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Gauge-invariant quantum kinetic equations for electrons in classical electromagnetic fields

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Abstract. Gauge-invariant quantum kinetic equations for interacting electrons are deduced using the Keldysh diagrammatic technique. The Dyson equations are transformed using a special type of the Wigner representation that produces gauge-invariant Green functions. As a result, they depend on the variables having a meaning of position and kinetic momentum. The Wigner representation used makes it necessary to modify the diagrammatic technique in such a way that it will be able to account for the momentum–energy exchange between the system and the electromagnetic field. The formalism obtained makes it possible to carry out many-particle calculations for non-linear systems in arbitrary electromagnetic fields. Some particular simple cases are considered. A special discussion is given regarding the meaning of the detailed balance in such a formulation.

1. Introduction

The kinetic equation, which plays the central role in non-equilibrium statistical mechanics, was derived by Boltzmann in 1872. Most of the theoretical analysis of transport processes in condensed matter has been based on this equation, whose validity depends on several assumptions. First, one assumes that the duration of a collision is much shorter than the mean-free time of the particle between collisions. The particles can be considered as being free between collisions that are well defined events in space and time. Second, the distribution function of the particles in phase space is assumed not to change during a time interval Δt that is much shorter than the mean-free time and much longer than the collision duration. This condition ensures that the rate of the distribution function variation depends only on its instantaneous value and not on its previous evolution. Third, in order that this rate at a given spatial point depends only on its value at this point, we assume that the distribution function does not change appreciably within the space volume crossed by the particle during the time interval Δt. Fourth is the assumption of molecular chaos. Correlations between the particles are neglected, and one assumes that a single-particle distribution function describes the system adequately so that no multi-particle distribution functions are needed to compute the collision integral.

When quantum effects are involved and the above assumptions are not met it is generally not possible to use the Boltzmann equation. It is then desirable to use another method that is applicable even when the above assumptions do not hold. A possible approach to the problem can be based on the quantum kinetic equations, which we discuss here within the framework of the Keldysh diagrammatic technique.

Quantum kinetic processes are in many cases treated by means of the Kubo (1957) linear response method. An alternative approach, based on the Keldysh (1965) diagrammatic

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technique, enables one to go rather easily beyond the linear approximation response. It has been shown that the difference of the Dyson equations and their conjugate produce, after some transformations, the Boltzmann equation in the classical limit. Hence one can hope to obtain quantum kinetic equations just by changing the variables of the two Dyson equations to Wigner variables.

The first to formulate kinetic equations, based on the real-time Green function technique, were Kadanoff and Baym (1962). Fleurov and Kozlov (1978) (see also Al'tshuler 1978) using the Keldysh formulation deduced two sets of linearized quantum kinetic equations, which may in principle give an exhaustive description of the dynamic and kinetic properties of a system of interacting Fermi particles. Since then, a number of papers were published on quantum kinetic equations, see for example, Tugushev and Fleurov (1983), Mahan (1987), Reizer and Sergeev (1987), Khan *et al* (1987), Reggiani *et al* (1987), Davies and Wilkins (1988), Bertoncini *et al* (1989), Rammer and Smith (1986), Garanin and Lutovinov (1992), and Gütter *et al* (1993) and references therein. However, the present formulation of the quantum kinetic equation still has some limitations. The technique in its present status cannot describe systems in an electromagnetic field with strong spatial or time dependencies. So far, the kinetic equations have been formulated almost exclusively for systems in static electromagnetic fields. One of the central problems is that in many cases these equations are written for quantities that are not explicitly gauge invariant.

Here we propose a derivation of the quantum kinetic equations for arbitrary classical electromagnetic fields and emphasize in particular its gauge-invariant form (section 2). Static and homogeneous fields and plane waves are considered as examples. The conventional Keldysh diagrammatic technique is modified in order to include the effects that the external fields have on the particle as it propagates in space and interacts with other particles (section 3). The meaning of the detailed balance in the quantum formulation will be considered in section 4. The derivation and some properties of macroscopic equations derived on the basis of the microscopic quantum kinetic equations is discussed in section 5. A short summary will be given in section 6.

2. Derivation of the kinetic equations

The diagrammatic technique proposed by Keldysh (1965) allows one to write the Dyson equation for a non-equilibrium quantum system in an arbitrary non-quantized electromagnetic field. A semiclassical Boltzmann equation, as well as its quantum versions, is obtained from this Dyson equation by making certain transformations and approximations. In the derivation to be presented below it is our aim to arrive at a quantum equation, avoiding approximations as much as possible. In this sense the validity of the equations to be obtained is equivalent to that of the Dyson equations.

Our point of departure is the Dyson equation

$$\hat{G}_0^{-1}(x)\hat{G}(x,x') = \delta^4(x-x')\sigma_x + \int \mathrm{d}^4x_1\sigma_x\hat{\Sigma}(x,x_1)\hat{G}(x_1,x') \tag{1}$$

written in differential form with the Green functions defined by Keldysh (1965) as

$$\tilde{G}(x,x') = \begin{pmatrix} G^c(x,x') & G^<(x,x') \\ G^>(x,x') & G^{\bar{c}}(x,x') \end{pmatrix} = \begin{pmatrix} -\mathrm{i}\langle T\psi(x)\psi^+(x')\rangle & \mathrm{i}\langle\psi^+(x')\psi(x)\rangle \\ -\mathrm{i}\langle\psi(x)\psi^+(x')\rangle & -\mathrm{i}\langle\tilde{T}\psi(x)\psi^+(x')\rangle \end{pmatrix}. \tag{2}$$

Here T and $\tilde{T}$ stand for the operators of the chronological and antichronological ordering, σ_x is the Pauli matrix, $x = (ct, r)$, $\psi(x)$ is the field operator of the elementary excitations

in the system and the angular brackets denote the averaging over the equilibrium statistic ensemble that is supposed to exist before the external fields and the interactions have been turned on.

It is often more convenient to use another representation for the Green function matrix

$$\hat{G} = \begin{pmatrix} 0 & G^a \\ G^r & G^K \end{pmatrix} \qquad \hat{\Sigma} = \begin{pmatrix} \Sigma^K & \Sigma^r \\ \Sigma^a & 0 \end{pmatrix} \tag{3}$$

which is obtained from the matrix (2) by a linear transformation, also proposed by Keldysh (1965).

The differential operator

$$\hat{G}_0^{-1}(x) = \left[i\hbar \frac{\partial}{\partial t} + e\varphi(x) - \frac{1}{2m}\left(-i\hbar\nabla^x - \frac{e}{c}A(x) \right)^2 \right] \tag{4}$$

in the left-hand side of (1) is defined in such a way as to obey

$$\hat{G}_0^{-1}(x)G_0(x, x') = \sigma_i \delta(x - x')$$

where G_0 is the matrix Green function for the system with all the interactions off but with the external electromagnetic $A(x)$ field on. The differential operator (4) is written for non-relativistic electrons with parabolic band dispersion. Here σ_i becomes σ_z if one chooses the representation (2) or σ_x in the representation (3).

The Dyson equation (1) contains all the information necessary for describing kinetic properties of the system. However, it should be first transformed into a more convenient form. One gains improved physical insight and a better possibility of comparison with the solutions of classical and semiclassical equations when introducing the Wigner variables $X = (cT, \boldsymbol{R}) = (x + x')/2$ and $y = (x' - x)$. These variables imply the distribution functions will depend on the spatial coordinate $\boldsymbol{R}$ at time T. The Fourier transform

$$G(P, X) = \int \mathrm{d}^4 y \, \mathrm{e}^{-(\mathrm{i}/\hbar) y^\mu P_\mu} G(y, X) \tag{5}$$

with respect to the variable y is usually made. Although this transform (5) seems to be quite obvious it possesses the important drawback of producing quantities that are not gauge invariant. The resulting conjugate variable $P = (\varepsilon, \boldsymbol{P})$ does not necessarily have the meaning of the kinetic 4-momentum.

As a result, it is rather problematic to ascribe certain physical meaning to the resulting equations and to quantities appearing in them. Mahan (1987, 1990) while deriving the kinetic equation overcomes this problem by introducing an artificial coordinate transformation applied in addition to the Fourier transform in order to recover a gauge-invariant form of the equations. This additional transformation was found using physical intuition, and should be made anew for each gauge. This problem can become particularly difficult when dealing with non-homogeneous fields in non-linear problems.

Fleurov and Kozlov (1978) applied a transform of the form

$$G(P, X) = \int \mathrm{d}^4 y \mathrm{e}^{-(\mathrm{i}/\hbar) y^\mu (P_\mu - A_\mu(X))} G(y, X) \tag{6}$$

which produces explicitly gauge-invariant quantities and equations in the linear approximation or in a non-linear case but for a static homogeneous electric field (Tugushev and Fleurov 1983). Here $A^\mu(x) = (\varphi(x), \boldsymbol{A}(x))$ is the 4-vector potential of the applied electromagnetic field.

