The Equilibrium Wigner Function in the Case of Nonparabolic Energy Bands

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Summary. By solving the Bloch equation the expression of the equilibrium Wigner function is obtained up to first order in the scaled Planck constant for arbitrary energy bands.

1 Introduction

Due to the extreme miniaturization of the electron devices, the simulation requires advanced transport models that take into account also quantum effects.

In [1] a model based on the maximum entropy principle has been proposed by including the quantum corrections with a Chapmann–Enskog expansion starting from the Wigner equation. In the drift-collision dominated regime an explicit form of the Wigner function has been obtained up to first order in the square of the scaled Planck constant in the effective mass approximation. A key point is constituted by the equilibrium Wigner function. It has been determined for the first time in [3] in the effective mass approximation while in [2] a procedure based on the Bloch equation has been devised.

In the present paper we write the Bloch equation for an arbitrary energy band assuming that it is defined in all the space, as appropriate for some analytical approximations like Kane's dispersion relation. The free streaming pseudo-differential operator is defined as a multiplication operator in the space of Fourier transforms. The general form of the solution up to second order terms in the scaled Plank is determined. In the case of the Kane dispersion relation an explicit formula is given and it shown that, at variance with the parabolic band, a quantum correction is present even in the bulk case.

2 The Bloch Equation

The physical situation is represented by an electron gas which is in equilibrium with a thermal bath of phonons at a constant temperature T_L. We suppose

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that the energy bands are represented by a function $\mathcal{E}(p)$ defined in $\Re^3$, which depends only on the modulus of the crystal momentum p and it is even. Several analytical approximation as the parabolic band and the Kane dispersion relation satisfy the previous conditions. Moreover we will work in the single electron approximation.

Under the previous assumptions the system is described by the density matrix $\rho(r,s)$ with r,s position vectors belonging to $\Re^3$. If we denote by H the Hamiltonian, the equilibrium is parametrized by the inverse of the temperature $\beta = \frac{1}{k_B T_L}$ and is defined, in the Boltzmann limit of the Fermi-Dirac statistics, by $\rho^{(eq)}(r,s,\beta) = \exp(-\beta H)$, where of course the exponential must be intended in the operatorial sense. Expanding the exponential gives an approximation of $\rho^{(eq)}(r,s,\beta)$ but the procedure is rather cumbersome.

An alternative way has been devised in [2]: starting from the Schrödinger equation one derives the following equation for the equilibrium density matrix $\rho^{(eq)}(r,s,\beta)$

$$\frac{\partial}{\partial \beta}\rho^{(eq)}(r,s,\beta) = -\frac{1}{2}\left(H\rho^{(eq)} + \rho^{(eq)}H\right), \tag{1}$$

called the Bloch equation, augmented by the condition $\rho^{(eq)}(r,s,0) = \delta(r-s)$

The Hamiltonian H is given for a general energy band $\mathcal{E}$ by

$$H(x,p) = \mathcal{E}(p) - qV(x) - \Phi \tag{2}$$

with q absolute electron charge and V the electrostatic potential. Φ is the quasi Fermi potential which is constant at equilibrium. In an operatorial sense $\mathcal{E}(p)$ acts as $\mathcal{E}(-i\hbar\nabla_x)$, e.g. in the parabolic case $\mathcal{E}(p) = p^2/(2m^*)$ the corresponding operator is $-(\hbar^2/2m^*)\Delta_x$, m^* being the effective electron mass. In the sequel in order to simplify the notation the same symbol will be used both for the operator and its symbol.

After the change of variables

$$\begin{cases} r = x + \frac{\hbar}{2}\eta, \\ s = x - \frac{\hbar}{2}\eta \end{cases}$$

we introduce the Wigner function

$$w(x,p,t) = \mathcal{F}^{-1}[\rho(r,s,t)](x,p,t) = \frac{1}{(2\pi)^3}\int_{\Re^3_\eta} \rho\left(x + \frac{\hbar}{2}\eta, x - \frac{\hbar}{2}\eta\right) e^{ip\cdot\eta}\, d\eta,$$

with $\mathcal{F}$ the Fourier transform and $\mathcal{F}^{-1}$ its inverse. In particular $w^{(eq)}(x,p,\beta)$ is the equilibrium Wigner function given by $\mathcal{F}^{-1}[\rho^{(eq)}](x,p,\beta)$.

