QUANTUM PHYSICS OF RETARDED TRANSPORT

J. Barker

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Abstract: Many problems in hot electron physics, in particular the transport properties of sub-micron devices, involve space and time scales such that the semi-classical Boltzmann transport theory is invalid. Here we examine the temporal and spatial retardation effects associated with the evolution of the microscopic Wigner distributions for carriers using many-body Green function techniques applicable to inhomogeneous high field quasi-particle transport.

1. Introduction: Boltzmann transport theory is widely deployed in hot electron physics, yet there are a number of circumstances where its validity is questionable [1,2,3] and we have to make recourse to a deeper theory. In the present paper we attempt to focus on a particular problem: the spatio-temporal response of the carrier and phonon distribution functions. It is already well appreciated that the macroscopic integrals of motion e.g. average velocity, temperature, calculated within the Boltzmann theory, show retardation effects in space and time when the conditions for a steady state are violated, or when the driving fields have high frequency components [1,4]. Thus overshoot and other transient relaxation effects occur on time scales for which the considered transit time is less than or comparable to the classical momentum and energy relaxation times within the system. In these circumstances the time evolution of the average response is not Markovian: some memory of the initial transients and state preparation persists. An extreme case is the idealised situation of true ballistic transport where it is supposed that no collisions occur so that the carrier dynamics are strictly time-reversible [4,5]. On the other hand, overshoot, ballistic transport etc cannot be rigorously handled by Boltzmann transport theory because the time/space scales on which these effects occur, are generally too short for the Boltzmann equation itself to be valid, although the required modification may only be perturbative [6-8]. In previous
studies [1-8], the emphasis has been on the retarded quantum transport physics of bare electrons and phonons within a homogeneous region of semiconductor material. But in sub-micron configured high field devices, where transient effects are the norm, it is not sufficient to consider the intra-device volume alone. For example, carriers within the device volume are generally swept into the channel from states within the contact regions where the land structure, scattering environment and electric fields are very different from the channel itself. This is also true for hot electron injection from semiconductors at insulators and vice-versa. Now within any homogeneous region it is usual to describe the carrier/phonon states as re-normalised states, particularly in polar media where the dressing effects of the screening, and electron-phonon interactions may be substantial in so far as they effect the quasi-particle masses and lifetimes, and indeed the effective strength of the quasi-particle scattering interactions. The question which we wish to address concerns how the "memory" of the dynamical states of carriers/phonons within a source region (e.g. a contact) is lost or preserved when the carriers/phonons are swept into a different channel region. This and related questions cannot be posed within Boltzmann transport theory, nor indeed within the previously deployed quantum kinetic equations [2] based on single time Green functions (Wigner functions). Instead we shall use the language of non-equilibrium double-time thermodynamic Green functions first studied for linear transport problems by Kadanoff and Baym [9]. The structure of the general non-linear theory is outlined in an accompanying paper [10]. Here we focus on the nature and origin of the retardation of response to inhomogeneous systems of coupled electrons and phonons.

2. The exact quantum transport equations

Following our previous studies [2], we work entirely with the single carrier Wigner distribution \( f(p,R,t) \), which is related to the more fundamental double-time retarded Green function \( G^R(1,1') \) where \((1,1') \equiv (r_1,t_1;r_2,t_2)\) or in terms of Wigner coordinates: \( R = (r_1 + r_2)/2, r = r_1 - r_2, T = (t_1 + t_2)/2, t = t_1 - t_2 - \)

\[
G^R(r,t;R,t) = \int \frac{d\omega}{2\pi} G^R(p,\omega;R,T) \left\{ \int d^3re^{-ip\cdot r} \langle \psi^+(R-r/2,T)\psi(R+r/2,T) \rangle \right\}
\]

