Journal of Statistical Physics, Vol. 86, Nos. 5/6, 1997

Generalized Gradient Expansions in Quantum Transport Equations

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Received March 22, 1996; final August 22, 1996

Gradient expansions in quantum transport equations of a Kadanoff–Baym form have been reexamined. In a consistent approach the expansion should be performed also inside the self-energy in the scattering integrals of these equations. In the first perturbation order this internal expansion gives new correction terms to the generalized Boltzmann equation. These correction terms are found here for several typical systems. Possible corrections to the theory of a linear response to weak electric fields are also discussed.

KEY WORDS: Nonequilibrium Green's functions; generalized Boltzmann equation; gradient corrections; T-matrix approximation; shielded potential approximation.

1. INTRODUCTION

Time-dependent transport phenomena in quantum many-body systems can be described by the nonequilibrium Green's function formalism (NGF) of Kadanoff and Baym[1] or Keldysh.[2] The Kadanoff–Baym transport equations for nonequilibrium correlation functions can be obtained by analytic continuation to real times[3] of the Dyson equation for Matsubara Green's functions in purely complex times.[4, 5] The differential form of these equations has been applied in many systems.[6–9] Usually it is necessary to approximate the equations on several levels,[1] although in some systems the equations can be directly solved by powerful numerics.[10] The integral form of the Kadanoff–Baym equations has been less exploited because approximations in a time domain are not so familiar here.[11] Both

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0022-4715/97/0300-1337$12.50/0

approaches also have been used to develop a linear response theory for quantum systems in weak dc and ac electric fields. Here the integral version[12] seems to be more direct than the older differential versions[13, 14]

All functions in the Kadanoff–Baym equations depend separately on two time and two space arguments $(r_1, r_2; t_1, t_2)$. This two-argument structure, which results in nonequilibrium many-body systems with time or space nonlocal scattering, is the main obstacle in solving the transport equations. An approximate one-argument form of the equations can be obtained in systems with not very strong interactions.[15] Most older transport methods have a one-argument structure because they usually implicitly consider the presence of weak interactions.

A different simplification can be obtained in all types of systems if external excitation fields vary slowly in time and space. Then it is useful to subtract two equivalent sets of Kadanoff–Baym equations differentiated over the first (r_1, t_1) and second variables (r_2, t_2) and perform the so-called gradient expansion[1] in the new equations transformed to the center-of-mass system (CMS)

$$\xi = (x, X) = (r, t; R, T) = \left(r_1 - r_2, t_1 - t_2; \frac{r_1 + r_2}{2}, \frac{t_1 + t_2}{2} \right)$$

In the transformed equations various terms have second arguments with uppercase variables (R, T) shifted by different fractions of the lowercase variables (r', t'). The Taylor expansion of these terms in the small variables around the common values of the big variables is the gradient expansion. This expansion in powers of derivatives over (R, T) multiplied by (r', t') can be *unambiguously* and *consistently* stopped at chosen perturbation orders. In this way the two sets of CMS variables (R, T) and (r', t') can be step-by-step decoupled. By this decoupling memory effects are cut, so that the nonequilibrium dynamics becomes quasilocal and the equations get a quasiequilibrium form. Far from equilibrium this approach evidently fails, because the nonlocal scattering, leading (in equilibrium) to quasiparticles with a (k, ω)-dependent self-energy, should be reflected in the nonlocality of the nonequilibrium dynamics.

In the zeroth order of the gradient expansion the transport equations get a local dynamics. Stopping the gradient expansion in the first order gives corrections to the equations which partially restore memory effects peculiar to the nonlocal dynamics. Such an equation is called a generalized Boltzmann equation[1] (GBE). The GBE is not limited to weak interactions, but it can only describe slow dynamics close to equilibrium. The weaker the scattering, the better is the description far from equilibrium. When the scattering processes can be considered extremely weak, then the

nonequilibrium correlation functions in the GBE can be substituted by a deltalike spectral function multiplied by a distribution function for momenta.[1] As a result the GBE reduces to the Boltzmann equation (BE), which differs from its classical counterpart only by the degeneracy of the described gases. It is interesting that the integral version of the quantum transport equations[16] approximated by low orders of the gradient expansion do not give the BE. It is also worth mentioning that the gradient expansions in quantum transport equations are analogous to expansions in the classical Enskog equation or the more general BBGKY equations.[17]

The gradient corrections in the GBE described in the past[1] do not fully reflect the character of scattering processes because the self-energy in the scattering integrals of the transport equations is considered as a structureless entity. We realized[18] that a consistently performed gradient expansion should include also expansion of the self-energy *itself* as soon as the self-energy includes additional scattering events separated by internal vertices.[4] In the first order this *internal* expansion gives new correction terms to the GBE which are determined by the character of many-body scattering processes.

In this work phenomenological rules are presented which allow one to perform these internal gradient expansions. The rules are applied to derive consistently the GBE with all correction terms. These correction terms are found in three examples of the self-energy: the averaged T-matrix approximation for the self-energy in electron scattering on local potentials, the local T-matrix approximation, and the shielded potential approximation for the self-energy of interacting spinless fermions. The importance of the internal gradient corrections for the linear response to weak electric fields is also briefly discussed.

2. GRADIENT EXPANSIONS IN QUANTUM TRANSPORT EQUATIONS

In slowly changing fields the two differential forms of the Kadanoff–Baym equations in (B.7) can be subtracted and the gradient expansion can be performed in the resulting equations. The right sides of the subtracted equations include scattering terms of the form

$$\Sigma^{\alpha}(x_1, \bar{x}_3)\, G^{\beta}(\bar{x}_3, x_2), \qquad G^{\alpha}(x_1, \bar{x}_3)\, \Sigma^{\beta}(\bar{x}_3, x_2), \quad x_i = (r_i, t_i) \tag{1}$$

where the analytical structure of the self-energy Σ and the Green's function G in (1) are determined by the indexes α, $\beta = r$, a, $<$, and $>$ (see Appendix A).

