, we derive the EOM within the framework of the Keldysh perturbation formalism. It will become clear in the final result that the singularity defined in our formulation is consistent with the Keldysh statistical ensemble.

3. Singularities in the EOM

Let us start with the EOM for the retarded GF

$$i\frac{\partial}{\partial t_2}\langle\langle A(t_2), B(t_1)\rangle\rangle^r = \delta(t_1 - t_2)\langle[A(t_1), B(t_1)]\rangle + \langle\langle[A(t_2), H] \mid B(t_1)\rangle\rangle^r \quad (8)$$

which is independent of the details of the statistical ensemble and can be derived directly from the Heisenberg equation of motion. The interaction Hamiltonian represents all many-body interactions in the many-particle system. Suppose that the general forms of operators A and B are products of creation and annihilation operators. The commutator $[A(t_2), H_0]$ can easily be evaluated with the result $\sum \lambda_i \varepsilon_i A(t_2)$ where $\lambda_i = +1(-1)$ for the annihilation (creation) operator which is being interchanged with H_0. Hence only the commutator $[A(t_2), H_1]$ is retained in the equation. We now apply the Fourier transformation to the resulting equation,

combine the two terms involving the Green function $\langle\!\langle A, B \rangle\!\rangle^r_\omega$ and then Fourier transform the equation back. Equation (8) finally becomes

$$\langle\!\langle A(t_2), B(t_1) \rangle\!\rangle^r = g^r_a(t_2 - t_1)\langle[A(t_1), B(t_1)]\rangle + \int dt' g^r_a(t_2 - t')\langle\!\langle[A(t'), H_1] \mid B(t_1)\rangle\!\rangle^r \quad (9a)$$

where

$$g^r_a(t_2 - t_1) = -i\theta(t_2 - t_1)\exp\left[-i\sum_i \lambda_i \varepsilon_i (t_2 - t_1)\right] \quad (9b)$$

is the retarded GF for free particles when $[A, B] = 1$.

In a similar fashion, we can derive the EOM for the distribution GF from Heisenberg equation and find

$$i\frac{\partial}{\partial t_2}\langle\!\langle A, B(t_1) \rangle\!\rangle^< = \langle\!\langle[A(t_2), H] \mid B(t_1)\rangle\!\rangle^<. \quad (10a)$$

The Fourier transform of equation (10a) is

$$\left(\omega - \sum \lambda_i \varepsilon_i\right)\langle\!\langle A, B \rangle\!\rangle^<_\omega = \langle\!\langle[A, H_1], B \rangle\!\rangle^<_\omega. \quad (10b)$$

In order to find the distribution GF, we must divide (10b) by $\left(\omega - \sum \lambda_i \varepsilon_i\right)$. This yields [30]

$$\langle\!\langle A, B \rangle\!\rangle^<_\omega = \left(\omega - \sum \lambda_i \varepsilon_i\right)^{-1}\langle\!\langle[A, H_1], B \rangle\!\rangle^<_\omega + a(\omega)\delta\left(\omega - \sum \lambda_i \varepsilon_i\right)^{-1}. \quad (10c)$$

However, both the arbitrary function $a(\omega)$ and the integration contour of $\left(\omega - \sum \lambda_i \varepsilon_i\right)^{-1}$ remain unknown. In the time-loop formalism, as we shall see, the exact expression of the unknown function $a(\omega)$ as well as the contour to integrate $\left(\omega - \sum \lambda_i \varepsilon_i\right)^{-1}$ are determined naturally, and the result is consistent with the initial adiabatic preparation. As a matter of fact, it contains all the necessary statistical information on the system.