where \( \psi^+ \), \( \psi \) are electron field operators defined within the Heisenberg representation such that the ensemble average \( < > \) involves a many body trace over the initial system density matrix at time \( T = 0 \). It is supposed here for simplicity that the external fields are initiated at \( T > 0 \), so that \( \psi, \psi^+ \) evolve under a Hamiltonian which contains the coupling to an external applied potential \( \phi_a(R,T) \). Note that \( G^R(p\omega RT) \) is the space-time Fourier transform over the relative coordinates \( n,t \) of
\[ G^R(x,t;RT) \] We also observe that \( G^R \) and the advanced Green function \( G^A \) are related to the full Green function \( G \) defined by

\[ G(1,1') = -i \langle \hat{T} \psi(1) \psi^+(1') \rangle \] (2)

where \( \hat{T} \) is the fermion time-ordering operator, \( G, G^R, G^A \) maybe most conveniently analysed by constructing equation of motion for an analogous imaginary time Green function \( G(1,1',S) \) defined by:

\[ G(1,1',S) = -i \langle \hat{T} S \psi(1) \psi^+(1') \rangle / \langle \hat{T} S \rangle \] (3)

where

\[ S = \exp[-\int_{t_0}^{t_o-i\beta} d\phi_\alpha(2)n(2)] \] (4)

\( n(2) \) is the number density operator, \( \beta = 1/kT \) (initial temperature), and the times are defined in the imaginary time domain: \( 0 < i(t-t_o) < \beta \) (\( t_o \) real). \( G(1,1',S) \) involves a system evolving from an inhomogeneous equilibrium density matrix

\[ \rho = \exp[-\beta(H + \int dr n(x,t) \phi(x,t))] \] (5)

It maybe shown [9,11,12], that \( G(1,1') \) is just the analytic continuation of \( G(1,1',S) \) to the real time domain provided \( t_o \rightarrow -\infty \).

The equation of motion for \( G(1,1',S) \) may be formally derived by functional derivative techniques to have an "apparently" closed form by introducing the self-energy \( \Sigma \) for the carriers:

\[ [i\partial_{l_1} + \gamma^2/2m - \phi(l,t_o)]G(1,1',S) = \delta(1-1') + \int_{t_o}^{t_o-i\beta} dl'' \Sigma(1,1'',S)G(1'',1',S) \] (6)

where \( \phi \) is the effective total driving potential comprising the induced field potentials plus the applied potential. If we perform the analytic continuation, the exact equation of motion for \( G^R(pw;RT) \) is obtained from:

\[ [i\partial_{l_1} + i\partial_{l_1} - \gamma^2/2m - \phi(l) + \phi(l')]G^R(1,1') = \]

\[ \int_{-\infty}^{t_1} dl'' \Sigma^R(1,1'')G^R(1'',1') \]

\[ + \int_{-\infty}^{t_1} dl'' \Sigma^R(1,1'') (G^A - G^R)[1'',1'] \]

\[ - \int_{-\infty}^{t_1} dl'' \Sigma^R(1,1'') (G^A - G^R)[1'',1'] \]

\[ - \int_{-\infty}^{t_1} dl'' \Sigma^R(1,1'') (G^A - G^R)[1'',1'] \] (7)
3. The Boltzmann limit

The Boltzmann transport theory may be recovered from (7) by: (a) assuming slowly varying disturbances; (b) taking the asymptotic limit \( T \rightarrow \infty \). Let us first examine the appearance of the local driving force, i.e. of the normal form

\[
[\partial_T + v \cdot \partial_R + eE \cdot \partial_D]f(p, R, T) \tag{8}
\]

We note first that the LHS of (7) has the Wigner coordinate form:

\[
[i\partial_T + \partial_R \cdot \mathbf{x}]/\hbar - \phi(R + x/2, T + t/2) + \phi(R - x/2, T - t/2)]G^R_{\omega R T} \tag{9}
\]

In thermal equilibrium, the undressed version of \( G^R \) is diagonal, and has a spatial range of the order of a thermal wavelength \( \lambda \sim (\hbar^2/2m)^{1/2} \), and a temporal decay time of the order \( \hbar^2/2m \).

