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# A quantum kinetic equation for high-field transport in semiconductors

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**Abstract.** Our aim is the formulation of a tractable quantum theory capable of dealing properly with the length and time scales relevant to modern submicron devices. The Kadanoff–Baym–Keldysh non-equilibrium Green function method is employed to develop a formalism appropriate for high fields. No perturbation expansion arguments are employed. The equivalence of the two Kadanoff–Baym equations for the correlation function  $G^<$  for these systems is demonstrated. A relation analogous to the equilibrium case between  $G^<$ , the spectral function  $A$  and the quantum distribution function  $f$  is derived at high fields without the loss of the intracollisional field effect.

## 1. Introduction

In the semiclassical theory, transport phenomena are described by a distribution function  $f(\mathbf{p}, \mathbf{R}, t)$  which is the density of particles with momentum  $\mathbf{p}$  at the point  $\mathbf{R}$  and time  $t$ . Obviously, this assumes that the position and momentum of the particle can be defined simultaneously. If quantum effects are important, this description is no longer valid. Quantum mechanical situations are found in submicrometre devices where the mean free times can be of the order of  $10^{-14}$  s and the mean free paths are about  $50 \text{ \AA}$  [1]. One, then, needs to take into account the uncertainty relations and include the broadening of the energy and momentum states caused by the scattering processes [2]. Energy ( $\hbar\omega$ ) and momentum must now be considered as independent variables and we need a distribution function  $f(\mathbf{p}, \mathbf{R}, \omega, t)$  that depends on four variables in place of the semiclassical  $f$  which depends on  $(\mathbf{p}, \mathbf{R}, t)$  only. Of course, we can always remove the effects due to the uncertainty principle by performing some coarse-graining average in phase space, for instance by summing  $f(\mathbf{p}, \mathbf{R}, \omega, t)$  over all energy states [3]. A theory of transport capable of overcoming the limitations of the semiclassical approach can be formulated within the Green function formalism as developed by Kadanoff and Baym [4], Keldysh [5] and Langreth [6, 7] although, so far, none of the approaches that have used this technique are able to account properly for the high-field behaviour of quantum systems. Here, we would like to clarify the nature of the problems encountered in the description of non-equilibrium transport phenomena, and propose a new line of approach based on an Airy space formulation.

The various Green functions express the correlation between the field operator  $\hat{\psi}$  (1) of the particle at the space-time point  $(\mathbf{r}_1, t_1)$  and the conjugate field operator  $\hat{\psi}^\dagger(2)$  at another point  $(\mathbf{r}_2, t_2)$ , namely

$$\begin{aligned} G^>(1, 2) &= -(i/\hbar)\langle\hat{\psi}(1)\hat{\psi}^\dagger(2)\rangle & G^<(1, 2) &= \pm(i/\hbar)\langle\hat{\psi}^\dagger(2)\hat{\psi}(1)\rangle \\ G^r(1, 2) &= -(i/\hbar)\langle[\hat{\psi}(1), \hat{\psi}^\dagger(2)]_\pm\rangle\delta(t_1 - t_2) & G^a(1, 2) &= (i/\hbar)\langle[\hat{\psi}(1), \hat{\psi}^\dagger(2)]_\pm\rangle. \end{aligned}$$

Here the + (−) sign refers to fermions and anticommutation (bosons and commutation). The angular bracket  $\langle \dots \rangle$  indicates a thermodynamic average for equilibrium situations and an average over the available states for non-equilibrium systems. The interactions of the particles with the crystal are represented by the equivalent self-energy functions  $\Sigma^{r,a,<,>}$  [4–7]. Another important function is the spectral density

$$A(1, 2) = \langle\{\hat{\psi}(1), \hat{\psi}^\dagger(2)\}\rangle.$$

If  $A$  is a function only of the difference of its arguments, its Fourier transform  $A(\mathbf{p}, \omega)$  gives the probability that a particle with momentum  $\mathbf{p}$  will have energy  $\hbar\omega$  [3, 4].

From its definition,  $G^<$  is proportional to the density of particles and therefore has the character of a distribution function. Indeed, the average value  $\langle Q \rangle$  of any operator  $Q$  that is the sum of one-body terms can be expressed immediately in terms of  $G^<$ . In fact, when such a quantity is written in the second-quantisation formalism, from the commutation properties of the field operators, we have [8]

$$\langle Q(t) \rangle = \int d\mathbf{r} \langle \hat{\psi}^\dagger(\mathbf{r}, t) Q(\mathbf{r}, t) \hat{\psi}(\mathbf{r}, t) \rangle = \pm i\hbar \int d\mathbf{r} \lim_{t \rightarrow t'} Q(\mathbf{r}, t) G^<(\mathbf{r}, t; \mathbf{r}', t). \quad (1.1)$$

The equations of motion for the Green function defined above follow directly, and exactly, from the Schrödinger equations for the field operators  $\hat{\psi}$  and  $\hat{\psi}^\dagger$ . They can be expressed, by using the matrix notation [9]

$$\tilde{\mathbf{G}} = \begin{pmatrix} G_t & -G^< \\ G^> & -G_{\bar{t}} \end{pmatrix} \quad \tilde{\Sigma} = \begin{pmatrix} \Sigma_t & -\Sigma^< \\ \Sigma^> & -\Sigma_{\bar{t}} \end{pmatrix}$$

( $G_t = G^< + G^r$ ,  $G_{\bar{t}} = G^< - G^a$  and analogously for  $\Sigma_{t,\bar{t}}$ ) as

$$\left(i\hbar \frac{\partial}{\partial t_1} - H(1)\right) \tilde{\mathbf{G}}(1, 2) = \delta^4(1 - 2) \tilde{\mathbf{I}} + \int d3 \tilde{\Sigma}(1, 3) \tilde{\mathbf{G}}(3, 2) \quad (1.2a)$$

$$\left(i\hbar \frac{\partial}{\partial t_2} - H(2)\right) \tilde{\mathbf{G}}(1, 2) = \delta^4(1 - 2) \tilde{\mathbf{I}} + \int d3 \tilde{\mathbf{G}}(1, 3) \tilde{\Sigma}(3, 2). \quad (1.2b)$$

$\tilde{\mathbf{I}}$  is the identity matrix and the Hamiltonian contains only the non-interacting terms, that is, the kinetic energy operator and the external fields.

Because of the multiple integrations, these equations are quite difficult to solve. They simplify considerably for homogeneous systems in equilibrium, where the arguments of the Green functions and self-energies depend only upon the difference of their arguments:  $(1, 2) = (1-2)$ . In these cases, the Fourier transforms of these quantities will

be diagonal in both  $\mathbf{p}$  and  $\omega$  and (1.2) will be just algebraic equations that can be easily solved [10] and each leads to the same result

$$G^<(\mathbf{p}, \omega) = G^r(\mathbf{p}, \omega) \Sigma^a(\mathbf{p}, \omega) G^a(\mathbf{p}, \omega)$$

or, equivalently

$$G^<(\mathbf{p}, \omega) = A(\mathbf{p}, \omega) f(\mathbf{p}, \omega)$$

where the relation

$$A(\mathbf{p}, \omega) = -2 \operatorname{Im} G^r(\mathbf{p}, \omega)$$

and the definition

$$f(\mathbf{p}, \omega) = -\Sigma^<(\mathbf{p}, \omega)/2 \operatorname{Im} \Sigma^r(\mathbf{p}, \omega)$$

have been used.