By substituting the expression of H into (1) and applying $\mathcal{F}^{-1}$ one has

$$\begin{aligned} \frac{\partial}{\partial \beta} w^{(eq)}(x,p,\beta) = & -\frac{1}{2}\mathcal{F}^{-1}\left[\mathcal{E}(-i\hbar\nabla_r)\rho^{(eq)} + \mathcal{E}(-i\hbar\nabla_s)\rho^{(eq)}\right] \\ & + \frac{q}{2}\mathcal{F}^{-1}\left[\left(V(r) + V(s)\right)\rho^{(eq)}\right] + \Phi w^{(eq)}. \end{aligned} \tag{3}$$

By introducing the convolution operator $f * g = \int f(x-t)g(t)dt$, we have

$$\begin{aligned}
&\mathcal{F}^{-1}\left[(V(r)+V(s))\,\rho^{(eq)}\right](x,p,\beta)\\
&= \mathcal{F}^{-1}\left[(V(r)+V(s))\right] * w^{(eq)}(x,p,\beta)\\
&= \int_{\Re^3_q} \mathcal{F}^{-1}\left[(V(r)+V(s))\right](x,p-q,\beta)w^{(eq)}(x,q,\beta)\,dq\\
&= \frac{1}{(2\pi)^3}\int_{\Re^3_q\times\Re^3_\eta}[V(x+\frac{\hbar}{2}\eta)+V(x-\frac{\hbar}{2}\eta)]w^{(eq)}(x,q,\beta)e^{i(p-q)\cdot\eta}dqd\eta.
\end{aligned} \tag{4}$$

Similarly, since $i\hbar\nabla_r = i\frac{\hbar}{2}\nabla_x + i\nabla_\eta$ and $i\hbar\nabla_s = i\frac{\hbar}{2}\nabla_x - i\nabla_\eta$, by taking into account that p and η are conjugate variables, we define

$$\begin{aligned}
&\mathcal{F}^{-1}\left[\mathcal{E}(-i\hbar\nabla_r)\rho^{(eq)} + \mathcal{E}(-i\hbar\nabla_s)\rho^{(eq)}\right](x,p,\beta)\\
&= (2\pi)^{-3}\int_{\Re^3_\nu\times\Re^3_{x'}}\left[\mathcal{E}\left(p+\frac{\hbar\nu}{2}\right)+\mathcal{E}\left(p-\frac{\hbar\nu}{2}\right)\right]\\
&\quad w^{(eq)}(x',p,\beta)e^{i(x-x')\cdot\nu}\,d\nu dx'.
\end{aligned} \tag{5}$$

By expanding up to first order in $\hbar^2$, one has

$$\mathcal{E}\left(p+\frac{\hbar\nu}{2}\right)+\mathcal{E}\left(p-\frac{\hbar\nu}{2}\right) = 2\mathcal{E}(p) + \frac{1}{4}\frac{\partial^2\mathcal{E}}{\partial p_i\partial p_j}\nu_i\nu_j\hbar^2 + o(\hbar^2),$$

$$V(x+\frac{\hbar}{2}\eta)+V(x-\frac{\hbar}{2}\eta) = 2V(x) + \frac{1}{4}\frac{\partial^2 V}{\partial x_i\partial x_j}\eta_i\eta_j\hbar^2 + o(\hbar^2),$$

where summation over repeated indexes is understood, and the Bloch equation up to first order in $\hbar^2$ reads

$$\begin{aligned}
\frac{\partial}{\partial\beta}w^{(eq)}(x,p,\beta) &= -\mathcal{E}(p)w^{(eq)}(x,p,\beta) + \frac{\hbar^2}{8}\frac{\partial^2\mathcal{E}}{\partial p_i\partial p_j}\frac{\partial^2 w^{(eq)}(x,p,\beta)}{\partial x_i\partial x_j}\\
&+qV(x)w^{(eq)}(x,p,\beta) - \frac{q\hbar^2}{8}\frac{\partial^2 V}{\partial x_i\partial x_j}\frac{\partial^2 w^{(eq)}(x,p,\beta)}{\partial p_i\partial p_j} + \Phi w^{(eq)}(x,p,\beta),
\end{aligned} \tag{6}$$

with initial condition $w^{(eq)}(x,p,0)=1$.