2.1. External Expansions

Consider as an example the gradient expansion in the term $\Sigma^{\alpha}(x_1, \bar{x}_3)\, G^{\beta}(\bar{x}_3, x_2)$ from (1), where the many-body structure of Σ^{α} is neglected.[1] The expansion gives, in the CMS coordinates $\chi = (x, X) = (r, t; R, T)$,

$$\int dx_3\, \Sigma^{\alpha}(x_1, x_3)\, G^{\beta}(x_3, x_2)$$

$$= \int dx_3\, \Sigma^{\alpha}\left(x_1 - x_3, \frac{x_1 + x_3}{2}\right) G^{\beta}\left(x_3 - x_2, \frac{x_3 + x_2}{2}\right)$$

$$= \int d\bar{x}\, \Sigma^{\alpha}\left(\bar{x}, X + \frac{x - \bar{x}}{2}\right) G^{\beta}\left(x - \bar{x}, X - \frac{\bar{x}}{2}\right)$$

$$= \int d\bar{x}\, \Sigma^{\alpha}(\bar{x}, X)\, G^{\beta}(x - \bar{x}, X) + \int d\bar{x}\, \frac{\partial \Sigma^{\alpha}(\bar{x}, X)}{\partial X}\left(\frac{x - \bar{x}}{2}\right) G^{\beta}(x - \bar{x}, X)$$

$$+ \int d\bar{x}\, \Sigma^{\alpha}(\bar{x}, X)\, \frac{\partial G^{\beta}(x - \bar{x}, X)}{\partial X}\left(-\frac{\bar{x}}{2}\right) + \cdots \tag{2}$$

The new coordinates are $x = x_1 - x_2$, $\bar{x} = x_1 - x_3$, $X = (x_1 + x_2)/2$. A Fourier transform of the last expression in (2) from the coordinates $x = (r, t)$ to $q = (k, \omega)$ gives the following expansion in a series of Poisson brackets[9]:

$$\exp\left(\frac{i}{2} D(\xi, \xi')\right) \Sigma^{\alpha}(\xi)\, G^{\beta}(\xi')$$

$$\equiv \Sigma^{\alpha}(\xi)\, G^{\beta}(\xi) + \frac{i}{2}\left(\frac{\partial \Sigma^{\alpha}(\xi)}{\partial R}\frac{\partial G^{\beta}(\xi)}{\partial k} - \frac{\partial \Sigma^{\alpha}(\xi)}{\partial k}\frac{\partial G^{\beta}(\xi)}{\partial R}\right.$$

$$\left. - \frac{\partial \Sigma^{\alpha}(\xi)}{\partial T}\frac{\partial G^{\beta}(\xi)}{\partial \omega} + \frac{\partial \Sigma^{\alpha}(\xi)}{\partial \omega}\frac{\partial G^{\beta}(\xi)}{\partial T}\right) + \cdots$$

$$= \Sigma^{\alpha}(\xi)\, G^{\beta}(\xi) + \frac{i}{2}[\Sigma^{\alpha}(\xi), G^{\beta}(\xi)] + \cdots, \qquad \xi = (q, X) = (k, \omega; R, T) \tag{3}$$

The gradient expansion of the scattering term $\Sigma^{\alpha}(x_1, \bar{x}_3)\, G^{\beta}(\bar{x}_3, x_2)$ has been obtained in (3) without taking into account the many-body structure of the self-energy Σ^{α}. Therefore this expansion can be called *external*. The first order of this expansion includes only the first Poisson bracket in (3).

One can similarly perform the gradient expansion in driving terms of the quantum transport equations.

2.2. Internal Expansions

In many systems the self-energy is approximated by Feynman diagrams formed by ladders or bubbles of fermion and boson Green's functions.[1, 8, 19] This nontrivial functional of Green's functions, connected by internal integrations, can substitute the self-energy in any step of the calculations. The internal structure of the functional was not taken into account in the gradient expansion (3). Does it contribute new terms in the gradient expansion? It is obvious that this question can be answered if a systematic gradient expansion is performed in the expressions (1) where the self-energy is substituted by the functional of the Green's functions.

Consider for simplicity that the self-energy describes electron scattering on the localized potentials $V(r) = \sum_{r_i} V_0\, \delta(r - r_i)$. Assume further that V_0 is of moderate strength, but the number of random coordinates r_i is relatively small. Then a suitable self-energy for this problem results from the averaged T-matrix approximation (ATA)[20]

$$\Sigma(t_1, t_2) = c\{V_0 + V_0^2 G(t_1, t_2) + V_0^3 G(t_1, \bar{t}_3)\, G(\bar{t}_3, t_2) + \cdots\} = c\theta(t_1, t_2) \tag{4}$$

Here c represents the weak concentration of the potentials V_0 and θ is the local T-matrix. The Green's functions in (4) depend only on the time variables because the space variables have been integrated out due to the local scattering.

Analytical continuation of the self-energy (4) gives the propagator and correlation functions for the self-energy in the form (see Appendix B)[1]

$$\begin{aligned}\Sigma^r(t_1, t_2) &= c\{V_0 + V_0^2 G^r(t_1, t_2) + V_0^3 G^r(t_1, \bar{t}_3)\, G^r(\bar{t}_3, t_2) + \cdots\} \\ &= c\theta^r(t_1, t_2)\end{aligned} \tag{5}$$

$$\begin{aligned}\Sigma^<(t_1, t_2) &= c\theta^r(t_1, \bar{t}_3)\, G^<(\bar{t}_3, \bar{t}_4)\, \theta^a(\bar{t}_4, t_2) \\ &= c\theta^<(t_1, t_2)\end{aligned} \tag{6}$$

Each term in the expressions for $\Sigma^{r,<}$ in (5)–(6) is formed by several propagators or a correlation function with time arguments in "series" (see Appendix B).

Let us study in detail the gradient expansion of the scattering terms in (1) for the self-energy in (5)–(6). Assume first that the self-energy in the first expression from (1) is substituted by one of the terms from (5)–(6)

which has two Green's functions, $\Delta\Sigma(t_1, t_3) = cV_0^3 G^\alpha(t_1, \bar{t}_2)\, G^\beta(\bar{t}_2, t_3)$ (no index is used on the contribution to the self-energy $\Delta\Sigma$, to show its analytical structure). Then the expression $\Delta\Sigma(t_1, \bar{t}_2)\, G^\gamma(\bar{t}_2, t_3)$ can be transformed to the CMS coordinates as follows (we suppress the prefactor cV_0^3 and neglect the fact that the function G^γ depends also on space variables):

$$
\begin{aligned}
&G^\alpha(t_1, \bar{t}_2)\, G^\beta(\bar{t}_2, \bar{t}_3)\, G^\gamma(\bar{t}_3, t_4) \\
&\quad = G^\alpha\left(t_1 - \bar{t}_2, \frac{t_1 + \bar{t}_2}{2}\right) G^\beta\left(\bar{t}_2 - \bar{t}_3, \frac{\bar{t}_2 + \bar{t}_3}{2}\right) G^\gamma\left(\bar{t}_3 - t_4, \frac{\bar{t}_3 + t_4}{2}\right) \\
&\quad = G^\alpha\left(\bar{\tau}_\mathrm{I}, T + \frac{\tau - \bar{\tau}_\mathrm{I} - \bar{\tau}_\mathrm{II}}{2} + \frac{\bar{\tau}_\mathrm{II}}{2}\right) G^\beta\left(\bar{\tau}_\mathrm{II}, T + \frac{\tau - \bar{\tau}_\mathrm{I} - \bar{\tau}_\mathrm{II}}{2} - \frac{\bar{\tau}_\mathrm{I}}{2}\right) \\
&\qquad \times G^\gamma\left(\tau - \bar{\tau}_\mathrm{I} - \bar{\tau}_\mathrm{II}, T - \frac{\bar{\tau}_\mathrm{I}}{2} - \frac{\bar{\tau}_\mathrm{II}}{2}\right), \qquad \alpha, \beta, \gamma = r, a, <, >
\end{aligned} \tag{7}
$$

where $(\tau, T) \equiv (t_1 - t_4, (t_1 + t_4)/2)$ and $\bar{\tau}_\mathrm{I} = t_1 - \bar{t}_2$, $\bar{\tau}_\mathrm{II} = \bar{t}_2 - \bar{t}_3$. In expression (7) a Taylor expansion in the τ coordinates can be performed around the T coordinates as in (2). In first order each of the Green's functions differentiated over T has multiplicative coefficients formed by the τ coordinates of the remaining two Green's functions in the series. Therefore in this structure of the arguments the Green's functions are equivalent from the point of view of gradient expansions.