In non-equilibrium conditions, unfortunately, this is no longer the case and we have to consider functions of their separate arguments. This is particularly true at high electric fields that cannot be treated perturbatively. In steady-state conditions, the time-translational invariance does persist [11], and all of the time variables have to depend only upon the difference of the two values  $t_1 - t_2$ . This is, as a matter of fact, an expression of the principle of causality: the effect at time  $t_1$  depends on the cause only at preceding times  $t_2$ . This is obvious because the Green functions are sums of correlation functions of two operators, and for a system that has the same dynamic properties at all times, the correlation between two observables at different times will depend only upon the time elapsed between them. This principle is, of course, universal, as true in classical as in quantum physics. It leads to some useful and interesting properties of the temporal Fourier transforms of the causal  $G^r$  in the plane of the variable  $\omega$ , including the relation  $A(\mathbf{p}, \omega) = -2 \operatorname{Im} G^r(\mathbf{p}, \omega)$ .

The space-translational invariance along the direction of the applied field is, however, violated. This is particularly clear when the applied electric field is represented in the scalar-potential gauge. The particle momentum, in this direction, then, is no longer a good quantum number. This complication makes the Fourier transform in space impractical for the solution of (1.2) because of the mixing of space and time coordinates that appears when the interactions with the crystal are modified by the strong electric field. The use of the vector-potential gauge, used by many authors [12–18] to represent the field, does not simplify the problem since this choice artificially breaks the time-translation invariance which is an essential feature of a system in the steady-state regime, as discussed before.

For all these reasons, the description of non-linear transport phenomena is a difficult, long-standing and much debated theoretical problem [19, 20]. All of the models presented so far [21–26] in the literature and that do not make use of the methods of many-particle physics, are approximations that are not able to describe adequately the simultaneous presence of an external field and of collisions (with phonons or impurities) in the electronic system. Most Green function approaches, although rigorous in principle, have been limited to weak fields by the use of the gradient expansion, which does not describe situations beyond linear response. Furthermore, the way the centre-of-mass coordinates  $(\mathbf{r}, \mathbf{R}, \tau, T)$  [4] are employed in these approaches makes them unsuitable for the description of the fluctuation phenomena that appear at length scales shorter than the inelastic mean free path [27]. In fact, the spatial and temporal dependence of the correlation function  $G^<$  describes how the concomitance of an

external field and the scattering processes affects the phase-coherent properties of the system, even in a homogeneous, steady-state system. The time and spatial scales pertinent to these properties are the inelastic mean free time and the inelastic mean free path, respectively [28]. When the centre-of-mass coordinates are employed, the relevant time axis is the centre-of-mass time  $T$  and the relevant coordinate is the centre-of-mass position  $\mathbf{R}$ . Then, the assumption that spatially ‘homogeneous’ and steady-state systems are independent of  $\mathbf{R}$  and  $T$  [10–18] is equivalent to coarse-graining the system over time and space scales corresponding to the inelastic mean free time and the inelastic mean free path. As a consequence, none of the fluctuation phenomena that appear on a scale smaller than these coarse-graining times and lengths can be taken into account by these methods.

In a recent paper [29], we have proposed a different technique to include high, homogeneous electric fields exactly. There we used Airy transforms, instead of Fourier transforms, to handle the position dependence parallel to the applied electric field. In this way, an analytic model was obtained for the spectral density. This model includes both the intracollisional field effect and collisional broadening [30, 31]. Furthermore, *in the assumption of the diagonality of the functions with respect to our new ‘Airy coordinates’*  $s$ , we were able to derive an integral kinetic equation for the correlation function  $G^<$  [32] starting from the sum of the two equations (1.2). Here, we want to show that it is possible to generalise those results to non-diagonal  $G^<$  and  $\Sigma^<$ . We will also show that even in this case the two Kadanoff–Baym equations (1.2) lead to the same relation  $G^< = Af$  between  $G^<$  and the quantum distribution function  $f$ , whether they are added, subtracted or solved independently.

In section 2, we will briefly review the ‘Airy function’ technique and summarise the results already presented elsewhere. In section 3, we will generalise these results by deriving a quantum kinetic equation valid at high fields and scattering mechanisms described by a momentum-independent self-energy. In section 4 we will discuss the results obtained and will clarify some obscure points of the previous papers.

## 2. The Airy representation formalism

As mentioned before, we do not try to solve (1.2) by writing them in terms of the centre-of-mass coordinates  $\mathbf{r}$ ,  $\mathbf{R}$ ,  $\tau$ ,  $T$  and then Fourier transforming with respect to  $\mathbf{r}$  and  $\tau$ , as done in previous approaches. Instead, we include the electric field (given by the scalar potential  $\varphi = eEz$ ) as a part of the unperturbed Hamiltonian [14] and choose, as our basis set, plane waves on the plane normal to the field and continuous set of Airy functions of the first kind along the direction of the field. This is the Hilbert space of the normalised eigenfunctions of an electron in a uniform electric field. In this space, we define a transformation

$$F(\mathbf{p}_\perp, s_1, s_2) = \int \frac{dx dy}{2\pi} \int \frac{dz_1 dz_2}{L^2} \exp\left(\frac{i}{\hbar} \mathbf{p}_\perp \cdot \mathbf{r}_\perp\right) \text{Ai}\left(\frac{z_1 - s_1}{L}\right) \\ \times \text{Ai}\left(\frac{z_2 - s_2}{L}\right) f(\mathbf{p}_\perp, z_1, z_2) \quad (2.1)$$

by which a function  $f$ , translationally invariant in the transverse direction (as expressed by the single transverse position vector  $\mathbf{r}_\perp$ ), but not in the direction  $z$  of the electric field,

is written in terms of its transverse momentum  $\mathbf{p}_\perp$  and of the ‘Airy variables’  $s$  and  $s'$ . The Airy coordinate  $s$  varies continuously and thus corresponds to the classical turning point in  $z$  of an electron with energy  $\varepsilon_{\mathbf{p}_\perp, s} = \mathbf{p}_\perp^2/2m + eEs$ .  $L = \hbar^2/2meE^{1/3}$  is a normalisation length. As demonstrated in [32], a function diagonal in the  $s$ -variable is not translationally invariant along the  $z$  direction. This is a very useful property because it allows the use of diagonal functions while maintaining the lack of translational invariance along the direction of the applied field. In terms of these new variables  $(\mathbf{p}_\perp, s)$ , the first of (1.2), for the ‘unperturbed’, field-dependent retarded Green function  $G_E^r$ , in the absence of the two particle interaction  $\Sigma$ , leads to

$$G_E^r(\mathbf{p}_\perp, s_1, \tau) = -i/\hbar \vartheta(\tau) \exp[-(i/\hbar)\varepsilon_{\mathbf{p}_\perp, s_1} \tau] \tag{2.2}$$

and the second gives  $G_E^r(\mathbf{p}_\perp, s_2, \tau)$ . The corresponding spectral density function can be immediately found [32]:

$$A_E(\mathbf{p}_\perp, s, \omega) = -2 \text{Im} G_E^r = 2\pi\delta(\hbar\omega - \varepsilon_{\mathbf{p}_\perp, s}). \tag{2.3}$$