The aim of this paper is to propose an explicitly gauge-invariant procedure that holds for an arbitrary classical electromagnetic field. This can be achieved by making use of the transform

$$G(P,X)=\int \mathrm{d}^4y \exp\left(-\frac{\mathrm{i}}{\hbar}Py+\frac{\mathrm{i}e}{c\hbar}\int_{-1/2}^{1/2} y^\mu A_\mu(X+sy)\mathrm{d}s\right)G(y,X). \tag{7}$$

The phase factors generated by the wavefunctions

$$\psi(x)\to\psi(x)\mathrm{e}^{(\mathrm{i}e/\hbar c)\Lambda(x)} \tag{8}$$

under the local gauge transformation

$$A_\mu(x)\to A_\mu(x)-\partial_\mu\Lambda(x) \tag{9}$$

defined by means of an arbitrary real function $\Lambda(x)$, are cancelled by the integral in the exponent of (7) and the Green function $G(P,X)$ remains unchanged. In the definition (7) the integration path is taken as a straight line between the points $X-y/2$ and $X+y/2$. Different choices of this path will lead to different meanings of P and to changing the form of the quantum kinetic equations. If one chooses the variables P to be the kinetic momentum of the particles the straight line between the points $X-y/2$ and $X+y/2$, (Vasak *et al* 1987, Elze *et al* 1986 and Serimaa *et al* 1986) must be chosen as the integration path. This certainly produces a restriction on the topology of the electromagnetic field. However, we are not going to address here the problem of spaces that are not simply connected, and the latter choice of the path will be used throughout.

The Wigner quasi-distribution function (see, for example, Hillery *et al* 1984) can be defined as $f(P,X)=-\mathrm{i}G^<(P,X)$ where $G^<(P,X)$ is obtained from the Green function $G^<(y,X)$ by means of the transform (7). Macroscopic quantities of the system can be calculated by means of this function. Hence, in most of the problems one is interested in, one needs quantum kinetic equations to obtain the Wigner quasi-distribution function $f(P,X)$.

These quantum kinetic equations are obtained according to the following procedure.

(i) The sum and the difference of the Dyson equations (1) and their Hermitian conjugate are formed.

(ii) The integral in the transform (7) is represented as

$$\int \mathrm{d}^4y\mathrm{e}^{-(\mathrm{i}/\hbar)Py}[\cdots]\to\int \mathrm{d}^4(p'-p)\mathrm{e}^{(\mathrm{i}/\hbar)(p'-p)X}\int \mathrm{d}^4x\mathrm{d}^4x'\mathrm{e}^{(\mathrm{i}/\hbar)(px-p'x')}[\cdots]. \tag{10}$$

(iii) Integrating by parts and using the equalities

$$\partial_\lambda^x\left(\frac{\mathrm{i}e}{c\hbar}\int_{-1/2}^{1/2} y^\mu A_\mu(X+sy)\mathrm{d}s\right)=-A_\lambda(X-\tfrac{1}{2}y)+y^\mu\int_{-1/2}^{1/2}\mathrm{d}s(\tfrac{1}{2}-s)F_{\lambda\mu}(X+sy) \tag{11}$$

and

$$\partial_\lambda^{x'}\left(\frac{\mathrm{i}e}{c\hbar}\int_{-1/2}^{1/2} y^\mu A_\mu(X+sy)\mathrm{d}s\right)=A_\lambda(X+\tfrac{1}{2}y)+y^\mu\int_{-1/2}^{1/2}\mathrm{d}s(\tfrac{1}{2}+s)F_{\lambda\mu}(X+sy) \tag{12}$$

where

$$\partial_\lambda^x=\tfrac{1}{2}\partial_\lambda^X-\partial_\lambda^y \qquad \partial_\lambda^{x'}=\tfrac{1}{2}\partial_\lambda^X+\partial_\lambda^y.$$

The equations are expressed in terms of the electromagnetic tensor

$$F_{\mu\nu}(x) = \partial_\mu^x A_\nu(x) - \partial_\nu^x A_\mu(x).$$

The notation $\partial_\nu^x = \partial/\partial x^\nu$ is used throughout this paper and we write the differential variable as the superscript of the ∂ or ∇ symbols.

(iv) Use is made of the two formal equalities

$$F_{\lambda\mu}(X + sy) = e^{sy\partial^X} F_{\lambda\mu}(X) \tag{13}$$

$$\int d^4y e^{-(i/\hbar)Py} f(y)g(y) = f(i\hbar\partial^P) \int d^4y\, e^{-(i/\hbar)Py} g(y) \tag{14}$$

so that the variable y does not appear explicitly in the equations.

(v) Finally, the integration with respect to the variable s is carried out in the left-hand side of the equations.

This five-step procedure leads to two matrix equations of the form

$$\begin{aligned}
&\Big[2\varepsilon + e\hbar j_1(\tfrac{1}{2}\Delta)F_{0\mu}(X)\partial^{P\mu} - \frac{1}{m}\Big(P_\lambda + \frac{e\hbar}{2c} j_1(\tfrac{1}{2}\Delta)F_{\lambda\mu}(X)\partial^{P\mu}\Big)^2 \\
&\qquad - \frac{\hbar^2}{4m}\Big(\nabla_\lambda^X + \frac{e}{c} j_0(\tfrac{1}{2}\Delta)F_{\lambda\mu}(X)\partial^{P\mu}\Big)^2 \\
&\qquad + \frac{\hbar^2 e}{mc}\Big(\tfrac{1}{2} j_0(\tfrac{1}{2}\Delta) - \frac{1}{\Delta} j_1(\tfrac{1}{2}\Delta)\Big)\nabla^{X\lambda}F_{\lambda\mu}(X)\partial^{P\mu}\Big]\hat{G}(P, X) \\
&\quad = \int d^4(p' - p) e^{(i/\hbar)(p'-p)X} \int d^4x d^4x' e^{(i/\hbar)(px - p'x')} \\
&\qquad \times \exp\Big(\frac{ie}{c\hbar}\int_0^1 (x' - x)^\mu A_\mu\big(x + s(x' - x)\big)ds\Big) \\
&\qquad \times \Big(2\delta^4(x - x')\sigma_x + \int d^4x_1\big(\sigma_x\hat{\Sigma}(x, x_1)\hat{G}(x_1, x') + \hat{G}(x, x_1)\hat{\Sigma}(x_1, x')\sigma_x\big)\Big)
\end{aligned} \tag{15}$$

and

$$\begin{aligned}
&\Big[i\hbar\frac{\partial}{\partial T} + ie\hbar j_0(\tfrac{1}{2}\Delta)F_{0\mu}(X)\partial^{P\mu} + i\frac{e\hbar}{mc}P^\lambda j_0(\tfrac{1}{2}\Delta)F_{\lambda\mu}(X)\partial^{P\mu} \\
&\qquad + \Big(i\frac{\hbar}{m}P_\lambda + i\frac{\hbar^2 e}{4mc} j_1(\tfrac{1}{2}\Delta)F_{\lambda\mu}(X)\partial^{P\mu}\Big)\nabla^{X\lambda} \\
&\qquad - \frac{1}{2m}\Big(\frac{e\hbar}{c}\Big)^2 [j_0(\tfrac{1}{2}\Delta)F_{\lambda\mu}(X)\partial^{P\mu}][j_1(\tfrac{1}{2}\Delta)F_{\lambda\mu}(X)\partial^{P\mu}] \\
&\qquad + i\frac{e\hbar^2}{2mc} j_1(\tfrac{1}{2}\Delta)\big(\nabla^{X\lambda}F_{\lambda\mu}(X)\big)\partial^{P\mu}\Big]\hat{G}(P, X) \\
&\quad = \int d^4(p' - p) e^{(i/\hbar)(p'-p)X} \int d^4x d^4x' e^{(i/\hbar)(px - p'x')} \\
&\qquad \times \exp\Big(\frac{ie}{c\hbar}\int_0^1 (x' - x)^\mu A_\mu\big(x + s(x' - x)\big)ds\Big) \\
&\qquad \times \int d^4x_1\big(\sigma_x\hat{\Sigma}(x, x_1)\hat{G}(x_1, x') - \hat{G}(x, x_1)\hat{\Sigma}(x_1, x')\sigma_x\big)
\end{aligned} \tag{16}$$

where $j_0(x) = \sin(x)/x$ and $j_1(x) = \sin(x)/x^2 - \cos(x)/x$; the derivative with respect to X in the operator $\Delta = \hbar\partial^P\partial^X$ acts only on the electromagnetic tensor $F_{\mu\nu}$. These equations are equivalent to the Dyson equations and they give a correct physical description for kinetic processes of a many-particle system in arbitrary electromagnetic fields. We wrote two matrix equations which would correspond to six equations for complex functions. However, the number of really independent functions, and hence independent equations, is only two (see, for example, the discussion in Fleurov and Kozlov 1978). One can, for example, take an off-diagonal term in the matrix equation (15) in the representation (3) which would be an equation for, say, the retarded Green function G^r determining the spectrum of the system. The second equation can be produced from one of the diagonal terms of the matrix equation (16) (in the same representation) and this is the equation for the function G^K, which in the semiclassical approximation converts into the conventional Boltzmann equation.