3 The Equilibrium Wigner Function

We look for a solution of (6) of the form

$$w^{(eq)}(x,p,\beta) = w^{(0)}(x,p,\beta) + \hbar^2 w^{(1)}(x,p,\beta) + o(\hbar^2).$$

At zero order (6) gives

$$\frac{\partial}{\partial\beta}w^{(0)}(x,p,\beta) = -\mathcal{E}(p)w^{(0)}(x,p,\beta) + qV(x)w^{(0)}(x,p,\beta) + \Phi w^{(0)}(x,p,\beta).$$

where from $w^{(0)}(x,p,\beta) = \exp[-\mathcal{E}(p)\beta + \beta(\Phi + qV(x))]$.

At first order in $\hbar^2$ (6) gives

$$\frac{\partial}{\partial \beta} w^{(1)}(x,p,\beta) = -\mathcal{E}(p) w^{(1)}(x,p,\beta) + \frac{1}{8} \frac{\partial^2 \mathcal{E}}{\partial p_i \partial p_j} \frac{\partial^2 w^{(0)}(x,p,\beta)}{\partial x_i \partial x_j}$$
$$+ qV(x) w^{(1)}(x,p,\beta) - \frac{q}{8} \frac{\partial^2 V}{\partial x_i \partial x_j} \frac{\partial^2 w^{(0)}(x,p,\beta)}{\partial p_i \partial p_j}$$
$$+ \varPhi w^{(1)}(x,p,\beta). \tag{7}$$

We solve the last equation via separation of constants looking for solution of the form

$$w^{(1)}(x,p,\beta) = g(x,p,\beta) w^{(0)}(x,p,\beta)$$

with the function g satisfying the equation

$$\frac{\partial g}{\partial \beta} = \frac{1}{8 w^{(0)}} \frac{\partial^2 \mathcal{E}}{\partial p_i \partial p_j} \frac{\partial^2 w^{(0)}(x,p,\beta)}{\partial x_i \partial x_j} - \frac{q}{8 w^{(0)}} \frac{\partial^2 V}{\partial x_i \partial x_j} \frac{\partial^2 w^{(0)}(x,p,\beta)}{\partial p_i \partial p_j} \tag{8}$$

and the initial condition

$$g(x,p,0) = 0.$$

One finds

$$g(x,p,\beta) = \frac{q\beta^2}{8} \frac{\partial^2 \mathcal{E}}{\partial p_i \partial p_j} \frac{\partial^2 V}{\partial x_i \partial x_j} + \frac{q^2 \beta^3}{24} \left[\frac{\partial^2 \mathcal{E}}{\partial p_i \partial p_j} \frac{\partial V}{\partial x_i} \frac{\partial V}{\partial x_j} - \frac{\partial^2 V}{\partial x_i \partial x_j} v_i v_j \right], \tag{9}$$

where $v = \nabla_p \mathcal{E}(p)$ is the electron velocity. The equilibrium Wigner equation is therefore given by

$$w^{(eq)}(x,p,\beta) = \exp\left[-\mathcal{E}(p)\beta + \beta\left(\varPhi + qV(x)\right)\right] \left\{ 1 + \frac{q\beta^2 \hbar^2}{8} \frac{\partial^2 \mathcal{E}}{\partial p_i \partial p_j} \frac{\partial^2 V}{\partial x_i \partial x_j} \right.$$
$$\left. + \frac{q^2 \beta^3 \hbar^2}{24} \left[\frac{\partial^2 \mathcal{E}}{\partial p_i \partial p_j} \frac{\partial V}{\partial x_i} \frac{\partial V}{\partial x_j} - \frac{\partial^2 V}{\partial x_i \partial x_j} v_i v_j \right] \right\} + o(\hbar^2). \tag{10}$$