The local homogeneity approximation (LHA) [1], this supposes that if \( \phi \) varies slowly on these scales, we may expand \( \phi \) in a Taylor series to lowest order:

\[
\phi(R + x/2, T + t/2) \approx (1 + x/2 \partial_R + t/2 \partial_T) \phi(R, T) \tag{10}
\]

The driving term for \( f(p, R, T) \) is then easily obtained as expression (8). More generally, one should use the exact form:

\[
[\partial_T + (2/\hbar)H(p, R, T) \sin(\hbar \Lambda/2)]G^R_{p, \omega R T} \tag{11}
\]

where \( H = p^2/2m + \phi(R, T) \); \( \Lambda \equiv \partial_R \cdot \partial_R + \partial_D \cdot \partial_D + \partial_T \cdot \partial_T \). \( \Lambda \) is the generalised Poisson bracket operator [10]. Expression (10) is exact for constant, uniform fields.

If we use the LHA on the driving terms, and neglect all quantities of order \( t, r \) compared to \( R, T \) the RHS of (8), we find:

\[
[\partial_T + v \cdot \partial_R + \partial_D \cdot \partial_D + \partial_T \cdot \partial_T]G^R(p, \omega, R, T) =
\]

\[
G^A(p, \omega, RT) I^R(p, \omega, RT) - G^R(p, \omega, RT) I^A(p, \omega, RT) \tag{12}
\]

Now \( G^R \) is related to \( G^A \) via the special function \( A(p, \omega, RT) \)

\[
A = G^R - G^A \tag{13}
\]

From the equation of motion for \( G^R \) and \( G^A \) we thus obtain, within the same approximation:

\[
[\partial_T + v \cdot \partial_R + \partial_D \cdot \partial_D + \partial_T \cdot \partial_T]A = 0 \tag{14}
\]

It may also be shown (exactly) that

\[
G^R = A(p, \omega, RT) f(p, R, T) \tag{15}
\]

The linear transport study by Kadanoff and Baym [6] takes:

\[
A = 2\pi \delta(\omega - p^2/2m + \phi(R, T)) \tag{16}
\]

as the solution to (14). By taking the Born approximation to the self energy it is
then very easy to show that equation (12) reduces exactly to the Boltzmann equation with the aid of (13), (15), (16). This result is a weak coupling result and neglect all quasi-particle effects. Moreover, the deliberate local approximation made to the time and space dependence of the "collision integrals" or the RHS of (17), plus the local solution (16), are primarily responsible for the resulting Markovian (i.e. non-retarded) form of the Boltzmann equation. No intra-collisional field effects are visible despite the appearance of the field in (16).

4. Retarded transport

We have already seen from expression (9) that the driving forces are generally non-local in space and time. Let us now observe that the "collision" terms are ratio retarded. The appearance of retardation is intimately related to the degree of dissipativity within the system. Boltzmann transport is a dissipative theory; collisions occur as point events which are completed irreversibly.

To see how the collision integral contains retardation, let us go back to equation (7), and look at the limit $t = t_1 - t_1' + 0$, which we need to obtain the Wigner distribution $f$. Let us keep the same approximation for the spatial dependence of $E$, $G$ but treat the time-dependence exactly. The equivalent of the RHS of equation (12) is then found to be

$$2 \int_{-\infty}^{T} d\omega' d\omega'' \exp \left[ 2i(\omega' - \omega'')(T - \tau) \right] + c.c \times$$

$$\left\{ \mathcal{L}^A(p\omega', R, \tau) G^R(p, \omega'', R, \tau) - \mathcal{L}^R G^A \right\}$$

The asymptotic limit is now easily seen: if we let $T \to \infty$, the exponential factors collapse to a representation of a $\delta$-function, describing the conservation of energy:

$$2 \int_{-\infty}^{T} d\omega' d\omega'' \delta(\omega' - \omega'') \left\{ \mathcal{L}^A G^R R^A \mathcal{R}^R \right\}$$

Neglect of the time variation in the earlier approximation is thus equivalent to a time-coarse graining of the system.