It is interesting to look at some particular forms of the equations that are obtained for a given dependence of the electromagnetic fields on the coordinates.

2.1. Static and homogeneous fields

Here a simple case is considered when only static and homogeneous electric and/or magnetic fields are applied. All derivatives of the electromagnetic tensor with respect to the coordinates then vanish. One can easily verify for this case that

$$j_0(\tfrac{i}{2}\Delta)F_{\lambda\mu} = F_{\lambda\mu} \qquad j_1(\tfrac{i}{2}\Delta)F_{\lambda\mu} = 0$$

so that equations (15) and (16) become

$$\left[2\varepsilon - 2\left(\frac{P^2}{2m}\right) + \frac{\hbar^2}{4m}\left(\nabla^X + \frac{e}{c}B\times\nabla^P + eE\partial^\varepsilon\right)^2\right]\hat{G}(P,X)$$
$$= \int \mathrm{d}^4(x'-x)\exp\left\{-(\mathrm{i}/\hbar)(x'-x)^\mu\left[P_\mu - \frac{e}{c}A_\mu\left(\frac{x'+x}{2}\right)\right]\right\}\left(2\delta^4(x-x')\sigma_x\right.$$
$$\left. + \int \mathrm{d}^4x_1\left(\sigma_x\hat{\Sigma}(x,x_1)\hat{G}(x_1,x') + \hat{G}(x,x_1)\hat{\Sigma}(x_1,x')\sigma_x\right)\right) \tag{17}$$

$$\left[\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}T} + \mathrm{i}e\hbar E\nabla^P + \mathrm{i}\hbar\frac{P}{m}\left(\nabla^X + \frac{e}{c}B\times\nabla^P + eE\partial^\varepsilon\right)\right]\hat{G}(P,X)$$
$$= \int \mathrm{d}^4(x'-x)\exp\left\{-(\mathrm{i}/\hbar)(x'-x)^\mu\left[P_\mu - \frac{e}{c}A_\mu\left(\frac{x'+x}{2}\right)\right]\right\}$$
$$\left(\int \mathrm{d}^4x_1\left(\sigma_x\hat{\Sigma}(x,x_1)\hat{G}(x_1,x') - \hat{G}(x,x_1)\hat{\Sigma}(x_1,x')\sigma_x\right)\right). \tag{18}$$

For static and homogeneous fields the integral of the potential in the transform (7) simplifies and the whole transform converts into the transform (6). The previously cited papers on quantum kinetic equations were mainly concerned with static and homogeneous fields, hence methods for the evaluation of the right-hand side of these equations can be found in those papers. They all use the so-called gradient expansion (Kadanoff and Baym 1962) which appeared to be useful when treating the problem in the linear approximation or in the case of a static homogeneous electric field.

Sometimes the non-gauge-invariant Fourier transform (5) is used. Then the Green functions are expanded in Taylor series with respect to the variable X, which produces a series of derivatives of the Green functions (Rammer and Smith 1986). An additional transformation is necessary in this case in order to eliminate the gauge non-invariant terms

(Mahan 1990) appearing on the left-hand side. The latter step can be avoided by using the transform (6), which is gauge invariant for static homogeneous fields (Fleurov and Kozlov 1978, Tugushev and Fleurov 1983).

The second set of equations (18) has a structure similar to that of the Boltzmann equation, which usually is represented in the form

$$\frac{\partial}{\partial T} f + \frac{\boldsymbol{P}}{m} \cdot \nabla^X f + \boldsymbol{F} \cdot \nabla^P f = I_{\text{coll}} \tag{19}$$

where $\boldsymbol{F}$ is the force acting on the particle. In the quantum kinetic equation it corresponds to the Lorentz force $\boldsymbol{F} = e\boldsymbol{E} + e(\boldsymbol{P}/m) \times \boldsymbol{B}$. The one-particle distribution function is connected with the Green function by the relation

$$f(\boldsymbol{P}, T, \boldsymbol{R}) = -\mathrm{i} \int \mathrm{d}\varepsilon G^<(\varepsilon, \boldsymbol{P}, T, \boldsymbol{R}) = \frac{1}{2}\left(1 - \mathrm{iTr} \int \mathrm{d}\varepsilon G(\varepsilon, \boldsymbol{P}, \mathrm{T}, \boldsymbol{R})\right).$$

The Boltzmann equation (19) has been obtained by integrating the trace of equation (18) over the energy variable ε.

The additional term in the quantum equation comes from the energy variable ε in the Wigner quasi-distribution. Indeed, the first set of equations (17), in its linearized form, was used in the papers referred to above to find an equation for the retarded Green function, G^{r}, while the second set of equations (18) was used to find the Keldysh Green function, G^{K}. In the homogeneous and time-independent fields, the linear approximation produces

$$G^{\mathrm{r}} = (\varepsilon - \varepsilon_p - \Sigma^{\mathrm{r}})^{-1}$$

and

$$\boldsymbol{E} \cdot \frac{\boldsymbol{p}}{m} \frac{\mathrm{d}n(\varepsilon)}{\mathrm{d}\varepsilon} \frac{\mathrm{d}}{\mathrm{d}\varepsilon_p}\left(\eta A + 2\tan^{-1}\frac{2\eta}{\Gamma}\right) = \tfrac{1}{2}(\Gamma G^{\mathrm{K}} - \Sigma^{\mathrm{K}} A)$$

where $A = -2\mathrm{Im}\, G^{\mathrm{r}}$, $\Gamma = -2\mathrm{Im}\, \Sigma^{\mathrm{r}}$, $\eta = \varepsilon - \varepsilon_p - \mathrm{Re}\, \Sigma^{\mathrm{r}}$ and $n(\varepsilon)$ is the Fermi distribution function (Fleurov and Kozlov 1978). It should be noted that the left-hand side of the last equation, which is in fact the quantum analogue of the Boltzmann equation, contains terms that have been transferred from the right-hand side of (18). These are the so-called non-local terms.

2.2. *Plane electromagnetic wave*

We consider here electromagnetic fields whose dependence on the coordinates is assumed to be represented as

$$F_{\lambda\mu}(X) = \mathrm{e}^{\mathrm{i}KX} F_{\lambda\mu}(K).$$

The following equality can then be easily obtained:

$$j_0(\tfrac{1}{2}\Delta) F_{\lambda\mu}(X) \partial^{P\mu} \hat{G}(P, X) = (\hbar K^\mu)^{-1} F_{\lambda\mu}(X)[\hat{G}(P + \tfrac{1}{2}\hbar K, X) - \hat{G}(P - \tfrac{1}{2}\hbar K, X)]$$
$$\equiv (\hbar K^\mu)^{-1} F_{\lambda\mu}(X) \mathcal{D}(P, X, K)$$

$$j_1(\tfrac{1}{2}\Delta) F_{\lambda\mu}(X) \partial^{P\mu} \hat{G}(P, X) = -2(\hbar K^\mu)^{-1} F_{\lambda\mu}(X)$$
$$\times \left(\tfrac{1}{2}[\hat{G}(P - \tfrac{1}{2}\hbar K, X) + \hat{G}(P + \tfrac{1}{2}\hbar K, X)]\right.$$
$$\left. - \int_{-1/2}^{1/2} \mathrm{d}s \hat{G}(P - s\hbar K, X)\right) \equiv (\hbar K^\mu)^{-1} F_{\lambda\mu}(X) \mathcal{Z}(P, X, K).$$

The last lines of both these equalities are definitions of the functions $\mathcal{D}(P, X, K)$ and $\mathcal{Z}(P, X, K)$. We also define the wavelength vector

$$\bar{\lambda} = \lambda/2\pi = (K_0^{-1}, K_1^{-1}, K_2^{-1}, K_3^{-1})$$

and write the equality

$$(K^\mu)^{-1} F_{\lambda\mu}(X) = \big(\boldsymbol{\lambda} \cdot \boldsymbol{E}(X), \bar{\lambda}_0 \boldsymbol{E}(X) + \boldsymbol{\lambda} \times \boldsymbol{B}(X)\big).$$