After a Fourier transform over the small variables a symmetrical expression in the three functions $G^{\alpha,\beta,\gamma}$ with respect to the derivatives $(\partial/\partial X)(\partial/\partial q)$ can be obtained. Therefore the complete gradient expansion up to the linear order can be written as follows (the space variables have been included in G^γ):

$$
\begin{aligned}
&cV_0^3\{G^\alpha(\omega, T)\, G^\beta(\omega, T)\, G^\gamma(\xi) + \tfrac{1}{2}i[G^\alpha(\omega, T)\, G^\beta(\omega, T), G^\gamma(\xi)] \\
&\quad + \tfrac{1}{2}i[G^\alpha(\omega, T), G^\beta(\omega, T)]\, G^\gamma(\xi)\}, \qquad \xi = (k, \omega; R, T)
\end{aligned} \tag{8}
$$

where Poisson brackets have been used. Since the space coordinates (k, R) are integrated out in the present self-energy, gradient expansions cannot be performed in these variables. But in the general case both pairs of coordinates contribute in the way shown in (8).

The second term in (8) resulted as in (3) from the (external) gradient expansion of the expression $\Delta\Sigma(t_1, \bar{t}_2)\, G^\gamma(\bar{t}_2, t_3)$. The last term in (8) resulted from the gradient expansion of the internal structure of the self-energy contribution $\Delta\Sigma$. Therefore this expansion and the resulting term can be called *internal*. In (8) only contributions to the self-energy diagrams with two Green's functions were included. Analogously one can perform

the gradient expansion in terms with any number of Green's functions. This problem is solved in the next section in detail.

The *internal* gradient corrections can be easily physically understood from the previous example, where scattering processes can be seen as many consecutive events on the same center. If the system is excited by a time-dependent field, then scattering conditions on the center can change between these consecutive scattering events. Corrections to these changed scattering conditions are represented by the internal correction terms. For centers which are little smeared in space, nonzero internal gradient corrections result, even in excitation by static fields.

3. GRADIENT EXPANSIONS IN GENERAL

A gradient expansion in quantum transport equations can be *unambiguously* represented by a series of Poisson brackets of increasing order n. Physically this is a consistent expansion in powers of space (time) inhomogeneities, since the nth-order Poisson brackets are of the same order of magnitude as the terms $(k\sigma)^n$, where k is the inverse mean free path and σ is the range of space inhomogeneity (analogous terms apply for the time inhomogeneity). If $k\sigma \ll 1$, then the expansion can be stopped in the first order ($n = 1$), which is equivalent to inclusion of both *external* and *internal* corrections in the GBE [see also (8), (9), and (32)].

Gradient expansions can be performed also in classical transport equations describing dense systems. Such systems were first studied approximately by the Enskog equation,[17] which generalizes the Boltzmann equation by taking finite volumes of scattering particles. Since only binary collisions are included here, as in the BE, gradient expansions in this equation are analogous to the *external* expansions in quantum transport equations, giving the uncomplete quantum GBE.[1] Later, classical dense systems were described by the so-called BBGKY hierarchy of kinetic equations,[17] which can include multiple encounters of particles. Under some assumptions this set of equations can be reduced to a classical generalized Boltzmann equation,[17] which has scattering integrals with a structure analogous to that in the quantum transport equations. Therefore gradient expansions in this classical GBE are analogous to both the *external* and *internal* expansions leading to the complete quantum GBE (in the classical GBE, gradient expansions can be performed, while the quantum GBE is the result of the gradient expansions).

3.1. General Rules for Gradient Expansions

We formulate a set of phenomenological rules for performing *external* and *internal* gradient expansions in terms as in (1) appearing in quantum

transport equations. From now on the gradient expansions are stopped after the first perturbation order (higher order contributions can be found analogously). The following points specify and summarize the necessary steps for gradient expansions in concrete terms:

1. Analytic continuation to real times of the term is performed, to get an expression formed by propagators and correlation functions.
2. Each of the self-energy functions $\Sigma^{r,a,<,>}$ is resolved into a functional of full fermion and boson Green's functions $G^{r,a,<,>}$ and undressed matrix elements.
3. The whole term is transformed into CMS coordinates, and the uppercase coordinate X is linearized in the conjugate lowercase coordinate x. After a Fourier transform over the coordinates x, the linearization prefactors x become derivatives ∂_q, which produce a series of new terms. In each of these new terms just two derivatives appear (over X and q). The expansion should be performed on a hierarchical structure of levels, going more and more inside the structure of Σ (the vertices are the landmarks). Corrections for higher levels are done on lower levels. All objects which depend on some of the coordinates must be differentiated. The lowest objects are the full Green's functions and undressed coupling matrix elements.
4. "Parallel" objects with the same coordinates (x_i, x_j) can be considered in the derivatives as a single differentiated object, irrespective of the order of x_i and x_j. At the lower level some of the objects with the coordinates (x_i, x_j) can have still other internal coordinates, which can give further gradient corrections.
5. "Serial" objects with arguments as in (7) are differentiated in such a way that differentiation of one object over an uppercase coordinate X is accompanied by differentiation of the other objects in a series (one by one) over the conjugate lowercase coordinate q. Sign prefactors depend on the sequence of objects. Realization of this rule for terms with many Green's functions in a series can be done by a second functional derivative of the term over the objects in the series. This derivative is multiplied by a Poisson bracket of the two differentiating objects in the functional derivative.

In the previous section these rules have already been implicitly applied on a simple algebraic term from the self-energy [see (8)]. Analogously one can deal with other such algebraic terms or complex recursive terms. Before we come to these expansions we present a theorem. Application of the

above rules to scattering terms from transport equations which include a self-energy as in (8) gives the following formal expansion (stopped in the first perturbation order):

$$G^<(\xi)\,\Sigma(\xi) + \tfrac{1}{2}i[G^<(\xi), \Sigma(\xi)] + G^<(\xi)\,F_i[\Sigma](\xi) \tag{9}$$

Here $F_i[\Sigma](\xi)$ represents the internal gradient expansion in the self-energy Σ. Since the form (9) is fully general, it can be taken as a theorem:

- *Internal* expansion of a term with a self-energy results by the substitution of $\Sigma(\xi)$ by $\Sigma(\xi) + F_i[\Sigma](\xi)$ in the zeroth-order term.