4. EOM from the time-loop formalism

We attempt to derive the EOM for the retarded GF within the framework of the Keldysh perturbation formalism. It is expected from analytic continuation that the same procedure produces simultaneously EOM for the nonequilibrium distribution GF and retarded GF. Let us first define the following convention for convenience. When t_a is earlier than t_b on the loop, we have $t_a <_c t_b$, and we have $t_a >_c t_b$ otherwise. If we assume $t_a >_c t_b$ in the loop, then

$$\text{tr}\{\rho_0 T_c[A(t_a)B(t_b)H(t_1)\ldots H(t_n)]\}$$
$$= \text{tr}\{\rho_0[H_1(t_1)\ldots A(t_a)H_1(t_i)\ldots B(t_b)H_1(t_j)\ldots H_1(t_n)]\} = \text{tr}(\rho_0 W) \quad (11)$$

where we have defined $W = H_1(t_1)\ldots A(t_a)H_1(t_i)\ldots B(t_b)H_1(t_j)\ldots H_1(t_n)$ for simplicity. Equation (11) is written in the interaction picture in which we are going to develop the theory, and hence the subscript I is dropped from now on. We now move the operator $A(t_a)$ to the right within the trace by a complete cycle in order to find an equation the Green function has to satisfy. No additional sign is introduced due to the interchange of operators in the product even if we are dealing with fermions because the Fermi operators always appear in pairs in the Hamiltonian. When the operator $A(t_a)$ is moving to the right, we have

$$\text{tr}[\rho_0 W] = \text{tr}\{\rho_0[H_1(t_1)\ldots [A(t_a), H_1(t_i)]\ldots B(t_b)H_1(t_j)\ldots$$
$$\ldots H_1(t_n)]\} + \text{tr}\{\rho_0[H_1(t_1)\ldots H_1(t_i)A(t_a)\ldots B(t_b)H_1(t_j)\ldots H_1(t_n)]\}. \quad (12)$$

To work out the commutator $[A(t_0), H_1]$, we may define, for simplicity, the operators $A(t_a)$, $B(t_b)$ and $H_1(t_i)$ as

$$A(t_a) = \alpha_1 \ldots \alpha_l \, e^{i\lambda_{1\alpha}\varepsilon_{1\alpha}t_a} \ldots e^{i\lambda_{l\alpha}\varepsilon_{l\alpha}t_a} = \alpha_1 \ldots \alpha_l \, f_a(t_a) \tag{13a}$$

$$B(t_b) = \beta_1 \ldots \beta_m \, e^{i\lambda_{1\beta}\varepsilon_{1\beta}t_b} \ldots e^{i\lambda_{m\beta}\varepsilon_{m\beta}t_b} = \beta_1 \ldots \beta_m \, f_b(t_b) \tag{13b}$$

$$H(t_i) = h_1 \ldots h_p \, e^{i\lambda_{1h}\varepsilon_{1h}t_i} \ldots e^{i\lambda_{ph}\varepsilon_{ph}t_i} = h_1 \ldots h_p \, f_h(t_i) \tag{13c}$$

where α, β and h represent either creation or annihilation operators. The value for λ_i in the exponents is $+1$ (-1) for the corresponding creation (annihilation) operator. From the definitions in equations (13), it is easy to prove the commutation relation

$$[A(t_a), H_1(t_i)] = C(t_i) f_a(t_a - t_i) \tag{14a}$$

$$C(t_i) = [A(t_i), H_1(t_i)]. \tag{14b}$$

Inserting equations (14) in (12), we find after moving through all the operators on the left of $B(t_j)$

$$\mathrm{tr}\lfloor\rho_0 W\rfloor = \mathrm{tr}\{\rho_0[H_1(t_1)\ldots C(t_i)\ldots B(t_b)H_1(t_j)\ldots H_1(t_n)]\}f(t_a - t_i) + \cdots$$

$$\cdots + \mathrm{tr}\{\rho_0[H_1(t_1)\ldots C(t_{j-1})B(t_b)H_1(t_j)\ldots H_1(t_n)]\}f(t_a - t_{j-1})$$

$$+ \mathrm{tr}\{\rho_0[H_1(t_1)\ldots H_1(t_{j-1})A(t_a)B(t_b)H_1(t_j)\ldots H_1(t_n)]\}. \tag{15}$$