Substituting all these in (15) and (16) one obtains the quantum kinetic equations for electrons in the plane electromagnetic wave:

$$\begin{aligned}
&\left(2\varepsilon - \frac{P^2}{m} - \frac{(-i\hbar\nabla^X)^2}{4m}\right)\hat{G}(P, X) + \left(e\boldsymbol{\lambda}\cdot\boldsymbol{E}(X) - \frac{eP}{mc}\cdot\big(\bar{\lambda}_0 \boldsymbol{E}(X) + \boldsymbol{\lambda}\times\boldsymbol{B}(X)\big)\right)\mathcal{Z}(P, X, K) \\
&\quad - \frac{2}{m}\left(\frac{ie}{2c}\right)\big(\bar{\lambda}_0\boldsymbol{E}(X) + \boldsymbol{\lambda}\times\boldsymbol{B}(X)\big)\cdot\big[\tfrac{1}{2} - i\hbar\nabla^X + \tfrac{1}{2}\hbar K\big]\mathcal{D}(P, X, K) \\
&\quad - \frac{1}{m}\left(\frac{ie}{2c}\right)^2\big(\bar{\lambda}_0\boldsymbol{E}(X) + \boldsymbol{\lambda}\times\boldsymbol{B}(X)\big)^2\big(\mathcal{D}^2(P, X, K) + \mathcal{Z}^2(P, X, K)\big) \\
&\quad + \frac{8}{m}\frac{ie}{2c}\big(\bar{\lambda}_0\boldsymbol{E}(X) + \boldsymbol{\lambda}\times\boldsymbol{B}(X)\big)\cdot(\hbar\boldsymbol{K})\int \hat{G}(P + \tfrac{1}{2}s\hbar K, X)s\,ds \\
&\quad = \int \mathrm{d}^4(x' - x)\exp\left\{-\frac{i}{\hbar}(x' - x)^\mu\left[P_\mu - \frac{e}{c}A_\mu\left(\frac{x' + x}{2}\right)j_0\big(\tfrac{1}{2}K(x' - x)\big)\right]\right\} \\
&\quad \times\left(2\delta^4(x - x')\sigma_x + \int \mathrm{d}^4x_1\big(\sigma_x\hat{\Sigma}(x, x_1)\hat{G}(x_1, x') + \hat{G}(x, x_1)\hat{\Sigma}(x_1, x')\sigma_x\big)\right)
\end{aligned} \tag{20}$$

and

$$\begin{aligned}
&\left(i\hbar\frac{\mathrm{d}}{\mathrm{d}T} + \frac{i\hbar}{m}P\cdot\nabla^X\right)\hat{G}(P, X) + ie\left(\boldsymbol{\lambda}\cdot\boldsymbol{E}(X) + \frac{\boldsymbol{P}}{mc}\cdot\big(\bar{\lambda}_0\boldsymbol{E}(X) + \boldsymbol{\lambda}\times\boldsymbol{B}(X)\big)\right)\mathcal{D}(P, X, K) \\
&\quad - \frac{1}{m}\left(\frac{e}{2c}\right)\big(\bar{\lambda}_0\boldsymbol{E}(X) + \boldsymbol{\lambda}\times\boldsymbol{B}(X)\big)\cdot(-\tfrac{1}{2}i\hbar\nabla^X + \hbar\boldsymbol{K})\mathcal{Z}(P, X, K) \\
&\quad - \frac{2}{m}\left(\frac{ie}{2c}\right)^2\big(\bar{\lambda}_0\boldsymbol{E}(X) + \boldsymbol{\lambda}\times\boldsymbol{B}(X)\big)^2\mathcal{D}(P, X, K)\mathcal{Z}(P, X, K) \\
&\quad = \int \mathrm{d}^4(x' - x)\exp\left\{-\frac{i}{\hbar}(x' - x)^\mu\left[P_\mu - \frac{e}{c}A_\mu\left(\frac{x' + x}{2}\right)j_0\big(\tfrac{1}{2}K(x' - x)\big)\right]\right\} \\
&\quad \times\left(\int \mathrm{d}^4x_1\big(\sigma_x\hat{\Sigma}(x, x_1)\hat{G}(x_1, x') - \hat{G}(x, x_1)\hat{\Sigma}(x_1, x')\sigma_x\big)\right).
\end{aligned} \tag{21}$$

In the limit of large wavelengths and low frequencies ($K \to 0$) one finds that

$$\mathcal{Z}(P, X, K) \to 0 \qquad \bar{\lambda}_0\mathcal{D}(P, X, K) \to c\hbar\partial^\varepsilon\hat{G}(P, X)$$

and

$$\boldsymbol{\lambda}\mathcal{D}(P, X, K) \to \hbar\nabla^P\hat{G}(P, X).$$

Therefore, these equations convert into the kinetic equations for static and homogeneous fields (17) and (18). These quantum kinetic equations for a system under the plane electromagnetic wave were derived in a systematic way, taking care of their explicit gauge invariance. In the next subsection we will use these equations in order to consider the problem of linear response in such a system.

2.3. Linear response

The linear response of a system to an external perturbation is usually calculated along the lines of the Kubo (1957) formalism. According to Kubo the linear response is given in terms of correlation functions, which are calculated for equilibrium quantities. If the calculation of the correlation functions is done by means of a diagrammatic technique, the lines in the diagrams correspond to equilibrium Green functions. The linear response can be also found using the quantum kinetic equations (15) and (16).

The impulse response, $\hat{h}^{\mu\lambda}(x, x', x_1)$, of the system to the external electromagnetic field will be considered. The Green functions of the system can be written

$$\hat{G}(x, x') = \hat{G}(x, x')\big|_{F=0} + \int \hat{h}^{\mu\lambda}(x, x', x_1) F_{\mu\lambda}(x_1) \mathrm{d}^4 x_1 \tag{22}$$

where $\hat{G}(x, x')\big|_{F=0}$ are the Green functions of the system when no electromagnetic field is applied. It is possible to define the frequency response of the system, $\hat{H}^{\mu\lambda}(x, x', K)$, as the Fourier transform of $\hat{h}^{\mu\lambda}(x, x', x_1)$ with respect to the coordinate x_1. The Green function of the system can then be written in terms of the Fourier coefficients of the external field

$$\hat{G}(x, x') = \hat{G}(x, x')\big|_{F=0} + \int \hat{H}^{\mu\lambda}(x, x', K) F_{\mu\lambda}(K) \mathrm{d}^4 K. \tag{23}$$

This gives rise to the following question: what sort of Fourier transform should be used in order to write this equation in the Wigner representation? The functions $\hat{G}(x, x')\big|_{F=0}$ should be transformed by means of (5) since it corresponds to the system without external fields. The transform (7) contains a dependence on the external electromagnetic fields and if one uses it to transform $\hat{H}^{\mu\lambda}(x, x', K)$ the outcome will depend on the external fields as well. The response of the system should not depend on the external fields, and we conclude that one should use the transform (5). However, we emphasize that this is not the case for the terms that depend explicitly on the electromagnetic potentials, $\hat{G}_0^{-1}(x)\hat{G}(x, x')$, and usually appear in the kinetic equation.

The Green function of the system can be written in the linear approximation

$$\hat{G}(P, X) = \hat{G}(P, X)\big|_{F=0} + \int \hat{H}^{\mu\lambda}(P, X, K) F_{\mu\lambda}(K) \mathrm{d}^4 K. \tag{24}$$

If the system without the external fields is static and homogeneous, i.e.

$$\hat{G}(P, X)\big|_{F=0} = \hat{G}(P)\big|_{F=0}$$

then one immediately realizes that

$$\hat{h}^{\mu\lambda}(x, x', x_1) = \hat{h}^{\mu\lambda}(y, X - x_1)$$

and

$$\hat{H}^{\mu\lambda}(P, X, K) = \hat{H}^{\mu\lambda}(P, K) \exp(\mathrm{i}KX).$$

To find equations for the plane-wave response, one should substitute (24) in (20) and (21), take $F_{\mu\lambda}(K') \propto \delta(K' - K)$ and leave only the terms linear in the external field.