From this theorem it follows that the *internal* gradient expansion in terms with a self-energy can be directly found from the function $F_i[\Sigma](\xi)$.

3.2. Expansions of the Self-Energy

We can concentrate on this function $F_i[\Sigma](\xi)$ and evaluate if for several typical examples of a self-energy.

3.2.1. Static Averaged *T*-Matrix Approximation. The first example concerns the ATA self-energy (4) for electron scattering on local potentials. After application of rules 1–3, the zeroth-order propagator and correlation parts for the self-energy in the frequency representation are

$$\Sigma^r(\omega, T) = c\frac{V_0}{1 - G^r(\omega, T)\,V_0} = c\theta^r(\omega, T) \tag{10}$$

$$\Sigma^<(\omega, T) = c\theta^r(\omega, T)\,G^<(\omega, T)\,\theta^a(\omega, T) = c\theta^<(\omega, T) \tag{11}$$

Application of rule 5 to the retarded part in (5) gives the first-order term

$$F_i[\Sigma^r](\xi) = \frac{\delta^2\Sigma^r}{\delta G^r\,\delta G^r}(\xi)\,\frac{i}{2}\,[G^r(\xi), G^r(\xi)] = 0 \tag{12}$$

since only functional derivatives of Σ^r over the propagator Green's functions G^r can be applied here. Because the Poisson bracket from equivalent objects is zero, the function $F_i[\Sigma^r](\xi)$ does not contribute to the internal expansion. Analogously one can find the internal term for the correlated part in (6),

$$
\begin{aligned}
F_i[\Sigma^<](\xi) = & \frac{\delta^2 \Sigma^<}{\delta G^r \, \delta G^<}(\xi) \frac{i}{2}[G^r(\xi), G^<(\xi)] \\
& + \frac{\delta^2 \Sigma^<}{\delta G^< \, \delta G^a}(\xi) \frac{i}{2}[G^<(\xi), G^a(\xi)] \\
& + \frac{\delta^2 \Sigma^<}{\delta G^r \, \delta G^a}(\xi) \frac{i}{2}[G^r(\xi), G^a(\xi)] \\
= & -c \operatorname{Im}\{[\theta^r(\omega, T)]^2 \theta^a(\omega, T)[G^r(\omega, T), G^<(\omega, T)]\} \\
& - \frac{c}{2} |\theta^r(\omega, T)|^4 G^<(\omega, T) \\
& \times \int \frac{d\bar{\omega}}{2\pi} \frac{1}{\omega - \bar{\omega}} \left(\frac{\partial A(\bar{\omega}, T)}{\partial \bar{\omega}} \frac{\partial A(\omega, T)}{\partial T} - \frac{\partial A(\bar{\omega}, T)}{\partial T} \frac{\partial A(\omega, T)}{\partial \omega} \right)
\end{aligned}
\tag{13}
$$

The term $F_i[\Sigma^>](\omega, T)$ can be evaluated in the same way. In the first expression in (13) only the nonzero functional derivatives have been considered, which result from differentiation over Green's functions of different analytical structures. The order of derivatives and terms in Poisson brackets is the same as the order of these functions in (6). The second expression results by integration by parts in the Poisson bracket $[G^r(\xi), G^a(\xi)]$ and some simple algebra.

3.2.2. Dynamic *T*-Matrix Approximation. Another T-matrix approximation is used[1, 19] if the mutual interaction of electrons is studied. This approximation gives a self-energy of a very similar structure to the ATA self-energy in (4), but the internal dynamics is more complicated here. For spinless fermions the self-energy can be written as[1]

$$
\Sigma(t_1, t_2) = -i\Theta(t_1, t_2) \, G(t_2, t_1) \tag{14}
$$

where Θ is the dynamic T-matrix

$$
\begin{aligned}
\Theta(t_1, t_2) &= V \delta(t_1 - t_2) + V R_0(t_1, \bar{t}_3) \, \Theta(\bar{t}_3, t_2) \\
R_0(t_1, t_2) &= iG(t_1, t_2) \, G(t_1, t_2)
\end{aligned}
\tag{15}
$$

In this self-energy the singular Hartree term is included ($t_2 - t_1^-$), but the exchange terms have been neglected for simplicity.

Analytical continuation to real times of (15) gives the propagators and correlation functions (see Appendix B)

$$\begin{aligned} R_0^r(t_1, t_2) &= G^r(t_1, t_2)\, G^>(t_1, t_2) - G^<(t_1, t_2)\, G^r(t_1, t_2) \\ R_0^<(t_1, t_2) &= G^<(t_1, t_2)\, G^<(t_1, t_2) \end{aligned} \tag{16}$$

and

$$\begin{aligned} \Theta^r(t_1, t_2) &= V\,\delta(t_1 - t_2) + V R_0^r(t_1, \bar{t}_3)\, \Theta^r(\bar{t}_3, t_2) \\ \Theta^<(t_1, t_2) &= V[\Theta^r(t_1, \bar{t}_3)\, R_0^<(\bar{t}_3, t_2) + \Theta^<(t_1, \bar{t}_3)\, R_0^a(\bar{t}_3, t_2)] \end{aligned} \tag{17}$$

After application of rule 3 in (16)–(17) the zeroth-order terms can be completed in a form similar to the θ-functions in (10)–(11),

$$\begin{aligned} \Theta^r(\omega, T) &= \frac{V}{1 - R_0^r(\omega, T)\, V} \\ \Theta^<(\omega, T) &= \Theta^r(\omega, T)\, R_0^<(\omega, T)\, \Theta^a(\omega, T) \end{aligned} \tag{18}$$

The zeroth-order contributions to the propagator and correlated parts of the self-energy (14) result from these functions as follows:

$$\begin{aligned} \Sigma^r(\omega, T) &= \Theta^r(\omega + \bar{\omega}, T)\, G^<(\bar{\omega}, T) - \Theta^<(\omega + \bar{\omega}, T)\, G^a(\bar{\omega}, T) \\ \Sigma^<(\omega, T) &= \Theta^<(\omega + \bar{\omega}, T)\, G^>(\bar{\omega}, T) \end{aligned} \tag{19}$$

We can continue with the internal gradient expansion in the self-energy (14). The separate Green's function in (19) is on the highest level, so it is excluded from the internal expansion. The remaining functions Θ^r and $\Theta^<$ can be independently expanded after rule 4 and give $F_i[\Theta^r](\xi)$ and $F_i[\Theta^<](\xi)$, respectively.