This can be shown [33] to be equivalent to the result

$$A_E(\mathbf{p}, \tau) = (1/\hbar) \exp\{-(i/\hbar)[(p^2/2m)\tau + (e^2E^2/24m)\tau^3]\},$$

obtained by using the centre-of-mass coordinates in the gauge invariant formulation [14, 34].

In order to determine the interacting, retarded Green function from (1.2), we need a model for  $\Sigma^r$ , describing the interactions of the electrons with the crystal. For non-degenerate electrons and weak electron–phonon interaction,  $\Sigma^r$  can be written in the Born approximation as

$$\Sigma^r(1, 2) = D_0^\rhd(1, 2)G^r(1, 2). \tag{2.4}$$

At low densities, the electrons are not expected to influence the phonons, so for  $D_0^\rhd$  we can use the equilibrium phonon Green function

$$D_0^\rhd(1, 2) = (i/\hbar)\langle\hat{\varphi}(1)\hat{\varphi}^\dagger(2)\rangle$$

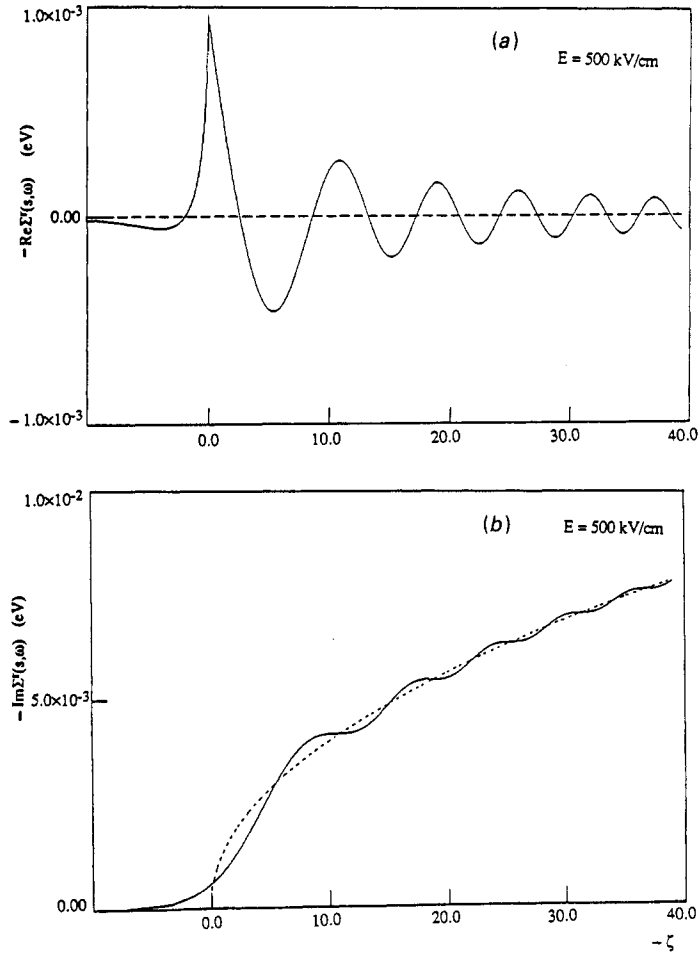
with  $\varphi$  the Boson field operator representing the displacement from equilibrium of the ions in the solid at position  $(\mathbf{r}_1, t_1)$  in space–time. For non-polar optical phonons and the one-phonon scattering process,  $G^r = G_E^r$  in (2.3), the retarded self-energy in  $(\mathbf{p}_\perp, s)$  coordinates is given by [32]

$$\Sigma^r(s, \omega) = \frac{2\pi}{\hbar} |V|^2 \sum_{\eta=\pm 1} \left(N_0 + \frac{\eta + 1}{2}\right) F(s, \omega)$$

$$\begin{aligned} \text{Re}[F(s, \omega)] = & -(1/\sqrt{\pi})(m^{3/2}/\hbar^2)\Theta^{1/2}[\text{Ai}'(\zeta)\text{Bi}'(\zeta) - \zeta\text{Ai}(\zeta)\text{Bi}(\zeta) \\ & + \sqrt{\zeta/\pi}\vartheta(\zeta)] \end{aligned} \tag{2.5}$$

$$\text{Im}[F(s, \omega)] = -(1/\sqrt{\pi})(m^{3/2}/\hbar^2)\Theta^{1/2}(\text{Ai}'^2(\zeta) - \zeta\text{Ai}^2(\zeta))$$

where  $\Theta = 3^{1/3}eEL$ ,  $\zeta = -[eEs - \hbar(\omega - \eta\omega_0)]/\Theta$ , and  $|V|$  is the electron–phonon matrix element and  $\eta = +1$  ( $-1$ ) corresponds to emission (absorption) of a phonon of



**Figure 1.** (a) The real part of the self-energy as a function of the reduced energy  $\zeta$ , for emission processes. (b) The imaginary part of the self-energy. The broken curve refers to the free-electron case. The parameters are those for silicon.

frequency  $\omega_0$  by the electron. The self-energy above is shown in figure 1. (We use parameters appropriate to Si: an optical phonon energy  $\hbar\omega_0 = 0.039$  eV,  $m = 0.295 m_0$ , where  $m_0$  is the free-electron mass. The electron-phonon interaction is given by a deformation potential parameter  $D_t = 6.85 \times 10^{10}$  eV m $^{-1}$ .)