In the particular case of a parabolic band

$$\mathcal{E}(p) = \frac{p^2}{2m^*}, \quad v = \frac{p}{m^*}$$

with m^* electron effective mass, and one obtains the same results as in [3]

$$w^{(eq)}(x,p,\beta) = \exp\left[-\frac{\beta p^2}{2m^*} + \beta\left(\varPhi + qV(x)\right)\right] \left\{ 1 + \frac{q\beta^2 \hbar^2}{8m^*} \Delta V \right.$$
$$\left. + \frac{q^2 \beta^3 \hbar^2}{24 m^*} \left[|\nabla V|^2 - m^* \frac{\partial^2 V}{\partial x_i \partial x_j} v_i v_j \right] \right\} + o(\hbar^2).$$

It is convenient (see for example [1]) to parametrize $w^{(eq)}(x,p,\beta)$ in term of the local density instead of the quasi Fermi potential $\varPhi$.

By defining the density as

$$n(x,t) = \int_{\Re^3_p} w^{(eq)}(x,p,\beta)dp$$

and eliminating $\exp[\beta(qV+\phi)]$, one has

$$w^{(eq)}(x,p,\beta) = \frac{n(x,t)e^{-\beta\mathcal{E}}\exp}{A_0(\beta,m^*)}\left\{1+\hbar^2\left[\left(\frac{q\beta^2}{8}\frac{\partial^2 V}{\partial x_i\partial x_j}+\frac{q^2\beta^3\hbar^2}{24}\frac{\partial V}{\partial x_i}\frac{\partial V}{\partial x_j}\right)\right.\right.$$
$$\left.\left.\left(\frac{\partial^2\mathcal{E}}{\partial p_i\partial p_j}-\frac{A_{ij}(\beta,m^*)}{A_0(\beta,m^*)}\right)-\frac{q\beta^3\hbar^2}{24}\frac{\partial^2 V}{\partial x_i\partial x_j}\left(v_iv_j-\frac{B_{ij}(\beta,m^*)}{A_0(\beta,m^*)}\right)\right]\right\}+o(\hbar^2) \tag{11}$$

where

$$A_0(\beta,m^*) = \int_{\Re^3} e^{-\beta\mathcal{E}}\,dp,\quad A_{ij}(\beta,m^*) = \int_{\Re^3} e^{-\beta\mathcal{E}}\frac{\partial^2\mathcal{E}}{\partial p_i\partial p_j}\,dp,$$
$$B_{ij}(\beta,m^*) = \int_{\Re^3} e^{-\beta\mathcal{E}}v_iv_j\,dp.$$

4 The Case of the Kane Dispersion Relation

In the case of the Kane dispersion relation

$$\frac{p^2}{2m^*} = \mathcal{E}\,(1+\alpha\mathcal{E})$$

with α nonparabolicity factor while

$$v = \frac{p}{m^*(1+2\alpha\mathcal{E})}$$

and

$$\frac{\partial^2\mathcal{E}}{\partial p_i\partial p_j} = \frac{1}{m^*(1+2\alpha\mathcal{E})}\left[\delta_{ij}-\frac{2\alpha}{m^*(1+2\alpha\mathcal{E})^2}p_ip_j\right].$$

By expressing the elementary volume $d\,p$ as

$$dp = m^*\sqrt{2m^*\mathcal{E}(1+\alpha\mathcal{E})}(1+2\alpha\epsilon)\,d\mathcal{E}d\Omega,$$