The time arguments of the objects $R_0(t_1, t_2)$ in the function $\Theta(t_1, t_2)$ from (15) are in a series, so that the rule 5 can be directly applied. The expansion of the propagator function in terms of R_0^r results in zero, similarly as in (12),

$$F_i[\Theta^r](\xi) = \frac{\delta^2 \Theta^r}{\delta R_0^r\, \delta R_0^r}(\xi)\, \frac{i}{2}\, [R_0^r(\xi), R_0^r(\xi)] = 0 \tag{20}$$

The internal expansions of the correlation function $\Theta^<$ is formed by terms analogous to those in (13),

$$
\begin{aligned}
F_i[\Theta^<](\xi) &= \frac{\delta^2\Theta^<}{\delta R_0^r\,\delta R_0^<}(\xi)\frac{i}{2}[R_0^r(\xi), R_0^<(\xi)] \\
&\quad + \frac{\delta^2\Theta^<}{\delta R_0^<\,\delta R_0^a}(\xi)\frac{i}{2}[R_0^<(\xi), R_0^a(\xi)] \\
&= \frac{\delta^2\Theta^<}{\delta R_0^r\,\delta R_0^a}(\xi)\frac{i}{2}[R_0^r(\xi), R_0^a(\xi)] \\
&= -\operatorname{Im}((\Theta^r(\omega, T))^2\,\Theta^a(\omega, T)[R_0^r(\omega, T), R_0^<(\omega, T)]) \\
&\quad -2\,|\Theta^r(\omega, T)|^4\,R_0^<(\omega, T) \\
&\quad \times \int \frac{d\bar{\omega}}{2\pi}\frac{1}{\omega-\bar{\omega}}\left(\frac{\partial \operatorname{Im} R_0^r(\bar{\omega}, T)}{\partial\bar{\omega}}\frac{\partial \operatorname{Im} R_0^r(\omega, T)}{\partial T}\right. \\
&\quad \left. -\frac{\partial \operatorname{Im} R_0^r(\bar{\omega}, T)}{\partial T}\frac{\partial \operatorname{Im} R_0^r(\omega, T)}{\partial\omega}\right)
\end{aligned}
\tag{21}
$$

The function $F_i[\Theta^>(\xi)]$ results from the change of the index "$<$" by "$>$" in all places of (21). Finally, the internal expansions $F_i[\Sigma^r](\xi)$ and $F_i[\Sigma^<](\xi)$ can be obtained if the functions $\Theta^r(\xi)$ and $\Theta^<(\xi)$ in the zeroth-order self-energy (19) are substituted by $F_i[\Theta^r](\xi)$ and $F_i[\Theta^<](\xi)$ from (20)–(21):

$$
\begin{aligned}
F_i[\Sigma^r](\omega, T) &= F_i[\Theta^<](\omega+\bar{\omega}, T)\,G^a(\bar{\omega}, T) \\
F_i[\Sigma^<](\omega, T) &= F_i[\Theta^<](\omega+\bar{\omega}, T)\,G^>(\bar{\omega}, T)
\end{aligned}
\tag{22}
$$

Here the fact that $F_i[\Theta^r](\xi)=0$ in (20) has been taken into account.

3.2.3. Shielded Potential Approximation. Particle interactions are often long range, as in the Coulomb potential. If free particles are available in the system, then screening can shorten the range of the interaction (give a much more localized potential). The shielded potential approximation of the self-energy[1] does not include ladders, as in the above-studied examples, but rows of electron–hole bubbles screening the potential. Localization of the potential by screening has a dynamical character. Therefore it would be interesting to know the time-dependent behavior of screening in nonequilibrium processes. Recently the dynamics of ultrafast screening processes has been studied by NGF.[21, 22] Close to equilibrium these systems can be described by the GBE, where the internal corrections to the screening dynamics can play an important role.

The shielded approximation for the self-energy can be written in the form[1]

$$\Sigma(1, 2) = iV_s(1, 2)\, G(1, 2) \tag{23}$$

where the singular Fock term is included ($t_2 \to t_1^+$). In the lowest order of perturbation theory the screened potential V_s is related to the unscreened one V by the polarization function L_0 as follows:

$$\begin{aligned} V_s(1, 2) &= V(1, 2) - V(1, \bar{3})\, L_0(\bar{3}, \bar{4})\, V_s(\bar{4}, 2) \\ V(1, 2) &= V(r_1 - {}_2)\, \delta(t_1 - t_2) \\ L_0(1, 2) &= iG(1, 2)\, G(2, 1) \end{aligned} \tag{24}$$

The propagators and correlation functions for the polarization function L_0 in (24) can be found by the rules in Appendix B:

$$\begin{aligned} L_0^r(1, 2) &= -[G^r(1, 2)\, G^<(2, 1) + G^<(2, 1)\, G^a(2, 1)] \\ L_0^<(1, 2) &= -G^<(1, 2)\, G^>(2, 1) \end{aligned} \tag{25}$$

and the functions V_s^r and $V_s^<$ result analogously to Θ^r and $\Theta^<$ in (17).

Therefore after the application of rule 3 in (25), the zeroth order of the gradient expansion can be obtained as in (18) [the full CMS coordinates $\xi = (k, \omega; R, T)$ are considered, since the interaction is nonlocal]

$$V_s^r(\xi) = \frac{V(k)}{1 + L_0^r(\xi)\, V(k)}, \qquad V_s^<(\xi) = V_s^r(\xi)\, L_0^<(\xi)\, V_s^a(\xi) \tag{26}$$

Similarly, the zeroth-order gradient contributions to the propagator and correlated parts of the self-energy (23) yield

$$\begin{aligned} \Sigma^r(k, \omega; R, T) &= G^r(k - \bar{k}, \omega - \bar{\omega}; R, T)\, V_s^>(\bar{k}, \bar{\omega}; R, T) \\ &\quad - G^<(k - \bar{k}, \omega - \bar{\omega}; R, T)\, V_s^a(\bar{k}, \bar{\omega}; R, T) \\ \Sigma^<(k, \omega; R, T) &= G^<(k - \bar{k}, \omega - \bar{\omega}; R, T)\, V_s^<(\bar{k}, \bar{\omega}; R, T) \end{aligned} \tag{27}$$

The structure of the internal corrections to the self-energy (24) is also similar to the previous example. The main difference is that here the potential $V(k)$ depends on the wave vector k, so that new corrections terms are included:

$$F_i[V_s^r](\xi) = \frac{\delta^2 V_s^r}{\delta L_0^r \delta L_0^r}(\xi)\frac{i}{2}[L_0^r(\xi), L_0^r(\xi)]$$
$$+\frac{\delta^2 V_s^r}{\delta L_0^r \delta V}(\xi)\frac{i}{2}[L_0^r(\xi), V(k)]$$
$$+\frac{\delta^2 V_s^r}{\delta V \delta L_0^r}(\xi)\frac{i}{2}[V(k), L_0^r(\xi)] = 0 \qquad (28)$$

The potential V in the last two terms is either more "right" or more "left" than L_0 in the series (24) [see also comment below (13)]. Since the second functional derivative is symmetrical in the differentiating functions, these two terms counteract each other. In the Poisson brackets from (28) derivatives over space-momentum coordinates are also performed [see (3)], but the potential $V(k)$ can be differentiated only over the momentum.

