Electron transport in semiconductors

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Previous calculations of macroscopic electron transport based on an exact integro-differential equation of motion yield a set of three coupled equations. These were solved with the assumption of a single thermalizing time. We show that when we supplement the three equations with a generalized Fokker-Planck equation their solution is fully determined without the additional assumption. The final result is the same thermalizing processes and macroscopic transport coefficients as reported earlier.

In two previous publications the density matrix propagator of a single electron interacting with lattice vibrations was given by the Fourier representation[1,2]

$$\rho_w(\vec{r},\vec{u};\vec{r}_0,\vec{u}_0;t) = (2\pi)^{-6}\int\int d^3k\, d^3w \exp[i\vec{k}\cdot(\vec{u}-\vec{u}_0e^{-\beta t})] \times e^{i\vec{w}\cdot\vec{P}}\hat{p}(\vec{k},\vec{w},t) \ , \tag{1a}$$

$$\vec{P}\equiv\vec{r}+\frac{\vec{u}}{\beta}-\vec{r}_0-\frac{\vec{u}_0}{\beta} \ , \tag{1b}$$

$$\hat{p}(\vec{k},\vec{w},t)\equiv\exp F \ , \tag{1c}$$

$$F\equiv-\tfrac{1}{2}[B(t)k^2-2H(t)\vec{k}\cdot\vec{w}+A(t)w^2] \ . \tag{1d}$$

Here $\vec{r},\vec{u}$ are the electron's position and velocity Wigner coordinates at final time t, and $\vec{r}_0,\vec{u}_0$ at initial time zero, and we are retaining dimensions. Upon asymptotic expansion in wave vectors $\vec{k}$ and $\vec{w}$ three coupled differential equations for the functions $A(t)$, $B(t)$, $H(t)$ were obtained from the original Liouville equation of motion.

In our development we have made for convenience one assumption right from the beginning, namely, that the initial velocity $\vec{u}_0$ would be thermalized as $\vec{u}_0e^{-\beta t}$, β^{-1} a thermalizing time. By convenience we mean that the assumption allowed us to carry through all steps, including the transformation to Wigner variables in the many-coordinate formulation in II in a prescribed way, and extract a solution to the Liouville equation. We are not concerned here with the exponential form for thermalizing $\vec{u}_0$. Perusal of II will indicate that other functional forms are not possible if a "closed" propagator depending only on the overall time t, i.e., a density function, is to exist. However, if we make no assumptions about time constants in $B(t)$ and $H(t)$ then we find that our asymptotic procedure for finding ρ leaves us with three coupled equations for $A(t)$, $B(t)$, $H(t)$, with yet a fourth unknown, the extraneous parameter β.

Some additional information must be introduced. One obvious requirement is physical continuity. However, we shall show below that this follows automatically from our equations for A, B, and H. In I we suggested resorting to some general statistical result, such as a Maxwell distribution for electron velocities. However, such statistical results actually only apply when particles interact weakly, and here their insertion leads to error when the coupling is not vanishingly small (see II). In II it was taken for granted that the exponential decays found in $B(t)$, $H(t)$ also depict thermalizing processes, and must be characterized by the same β^{-1} as the thermalization of the initial velocity $\vec{u}_0$ in the formal solution, Eqs. (1). This procedure leads to a unique asymptotic solution. Since the question of the uniqueness of the solution plays such a key role in our arguments, a more complete treatment appears worthwhile. The utilization of a (single) thermalizing time was inspired by classical Brownian motion, and the Smoluchowski and Fokker-Planck equations. We shall turn to these equations, and their derivation, and, thereby, succeed in resolving the situation.