Keeping in mind that $\hat{G}(P,X)\big|_{F=0}=\hat{G}(P)\big|_{F=0}$ one arrives at the following equations:

$$\left(2\varepsilon-\frac{P^2}{m}-\frac{(\hbar K)^2}{4m}\right)\hat{H}^{\mu\lambda}(P,K)$$
$$+\left(e\boldsymbol{\lambda}\cdot\boldsymbol{E}(X)-\frac{e\boldsymbol{P}}{mc}\cdot\left(\lambda_0\boldsymbol{E}(X)+\boldsymbol{\lambda}\times\boldsymbol{B}(X)\right)\right)\mathcal{Z}(P,K)\big|_{F=0}$$
$$-\frac{2}{m}\left(\frac{ie}{2c}\right)\left(\lambda_0\boldsymbol{E}(X)+\boldsymbol{\lambda}\times\boldsymbol{B}(X)\right)\cdot\tfrac{1}{2}\hbar\boldsymbol{K}\mathcal{D}(P,K)\big|_{F=0}$$
$$+\frac{8}{m}\frac{ie}{2c}\left(\lambda_0\boldsymbol{E}(X)+\boldsymbol{\lambda}\times\boldsymbol{B}(X)\right)\cdot(\hbar\boldsymbol{K})\int s\hat{G}(P+\tfrac{1}{2}s\hbar K)\big|_{F=0}\,\mathrm{d}s$$
$$=\sigma_x\hat{\Sigma}(P-K/2)\big|_{F=0}\hat{H}^{\mu\lambda}(P,K)+\hat{H}^{\mu\lambda}(P,K)\hat{\Sigma}(P+K/2)\big|_{F=0}\sigma_x$$
$$+\sigma_x\hat{\Omega}^{\mu\lambda}(P,K)\hat{G}(P+K/2)\big|_{F=0}+\hat{G}(P-K/2)\big|_{F=0}\hat{\Omega}^{\mu\lambda}(P,K)\sigma_x \qquad (25)$$

and

$$\left(-\hbar\omega-\frac{\hbar}{m}\boldsymbol{P}\cdot\boldsymbol{K}\right)\hat{H}^{\mu\lambda}(P,K)$$
$$+ie\left(\boldsymbol{\lambda}\cdot\boldsymbol{E}(X)+\frac{\boldsymbol{P}}{mc}\cdot\left(\lambda_0\boldsymbol{E}(X)+\boldsymbol{\lambda}\times\boldsymbol{B}(X)\right)\right)\mathcal{D}(P,K)\big|_{F=0}$$
$$-\frac{1}{m}\left(\frac{e}{2c}\right)\left(\lambda_0\boldsymbol{E}(X)+\boldsymbol{\lambda}\times\boldsymbol{B}(X)\right)\cdot\hbar\boldsymbol{K}\mathcal{Z}(P,K)\big|_{F=0}$$
$$=\sigma_x\hat{\Sigma}(P-K/2)\big|_{F=0}\hat{H}^{\mu\lambda}(P,K)-\hat{H}^{\mu\lambda}(P,K)\hat{\Sigma}(P+K/2)\big|_{F=0}\sigma_x$$
$$+\sigma_x\hat{\Omega}^{\mu\lambda}(P,K)\hat{G}(P+K/2)\big|_{F=0}-\hat{G}(P-K/2)\big|_{F=0}\hat{\Omega}^{\mu\lambda}(P,K)\sigma_x. \qquad (26)$$

Here $\hat{\Omega}^{\mu\lambda}(P,X,K)$ represents the linear response of the mass operator $\hat{\Sigma}(P,X)$. This can be connected with the linear response, $\hat{H}^{\mu\lambda}(P,X,K)$, of the Green function using the Ward identity. The latter, after the transform (5), takes the form

$$\hat{\Omega}^{\mu\lambda}(P,X,K)=-\frac{\mathrm{i}}{2}\int\int L(P,X,P_0,X_0)\hat{H}^{\mu\lambda}(P_0,X_0,K)\,\mathrm{d}^4X_0\mathrm{d}^4P_0 \qquad (27)$$

where $L(P,X,P_0,X_0)$ is the bimatrix, representing the aggregate of all irreducible skeleton diagrams.

It seems to be instructive here to discuss briefly the case of an alternating electric field when $K=(\omega/c,\mathbf{0})$. Then (25) and (26) become

$$\left(2\varepsilon-\frac{P^2}{m}\right)\hat{H}^{\mu\lambda}(P,K)=\sigma_x\hat{\Sigma}(\varepsilon-\omega/2,P)\big|_{F=0}\hat{H}^{\mu\lambda}(P,\omega,\mathbf{0})$$
$$+\hat{H}^{\mu\lambda}(P,\omega,\mathbf{0})\hat{\Sigma}(\varepsilon+\omega/2,P)\big|_{F=0}\sigma_x$$
$$+\sigma_x\hat{\Omega}^{\mu\lambda}(P,\omega,\mathbf{0})\hat{G}(\varepsilon+\omega/2,P)\big|_{F=0}+\hat{G}(\varepsilon-\omega/2,P)\big|_{F=0}\hat{\Omega}^{\mu\lambda}(P,\omega,\mathbf{0})\sigma_x \qquad (28)$$

and

$$-\hbar\omega\hat{H}^{\mu\lambda}(P,K)+ie\hbar\boldsymbol{E}\nabla^P\hat{G}(P)\big|_{F=0}$$
$$+\frac{\boldsymbol{P}}{m}\frac{1}{\omega}\left(\hat{G}(\varepsilon+\hbar\omega/2c,P)\big|_{F=0}-\hat{G}(\varepsilon-\hbar\omega/2c,P)\big|_{F=0}\right)$$
$$=\sigma_x\hat{\Sigma}(\varepsilon-\omega/2,P)\big|_{F=0}\hat{H}^{\mu\lambda}(P,\omega,\mathbf{0})-\hat{H}^{\mu\lambda}(P,\omega,\mathbf{0})\hat{\Sigma}(\varepsilon+\omega/2,P)\big|_{F=0}\sigma_x$$
$$+\sigma_x\hat{\Omega}^{\mu\lambda}(P,\omega,\mathbf{0})\hat{G}(\varepsilon+\omega/2,P)\big|_{F=0}-\hat{G}(\varepsilon-\omega/2,P)\big|_{F=0}\hat{\Omega}^{\mu\lambda}(P,\omega,\mathbf{0})\sigma_x. \qquad (29)$$

This result is compared with the equations obtained in Wu and Mahan (1984) (see also Mahan 1987) where quantum kinetic equations for non-static but homogeneous fields are considered. Contrary to the derivation presented here they use the representation corresponding to the transform (5). It leads to quantities that are not explicitly gauge invariant, and one has to take special care for the gauge invariance of the final results. As a result our equations (28) and (29) differ in some details from the corresponding equations of Mahan (1987) (equations (77), (78), (82)). The term $(1 - \delta\sigma)$ should be substituted by $\delta\sigma$ and the term proportional to ∇^P is missing. It is important, however, to note that these differences have fortunately not influenced the results of the calculations presented in this paper, since the corresponding integrals have appeared to be zero. It seems that using an explicitly gauge-invariant equation could have saved the necessity of considering these terms at all.

Equations (25) and (26) give an exhaustive description of the linear response for systems of interacting particles. The function $L(P, P_0)$ can be calculated by means of a diagrammatic technique and the equations obtained for $\hat{H}^{\mu\lambda}(P, K)$ are integral equations. These equations offer an alternative method to the Kubo formalism for calculating the linear response.

3. Diagrammatic techniques

The right-hand side of the quantum kinetic equations (15) and (16) contains the mass operator $\hat{\Sigma}(x, x')$, which within the Keldysh formulation is obtained by means of a diagrammatic technique. The problem lies in the fact that this formulation assumes Green functions and other quantities to be in the (x, x') representation while the equations deduced above use Fourier transformed functions, i.e. the Wigner representation, (P, X). Coordinate and time homogeneity is now absent and the momentum–energy conservation in an individual vertex is violated. Moreover, the transform (7), producing gauge-invariant functions, involves the potential of the electromagnetic field. As a result, the standard formulation of the Keldysh diagrammatic technique is to be correspondingly modified in order to describe non-equilibrium systems in the electromagnetic fields in gauge-invariant form. This modified formulation is described below.

3.1. Diagrammatic expansion

As mentioned above, the difficulties in formulating the diagrammatic technique are due to the inhomogeneity of the system and the inclusion of the electromagnetic field in the gauge-invariant Green function

$$G(p, p') = \int \mathrm{d}^4x\mathrm{d}^4x' \exp[(\mathrm{i}/\hbar)(px - p'x')] \times \exp\left(\frac{\mathrm{i}e}{\hbar}\int_0^1 (x' - x)^\lambda A_\lambda\big(x + s(x' - x)\big)\mathrm{d}s\right) G(x, x') \tag{30}$$

which depends now on two variables p and p' due to the lack of momentum–energy conservation. The second function that it is necessary to introduce can be called the phase-loop function. It appears for every electronic loop in the diagram and describes the momentum–energy transfer between the electron propagating in the loop and the

electromagnetic field. The phase-loop function that corresponds to an electronic loop with N vertices is defined by the equation

$$M(\pi \mid N, F(X)) = M(\{\pi_i\}_{i=1}^N \mid F(X)) = \int d^4x_1 \cdots d^4x_N \exp\left(\frac{i}{\hbar}\sum_{i=1}^N \pi_i x_i\right) \exp\left(\frac{ie}{c\hbar}\Phi(\{x_i\}_{i=1}^N)\right) \tag{31}$$

where

$$\Phi(\{x_i\}_{i=1}^N) = \sum_{i=1}^N y_k^\mu \int_{-1/2}^{1/2} A_\mu(X_k + s_k y_k) ds_k \tag{32}$$

and $y_k = x_{k+1} - x_k$, $X_k = (x_{k+1} + x_k)/2$ with cyclic conditions $x_{N+1} = x_1$ being assumed. The phase-loop function depends on N variables $\{\pi_i\}_{i=1}^N$, on the electromagnetic field $F(X)$ and is explicitly gauge-invariant. Applying the transform (9) does not affect the phase-loop function since the line integral in (32) is taken along a closed trajectory (the number of electrons is conserved). The gauge-invariance can be seen more transparently if one transforms the line integral, $\Phi(\{x_i\}_{i=1}^N)$, into integrals of differential forms which depend explicitly on the electromagnetic field rather than on the vector potential (see, for example, Eguchi *et al* 1980).