The correlation function $V_s^<$ gives more interesting internal contributions. We write only terms with nonzero Poisson brackets and also neglect terms analogous to those in (28), where both functions originate from one of the propagators $V_s^{r,a}$. The fact that the differentiating functions V, $L_0^{r,a}$ originate from different full potential propagators $V_s^{r,a}$ is symbolized by an index on the potentials $V^{(r)}$, $V^{(a)}$ to show which side they originate from. The nonzero terms are

$$F_i[V_s^<](\xi) = \frac{\delta^2 V_s^<}{\delta L_0^r \delta L_0^<}(\xi)\frac{i}{2}[L_0^r(\xi), L_0^<(\xi)]$$
$$+\frac{\delta^2 V_s^<}{\delta L_0^< \delta L_0^a}(\xi)\frac{i}{2}[L_0^<(\xi), L_0^a(\xi)]$$
$$+\frac{\delta^2 V_s^<}{\delta L_0^r \delta L_0^a}(\xi)\frac{i}{2}[L_0^r(\xi), L_0^a(\xi)]$$
$$+\frac{\delta^2 V_s^<}{\delta L_0^r \delta V^{(a)}}(\xi)\frac{i}{2}[L_0^r(\xi), V(k)]$$
$$+\frac{\delta^2 V_s^<}{\delta V^{(r)} \delta L_0^a}(\xi)\frac{i}{2}[V(k), L_0^a(\xi)]$$
$$+\frac{\delta^2 V_s^<}{\delta L_0^< \delta V^{(a)}}(\xi)\frac{i}{2}[L_0^<(\xi), V(k)]$$
$$+\frac{\delta^2 V_s^<}{\delta V^{(r)} \delta L_0^<}(\xi)\frac{i}{2}[V(k), L_0^<(\xi)] \qquad (29)$$

The first three terms on the right-hand side of (29) are analogous those in (21), but there are additional space-momentum derivatives present in the Poisson brackets here. The next two terms in (29) are evidently nonzero, because the derivatives and the Poisson brackets are different and nonzero. In the remaining two terms the Poisson brackets are opposite to each other, but the functional derivatives are different, because the potentials are taken from different sides.

We can evaluate the above functional derivatives and collect all the terms:

$$\begin{aligned} F_i[V_s^<](\xi) = \operatorname{Im}\Bigg\{ & (V_s^r(\xi))^2 V_s^a(\xi) \\ & \times\left([L_0^r(\xi), L_0^<(\xi)] - \frac{1}{V(k)^2}[V(k), L_0^<(\xi)]\right)\Bigg\} \\ & + (V_s^r(\xi))^2 L_0^<(\xi)(V_s^a(\xi))^2 \\ & \times\frac{i}{2}\left([L_0^r(\xi), L_0^a(\xi)] + \frac{1}{V(k)^2}[V(k), L_0^r(\xi) - L_0^a(\xi)]\right) \end{aligned} \tag{30}$$

The function $F_i[V_s^>(\xi)]$ results from the change of the index "$<$" by "$>$" in all places of (30).

As before, the internal expansions $F_i[\Sigma^r](\xi)$ and $F_i[\Sigma^<](\xi)$ can be obtained if the functions $V_s^{r,a}(\xi)$ and $V_s^{<,>}(\xi)$ in the zeroth-order self-energy (27) are substituted by $F_i[V_s^{r,a}](\xi)$ and $F_i[V_s^{<,>}](\xi)$ from (28)–(30):

$$\begin{aligned} F_i[\Sigma^r](k, \omega; R, T) &= G^r(k-\bar{k}, \omega-\bar{\omega}; R, T)\, F_i[V_s^>](\bar{k}, \bar{\omega}; R, T) \\ F_i[\Sigma^<](k, \omega; R, T) &= G^<(k-\bar{k}, \omega-\bar{\omega}; R, T)\, F_i[V_s^<](\bar{k}, \bar{\omega}; R, T) \end{aligned} \tag{31}$$

The fact that $F_i[V_s^{r,a}](\xi) = 0$ in (28) has again been taken into account.

4. TRANSPORT EQUATIONS WITH INTERNAL CORRECTIONS

Internal corrections can appear in all kinds of equations derived by the gradient expansions from the Kadanoff–Baym equations.

4.1. Generalized Boltzmann Equation

The complete generalized Boltzmann equation with both the *external* and *internal* gradient corrections can be found directly when the above theorem is implemented in its derivation from Appendix B. The theorem

says that the internal terms result from the substitution of $\Sigma^{<(>)}(\xi)$ by $\Sigma^{<(>)}(\xi)+F_i[\Sigma^{<(>)}](\xi)$ in the zeroth-order terms. Therefore after a Fourier transform the complete GBE has the form

$$\left(\frac{\partial}{\partial T}+\frac{\mathbf{p}\cdot\nabla_R}{m}-\nabla_R U_{\text{eff}}(\xi)\cdot\nabla_{\mathbf{p}}+\frac{\partial U_{\text{eff}}(\xi)}{\partial T}\frac{\partial}{\partial\omega}\right)G^<(\xi)$$
$$-[\operatorname{Re}\Sigma^r(\xi), G^<(\xi)]+[\operatorname{Re}G^r(\xi), \Sigma^<(\xi)]$$
$$=-(\Sigma^>(\xi)+F_i[\Sigma^>(\xi)])\,G^<(\xi)+(\Sigma^<(\xi)$$
$$+F_i[\Sigma^<(\xi)])\,G^>(\xi) \tag{32}$$

The equation for the correlation function $G^>(\xi)$ can be found similarly. The singular (Hartree–Fock) contributions in (32) are included in the effective potential $U_{\text{eff}}(\xi)$. The propagator functions $G^{r(a)}(\xi)$ and $\Sigma^{r(a)}(\xi)$ in (32) are related to the correlated parts $G^<(\xi)$, $G^>(\xi)$ and $\Sigma^<(\xi)$, $\Sigma^>(\xi)$ by the Hilbert transform (A.7). Therefore it is not necessary to find separate transport equations for these propagator functions, which would eventually include the nonzero internal terms $F_i[\Sigma^{r(a)}(\xi)]$. The *internal* terms in (32) contribute to the dynamics (not the renormalization) of the studied system, so that they cannot be neglected in the transport equations. Conservation laws for the GBE in (32) can be proven in the same way as for the exact Kadanoff–Baym equations.[1]

In the above example of the ATA self-energy the expressions $F_i[\Sigma^{<(>)}(\xi)]$ in (32) should be substituted by (13). For the dynamic T-matrix approximation the terms (22) fulfill this role (the Hartree term should be taken once). In both these examples the CMS coordinates in the functions $F_i[\Sigma^{<(>)}(\omega, T)]$ are reduced with respect to the other terms in (32), where $\xi=(k, \omega; R, T)$. This reduction results from the local form of the T-matrix approximations studied here. In the shielded potential approximation for the self-energy the expressions $F_i[\Sigma^{<(>)}(\xi)]$ from (31) with full CMS coordinates can be used in the GBE. In all these cases the complete GBE with internal correction terms becomes quite complicated. Nevertheless, we believe that it can be handled by approximate numerical methods.