We next observe that the asymptotic limit cannot be taken without examining the asymptotic behaviour of $E$ and $G$. Indeed since both $E$ and $G$ can be expressed entirely in terms of the spectral function $A(p\omega RT)$ and the Wigner function $f(p\omega RT)$ (and the phonon distribution in general cases), to get an explicit form for the collision integral we must have an approximation for $A$. If we go back to equation (14) for example, it is obvious that Kadanoff and Baym's solution is not correct except for thermal equilibrium. To see this we transform equation (14) to path variable form [2]:

$$\frac{d}{d\tau} A[p(\tau), R(\tau), T(\tau), \omega(\tau)] = 0$$
where \( \frac{dT}{d\tau} = 1; \frac{dR}{d\tau} = p(\tau)/m; \frac{dp}{d\tau} = -\partial_{R}\phi(R(\tau),T(\tau)); \frac{d\omega}{d\tau} = \partial_{R}\phi(R,T). \) The general solution to (19) is in fact \( A(t) = \text{constant}. \) Thus if \( A \) has the boundary condition (initial) value \( A = 2\pi(\omega-e[p]), \) \( e[p] = p^2/2m \) we find:

\[
A(p,\omega,R,T) = 2\pi \delta(\omega - e[p])
\]

where the tildas refer to retarded quantities:

\[
\tilde{p} = p - \int_{0}^{T} dt eE(R(\tau),\tau)
\]

If eqn (20) is inserted into the Born approximation for \( \Sigma, \) and then into equation (17) we recover exactly the generalised kinetic equation of Barker and Ferry [3], showing the temporal retardation of the position, momentum and time dependence of the differential scattering rates plus the intra-collisional field effect [1]. For electron-phonon scattering the equation for \( f \) reads (homogeneous case):

\[
[\partial_{T} + eE \partial_{p}] f = \int_{0}^{T} dt \int_{p}^{p'} \{ S(\tilde{p},\tilde{p}',\tau)f(\tilde{p}',T-\tau) - S(\tilde{p}',\tilde{p},\tau)f(\tilde{p},T-\tau) \}
\]

\[
S(\tilde{p},\tilde{p}') = Re \frac{2\pi}{\hbar} \frac{1}{\epsilon(q)} \exp \left[ -\frac{(T-\tau)}{\tau_{e}} \right] (N_{q} + \frac{1}{2} + \frac{1}{2}) |V(q)|^{2} \delta_{p,p'} + \eta \tilde{p}
\]

\[
\exp[-i \int_{T}^{T'} dt eE(\tau)\{ e[p(\tau')] - e[p'(\tau')] + \eta \delta_{p,p'} \}]
\]

\[
\tilde{p}(\tau) = p - \int_{0}^{T} dt eE(\tau')
\]

In this case, taking the asymptotic limit \( T \to \infty, \) does not recover the sharp energy conservation of Boltzmann transport theory even for constant uniform fields, because the scattering is described between accelerating states; the states \( p, p' \) are thus shifted and smeared out by level shift and broadening effects due to the transition induced by the field within the collision duration [1].