The gauge-invariant Wigner representation $\hat{G}(P, X)$, which we actually need, is connected with the Green function defined in (30) by means of the equation

$$\hat{G}(P, X) = \int d^4(p' - p) e^{(i/\hbar)(p'-p)X} \hat{G}(p, p'). \tag{33}$$

However, we use the functions (30) since for these the perturbation series can be represented in diagrammatic form. It can be constructed just by substituting the standard Keldysh diagrammatic expansion of $\hat{G}(x, x')$ in the definition of $\hat{G}(p, p')$. Such an expansion will contain all the interactions existing in the system including, first of all, electron–electron and electron–phonon interactions. Each Green function in the expansion ($G(x_i, x_j)$ for electrons, $D(x_i, x_j)$ for phonons, and so on, with x_i and x_j corresponding to the vertices of the diagram) is then expressed via the Green function that depends on two momenta ($G(p_k, p_k')$ for electrons, $D(p_k, p_k')$ for phonons, and so on, where k enumerates the electron lines of the diagram). The exponential functions containing the field can be collected in groups forming phase-loop functions $M(\pi \mid N, F(X))$ (to be discussed below). As a result one can formulate the rules for the diagrammatic expansion of the function $\hat{G}(p, p')$.

As we know, the Keldysh diagrams are constructed according to the conventional Feynman rules with the only difference being that each Green function becomes a matrix of the functions. The electromagnetic field introduces some additional features, which are outlined below.

(i) Each line of the diagram stands for the corresponding Green function matrix: $\hat{G}(p, p')$ for electrons, $\hat{D}(q, q')$ for phonons, etc. Hence each internal line is labelled by two momenta, meaning that the momentum is not conserved between the interactions.

(ii) A function $M(\pi \mid N, F(X))$ is attached to each closed electron loop and to the two free ends of each diagram. Each variable π_i corresponds to a vertex in the closed electron loop or in the electron line connecting the two free ends of the diagram.

(iii) The energy and momentum conservation is maintained if the 4-momentum of the electromagnetic field is accounted for. It means that the sum of all 4-momenta entering the

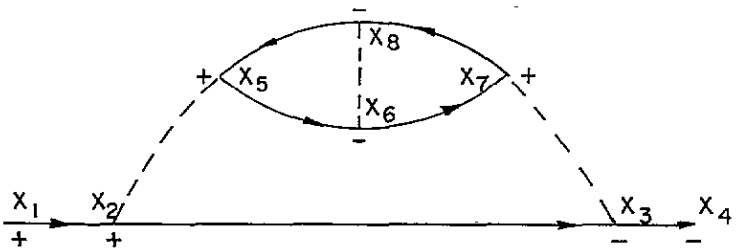

Figure 1. An example of a Keldysh diagram. The vertices are denoted by x_i.

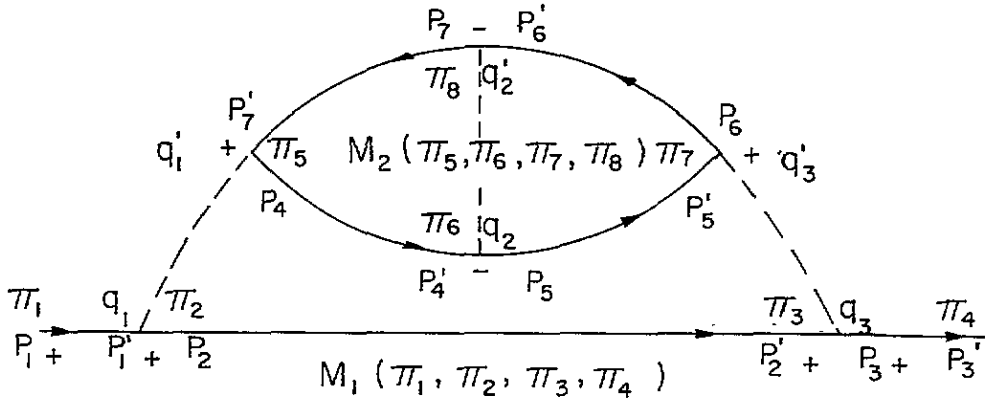

Figure 2. An example of a diagram in the double momentum space that corresponds to the Keldysh diagram in figure 1. The momentum of the Green functions are written near the vertices as well as the field momenta, π_i.

vertex minus the sum of all momenta leaving the vertex should equal the corresponding electromagnetic 4-momentum π_i.

All the other rules coincide with those of the conventional Keldysh formulation.

Figure 1 shows an example of a Keldysh diagram for a Green function $G(x, x')$ while figure 2 shows the corresponding diagram for $G(p, p')$. The full lines and curves in these figures represent electron Green functions, and the broken lines and curves stand for boson-type excitations (e.g. phonons) which are usually chargeless. Every vertex i in the diagram for $G(x, x')$ (figure 1) is characterized by the coordinate (x_i) and its location on the time contour (+ or −). As for the vertex in the diagram for $G(p, p')$ (figure 2), it is characterized by its location on the time contour (+ or −), by the momentum (π_i) transferred by the field and by the momenta of all the Green functions entering (p_i') or leaving (p_i) it.

The phase-loop functions M_2 and M_1 are attached to the electron loop and to the two free ends of the diagram (figure 2). The function M_1 exists in every electron diagram regardless of whether the diagram contains electron loops or not. As for the function M_2, it is attached to the electron loop. Additional functions of this sort would have appeared if the diagram had contained more electron loops. It should be emphasized that in order to have a non-trivial contribution the loop should contain more than one pair of vertices. That is why there is the bosonic line $D(q_2, q_2')$ in figure 2.

If a diagram without such a bosonic line were considered when the electron loop had only one pair of vertices, the phase-loop function would become

$$M_2(\pi_5, \pi_7|2, F(X)) = \delta(\pi_5)\delta(\pi_7). \tag{34}$$

It means that no exchange of momenta between the electrons and the field takes place, and the phase-loop function can be discarded.

3.2. The phase-loop function

Let us take a closer look at the phase-loop function. Using the equalities (13) and (14), this can be written in the form

$$M(\pi \mid N, F(X)) = \exp\left(\frac{ie}{c\hbar}\sum_{i=1}^{N}[i\hbar(\partial^{\pi_{i+1}} - \partial^{\pi_i})]^{\mu} \times \left\{j_0[\tfrac{1}{2}i\hbar(\partial^{\pi_{i+1}} - \partial^{\pi_i})^{\lambda}\partial_{\lambda}^{X}]A_{\mu}(X)\big|_{X=(i\hbar/2)(\partial^{\pi_{i+1}}+\partial^{\pi_i})}\right\}\right)\delta(\pi) \tag{35}$$

with cyclic conditions $\pi_{N+1} = \pi_1$ being assumed. This form of the phase-loop function is gauge invariant, and does not change under the transformation (9). It also shows in a relatively simple way how the field interferes with momentum conservation at the vertices. Derivatives of the delta function mean that derivatives of the Green functions and of the vertex functions appear in the analytical expressions for the diagrams. Hence momentum conservation is maintained not only between the Green functions themselves, but also between them and their derivatives. Physically, it corresponds to the fact that only the momentum of the whole system is conserved, which includes both the momenta of the quasi-particles and that of the electromagnetic field.

The line integral vanishes when no field is applied or if the loop consists only of two vertices (see the example in the previous subsection); the phase-loop function then becomes just a product of delta functions

$$M(\pi \mid N, F(X)) = \prod_{i=1}^{N}\delta(\pi_i). \tag{36}$$

In this case momentum conservation is maintained without the electromagnetic field and the phase-loop function can be discarded.