4.2. Linearized Transport Equations

The internal gradient corrections can appear also in linearized transport equations derived from the GBE in weak dc electric fields.[13] It has already been mentioned[23] that these linearized equations should include further correction terms for complicated scattering.

The left-hand side of the GBE in (32) reads, for dc electric fields, as follows:

$$\left[\frac{\partial}{\partial T}+\frac{1}{m}(\mathbf{k}+eT\mathbf{E}_0)\cdot\left(\nabla_R+e\mathbf{E}_0\frac{\partial}{\partial\omega}\right)\right]G^<(\xi) \tag{33}$$

To diminish the explicit time dependence in (33), not present in dissipative systems in weak dc fields, the following transform should be performed[13]

$$\mathbf{Q}\to\mathbf{k}+e\mathbf{E}_0T,\qquad \frac{\partial}{\partial T}\to\frac{\partial}{\partial T}+e\mathbf{E}_0\cdot\nabla_{\mathbf{Q}} \tag{34}$$

where $\mathbf{E}_0$ is the intensity of the dc electric field. Application of this transform to the Poisson brackets in the second line of (32) gives mixed terms of the following form:

$$[A,B]\to[A,B]+e\mathbf{E}_0\cdot\left(\frac{\partial A}{\partial\omega}\nabla_{\mathbf{Q}}B-\nabla_{\mathbf{Q}}A\frac{\partial B}{\partial\omega}\right) \tag{35}$$

If this transform is applied also to the Poisson brackets in the internal corrections $F_i[\Sigma^{<(>)}(\xi)]$ in (32), further new terms can result.

When the self-energy $\Sigma(\xi)$ depends only on (ω, T) variables, as in the space-localized scattering (4) or (14), then only the external terms

$$\frac{\partial\,\mathrm{Re}\,\Sigma^r(\omega)}{\partial\omega}\frac{\partial G^{<(>)}(k,\omega)}{\partial k}\qquad\text{and}\qquad\frac{\partial\Sigma^{<(>)}(\omega)}{\partial\omega}\frac{\partial\,\mathrm{Re}\,G^r(k,\omega)}{\partial k}$$

result from the transform (35). Application of this transform in the terms $F_i[\Sigma^{<(>)}(\xi)]$ from (13) and (22) gives nothing because only k-independent Green's functions are present there. If a nonlocal ATA self-energy[24] is used, generalizing (for neutral smeared imperfections) the local form (4), then new terms would result from application of the transform (35) in the k-dependent internal corrections $F_i[\Sigma^{<(>)}(\xi)]$. Nonlocal scattering results, for example, also from charged impurities,[25] where it is reasonable to screen the impurity potential,[26] similar to the self-energy (23). In both these examples internal and external corrections in (32) are nonzero. Since evaluation of these terms is direct, we do not write them or the resulting complicated linearized equations.

The question is how the internal corrections can contribute in the case of the linear response to weak ac electric fields, where we would expect that also the space-local interactions (4), (14) give new correction terms. The linearized transport equations in ac electric fields have been studied,[14] but the transform to new coordinates[13] was not performed. Therefore no

gradient corrections would seemingly contribute new terms. In fact it is probably hard to find the above transform in the ac case. Moreover, in the ac case it is not sufficient to stop the gradient expansions in the lowest orders. Therefore a new gauge-invariant approach has been developed[27] to study the linear response to weak ac and dc electric fields where no additional transforms are necessary. Unfortunately, the resulting equations are still quite complicated. Recently a relatively simple consistent approach has been devised[12] which starts from the integral version of the Kadanoff–Baym equations.

5. CONCLUSION

We have found new gradient corrections in the generalized Boltzmann equation.[1] These corrections result if the gradient expansion is performed also inside the self-energy in scattering integrals of the quantum transport equations. We call these corrections *internal* because they reflect the many-body character of scattering processes represented by the internal structure of the self-energy. Analogously the standard gradient corrections,[1] which do not take into account the internal structure of the self-energy, are called here *external.*

The generalized Boltzmann equation with all correction terms has been derived. The internal corrections to the GBE have been calculated for electron scattering on localized static potentials, which is described by the ATA self-energy. More complex corrections have been obtained for interacting spinless fermions, where the self-energy is described either by a local T-matrix approximation or by a nonlocal shielded potential approximation. We believe that the GBE with the new correction terms might be a proper tool for studies of relaxation to equilibrium in systems with nontrivial electron interactions. We are planning to investigate some of these systems in the future.

We have also discussed the importance of the internal corrections in the linearized transport equations in weak electric fields,[13] which can be derived from the GBE. The presence of new correction terms in the dc version of these equations has been clarified by examples. The internal corrections might be important in many other physical problems where the self-energy includes multiple scattering events.

APPENDIX A

The causal fermion ($O = \psi$) or boson ($O = A$) Green's functions in real time are defined by (Matsubara Green's functions in complex time are analogous)[4,5]

$$G^t(1,2) = -\frac{i}{\hbar}\langle T[O(1)\, O^+(2)]\rangle, \qquad j \equiv (r_j, t_j) \qquad (j = 1, 2) \qquad \text{(A.1)}$$

Correlation functions are related to the causal function as follows:

$$\begin{aligned} ihG^{t}(1,2) &= G^{>}(1,2) = \langle O(1)\, O^{\dagger}(2)\rangle, \qquad t_1 > t_2 \\ \mp ihG^{t}(1,2) &= G^{<}(1,2) = \langle O^{\dagger}(2)\, O(1)\rangle, \qquad t_1 < t_2 \end{aligned} \tag{A.2}$$

where the upper (lower) sign applies to fermions (bosons).

The retarded and advanced Green's functions are defined by

$$\begin{aligned} G^{r}(1,2) &= -\frac{i}{h}\theta(1-2)[G^{>}(1,2) \pm G^{<}(1,2)] \\ G^{a}(1,2) &= \frac{i}{h}\theta(2-1)[G^{>}(1,2) \pm G^{<}(1,2)] \end{aligned} \tag{A.3}$$

where the theta function is $\theta(t) = 0$, $t < 0$; $\theta(t) = 1$, $t \geqslant 0$.