We can choose either the commutation or anticommutation relation when the position of operators A and B are interchanged, depending on the statistics of the particle. In any case, we represent the commutator (or anticommutator) by

$$D = [A, B]_\pm. \tag{16}$$

Then, equation (15) becomes

$$\mathrm{tr}[\rho_0 W] = \mathrm{tr}\{\rho_0[H_1(t_1)\ldots C(t_i)\ldots B(t_b)H_1(t_j)\ldots H_1(t_n)]\}f(t_a - t_i) + \cdots$$

$$\cdots + \mathrm{tr}\{\rho_0[H_1(t_1)\ldots C(t_{j-1})B(t_b)H_1(t_j)\ldots H_1(t_n)]\}f(t_a - t_{j-1})$$

$$+ \mathrm{tr}\{\rho_0[H_1(t_1)\ldots H_1(t_{j-1})D(t_b)H_1(t_j)\ldots H_1(t_n)]\}f(t_a - t_b)$$

$$\mp \mathrm{tr}\rho_0[H_1(t_1)\ldots H_1(t_{j-1})B(t_b)A(t_a)H_1(t_j)\ldots H_1(t_n)]. \tag{17}$$

If we keep moving the operator A to the right, we eventually reach the result

$$\mathrm{tr}[\rho_0 W] = \mathrm{tr}\{\rho_0[H_1(t_1)\ldots C(t_i)\ldots B(t_b)H_1(t_j)\ldots H_1(t_n)]\}f(t_a - t_i) + \cdots$$

$$\cdots + \mathrm{tr}\{\rho_0[H_1(t_1)\ldots C(t_{j-1})B(t_b)H_1(t_j)\ldots H_1(t_n)]\}f(t_a - t_{j-1})$$

$$+ \mathrm{tr}\{\rho_0[H_1(t_1)\ldots H_1(t_{j-1})D(t_b)H_1(t_j)\ldots H_1(t_n)]\}f(t_a - t_b)$$

$$\mp \mathrm{tr}\{\rho_0[H_1(t_1)\ldots H_1(t_{j-1})B(t_b)C(t_j)\ldots H_1(t_n)]\}f_q(t_a - t_j)$$

$$\mp \cdots \mp \mathrm{tr}\{\rho_0[H_1(t_1)\ldots H_1(t_{j-1})B(t_b)H_1(t_j)\ldots C(t_n)]\}f(t_a - t_n)$$

$$\mp \mathrm{tr}\{\rho_0[H_1(t_1)\ldots H_1(t_{j-1})B(t_b)H_1(t_j)\ldots H_1(t_n)A(t_a)]\}. \tag{18}$$

The last term of the above equation can be rewritten as

$$\mp \mathrm{tr}\{A(t_a)\rho_0[H_1(t_1)\ldots H_1(t_{j-1})B(t_b)H_1(t_j)\ldots H_1(t_n)]\}. \tag{19}$$

Since all kinds of particle in the system are initially in their own equilibrium states characterized by different temperatures and chemical potentials, we may assume the most general case of a grand canonical ensemble. Thus, we take the density operator

$$\rho_0 = Z_0^{-1} \exp\left[-\sum_i \beta_i(\varepsilon_i - \mu_i)n_i\right] \tag{20}$$

with the grand partition function Z_0 for a noninteracting system and obtain after a little algebra

$$A(t_a)\rho_0 = e^{\lambda_{1\alpha}\beta_1(\varepsilon_{1\alpha}-\mu_{l\alpha})} \dots e^{\lambda_{l\alpha}\beta_l(\varepsilon_{l\alpha}-\mu_{l\alpha})} = F_a\rho_0 A(t_a) \tag{21a}$$

where we have defined

$$F_a = e^{\lambda_{1\alpha}\beta_1(\varepsilon_{1\alpha}-\mu_{l\alpha})} \dots e^{\lambda_{l\alpha}\beta_l(\varepsilon_{l\alpha}-\mu_{l\alpha})}. \tag{21b}$$