The approximation  $G^r = G_E^r$  does not neglect physical effects such as collisional broadening, as one might be led to think, because the retarded Green function must still be determined self-consistently in (1.2), and the presence of the field in  $G_E^r$  introduces high-field effects in the total Green function  $G^r$ . With this model for  $\Sigma^r$ , equations (1.2) are multiplicative equations and both lead to

$$G^r(\mathbf{p}_\perp, s_1, s_2; \omega) = \delta(s_1 - s_2) / (\hbar\omega - \varepsilon_{\mathbf{p}_\perp, s_1} - \Sigma^r(s, \omega)). \quad (2.6)$$

This generalises to high fields the result that Mahan and co-workers [11] obtained in the linear response regime: equations (1.2) are satisfied by the same function  $G^r$ , which has

the equilibrium form. However, the field is now included exactly, to all orders, in both the energy  $\varepsilon_{p_{\perp},s}$  and the self-energy  $\Sigma^r(s, \omega)$ . The spectral density can be immediately found to be

$$A(\mathbf{p}_{\perp}, s, \omega) = -2\text{Im}\Sigma^r(s, \omega) / [(\hbar\omega - \varepsilon_{p_{\perp},s} - \text{Re}\Sigma^r(s, \omega))^2 + (\text{Im}\Sigma^r(s, \omega))^2] \quad (2.7)$$

which, again, has the equilibrium form. Equation (2.7) is shown in figure 2. In this representation  $A(\mathbf{p}_{\perp}, s, \omega)$  is positive definite and satisfies the normal sum rules [4, 34]. The integral over  $\mathbf{p}_{\perp}$  of (2.7) gives the density of states (in this case a two-dimensional density of states)

$$\rho(s, \omega) = \frac{1}{\pi} \int d\mathbf{p}_{\perp} A(\mathbf{p}_{\perp}, s, \omega) = 4m \left[ \frac{\pi}{2} + \tan^{-1} \left( \frac{\hbar\omega - eEs - \text{Re}\Sigma^r(s, \omega)}{\text{Im}\Sigma^r(s, \omega)} \right) \right] \quad (2.8)$$

which is plotted in figure 3.

### 3. Quantum kinetic equations

Because of the problems discussed in the introduction, it is not an easy problem to derive a model for the spectral function that includes both collisional broadening and the intracollisional field effect. So far, to the best of our knowledge, this has been accomplished only through the Airy representation formalism discussed in the previous section.

In order for the spectral function  $A(\mathbf{p}_{\perp}, s, \omega)$  to be of utility in transport problems, however, we must also find (and solve!) a kinetic equation for the correlation function  $G^<$ , or for a quantum mechanical distribution function related to it, within this new formalism. That is, we have to solve the Kadanoff–Baym equations (1.2) for  $G^<$  in terms of the variables  $(\mathbf{p}_{\perp}, s, \omega)$ . Explicitly, equations (1.2) read

$$\begin{aligned} \left( i\hbar \frac{\partial}{\partial t_1} - H(\mathbf{r}_1, t_1) \right) G^<(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2) &= \int_{-\infty}^{\infty} d\mathbf{r}_3 dt_3 (\Sigma^r(\mathbf{r}_1, t_1; \mathbf{r}_3, t_3) \\ &\times G^<(\mathbf{r}_3, t_3; \mathbf{r}_2, t_2) + \Sigma^<(\mathbf{r}_1, t_1; \mathbf{r}_3, t_3) G^a(\mathbf{r}_3, t_3; \mathbf{r}_2, t_2)) \end{aligned} \quad (3.1a)$$

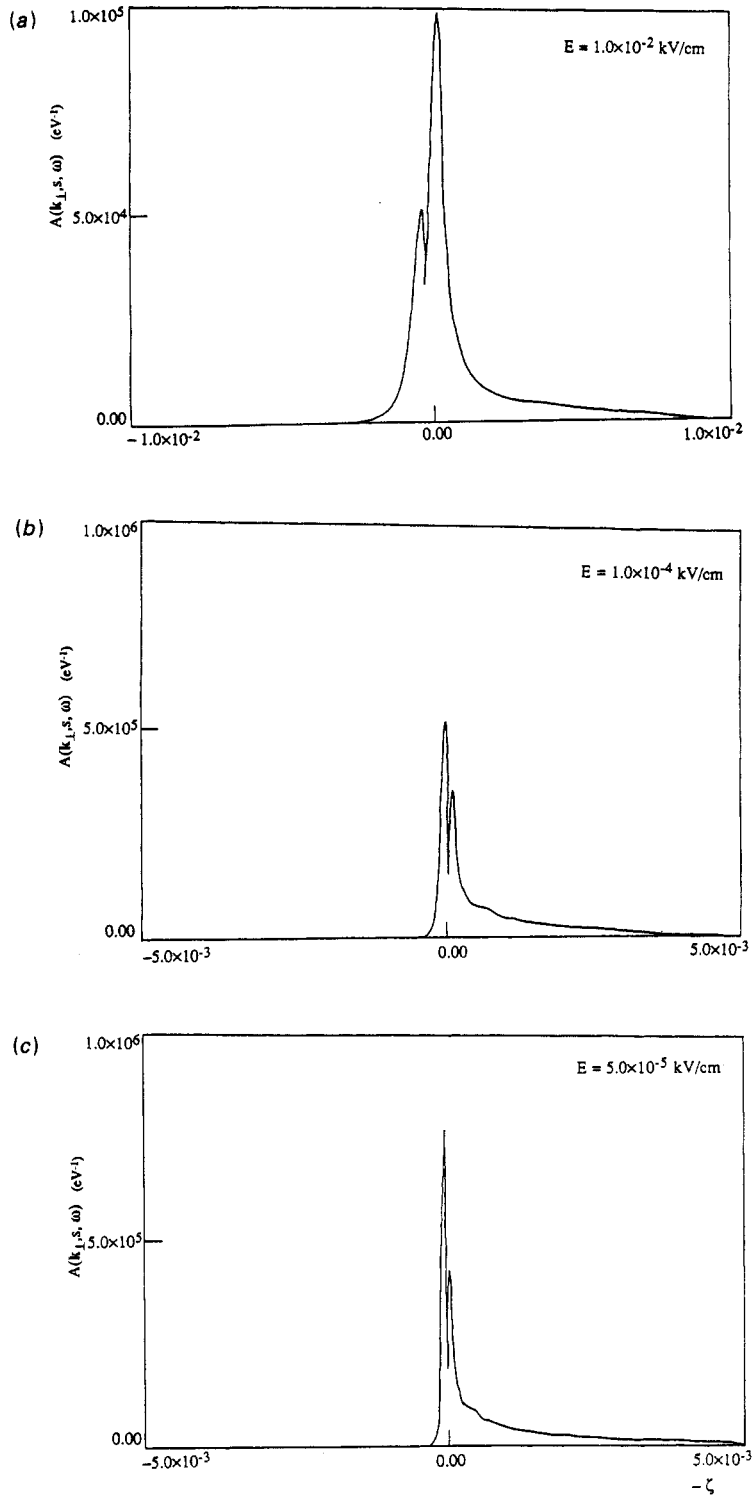
$$\begin{aligned} \left( -i\hbar \frac{\partial}{\partial t_2} - H(\mathbf{r}_2, t_2) \right) G^<(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2) &= \int_{-\infty}^{\infty} d\mathbf{r}_3 dt_3 (G^r(\mathbf{r}_1, t_1; \mathbf{r}_3, t_3) \\ &\times \Sigma^<(\mathbf{r}_3, t_3; \mathbf{r}_2, t_2) + G^<(\mathbf{r}_1, t_1; \mathbf{r}_3, t_3) \Sigma^a(\mathbf{r}_3, t_3; \mathbf{r}_2, t_2)). \end{aligned} \quad (3.1b)$$