$d\,\Omega$ being the elementary solid angle, the coefficients appearing in the Wigner function can be written as

$$\begin{aligned}A_0(\beta,m^*) &= 4\pi m^*\sqrt{2m^*}\int_0^\infty e^{-\beta\mathcal{E}}\sqrt{\mathcal{E}(1+\alpha\mathcal{E})}\mathcal{E}(1+2\alpha\mathcal{E})\,d\mathcal{E}\\ &= 4\pi m^*\sqrt{2m^*}\;d_0(\beta),\end{aligned}$$
$$A_{ij}(\beta,m^*) = 4\pi\sqrt{2m^*}\;\delta_{ij}\int_0^\infty e^{-\beta\mathcal{E}}\left[\sqrt{\mathcal{E}(1+\alpha\mathcal{E})}-\frac{4\alpha\left[\mathcal{E}(1+\alpha\mathcal{E})\right]^{3/2}}{3(1+2\alpha\mathcal{E})^2}\right]d\mathcal{E},$$
$$B_{ij}(\beta,m^*) = \frac{8\pi}{3}\sqrt{2m^*}\;\delta_{ij}\int_0^\infty e^{-\beta\mathcal{E}}\frac{\left[\mathcal{E}(1+\alpha\mathcal{E})\right]^{3/2}}{(1+2\alpha\mathcal{E})}\,d\mathcal{E},$$

obtaining the equilibrium Wigner function

$$w^{(eq)}(x,p,\beta) = \frac{n(x,t)e^{-\beta\mathcal{E}}}{4\pi m^* \sqrt{m^*} d_0(\beta)} \left\{ 1 + \hbar^2 \left[\left(\frac{q\beta^2}{8} \frac{\partial^2 V}{\partial x_i \partial x_j} + \frac{q^2\beta^3}{24} \frac{\partial V}{\partial x_i} \frac{\partial V}{\partial x_j} \right) \right. \right.$$
$$\left[\frac{\delta_{ij}}{m^*(1+2\alpha\mathcal{E})} - \frac{2\alpha p_i p_j}{(m^*)^2(1+2\alpha\mathcal{E})^3} - \frac{\delta_{ij}}{m^* d_0(\beta)} \right.$$
$$\left. \int_0^{+\infty} e^{-\beta\mathcal{E}} \left(\sqrt{\mathcal{E}(1+\alpha\mathcal{E})} - \frac{4\alpha}{3} \frac{[\mathcal{E}(1+\alpha\mathcal{E})]^{3/2}}{(1+2\alpha\mathcal{E})^2} \right) d\,\mathcal{E} \right]$$
$$- \frac{q\beta^3}{24} \frac{\partial^2 V}{\partial x_i \partial x_j} \left(v_i v_j - \frac{2\delta_{ij}}{3m^* d_0(\beta)} \right.$$
$$\left. \left. \left. \times \int_0^{\infty} e^{-\beta\mathcal{E}} \frac{[\mathcal{E}(1+\alpha\mathcal{E})]^{3/2}}{1+2\alpha\mathcal{E}} \, d\mathcal{E} \right) \right] \right\}.$$

Remark 1. In the bulk case the $\hbar^2$ correction vanishes in the parabolic band approximation and $w^{(eq)}(x,p,\beta)$ reduces to the semiclassical Maxwellian. Instead when the energy bands are described by the Kane dispersion relation, $w^{(eq)}(x,p,\beta)$ in the bulk case is given by

$$w^{(eq)}(x,p,\beta) = \frac{n(x,t)e^{-\beta\mathcal{E}}}{4\pi m^* \sqrt{m^*} d_0(\beta)} \left\{ 1 + \hbar^2 \frac{q^2\beta^3}{24} E_i E_j \right.$$
$$\left[\frac{\delta_{ij}}{m^*(1+2\alpha\mathcal{E})} - \frac{2\alpha p_i p_j}{(m^*)^2(1+2\alpha\mathcal{E})^3} - \frac{\delta_{ij}}{m^* d_0(\beta)} \right.$$
$$\left. \left. \int_0^{+\infty} e^{-\beta\mathcal{E}} \left(\sqrt{\mathcal{E}(1+\alpha\mathcal{E})} - \frac{4\alpha}{3} \frac{[\mathcal{E}(1+\alpha\mathcal{E})]^{3/2}}{(1+2\alpha\mathcal{E})^2} \right) d\,\mathcal{E} \right] \right\},$$

with $E_i = -\partial V/\partial x_i$ the components of the electric field. This implies that the quantum correction affects all the transport parameters even in the bulk case when more realistic approximations of the energy bands are used.

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