In the case of a plane wave, $A_{\mu}(X) = A_{\mu}(0)\exp(iKX)$, the expression for $M(\pi \mid N, F(X))$ becomes

$$M(\pi \mid N, F(X)) = \exp\left(\frac{ie}{c\hbar}\sum_{i=1}^{N}\frac{(\partial^{\pi_{i+1}} - \partial^{\pi_i})^{\mu}A_{\mu}(0)}{(\partial^{\pi_{i+1}} - \partial^{\pi_i})^{\lambda}K_{\lambda}}(e^{i\hbar K\partial^{\pi_{i+1}}} - e^{i\hbar K\partial^{\pi_i}})\right)\delta(\pi). \tag{37}$$

Taking the limit of long wavelength and neglecting the spatial dependence of the field, $K = (\omega/c, \mathbf{0})$, one arrives at the limit of alternating electric field and the 4-potential can be taken as $A = (\varphi, \mathbf{0})$. One then finds that the phase-loop function is just a product of delta functions (36), showing that the field does not participate in the momentum conservation. It also means that the interactions are not influenced by the field. The same result is obtained for static and homogeneous fields (the limit $K \to 0$), and for very weak fields (the limit $A \to 0$). More generally, one may say that the phase-loop function takes its trivial shape (36) for any conservative electric field ($\nabla \times E = 0$) and/or static and homogeneous magnetic field.

4. Principle of detailed balance

The principle of the detailed balancing of the processes that occur in the system by their reverse processes can be applied (Dirac 1924) to formulate general conditions for the system in statistical equilibrium. It is clear that the condition of detailed balance is much stronger than just nullification of the collision integral. The detailed balance for the linearized quantum kinetic equation was discussed by Fleurov and Kozlov (1978), who showed how the detailed balance followed from the properties of the Keldysh diagrams. This section will discuss the detailed balance for the collision integral of the more general quantum kinetic equation (16), which is valid for any classical electromagnetic field. Actually the aim is to find the necessary conditions that the Green function must obey in order that the collision integral becomes zero.

Following from (16), the quantum collision integral is

$$I_{\mathrm{coll}}(P, X) = \int \mathrm{d}\varepsilon \, D_{\mathrm{coll}}(P, X). \tag{38}$$

Here

$$D_{\mathrm{coll}}(P, X) = -\frac{1}{2\hbar} \int \mathrm{d}^4(p' - p) \mathrm{e}^{(\mathrm{i}/\hbar)(p'-p)X} \int \mathrm{d}^4x \mathrm{d}^4x' \mathrm{e}^{(\mathrm{i}/\hbar)(px - p'x')} \times \exp\left(\frac{\mathrm{i}e}{c\hbar} \int_0^1 (x' - x)^\mu A_\mu\big(x + s(x' - x)\big) \mathrm{d}s \right) \tilde{D}_{\mathrm{coll}}(x, x') \tag{39}$$

and

$$\tilde{D}_{\mathrm{coll}}(x, x') = \int \mathrm{d}^4x_4 \, \mathrm{Tr}(\sigma_i \Sigma G - G \Sigma \sigma_i). \tag{40}$$

Using the representation (2) ($\sigma_i = \sigma_z$) the quantity $\tilde{D}_{\mathrm{coll}}(x, x')$ can be written as

$$\begin{aligned} \tilde{D}_{\mathrm{coll}}(x, x') = \int \mathrm{d}^4x_1 [& \Sigma^c(x, x_1) G^c(x_1, x') - G^c(x, x_1) \Sigma^c(x_1, x') \\ & + G^{\tilde{c}}(x, x_1) \Sigma^{\tilde{c}}(x_1, x') - \Sigma^{\tilde{c}}(x, x_1) G^{\tilde{c}}(x_1, x') \\ & + \Sigma^<(x, x_1) G^>(x_1, x') - G^<(x, x_1) \Sigma^>(x_1, x') \\ & + G^>(x, x_1) \Sigma^<(x_1, x') - \Sigma^>(x, x_1) G^<(x_1, x')]. \end{aligned} \tag{41}$$

The expression in square brackets in (41) is transformed into the double-momentum representation (p, p') and expanded diagrammatically as explained in the previous section. The resulting diagrams can be arranged into pairs. One just has to take any pair of expressions from a line in the square brackets in (41), say $\Sigma^c(x, x_1)G^c(x_1, x')$ and $G^c(x, x_1)\Sigma^c(x_1, x')$, or $G^>(x, x_1)\Sigma^<(x_1, x')$ and $\Sigma^>(x, x_1)G^<(x_1, x')$. For each such pair a diagram of a certain order and topology is drawn. Then one can easily see that two such diagrams in each pair differ from each other only by the directions of the arrows in the lines. It means that such a pair of diagrams represents the same elementary process reversed in time.

Detailed balance exists in the system when each process is balanced by its time-reversed counterpart. Hence *we shall look for the conditions under which the two analytical expressions of the diagrams in the pair cancel each other* (figure 3).

When the arrows in the diagram are reversed, two changes in the corresponding analytical expression occur. First, each time-directed Green function ($G^<$, $G^>$, $D^<$, $D^>$

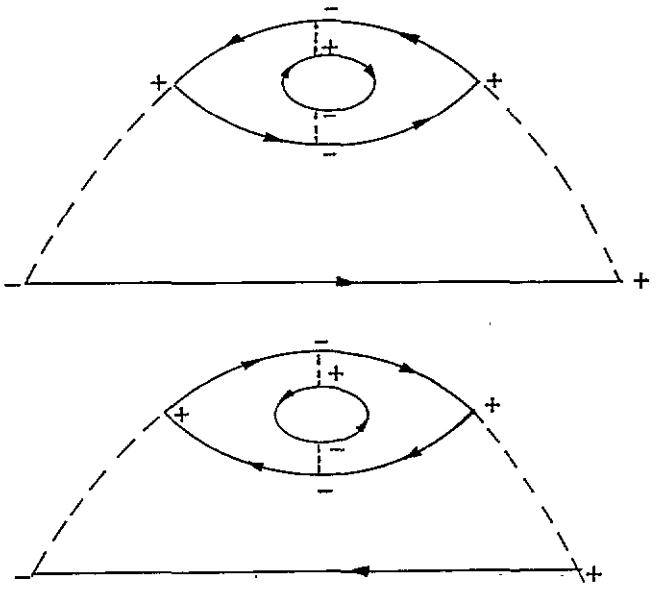

Figure 3. An example of a pair of diagrams that represent processes in opposite directions in time.

and so on) changes to the opposite one ($G^>$, $G^<$, $D^>$, $D^<$ and so on). Second, momenta in the delta functions standing for momentum conservation at each vertex, are permuted, $p_k \leftrightarrow p'_k$ ($q_k \leftrightarrow q'_k$ for phonons and so on) where k enumerates the Green functions. No changes happen in the phase-loop functions. Therefore one can conclude that a sufficient condition for the system to be detailed balanced is that all the time-directed Green functions of the system obey the relation

$$G^<(p, p') = -G^>(-p', -p) \tag{41a}$$

for fermions and

$$D^<(q, q') = D^>(-q', -q) \tag{41b}$$

for bosons.

As an example, we can look at the simple case of a system in equilibrium with no electromagnetic fields applied. In this case we can specify the Green functions completely. The function $M(\pi \mid N, F(X))$ is now just a product of delta functions. Assuming now that the momentum is conserved in each elementary process one can show that each pair of diagrams cancel each other if the condition

$$G^>(P) = -\exp(P^\mu c_\mu) G^<(P) \tag{42}$$

for fermions and

$$D^>(P) = \exp(P^\mu c_\mu) D^<(P) \tag{43}$$

for bosons holds. Here c is a constant 4-vector. If one substitutes $G^<$, $G^>$ for $G^>$, $G^<$ in the analytical expressions for the diagrams, the exponentials $\exp(P^\mu c_\mu)$ make products equal to unity. It reflects the energy–momentum conservation in the system. The two expressions for the two diagrams of a pair are then equal.

Combining the two conditions one finds that the Green functions have the form

$$G^{>}(P) = -in(P^{\mu}c_{\mu})A(P) \tag{44}$$

and

$$D^{>}(P) = iN(P^{\mu}c_{\mu})B(P). \tag{45}$$

This structure resembles the equations for the equilibrium Green functions since n and N are Fermi and Bose functions respectively. However, no conditions on the spectral functions $A(P)$ and $B(P)$ are imposed and they can be non-equilibrium.

A physical example of such a situation is the well known phonon drag effect proposed by Peierls (see, for example, Ziman 1960). The Green functions (44) and (45) correspond to a system moving as a whole with momentum c (a current flow) and having an effective inverse temperature $\beta = c_0$. However, if the momentum is not conserved (if there are impurities in the system, the phonon subsystem is kept at equilibrium, or U processes are of importance) the system momentum c must relax to zero and the effective temperature will become equal to the bath temperature, $c_0 = \beta$. Then we arrive at the conditions considered in Fleurov and Kozlov (1978).