Substituting equation (21) in (19) and moving the operator A further to the right until it returns to its initial position, we find finally that equation (18) becomes

$$
\begin{aligned}
\mathrm{tr}[\rho_0 W] = {}& \frac{f_a(t_a - t_b)}{1 \pm F_a}\mathrm{tr}\{\rho_0[H_1(t_1)\dots D(t_b)H_1(t_j)\dots H_1(t_n)]\} \\
&+ \sum_{t_j\leqslant_c t_k<_c t_i}\frac{f_a(t_a - t_k)}{1 \pm F_a}\mathrm{tr}\{\rho_0[H_1(t_1)\dots C(t_k)\dots B(t_b)H_1(t_j)\dots H_1(t_n)]\} \\
&\mp \sum_{t_k\leqslant_c t_j}\frac{f_a(t_a - t_k)}{1 \pm F_a}\mathrm{tr}\{\rho_0[H_1(t_1)\dots B(t_b)\dots C(t_k)\dots H_1(t_j)\dots H_1(t_n)]\} \\
&\mp \sum_{t_k>_c t_i}\frac{F_a f_a(t_a - t_k)}{1 \pm F_a}\mathrm{tr}\{\rho_0[H_1(t_1)\dots C(t_k)\dots B(t_b)H_1(t_n)]\}. \tag{22a}
\end{aligned}
$$

The second and third terms in equation (22a) can be combined into a single term by means of the time ordering operator if we note that the only difference between them is the order of t_k relative to other times. Hence, we have

$$
\begin{aligned}
\mathrm{tr}[\rho_0 W] = {}& \frac{f_a(t_a - t_b)}{1 \pm F_a}\mathrm{tr}\{\rho_0 T_c[D(t_b)H_1(t_1)\dots H_1(t_n)]\} \\
&+ \sum_{t_k\leqslant_c t_a}\frac{f_a(t_a - t_k)}{1 \pm F_a}\mathrm{tr}\{\rho_0 T_c[C(t_k)B(t_b)H_1(t_1)\dots H_1(t_n)]\} \\
&\mp \sum_{t_a<_c t_k}\frac{F_a f_a(t_a - t_k)}{1 \pm F_a}\mathrm{tr}\{\rho_0 T_c[C(t_k)B(t_b)H_1(t_1)\dots H_1(t_n)]\}. \tag{22b}
\end{aligned}
$$

It is interesting to remark that the coefficient before the trace in every term of equation (22b) is only determined by the relative time order. For $t_a >_c t_k$ it is $f_a(t_a - t_k)/(1 \pm F_a)$, and for $t_a <_c t_k$ it is $\mp F_a f_a(t_a - t_k)/(1 \pm F_a)$ where the upper (lower) sign is for fermions (bosons). As a consequence, we can define formally a single particle time-loop Green function for different relative orders of t_1 and t_2, namely,

$$\mathrm{i}g_a(t_2 - t_1) = \frac{f_a(t_2 - t_1)}{1 \pm F_a} \qquad t_2 >_c t_1 \tag{23a}$$

$$\mathrm{i}g_a(t_2 - t_1) = \mp\frac{F_a f_a(t_2 - t_1)}{1 \pm F_a} \qquad t_2 <_c t_1. \tag{23b}$$

With the help of equations (4) and (5), it is a simple matter to show that equations (23) are related to the retarded GF as given by (9b). In terms of these single-particle Green functions, (22b) takes the form

$$
\begin{aligned}
\mathrm{tr}[\rho_0 W] = {}& \mathrm{i}g_a(t_a - t_b)\mathrm{tr}\{\rho_0 T_c[D(t_b)H_1(t_1)\dots H_1(t_n)]\} \\
&+\mathrm{i}\sum_k g_a(t_a - t_b)\mathrm{tr}\{\rho_0 T_c[C(t_k)B(t_b)H_1(t_1)\dots H_1(t_n)]\}. \tag{24}
\end{aligned}
$$

Note that t_a and t_b are fixed but t_k is variable.