The three equations determining $A(t)$, $B(t)$, $H(t)$ are [Eqs. (6.5), (D.1), (D.2) in II]:

$$\frac{\dot{B}(t)}{2}+\Omega B(t)=Z \ , \tag{2a}$$

$$\beta B(t)+\dot{H}(t)+\Omega[H(t)-B(t)]=Y-Z \ , \tag{2b}$$

$$-\frac{\dot{A}(t)}{2}+(\Omega-\beta)H(t)=Y \ . \tag{2c}$$

In the notation of II, Ω, Y, Z are defined by

$$\Omega\equiv-G_2(1-e^{\beta T}) \ , \tag{3a}$$

$$Y\equiv G_1+G_2(A_2+H_2e^{\beta T}) \ , \tag{3b}$$

$$Z=G_2(H_2+B_2e^{\beta T})-G_1(e^{-\beta T}) \ , \tag{3c}$$

where, as in II, $T=t-s$, $A_2=A(t-s)$, etc., and G_1, G_2 imply integration over s from $-\infty$ to t of all functions of s in G_1 and G_2 themselves or appearing on their right. Thus, as in II, Ω, Y, Z are constants independent of t, since T goes from $-\infty$ to 0. The solution of these three differential equations subject to $A(0)=B(0)-H(0)=0$ is

$$\frac{\Omega A(t)}{2}=\beta t\left(\frac{\beta Z}{\Omega}-Z-Y\right)-\frac{(\Omega-\beta)}{\Omega^2}\{(2\beta Z-\Omega Z-\Omega Y)(e^{-\Omega t}-1)+\tfrac{1}{2}Z(\Omega-\beta)(e^{-2\Omega t}-1)\} \ , \tag{4a}$$

$$\Omega B(t)=Z(1-e^{-2\Omega t}) \ , \tag{4b}$$

$$\Omega H(t)=\left(Y-\frac{\beta Z}{\Omega}\right)(1-e^{-\Omega t})+(\beta-\Omega)Z(1-e^{-\Omega t})\frac{e^{-\Omega t}}{\Omega} \ . \tag{4c}$$

In Wigner variables continuity takes the form[1]

$$\frac{\partial}{\partial t}\int \rho_w(\vec{r},\vec{u};t)d^3u+\int \vec{u}\cdot\vec{\nabla}_r\rho_w(\vec{r},\vec{u};t)d^3u=0 \quad . \tag{5}$$

Substituting from Eqs. (1) into (5) we obtain

$$\beta B(t)+\beta H(t)+\tfrac{1}{2}\dot{B}(t)+\dot{H}(t)+\tfrac{1}{2}\dot{A}(t)=0 \quad . \tag{6}$$

We note that Eq. (6) follows directly by subtracting both sides of Eq. (2c) from the sums of both sides of Eqs. (2a) and (2b).

The development of the Fokker-Planck equation in both variables $\vec{r}$ and $\vec{u}$ incorporates letting $\vec{\Delta}r$ be given by $\vec{u}\Delta t$ in the distribution functions,[3] a procedure which lacks justification in a quantum calculation. However, if we integrate the distribution function over spatial coordinates, the corresponding development in u only becomes relevant. For a Markovian process one has the "Smoluchowski equation,"

$$\rho(\vec{u}_{N+1},\vec{u}_0;t+\tau)=\int \rho(\vec{u},\vec{u}_N;\tau)\rho(\vec{u}_N,\vec{u}_0;t)d^3u_N \quad , \tag{7}$$

where ρ is the propagator for velocity distribution functions. If we take τ small we obtain the differential equation[4]

$$\rho(\vec{u},\vec{u}_0;t)+\frac{\partial\rho}{\partial t}\tau=\int \rho(\vec{u},\vec{u}-\vec{\Delta}u;\tau) \times(\vec{u}-\vec{\Delta}u,u_0;t)d^3(\Delta u) \quad . \tag{8}$$

Expansion in $\vec{\Delta}u$ then leads to a Fokker-Planck equation. In our problem of an electron in a lattice we do not in general have Markovian factorization. The previous differential equation assumes the more general form

$$\rho(\vec{u},\vec{u}_0;t)+\frac{\partial\rho}{\partial t}\tau=\int \rho(\vec{u},\vec{u}-\Delta u,\vec{u}_{N-1},\ \ldots\ \vec{u}_0;t+\tau) \times d^3(\Delta u)d^3u_{N-1}\ldots d^3u_1 \quad . \tag{9}$$