In equilibrium and space-homogeneous systems the Green's functions depend only on the difference of coordinates $(r, t) = (r_1 - r_2, t_1 - t_2)$, so that they can be easily Fourier transformed to the (k, ω) representation as follows:

$$G(k,\omega) = \int d^{n}r \int dt \exp[i(\omega t - r\cdot k)]\, G(r_1 - r_2; t_1 - t_2) \tag{A.4}$$

Then the fermion and boson correlation functions can be expressed as[1]

$$\begin{aligned} G^{<}(k,\omega) &= n_{F,B}(h\omega)\, A(k,\omega) \\ G^{>}(k,\omega) &= (1 \mp n_{F,B}(h\omega))\, A(k,\omega) \end{aligned} \tag{A.5}$$

where n_F, n_B denote the Fermi–Dirac and Bose–Einstein distributions

$$n_{F,B}(h\omega) = \frac{1}{e^{h\omega/kT} \pm 1}$$

and the spectral function is defined by

$$A(k,\omega) \equiv -2\ \mathrm{Im}\, G^{r}(k,\omega) = G^{>}(k,\omega) \pm G^{<}(k,\omega) \tag{A.6}$$

The retarded Green's function can be calculated from the spectral function (A.6) as follows [(A.6)–(A.7) hold also in full CMS coordinates $\xi = (k, \omega; R, T)$]:

$$G^{r}(k,\omega) = \int_{-\infty}^{\infty} \frac{d\bar{\omega}}{2\pi} \frac{A(k,\bar{\omega})}{\omega - \bar{\omega} + i\delta} \tag{A.7}$$

Similar formulas can be applied for the self-energy.

APPENDIX B

The nonequilibrium Green's functions can be found by analytical continuation to real time of the Matsubara Green's functions in complex time.[1] In NGF it is often necessary to find the propagator or correlation part of a combination of functions. An example is the product

$$A(1,2) = B(1,2)\, C(1,2) \tag{B.1}$$

where A, B, C are one-particle causal Green's functions or self-energies. The required functions can be found by LW rules,[3] where the signs and prefactors result from the definitions (A.2)–(A.3). We have found the expressions for (B.1) in two cases, where the functions A, B, C correspond either to fermions (F) or to bosons (B) as follows: (1) $(A, B, C) = (\mathrm{F}, \mathrm{F}, \mathrm{B})$ (an example is the electron–phonon self-energy[5]) or (2) $(A, B, C) = (\mathrm{B}, \mathrm{F}, \mathrm{F})$ [an example is the function R_0 in (15)]. In both these cases the expressions result in

$$\begin{aligned}
A^<(1,2) &= -iB^<(1,2)\, C^<(1,2) \\
A^>(1,2) &= -iB^>(1,2)\, C^>(1,2) \\
A^r(1,2) &= -i(B^r(1,2)\, C^>(1,2) - B^<(1,2)\, C^r(1,2)) \\
A^a(1,2) &= -i(B^a(1,2)\, C^>(1,2) - B^<(1,2)\, C^a(1,2))
\end{aligned} \tag{B.2}$$

Similarly one can find the propagators and correlation functions for the expression

$$A(1,2) = B(1,2)\, C(2,1) \tag{B.3}$$

where the following possibilities have been chosen: (1) $(A, B, C) = (\mathrm{F}, \mathrm{B}, \mathrm{F})$ [an example is the self-energy (14)] or (2) $(A, B, C) = (\mathrm{B}, \mathrm{F}, \mathrm{F})$ [an example is the electron–hole bubble L_0 in (24)]. These possibilities, which, except for the order of B, F in (1), are the same as in (B.2), give the identities [(1) for (−), (2) for (+)]

$$\begin{aligned}
A^<(1,2) &= iB^<(1,2)\, C^>(2,1) \\
A^>(1,2) &= iB^>(1,2)\, C^<(2,1) \\
A^r(1,2) &= i(B^r(1,2)\, C^<(2,1) \mp B^<(1,2)\, C^a(2,1)) \\
A^a(1,2) &= i(B^a(1,2)\, C^<(2,1) \mp B^<(1,2)\, C^r(2,1))
\end{aligned} \tag{B.4}$$

The following structure appears also in most formulas:

$$A(1,2) = B(1,\bar{3})\, C(\bar{3},2) \tag{B.5}$$

where an overbar means integration over the whole real axis of these coordinates. The same expressions result, irrespective of the types of involved functions,

$$\begin{aligned} A^{<}(1,2) &= B^{r}(1,\bar{3})\, C^{<}(\bar{3},2) + B^{<}(1,\bar{3})\, C^{a}(\bar{3},2) \\ A^{>}(1,2) &= B^{r}(1,\bar{3})\, C^{>}(\bar{3},2) + B^{>}(1,\bar{3})\, C^{a}(\bar{3},2) \\ A^{r}(1,2) &= B^{r}(1,\bar{3})\, C^{r}(\bar{3},2) \\ A^{a}(1,2) &= B^{a}(1,\bar{3})\, C^{a}(\bar{3},2) \end{aligned} \tag{B.6}$$

In the text we use the term "parallel" for the structures of arguments in (B.1)–(B.4), while the structure (B.5)–(B.6) is termed "serial."

The Kadanoff–Baym equations can be found by application of the rules (B.6) to the differential Dyson equation, which can be written in two forms. If we take into account that $(G_0^{-1})^{<}(1,2) = 0$ and $\delta^{<}(1,2) = 0$, then the two forms of the Kadanoff–Baym equations are

$$\begin{aligned} (G_0^{r})^{-1}(1,\bar{3})\, G^{<}(\bar{3},2) &= \Sigma^{r}(1,\bar{3})\, G^{<}(\bar{3},2) + \Sigma^{<}(1,\bar{3})\, G^{a}(\bar{3},2) \\ G^{<}(1,\bar{3})(G_0^{a})^{-1}(\bar{3},2) &= G^{r}(1,\bar{3})\, \Sigma^{<}(\bar{3},2) + G^{<}(1,\bar{3})\, \Sigma^{a}(\bar{3},2) \end{aligned} \tag{B.7}$$

Analogous equations can be obtained for the correlation function $G^{>}$.

The generalized Boltzmann equation[1] can be derived by subtraction of the two sets of equations (B.7). In the resulting quantum transport equations for $G^{<,>}$ it is necessary to introduce CMS coordinates and perform the gradient expansion up to first order. Then a Fourier transform over the small coordinates is performed. It is helpful to resolve the propagators $G^{r,a}$ and $\Sigma^{r,a}$ from the right-hand side of (B.7) into real and imaginary parts. The imaginary parts of these propagators can be resolved with the help of the identity (A.6) (in CMS coordinates). Then the terms with equal correlation signs $<, <$ and $>, >$ fall out from the scattering side of the new equations and the GBE easily results [see its complete form in (32)].

ACKNOWLEDGMENTS

I thank B. Velický and V. Čápek for valuable comments.

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