By Fourier transforming the transverse variable  $\mathbf{r}_{\perp} = (\mathbf{r}_1 - \mathbf{r}_2)_{\perp}$  and Airy transforming the longitudinal variables  $z_1$  and  $z_2$  on both sides of (3.1a) and (3.1b), these can be written in  $(\mathbf{p}_{\perp}, s)$  space as

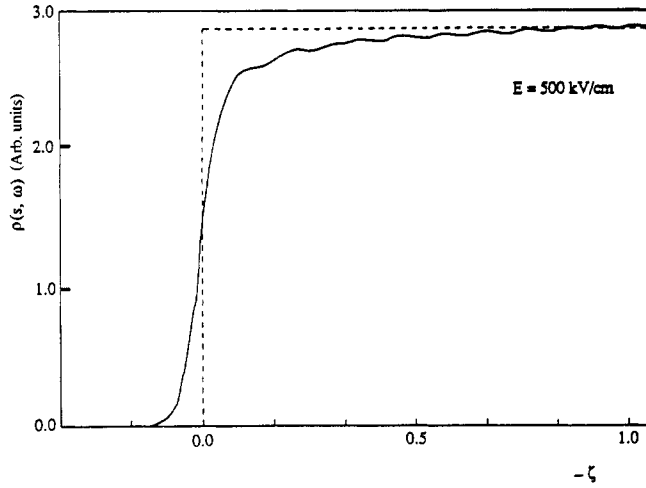
$$\begin{aligned} \left( i\hbar \frac{\partial}{\partial \tau} - \varepsilon_{p_{\perp},s_1} \right) G^<(\mathbf{p}_{\perp}, s_1, s_2; \tau) &= \int_{-\infty}^{\infty} d\tau' \int ds_3 (\Sigma^r(\mathbf{p}_{\perp}, s_1, s_3; \tau - \tau') \\ &\times G^<(\mathbf{p}_{\perp}, s_3, s_2; \tau') + \Sigma^<(\mathbf{p}_{\perp}, s_1, s_3; \tau - \tau') G^a(\mathbf{p}_{\perp}, s_3, s_2; \tau')) \end{aligned} \quad (3.2a)$$

$$\begin{aligned} \left( i\hbar \frac{\partial}{\partial \tau} - \varepsilon_{p_{\perp},s_2} \right) G^<(\mathbf{p}_{\perp}, s_1, s_2; \tau) &= \int_{-\infty}^{\infty} d\tau' \int ds_3 (G^r(\mathbf{p}_{\perp}, s_1, s_3; \tau - \tau') \\ &\times \Sigma^<(\mathbf{p}_{\perp}, s_3, s_2; \tau') + G^<(\mathbf{p}_{\perp}, s_1, s_2; \tau - \tau') \Sigma^a(\mathbf{p}_{\perp}, s_2, s_2; \tau')) \end{aligned} \quad (3.2b)$$





**Figure 2.** The spectral density function for three different values of the electric field. The broken curve refers to calculations with collisional broadening only.



**Figure 3.** The density of energy states compared with that of a two-dimensional free-particle system (broken curve). The presence of the electric field and of the collisions generates a series of damped oscillations for positive energies and a ‘tunnelling’ tail for negative energies. In the limit of high energies, both curves approach  $4\pi m$  (as required by (2.8)).

where the change of variables  $\tau = t_1 - t_2$  and  $\tau' = t_3 - t_2$  has also been performed.

For our system of electrons interacting with non-polar optical phonons in equilibrium, the self-energy  $\Sigma^<$ , which is, in general, given by

$$\Sigma^<(1, 2) = D_0^<(1, 2)G^<(1, 2),$$

is independent of momentum and can be expressed in  $s$ -coordinates as

$$\Sigma^<(s_1, s_2; \omega) = \frac{2\pi}{\hbar} \sum_{\eta} |V|^2 \left( N_0 + \frac{\eta + 1}{2} \right) \int d(\mathbf{p}_{\perp} - \mathbf{q}_{\perp}) ds_3 ds_4 \times G^<(\mathbf{p}_{\perp} - \mathbf{q}_{\perp}, s_3, s_4; \omega + \eta\omega_0) \begin{cases} -(1/2L^3)Y_0(2\sqrt{S}) & \text{if } S > 0 \\ (1/\pi L^3)K_0(2\sqrt{|S|}) & \text{if } S < 0 \end{cases}$$

where  $\mathbf{q}$  is the phonon momentum,  $S = [(s_1 + s_3) - (s_2 + s_4)][(s_1 - s_3)^2 - (s_2 - s_4)^2]$ , and  $Y_0$  and  $K_0$  are the Neumann and modified Bessel functions of order zero [35], respectively.

At this point, it is a standard procedure [4, 11, 14] to take the sum and the difference of these two equations (3.2). In our case, however, this turns out to yield exactly the same result. In order to show how this comes about, notice that the RHS of both (3.2a) and (3.2b) are sums of convolution products, so the Fourier transform in the time domain can be done trivially. Now we subtract (3.2b) from (3.2a) and use the model (2.5) for  $\Sigma^r$  and the result (2.6) for  $G^r$ . In this way, we obtain

$$eE(s_1 - s_2)G^<(\mathbf{p}_{\perp}, s_1, s_2; \omega) = (G^r(\mathbf{p}_{\perp}, s_1; \omega)\Sigma^<(s_1, s_2; \omega) + G^<(\mathbf{p}_{\perp}, s_1, s_2; \omega)\Sigma^a(s_2; \omega) - \Sigma^r(s_1; \omega)G^<(\mathbf{p}_{\perp}, s_1, s_2; \omega) - \Sigma^<(s_1, s_2; \omega)G^a(\mathbf{p}_{\perp}, s_2; \omega)) \quad (3.3a)$$

or, solving for  $G^<$ ,

$$\begin{aligned} G^<(\mathbf{p}_\perp, s_1, s_2; \omega) &= \frac{G^r(\mathbf{p}_\perp, s_1; \omega) - G^a(\mathbf{p}_\perp, s_2; \omega)}{eE(s_1 - s_2) + \Sigma^r(s_1; \omega) - \Sigma^a(s_2; \omega)} \Sigma^<(s_1, s_2; \omega) \\ &= G^r(\mathbf{p}_\perp, s_1; \omega) \Sigma^<(s_1, s_2; \omega) G^a(\mathbf{p}_\perp, s_2; \omega). \end{aligned} \quad (3.4a)$$