Inserting equation (24) into equation (7) we find that the time-ordered integral over $t_1\dots t_2$ in the first term can be carried out and the result is simply the time-average of $D(t_a)$, namely,

the first term yields $\mathrm{i}g_a(t_a - t_b)\langle D(t_b)\rangle$. The second term is more complicated. It is evaluated as follows.

$$\sum_{n=1}^{\infty} \frac{(-\mathrm{i})^n}{n!} \sum_k \int_c \mathrm{d}t_1 \ldots \int_c \mathrm{d}t_k \ldots \int_c \mathrm{d}t_n [\mathrm{i}g_a(t_a - t_k)] \mathrm{tr}\{\rho_0 T_c[C(t_k)B(t_b)H_1(t_1)\ldots H_1(t_n)]\}$$

$$= \sum_{n=1}^{\infty} \frac{(-\mathrm{i})^n}{n!} \sum_k \int_c \mathrm{d}t_k \mathrm{i}g_a(t_a - t_k)] \int_c \mathrm{d}t_1 \ldots \int_c \mathrm{d}t_{k-1} \int_c \mathrm{d}t_{k+1} \ldots$$

$$\ldots \int_c \mathrm{d}t_n \mathrm{tr}\{\rho_0 T_c[C(t_k)B(t_b)H_1(t_1)\ldots H_1(t_n)]\}$$

$$= \sum_{n=1}^{\infty} \frac{(-\mathrm{i})^n}{n!} n \int \mathrm{d}t [\mathrm{i}g_a(t_a - t)] \int_c \mathrm{d}t_1 \ldots$$

$$\ldots \int_c \mathrm{d}t_{n-1} \mathrm{tr}\{\rho_0 T_c[C(t)B(t_b)H_1(t_1)\ldots H_1(t_{n-1})]\}$$

$$= \mathrm{i} \int_c \mathrm{d}t\, g_a(t_a - t) \sum_{n=1}^{\infty} \frac{(-\mathrm{i})^n}{(n-1)!}(-\mathrm{i}) \int_c \mathrm{d}t_1 \ldots$$

$$\ldots \int_c \mathrm{d}t_{n-1} \mathrm{tr}\{\rho_0 T_c[C(t)B(t_b)H_1(t_1)\ldots H_1(t_{n-1})]\}$$

$$= \mathrm{i} \int_c \mathrm{d}t\, g_a(t_a - t) \langle\langle C(t) \mid B(t_b)\rangle\rangle \tag{25}$$

where we have made use of the fact that the integration of the trace over time variables $t_1 \ldots t_n$ is the same for any k and hence the sum over k results in n integrals of $(n-1)$ independent t variables. In the last step of equation (25), we have converted the equation from the interaction picture to the Heisenberg picture. With equation (25), we have finally

$$\langle\langle A(t_a), B(t_b)\rangle\rangle = g_a(t_a - t_b)\langle D(t_b)\rangle + \int_C \mathrm{d}t\, g_a(t_a - t)\langle\langle C(t)|, B(t_b)\rangle\rangle. \tag{26}$$

This is the EOM in the Heisenberg picture for the nonequilibrium GF, which incorporates statistical information in quantum mechanics. It differs from the usual Dyson equation in that it provides a general equation, independent of specific form of the Hamiltonian.