5. Quasi-particle effects

Let us now relax the spatial approximations to \( \Xi \) and \( G \) made in sections 3,4. We first evaluate these quantities at the same level of approximation as the driving terms i.e. use the LHA. Thus terms such as \( G(x',R-(x-x'))/2 \) which appear in (7) are approximated by

\[
G = G(x',R) - \frac{1}{2}(x-x') \partial_{R}G(x',R)
\]

The second term in (25) contributes two additional terms to equation (17). One has an asymptotic limit in the form of a Poisson bracket:

\[
-(Re\xi(pwRT), G_{R}(pwRT))
\]

where
\[
\{a, \beta\} = \sum_\omega a_\omega \beta^*_\omega - \sum_\omega a_\omega \beta - \sum_\omega a_\omega^*_\beta + \sum_\omega a_\omega^* \beta
\]  
(27)

Consequently, the terms in \(a_{\omega G}, a_{
\omega R}, a_{\omega P}\) can be returned to the RHS of equation (17) so as to renormalise the driving terms. Only one of these terms will be discussed here: the term in \(a_{\omega R}, \text{Re} \tilde{\omega} \tilde{a}_{\omega R}\). This term essentially renormalises the base velocity \(v = \frac{p}{m}\) to the quasi-particle velocity \(v \rightarrow \frac{p}{m} + \text{Re} \tilde{\omega}\). A similar modification follows through in the equation of motion for the spectral function. If the asymptotic limit is not taken we find that the quasi-particle velocity has a \emph{retarded} form with the structure.

\[
v = \frac{p}{m} + \int_{-\infty}^{T} d\tau M(\tau, \tau)
\]  
(28)

where \(M\) is a memory functional. If the driving fields are strong or vary rapidly in time \(v\) is found to reduce to \(\frac{p}{m}\). Only when the fields are slowly perturbative (adiabatic) does the equilibrium quasi-particle behaviour appear.

In addition, a further term is contributed by (25) which in its asymptotic form adds to (25) a term:

\[
(\text{Re} G_l) \tilde{l}\n\]
(29)

This asymptotic form describes the decay of initial correlations in the initial state at \(T = 0\). It does not appear to be significant for low frequency transport, but is dominant for frequencies in excess of the collisional relaxation frequencies \((\omega_{\tau} \gg 1)\) or for high magnetic fields \((\omega_{\tau} \gg 1)\). A discussion of this contribution has been given from a different point of view in ref. [1].

A rigorous treatment of the exact equation (7) has been made recently [12]. It requires that the basic modelling involve a dynamical approximation to the self-energy \(\Sigma\). The spectral functions and initial state are then evaluated self consistently with this approximation so as to validate the microscopic conservation laws (Ward identities [1]). In addition the level of time-space coarse graining (e.g. the LHA) is decided by examining within the model which time-space scale variations in the field or the heterojunction structure are comparable with the intrinsic time-space scales for quasi-particle dressing. As an example we quote the results for the case where the fields are sufficiently to modify energy conservation within collisions, but do not destroy the quasi-particle structure: this case assumes a homogeneous medium, but not necessarily homogeneous transport. We find that the dominant retardation process is fully described by the Barker-Ferry eqns. [3], but the momentum states appearing on the driving terms (group velocity) and collision integrals are modified to the field-dependent quasi-particle velocities. In addition the retarded collision integrals are modified by a quasi particle expotential decoy term. The latter is easily evaluated by solving for the spectral function from the rigorous equation of motion.
\[ \left( \frac{\partial}{\partial t} + v \cdot \nabla \right) \varphi - \nabla \cdot \left( \nabla \varphi + \varphi \nabla \omega \right) \right] A = \{ \text{Re} \Sigma, A \} + \{ \text{Re} G, \Gamma \} \quad (30) \]

where $\Gamma = \Sigma^A - \Sigma^R$ is the imaginary part of the self energy.

The resulting equations show for example, that the polaronic carriers in weak coupling media, are progressively stuffed to the bare land mass states (accelerating states) as high fields accelerate carriers beyond the often phonon threshold.

On the question of self-consistency, we find that the Born approximation to $\Sigma$ is never valid (see also [1]), but one can use the generalised Born approximations. The latter uses a self consistent form for the spectral function in the expression for the self energy, unlike the Born approximation which use the free carrier form. The effect is to give collisional level shifts in the energy conservation and to broaden the sharp energy conservation due to quasi-particle lifetime effects.

6. References