By summing, instead of subtracting, the two equations (3.2a) and (3.2b), and following the same procedure as indicated above, we have

$$\begin{aligned} [2\hbar\omega - \varepsilon_{\mathbf{p}_\perp} - eE(s_1 + s_2)]G^<(\mathbf{p}_\perp, s_1, s_2; \omega) &= G^r(\mathbf{p}_\perp, s_1; \omega) \Sigma^<(s_1, s_2; \omega) \\ &+ G^<(\mathbf{p}_\perp, s_1, s_2; \omega) \Sigma^a(s_2; \omega) + \Sigma^r(s_1; \omega) G^<(\mathbf{p}_\perp, s_1, s_2; \omega) \\ &+ \Sigma^<(s_1, s_2; \omega) G^a(\mathbf{p}_\perp, s_2; \omega) \end{aligned} \quad (3.3b)$$

and therefore

$$\begin{aligned} G^<(\mathbf{p}_\perp, s_1, s_2; \omega) &= \frac{G^r(\mathbf{p}_\perp, s_1; \omega) + G^a(\mathbf{p}_\perp, s_2; \omega)}{2\hbar\omega - \varepsilon_{\mathbf{p}_\perp} - eE(s_1 + s_2) - \Sigma^r(s_1; \omega) - \Sigma^a(s_2; \omega)} \Sigma^<(s_1, s_2; \omega) \\ &= G^r(\mathbf{p}_\perp, s_1; \omega) \Sigma^<(s_1, s_2; \omega) G^a(\mathbf{p}_\perp, s_2; \omega) \end{aligned} \quad (3.4b)$$

which is identical to (3.4a). The same result, however, can be obtained by solving (3.2a) and (3.2b) directly without going through the ‘subtraction’ and ‘addition’ procedure. In fact, the Fourier transform from  $\tau$  to  $\omega$  of (3.2a) and (3.2b) leads to

$$\begin{aligned} (\hbar\omega - \varepsilon_{\mathbf{p}_\perp, s_1})G^<(\mathbf{p}_\perp, s_1, s_2; \omega) &= \Sigma^r(s_1, \omega) G^<(\mathbf{p}_\perp, s_1, s_2; \omega) \\ &+ \Sigma^<(s_1, s_2; \omega) G^a(\mathbf{p}_\perp, s_2; \omega) \end{aligned} \quad (3.5a)$$

$$\begin{aligned} (\hbar\omega - \varepsilon_{\mathbf{p}_\perp, s_2})G^<(\mathbf{p}_\perp, s_1, s_2; \omega) &= G^r(\mathbf{p}_\perp, s_1; \omega) \Sigma^<(s_1, s_2; \omega) \\ &+ G^<(\mathbf{p}_\perp, s_1, s_2; \omega) \Sigma^a(s_2; \omega) \end{aligned} \quad (3.5b)$$

respectively. These can be solved for  $G^<$  and the result is precisely (3.4a). Note that the equivalence of the two Kadanoff and Baym equations is not dependent upon the choice of the type of phonon scattering, as it is a result based on (3.2), in which the phonon matrix elements appear only in general formal expressions.

Now, remembering that  $G^r = (G^a)^*$ , by substituting  $\text{Re } G^r$  and  $\text{Im } G^r$  in (3.4a), we obtain

$$G^<(\mathbf{p}_\perp, s_1, s_2; \omega) = A(\mathbf{p}_\perp, s_1; \omega) f_1(\mathbf{p}_\perp, s_1, s_2; \omega) \quad (3.6a)$$

where the ‘distribution function’  $f_1$  defined by

$$f_1(\mathbf{p}_\perp, s_1, s_2; \omega) = (G^r(\mathbf{p}_\perp, s_1; \omega)/G^r(\mathbf{p}_\perp, s_2; \omega))(-\Sigma^<(s_1, s_2; \omega)/2 \text{Im } \Sigma^r(s_2; \omega)). \quad (3.6b)$$

Equations (3.6) satisfy both (3.5a) and (3.5b) as can be verified by substitution.

The expression (3.6a) for  $G^<$  is quite interesting. It is an exact relation and has, in fact, the same formal structure of the non-equilibrium *ansätze* introduced in many earlier attempts to solve both the high-field and the linear-response-regime problem [3, 11, 12, 14–18]. Equation (3.6a) expresses a direct relationship between the correlation function  $G^<$  and a quantum mechanical distribution function  $f_1$ . In the present

form, however,  $f_1$  has no practical advantage with respect to  $G^<$  since it contains the same number of variables, and we might as well solve (3.6a) directly for  $G^<$  as can be easily realised by recalling the expression for  $\Sigma^<$  given above.

At this point, it should be noticed that the separation given by (3.6) is not unique, since, by substituting  $\text{Re } G^a$  and  $\text{Im } G^a$  in (3.4a), we can write

$$G^<(\mathbf{p}_\perp, s_1, s_2; \omega) = A(\mathbf{p}_\perp, s_2; \omega) f_2(\mathbf{p}_\perp, s_1, s_2; \omega) \tag{3.7a}$$

with

$$f_2(\mathbf{p}_\perp, s_1, s_2; \omega) = (G(\mathbf{p}_\perp, s_2; \omega)/G^a(\mathbf{p}_\perp, s_1; \omega))(-\Sigma^<(s_1, s_2; \omega)/2 \text{Im } \Sigma^r(s_1; \omega)) \tag{3.7b}$$

A unique quantum distribution function, however, is obtained when  $s_1 = s_2$ . Therefore, we have solved (3.6) by assuming diagonality of  $G^<$  with respect to the  $s$ -variable [32]:

$$G^<(s_1, s_2) \cong G^<(s_1)\delta(s_1 - s_2).$$

In this case, (3.6) reads

$$\begin{aligned} G^<(\mathbf{p}_\perp, s; \omega) &= A(\mathbf{p}_\perp, s; \omega) f(s; \omega) \\ f(s, \omega) &= -\frac{\Sigma^<(s, \omega)}{2 \text{Im } \Sigma^r(s, \omega)} = \sum_\eta \left( N_0 + \frac{\eta + 1}{2} \right) \\ &\quad \times \int_{-\infty}^\infty ds' \mathcal{F}(s, s'; \omega + \eta\omega_0) f(s'; \omega + \phi\omega_0) \end{aligned} \tag{3.8}$$

where

$$\mathcal{F}(s, s'; \omega) = 2\sqrt{3}\pi^2 \left( \frac{2\pi |V|}{\hbar L} \right)^2 \text{Ai}^2 \left( \frac{s - s'}{3^{1/3}L} \right) \frac{\rho(s'; \omega)}{\text{Im } \Sigma^r(s, \omega - \eta\omega_0)}.$$