Here

$$\rho(\vec{u},\vec{u}-\vec{\Delta}u,\vec{u}_{N-1},\ \ldots\ \vec{u}_0;t+\tau)$$

is the "open" propagator, i.e., the propagator in all $(N+1)$ $\vec{u}$ variables, obtainable from a path-integral kernel by integrating over all spatial coordinates. Underlying this derivation of the Fokker-Planck equation is that an "open" kernel exists, from which $\rho(\vec{u},\vec{u}_0;t)$ can be computed as a path integral. By definition, the path integral goes to a limit as the number of time intervals goes to infinity. If the left side of Eq. (9) represents $\rho(\vec{u},\vec{u}_0;t)$ calculated by dividing the propagation time t into N intervals, the right side implies $(N+1)$ intervals. This procedure is diammetrically opposed to the one used in II, where the time intervals were flexible, but their number was kept constant.

We now proceed by formally Fourier representing $\rho(\vec{u}_{N+1},\vec{u}_N\ \ldots\ \vec{u}_0;t)$, and again making a Taylor expansion in $\vec{\Delta}u$. We can focus on the small wave-vector components in the resulting linear differential equation. Here a Fourier representation of the open propagator is available from II. Because of our restriction to linear and quadratic terms in the wave vector we cut the expansion off at the second moment, as is usual. We shall not go explicitly through all the details with a many coordinate formulation as was done in II. What is relevant here is that a generalized Fokker-Planck equation can be written down. It serves to provide the needed information for a unique solution when an *a priori* thermalizing time is introduced, as we have done. Our further analysis serves as an illustration of this point.

We are now ready to complete the solution of our problem following the same kind of argument as in II. First we assume that the functions called $A_3(t)$, $B_3(t)$, $H_3(t)$ given there vanish. This assumption leads to a Markovian factorization of the propagator, reducing the generalized Fokker-Planck equation to its usual form. The well-known solution of this equation with a delta function initial condition is given by[9]

$$\rho(\vec{u},\vec{u}_0;t)=[2\pi B_{NN}(1-e^{-2\beta t})]^{-3/2} \times\exp\left[-\frac{(u-u_0e^{-\beta t})^2}{2B_{NN}(1-e^{-2\beta t})}\right] \quad . \tag{10}$$

The usual parameter q measuring the velocity fluctuation is here given by βB_{NN}, where B_{NN} is the leading coefficient in the Fourier representation of $\rho(\vec{u}_N,\vec{u}_{N-1}\ \ldots\ \vec{u}_0;t)$ (see II). We note that $\rho(\vec{u},\vec{u}_0;t)$ contains only one thermalizing time.

Upon integrating Eq. (1) over space variables we find that the general form for $\rho(\vec{u},\vec{u}_0;t)$ is given by

$$\rho(\vec{u},\vec{u}_0;t)=[2\pi B(t)]^{-3/2}\exp\left[\frac{-(\vec{u}-\vec{u}_0e^{-\beta t})^2}{2B(t)}\right] \quad . \tag{11}$$

Referring to Eq. (4b) and noting Eq. (10) we see that

$$\Omega=\beta \quad . \tag{12}$$

Equations (3a) and (12) yield Eq. (6.6G) in II, and with $\Omega=\beta$, Eqs. (4a) to (4c) also reduce to the previous results for $A(t)$, $B(t)$, $H(t)$, i.e., Eqs. (6.6a) to (6.6f) in II. Finally, as in II, we argue that since the more general problem, that is when A_3, B_3, H_3 are initially allowed to exist and the Fokker-Planck equation has its general form, again has a unique solution, that solution must be the one we are proposing here. This solution represents the asymptotic (macroscopic steady-state) limit, making use, as explained, of u thermalizing as $\exp(-\beta t)$. The calculation not only provides quantum formulae for finding the transport coefficients, but we view it as a basis for more detailed studies, for example, for obtaining initial transient behavior.

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