Following the Langreth theorem [31], we can change the integration over the loop in equation (26) to integration along the real time axis. This yields

$$\langle\langle A(t_a), B(t_b)\rangle\rangle^r = g_a^r(t_a - t_b)\langle[A(t_a), B(t_b)]_{\pm}\rangle$$
$$+ \int \mathrm{d}t\, g_a^r(t_a - t)\langle\langle[A(t), H_1(t)], B(t_b)\rangle\rangle^r \tag{27a}$$

$$\langle\langle A(t_a), B(t_b)\rangle\rangle^< = g_a^<(t_a - t_b)\langle[A(t_a), B(t_b)]_{\pm}\rangle$$
$$+ \int \mathrm{d}t\, g_a^r(t_a - t)\langle\langle[A(t), H_1(t)], B(t_b)\rangle\rangle^<$$
$$+ \int \mathrm{d}t\, g_a^<(t_a - t)\langle\langle[A(t), H_1(t)], B(t - b)\rangle\rangle^a. \tag{27b}$$

Before we discuss the physical meaning of equation (27b) and the graphical representation of perturbation theory, it is important to point out that we are dealing with many-particle Green functions here. An example of a two-particle GF and its graphic calculation can be found in the discussion of electrical conductivity of a metal in the presence of many impurities [32]. Each creation (annihilation) operator in $A(t_a)$ and $B(t_b)$ corresponds to a particle leaving (ending) the vertex at t_a and t_b, respectively. These particle and hole lines may exchange momentum at

any time during the interval $t_b - t_a$ because of the particle–particle interactions. The first term on the right-hand side of equation ($27b$) is the interaction-free contribution. The interaction part splits into two terms as we are dealing with time-loop GFs. In general, the integrands are products of a free-particle GF and a many-particle GF. This is understood as follows. The particle evolves freely from t_a until t when scattering occurs, and the resulting new Green function continues to develop until time t_b. The time variable t in the integrand may be in either the upper or the lower branch of the time loop, and the corresponding Green functions as defined in equation (3) can then be transformed into retarded and distribution Green functions. Hence the interaction leads to the last two terms in ($27b$). The integration over time includes all possible scattering paths. It is emphasized that the calculation of ($27b$) can be carried out directly without further approximation, and hence it is expected to yield new results. As a matter of fact, we have found the surprising inversion of the electron population in photon-assisted tunnelling through quantum wires and that the rotating-wave approximation is invalid when the quasi-particle transition is at resonance with incident light [33].

In the case of steady states, the Green functions depend only on the variable $t = t_a - t_b$, which is changed to ω by a Fourier transform. Thus, we have

$$\langle\!\langle A, B\rangle\!\rangle_\omega^r = g_a^r(\omega)\langle[A, B]_\pm\rangle + g_a^r(\omega)\langle\!\langle[A, H_1], B\rangle\!\rangle_\omega^r \tag{28a}$$

$$\langle\!\langle A, B\rangle\!\rangle_\omega^< = g_a^<(\omega)\langle[A, B]_\pm\rangle + g_a^r(\omega)\langle\!\langle[A, H_1], B\rangle\!\rangle_\omega^< + g_a^<(\omega)\langle\!\langle[A, H_1], B\rangle\!\rangle_\omega^a. \tag{28b}$$

Equation ($28a$) is just the Fourier transform of ($9a$), the EOM for the retarded GF, which can be found directly from the Heisenberg equation. Equation ($28b$) is the EOM for the distribution GF in which the singularity has already been expressed in the single-particle Green function $g_a^<(\omega)$ and $g_a^r(\omega)$, and can be used directly for theoretical calculations. With the explicit form of the g, equation ($28b$) can be rewritten as

$$\langle\!\langle A, B\rangle\!\rangle_\omega^< = \frac{\langle\!\langle[A, H_1], B\rangle\!\rangle_\omega^<}{\omega - \sum \lambda_i \varepsilon_i + i\eta} + 2\pi i P\delta\left(\omega - \sum \lambda_i \varepsilon_i\right)\langle[A, B]_\pm\rangle$$

$$+ 2\pi i P\delta\left(\omega - \sum \lambda_i \varepsilon_i\right)\langle\!\langle[A, H_1], B\rangle\!\rangle_\omega^a \tag{29}$$

where $P = \pm F_a/(1 \pm F_a)$. By comparing equation (29) with equation ($10c$) we see that the last two terms correspond to the arbitrary function $a(\omega)$ which indeed involves all the statistical information and cannot be obtained from the Heisenberg EOM alone. Besides, a positive imaginary part is added in $\omega - \sum \lambda_o \varepsilon_i + i\eta$ which fixes the original singularity.