Here  $\hbar(\omega + \eta\omega_0)$  represents the total electronic energy before the scattering event has occurred and  $s'$  and  $s$  are the electron turning points before and after the scattering event, respectively. Therefore, the kernel  $\mathcal{F}(s, s'; \omega + \eta\omega_0)$  is an operator that acts on the distribution function  $f(s'; \omega + \eta\omega_0)$  before the scattering, and transforms it to  $f(s; \omega)$ , the distribution function after the scattering. The integral equation was solved numerically by interaction and the quantity

$$G^<(s, \omega) = \int d\mathbf{p}_\perp G^<(\mathbf{p}_\perp, s, \omega). \tag{3.9}$$

proportional to the density of particles, is plotted in figure 4 as a function of the reduced energy  $\zeta$ . By anti-Airy transforming (3.9)

$$G^<(s; \omega) \Rightarrow G^<(z, z'; \omega)$$

and, according to (1.1), for  $z \rightarrow z'$ , we obtain  $G^<(z; \omega)$ , a quantity proportional to the density of particles in terms of the reduced position coordinate  $\xi = [z - \hbar(\omega + \eta\omega_0)/eE]/3^{1/3}L$ . The result is shown in figure 5. It should be noted that  $G^<(z; \omega)$  is actually a function of the single variable  $\xi$  which is essentially the shifted position  $(z - \hbar\omega/eE)$ . Integrating over  $\xi$  will, therefore, wash away its oscillatory nature. The fluctuation effects at the fine-grained scale  $(z - \hbar\omega/eE)$  will be averaged out and a uniform concentration will appear.

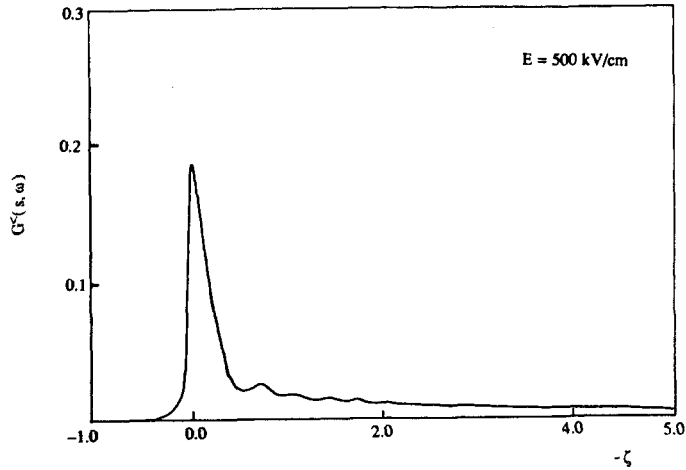


Figure 4. The correlation function (in natural units,  $\hbar/\omega_0 L^2$ ) as a function of  $\zeta$ .

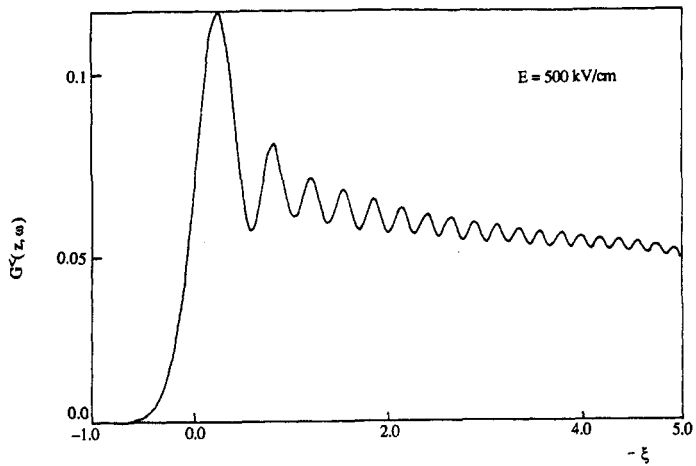


Figure 5. The correlation function (in natural units) as a function of the reduced position  $\xi$ .

It should further be noted that a momentum-independent distribution function can be obtained, in the non-diagonal case, by solving (3.4b) in a slightly different manner. In this case

$$G(\mathbf{p}_\perp, s_1, s_2; \omega) = (A(\mathbf{p}_\perp, s_1; \omega)A(\mathbf{p}_\perp, s_2; \omega))^{1/2} f_S(s_1, s_2; \omega) \quad (3.10a)$$

where  $f_S$  is the ‘symmetric distribution function’

$$f_S(s_1, s_2; \omega) = \frac{1}{2} \Sigma^<(s_1, s_2; \omega) / \sqrt{\text{Im}(\Sigma^r(s_1; \omega)) \text{Im}(\Sigma^r(s_2; \omega))}. \quad (3.10b)$$

Although the distribution function is now in a form reminiscent of that in equilibrium, this has been achieved at the expense of a more complicated ‘joint’ spectral function which is the geometric mean of the two spectral functions evaluated at  $s_1$  and  $s_2$ . In fact,

this is to be expected, and has a connection to results obtained using centre-of-mass coordinates. In the latter case,  $A(\mathbf{p}, \omega)$  depends upon  $p_z$  which is the spatial Fourier transform of the  $z_1 - z_2$  dependence. It must be remembered that the dependence upon only  $z_1 - z_2$  was achieved by an *ad hoc* assumption that the system was independent of  $z_1 + z_2$ . Indeed, this is only the case for  $z_1 + z_2 \gg \lambda$ , the inelastic mean free path [28]. In this case, the  $\mathbf{p}$ -dependence couples two positions  $z_1$  and  $z_2$  in the spectral density. This coupling is also present in (3.10a) since the 'joint' function now includes both  $z_1$  and  $z_2$  through  $s_1$  and  $s_2$ .

#### 4. Results and discussion

We have utilised the Kadanoff–Baym methods to develop a formalism that can be used for high, homogeneous fields. The aim was to derive a spectral density model and a quantum kinetic equation that account for both the energy dependence of the collision rate and the intracollisional field effect in a relatively simple and rigorous way. In order to accomplish this, we have introduced a representation in terms of Airy coordinates that replaces the usual momentum representation along the field direction [29, 32]. We point out that our technique differs from previous ones that have found solutions in terms of Airy functions. The introduction of the Airy transform, in fact, introduces the proper symmetry of the system from the beginning, thus yielding mathematically simpler equations with fewer coordinates and convolutions.

Furthermore, the possibility of dealing with functions that are diagonal in the transform variable  $s$ , while keeping their non-translational properties unaltered, allows us to avoid the coarse-graining procedure that was implied when the coordinates  $\mathbf{R}$  and  $T$  were set to zero [17, 18, 21] for homogeneous and steady-state systems, or the energy renormalisation ( $\hbar\Omega = \hbar\omega - e\mathbf{E} \cdot \mathbf{R}$ ) was performed [11], in those approaches that utilised the center-of-mass coordinates  $\mathbf{r}$ ,  $\tau$ ,  $\mathbf{R}$  and  $T$ . In our formalism, all components are kept in the calculation, but are associated with different values of the  $s$ -variable in transform space. This, therefore, makes it possible to account for the fluctuation phenomena that appear at length scales smaller than the inelastic mean free path. In fact, the appearance of fine-grained effects is confirmed by the presence of a series of damped oscillations in both the real and imaginary parts of the self-energy. They are a consequence of the inclusion of the correct symmetry of the system and of the non-perturbative treatment of the electric field.