We now address the same issue from another point of view. Generally, if the processes in the system are detailed balanced the collisions do not change the density matrix of the system. One can then say that the entropy of the system is at its maximum value. As is well known (see, for example, Alhassid and Levin 1979 and references therein) the entropy of the system at the maximum is

$$S = c^0 + c^{\mu}C_{\mu}$$

and its density matrix is given by

$$\rho = \exp(-c^0 - c^{\mu}\hat{C}_{\mu})$$

where C_{μ} are mean values of linearly independent but not necessarily commuting observables, $\hat{C}_{\mu}$, of the system; c_{μ} are constants that are determined by the conditions $1 = \mathrm{Tr}(\rho)$ and $C_{\mu} = \mathrm{Tr}(\rho\hat{C}_{\mu})$. The constants c_{μ} give an indication of the amount of information the mean values C_{μ} supply about the density matrix. If we have no knowledge about the mean value of an observable then this constant vanishes. For electrons we have only four possible observables: the three components of the momentum and the energy. The relation between the density operator and the electron Green function $G^{<}$ is given by the Wigner transformation. As a result, we see that the same dependence of these two quantities on the observables was obtained from maximum entropy considerations and from vanishing of the collision integral.

5. Equations for macroscopic quantities

The quantum kinetic equations provide us with the possibility of calculating Green functions. The latter, however, are not directly measurable; they are only used at certain steps of the calculations. The Green functions are quasi-distribution functions and macroscopic measurable quantities are calculated as their averages over the phase space. Although it is possible to deduce various equations for the macroscopic measurable quantities from the quantum kinetic equations, we shall consider only the two most important equations. It is shown in this section that all the Green functions that solve the quantum kinetic equations

result in macroscopic quantities that satisfy the *particle continuity equation* and the quantum mechanical equivalent of the classical *Hamilton–Jacobi equation.*

Macroscopic measurable quantities can be written in terms of space conditional moments. Hence, we start by defining the space conditional moments $\overline{\overline{P}}^n_\mu(X)$ as the means of $(P_\mu)^n$ for given X. These can be obtained from the equation

$$\overline{\overline{P}}^n_\mu(X) = -\frac{\mathrm{i}}{\rho(X)} \int \mathrm{d}^4 P (P_\mu)^n G^<(P, X) = -\frac{\mathrm{i}}{\rho(X)} \left(-\mathrm{i}\hbar \frac{\partial}{\partial y}\right)^n G^<(y, X)\Big|_{y\to 0} \tag{46}$$

where

$$\rho(X) = -\mathrm{i} \int \mathrm{d}^4 P G^<(P, X)$$

is the macroscopic particle density. Integrating the quantum kinetic equations with respect to the momenta, and using the equality (14), the two quantum kinetic equations become equations for space conditional moments.

The first equation we want to discuss is obtained from the trace of equation (16):

$$\frac{\partial}{\partial T}\rho(X) + \nabla^X(\rho(X)\overline{\overline{P}}(X)/m) = \int \mathrm{d}P I_{\mathrm{coll}}(P, X). \tag{47}$$

This electron density continuity equation (47) contains in its right-hand side the collision integral integrated over the momentum space. It stands for the transfer of electrons from and to a four-dimensional volume element, at X, caused by the collision processes.

One can readily see that the integral in the right-hand side of (47) is zero for any homogeneous system. This property is directly connected with the conservation of electron number in all the interaction processes. The integral is not necessarily zero for the case of inhomogeneous systems, which reflects local fluctuations of the electron number caused by scattering processes. However, we may consider the case when the inhomogeneity is weak on the scale of the free path length and time, l_{f}. The Green function and the mass operator can then be assumed to be approximately homogeneous :

$$G(x, x') \cong G(|x - x'|) + \mathrm{O}(1/l_{\mathrm{in}}) \tag{48}$$

and

$$\Sigma(x, x') \cong \Sigma(|x - x'|) + \mathrm{O}(1/l_{\mathrm{in}}) \tag{49}$$

on the scale l_{in}, which we assume to be larger than the mean free path and time, l_{f}. Using the fact that the integral converges on the scale $l_{\mathrm{f}} \ll l_{\mathrm{in}}$, the approximations (48) and (49) make the right-hand side of (47) vanish, i.e.

$$\int \mathrm{d}P I_{\mathrm{coll}}(P, X) = \int \mathrm{d}x_1 \mathrm{Tr}[\sigma_i \Sigma(\mathrm{X}, \mathrm{x}_1) G(\mathrm{x}_1, \mathrm{X}) - G(\mathrm{X}, \mathrm{x}_1)\Sigma(\mathrm{x}_1, \mathrm{X})\sigma_j] \cong 0. \tag{50}$$

We emphasize that this integral would not vanish if the inhomogeneity were strong on the scale of the free path length and/or time. The above coarse-graining procedure is then not applicable.

The conservation of total charge in the system can be seen after integrating (47) over the three-dimensional space, (compare, for example, Mahan 1987, Rammer 1991 and Green *et al* 1985). The corresponding integral is then *exactly* zero, regardless of the scale of the inhomogeneity.

Similarly one can multiply (16) by P or $P^2/2m$ and integrate it. Then equations for the *momentum and energy conservations* are derived (Kadanoff and Baym 1962).

The second equation is obtained from the $G^<$ component of (15):

$$\frac{\hbar^2}{8m\rho(X)}(\nabla^X)^2\rho(X) = \frac{\bar{\bar{P}}^2(X)}{2m} + \bar{\bar{\varepsilon}}_{\rm int}(X) - \bar{\bar{\varepsilon}}(X) \tag{51}$$

where

$$\bar{\bar{\varepsilon}}_{\rm int}(X) = \frac{1}{2\rho(X)}\int d^4x_1\big[\Sigma^c(X,x_1)G^<(x_1,X) + \Sigma^<(X,x_1)G^{\bar{c}}(x_1,X) - G^c(X,x_1)\Sigma^<(x_1,X) - G^<(X,x_1)\Sigma^{\bar{c}}(x_1,X)\big]$$

Equation (51) is compared with the quantum mechanical equivalent of the classical Hamilton–Jacobi equation (see, for example, Moyal 1949, equation (A4.5)). The time derivative of the Hamilton principal function is just the energy variable and the Hamilton principal function does not appear explicitly in the equation; $\bar{\bar{\varepsilon}}_{\rm int}(X)$ then gives a correction to the energy of the particle due to the interactions between the particles as a functional of the Green functions. In order to bring $\bar{\bar{\varepsilon}}_{\rm int}(X)$ to a more friendly form, we shall write it (using the representation (2)) as a sum of two terms:

$$\bar{\bar{\varepsilon}}_{\rm int}(X) = \frac{1}{4\rho(X)}\left(\int dx_1 {\rm Tr}[\sigma_z\tilde{\Sigma}(X,x_1)\tilde{G}(x_1,X) + \tilde{G}(X,x_1)\tilde{\Sigma}(x_1,X)\sigma_z] + \int dx_1 {\rm Tr}[\sigma_x\tilde{\Sigma}(X,x_1)\tilde{G}(x_1,X) - \tilde{G}(X,x_1)\tilde{\Sigma}(x_1,X)\sigma_x]\right). \tag{52}$$

The first term in the right-hand side of (52) is real since it is equal to its complex conjugate. This term can be represented as a sum of all unlinked connected skeleton diagrams that at equilibrium produce the interaction-induced variation of the ground-state energy (for example, Nozières 1964). Now we have a similar way to calculate this correction for systems that are not at equilibrium.

The second term is imaginary and is related to the fact that the local energy is not well defined due to the scattering processes. The structure of this term is similar to the integral in the right-hand side of (47) and it has the same properties: its integral over the whole space is zero, applying the coarse-graining procedure also makes it zero. It can be of importance only for strongly inhomogeneous systems. Using the same approach as in section 4 one can also show that this term is exactly zero for the detailed balanced systems.

6. Summary

Our aim in this study was to deduce quantum kinetic equations for interacting electrons written in terms of the momenta and the configuration coordinates in a gauge-invariant form for non-quantized arbitrary electromagnetic fields. This is achieved by making a transformation to the Wigner coordinates which includes the 4-potential of the electromagnetic field. As a result, the conventional Keldysh diagrams are to be reformulated and new phase-loop functions are introduced in order to account for the momentum and energy exchange between the electrons and the field. This phase-loop function becomes trivial for conservative electric fields and static homogeneous magnetic fields. However, the formulation obtained here in its general form allows one to treat inhomogeneous and non-linear problems.

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