The single-particle Green function $g^<(\omega) = 2\pi i P\delta\left(\omega - \sum \lambda_i \varepsilon_i\right)$ describes the initial statistical condition of the system. If it is possible to separate a term of the form $i\gamma \langle\!\langle A, B\rangle\!\rangle_\omega$ from the distribution GF $\langle\!\langle[A, H_1], B\rangle\!\rangle$, equation (29) can be rewritten as

$$\langle\!\langle A, B\rangle\!\rangle_\omega^< = \frac{2\pi i f\left(\sum \lambda_i \varepsilon_i\right)\left(\omega - \sum \lambda_i \omega_i\right)\delta\left(\omega - \sum \lambda_i \omega_i\right)\left[\langle[A, B]_\pm\rangle + \langle\!\langle[A, H_1], B\rangle\!\rangle_\omega^a\right]}{\omega - \sum \lambda \varepsilon_i + i\gamma_i}$$

$$+ \text{other terms from} \langle\!\langle[A, H_1], B\rangle\!\rangle_\omega^<. \tag{30}$$

The fact that the first term on the right vanishes justifies the usual phenomenological procedure in which a decay parameter γ is introduced instead of dealing with the singularity. This separation is always possible when the system is assumed to interact with an external reservoir. However, one then has to make further assumptions about the distribution function to decouple the reservoir which is valid only in the quasi-equilibrium approximation, or one still has to deal with a singularity in the EOM for the reservoir. On the other hand, the exact expression for the singularity is known in equation (29) which can then be employed for direct calculations without any phenomenological assumption.

This argument applies also to the transport problem in a mesoscopic system. The initial condition of the quasi-bound electrons is described by the first term of equation (30) and does

not contribute to the Green function. Hence the steady state solution is independent of the initial distribution of the quasi-bound electrons in the system. The same conclusion has been reached in the graphic analysis of the Green function [15].

5. Discussion and conclusion

We have seen that the EOM method is a powerful tool for the calculation of retarded GF for both the equilibrium and nonequilibrium systems. To find the distribution GF, however, the usual EOM approach from the Heisenberg equation yields undetermined singular terms. This does not cause any difficulty in the equilibrium case because the spectrum theorem can be applied to obtain the results. In the case of nonequilibrium problems, the traditional approach to avoid difficulties due to these singular terms is to introduce phenomenologically a decay parameter and then allow the system to interact with an external reservoir, which is valid only in the quasi-equilibrium approximation.

On the basis of the Schwinger–Keldysh perturbation formalism, both the nonequilibrium retarded GF and distribution GF follow simultaneously from the equation of motion approach. We have also derived the exact form of the singular terms and hence it is no longer necessary to introduce any parameter phenomenologically. It is different from the Dyson equation because it leads to a general equation that is independent of specific Hamiltonian. The procedure of calculation may be briefly outlined as follows. We first divide the system under consideration into parts with which different sets of statistical properties as the chemical potential and temperature can be associated. We then choose the Green function appropriate to the physical quantity in question. The difference from the equilibrium case is that we have to solve for distribution GF which involves the statistical information as well. In practice, a truncation procedure is required to achieve self-consistency. Thus the EOM method is more suitable for handling complicated problems for which the graphic method becomes impractical. The nonequilibrium GFs derived in this article are being employed to investigate quantum transport problems in mesoscopic structures with the presence of many-particle interactions as well as time-dependent external fields. Further studies of intersubband transitions in the photon-assisted tunnelling through a quantum well will be reported elsewhere in the near future.

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