It has been fashionable to ignore  $\mathbf{R}$  and  $T$  in steady-state systems that are homogeneous except for a constant, uniform field, but the present approach avoids this approximation. Both  $\mathbf{R}$  and  $T$  (depending upon the gauge choice) reflect the absolute phase relationship inherent in the Green functions. For lengths smaller than the inelastic mean free path, longitudinal inhomogeneity is recovered only after all transverse variations have been integrated out of the problem. Neglect, for instance, of the  $\mathbf{R}$ -variations is tantamount to smoothing these microfluctuations, and hence to coarse-graining over a dimension longer than the inelastic mean free path. The Airy transform approach discussed here avoids this process by retaining the exact treatment of the breakdown of translational invariance in the field.

The oscillations of the real part of the self-energy (which describes how the unperturbed energy  $\hbar\omega = \varepsilon_{\mathbf{p}_{\perp}, s}$  is modified by the presence of the interactions) denote regions in which the energy of the electron is raised (positive values of the self-energy) and regions in which the energy of the electron is lowered (negative values of the self-energy).

The net result is the existence of preferred energies for the electron, corresponding to alternating zero-crossing of  $\text{Re } \Sigma^r$ . The validity of the interpretation is reinforced by the step-like oscillations present in  $\text{Im } \Sigma^r$ . Since this quantity is proportional to the scattering rate [36], the plateaus are an indication of the quasi-two-dimensional sub-band tendencies mentioned above.

The presence of the intracollisional field effect and of collisional broadening produces a tail in  $\text{Im } \Sigma^r$  for  $\zeta < 0$ . The existence of such a tail to negative energies corresponds to the part with  $\zeta > 0$  in  $\text{Ai}(\zeta)$ , and represents tunnelling into the classically forbidden region. This smooths out the sharp threshold in energy of the scattering rate, making possible transitions that cannot occur in the absence of the field [2].

The spectral function  $A(\mathbf{p}_\perp, s, \omega)$  presents an interesting double-peak structure. The right peak would, then, describe the fact that the carrier has been accelerated during the emission of a phonon. The electron loses less energy to the phonon and exits the scattering process with an energy change greater than  $\hbar\omega_0$ . The left-hand peak, on the other hand, is a consequence of quantum-mechanical tunnelling and indicates the possibility for the electron to regain part of the energy lost to the phonon. It is as if the particle were decelerated by the field during the emission process, thus ending the collision with an energy loss smaller than  $\hbar\omega_0$ . The energy change in the lattice is always just the phonon energy, but the electron sees a modified energy by virtue of the field acting during the collision. This interpretation is supported by the fact that the height of the right-hand peak, relative to the left-hand one, decreases, as does their relative separation, until they merge to form the Lorentzian shape typical of the collisional broadening effect in the absence of a field [32]. Furthermore, the density of states  $\rho(s, \omega)$  shown in figure 3 indicates that the interaction of the field and the scattering processes is creating a quasi-two-dimensional behaviour in the electron system.

These physical effects present in  $\Sigma^r$  and  $A$  are embodied and synthesised in  $G^<(s; \omega)$ . Here again, we find the existence of particles with negative total energy as well as a series of preferred energy levels, indicated by the damped oscillations occurring at  $\zeta > 0$ . Furthermore, the presence of the high-energy tail suggests that a carrier can increase its kinetic energy even when it emits a phonon because of the collisional-broadening-induced Lorentzian-type tail of the spectral of the density function and because of the intracollisional field effect.

The oscillatory behaviour of the carrier  $G^<(z; \omega)$  indicates the existence of preferred positions for the particle, caused by the uncertainties introduced by the concomitance of collisional broadening and intracollisional field effect. This is a phenomenon that is, somehow, expected as a consequence of the non-conservation of momentum in inhomogeneous systems: the uncertainty in the definition of  $\mathbf{p}$  is ultimately responsible for the broadening of the electron position after each scattering event. This suggests the possibility of a discontinuous trajectory for the electron and that transport might, therefore, be, more appropriately, described in terms of the 'field-assisted hopping' in the  $z$  direction, between states described by discrete values of the Airy coordinate.

Another important result presented here is the derivation of the  $G^< = Af$  relation. For a space- and time-translationally invariant system, the spectral function  $A(x)$  is real and exactly related to the correlation functions  $G^<$  and  $G^>$  by [4]

$$G^>(\mathbf{p}, \omega) = A(\mathbf{p}, \omega)(1 + f(\omega)) \quad (3.11a)$$

$$G^<(\mathbf{p}, \omega) = A(\mathbf{p}, \omega)f(\omega) \quad (3.11b)$$

where  $f(\omega) = 1/[e^{\beta\hbar\omega} \pm 1]$ . These relations are an expression of the ‘fluctuation-dissipation’ theorem [37]. In fact, they relate the mean square fluctuation

$$\langle \hat{\psi}(\omega) \hat{\psi}^\dagger(\omega) \rangle = \int d\tau e^{i\omega\tau} \langle \hat{\psi}(\tau) \hat{\psi}^\dagger(0) \rangle \propto G^>(\omega)$$

of the field operators (or, more generally, of any appropriate operator) to  $\text{Im } G^r(\omega)$ , which is often proportional to the dissipation in the system [38]. This is a celebrated result, and because of its generality it is believed to hold also for non-equilibrium systems. However, for these cases, none of the previous approaches has been able to produce an expression that, through the distribution function, exactly relates the correlation function and the spectral function [39]. Even in the near-equilibrium gradient approximation only *ansätze* are available. In the previous treatment the use of the Wigner coordinates and the choice of the vector-potential gauge to represent the external fields led to systems whose temporal and spatial translational invariance was irrevocably lost. In our formalism, the time translational invariance of the system was preserved by the scalar-potential gauge. The broken homogeneity along the field direction was only formally restored by the assumption of the dependence of the retarded self-energy on just one Airy variable  $s$ . This, as already pointed out, does not imply any assumption of translational invariance in the real-space coordinate  $z$ . In this respect, the  $G = fA$  result (3.6) was derived at arbitrary fields in the Airy representation in a quite general manner.

This recovery of a fluctuation-dissipation theorem is rather general in another way: while our fundamental approximation is that the retarded (and thus also advanced) self-energy is diagonal in the Airy coordinate, we do not need to make any diagonal approximation for the other Green functions and self-energies ( $<$  and  $>$ ). In this non-diagonal case, it is possible to achieve the separation of (3.11) by introducing a ‘joint’ spectral density  $A(\mathbf{p}_\perp, s_1, s_2, \omega)$  defined as the geometrical mean of the spectral densities at  $s_1$  and  $s_2$ . This joint function fully retains the concept of the broken homogeneity and correlated fluctuations at points represented by  $s_1$  and  $s_2$ .

Closely linked to these results is the equivalence of the two Kadanoff–Baym equations in this representation. In the pure case, this suggests that when the time-translation invariance is not destroyed, the two equations give the same information, as is the case for the equilibrium systems.

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