Chapter 3

Wigner-Poisson Model of Quantum Transport

A description of quantum-transport in phase-space that is analogous to that of semi-classical transport is highly desirable. At first sight it may appear that defining a quantum-mechanical distribution function in phase-space is not possible because of the Heisenberg uncertainty principle. However, useful phase-space descriptions that do not violate the uncertainty relation can be developed. The starting point is to define a correspondence rule that associates an ordinary function with each quantum operator and vice-versa. Several phase-space descriptions are possible depending on the choice of the correspondence rule. Here we will use the Weyl correspondence rule. The Weyl transform of the density matrix is the Wigner function and it describes the state of the system in the quantum mechanical phase-space.

We follow Balescu (1973) in the discussion of the Weyl transform and the Wigner function. A discussion of the development of a quantum kinetic theory being beyond the scope of this work, the starting point is the single-particle reduced density matrix. It is shown that the Weyl transform allows quantum mechanical averages to be calculated just as in semiclassical transport, the Wigner function taking the place of the distribution function. This is an important reason for using the Wigner formulation of quantum mechanics. The equation of motion of the Wigner function is derived by considering the Weyl transform of the von Neumann equation of motion. Finally a relaxation time model is used to obtain a quantum kinetic equation. This is a closed

equation for the kinetic part of the one-particle reduced Wigner function, just as the Boltzmann equation describes the kinetic part of the classical distribution function (see, for example, (Balescu, 1973) for a discussion of kinetic equations).

After a general discussion of the Wigner transport equation, it is applied to heterostructure device simulation. In the past, Wigner function simulations have been restricted by the assumption of a spatially uniform parabolic energy band. Only recently have there been attempts to incorporate position-dependent energy bands into the Wigner transport simulation of heterostructure devices (Miller & Neikirk, 1991; Tsuchiya et al., 1991). It is shown that the equation derived by Tsuchiya et al. (1991) for transport in a position-dependent parabolic energy band is inconsistent with the Weyl transform. The equation of Miller and Neikirk (1991) does not satisfy current continuity. We present the equation of motion in a parabolic energy band that is consistent with the Weyl transform and also satisfies current continuity.

In this work the real bandstructure is expanded into its Fourier components and incorporated into the Wigner transport equation (the significance of the Fourier components of the bandstructure has been discussed in the previous chapter). In addition to allowing the incorporation of general energy bands into the transport equation, the approach taken here leads to a consistent discrete numerical model.

3.1 The Weyl transformation and the Wigner function

The average of a physical quantity corresponding to the operator $\hat{b}$ can be obtained as

$$\langle b \rangle = \int dz \, \langle z|\hat{\rho}\hat{b}|z\rangle \tag{3.1}$$

where $\hat{\rho}$ is the density matrix describing the state of the mixed quantum system and the position representation is used. The goal is to define a one-particle distribution function in quantum phase-space so that the calculation of averages

can be converted to a form that is analogous to the classical prescription. To this end, the quantum operator $\hat{b}$ is written as a Fourier transform (Balescu, 1973; Groot & Suttorp, 1972; Leaf, 1968):

$$\hat{b} = \int du\, dv\, \beta(u,v) e^{\imath(u\hat{z}+v\hat{k})} \tag{3.2}$$

$\hat{z}$ and $\hat{k}$ are the position and momentum operators respectively. Since $\hat{b}$ is Hermitian, we have that $\beta(-u,-v) = \beta^*(u,v)$. The Weyl rule states that associated with $\hat{b}$ is the Weyl transform $b(z,k)$ also written as a Fourier transform:

$$b(z,k) = \int du\, dv\, \beta(u,v) e^{\imath(uz+vk)} \tag{3.3}$$

with the same function $\beta(u,v)$ (Balescu, 1973). $b(z,k)$ is not always the classical function corresponding to the observable, as originally proposed by Weyl (Leaf, 1968). In general, the Weyl transforms $b(z,k)$ do not obey the commutative algebra of classical functions. The classical functions are obtained from the Weyl transforms in the limit $\hbar \to 0$, the limit being taken after the Weyl transform is expressed in terms of $p = \hbar k$. Of particular interest is the function $p^2/m^*(q)$ which is encountered in the study of heterostructure devices where the effective mass is a function of position. In this case the classical function and the Weyl transform are identical.

Invoking the Weyl correspondence rule for $\hat{b}$, Eq. 3.2 becomes

$$\langle b \rangle = \int du\, dv\, \beta(u,v) \int dz'\, dz\, \langle z|\hat{\rho}|z'\rangle \langle z'|e^{\imath(u\hat{z}+v\hat{k})}|z\rangle \tag{3.4}$$

Using $\hat{k} = -\imath\nabla_z$, expanding the exponential operator and performing the integration over z' gives

$$\langle b \rangle = \int du\, dv\, \beta(u,v) \int dz\, \langle z|\hat{\rho}|z+v\rangle e^{\imath(z+v/2)} \tag{3.5}$$

The Wigner function $f(q,k)$ is defined as (Groot & Suttorp, 1972)

$$\frac{1}{2\pi} \int dq\, dk\, e^{\imath(uq+vk)} f(q,k) = \int dz \langle z|\hat{\rho}|z+v\rangle e^{\imath u(z+v/2)} \tag{3.6}$$

Substituting this into Eq. 3.5 we get a prescription for the calculation of averages in quantum mechanical phase-space:

$$\langle b \rangle = \frac{1}{2\pi} \int dq\, dk\, b(q,k) f(q,k) \tag{3.7}$$

The averages of physical observables in phase-space can be calculated in a manner analogous to that in classical mechanics. The Wigner function $f(q,k)$ plays the role of the distribution function in classical transport, and is obtained from Eq. 3.6 by taking the inverse Fourier transform

$$f(q,k) = \int dv\, e^{-\imath k v} \langle\, q - v/2 | \hat{\rho} | q + v/2 \rangle \tag{3.8}$$

Equation 3.8 is another version of the Weyl transform and states that the Wigner function is obtained from the density matrix $\langle z' | \hat{\rho} | z \rangle$ by making the coordinate transformation

$$\begin{aligned} q &= \frac{1}{2}(z + z') \\ v &= z - z' \end{aligned} \tag{3.9}$$

and taking the Fourier transform with respect to the relative coordinate v. Although the Wigner function enters the calculation of averages as if it were a probability density, it cannot be interpreted as one because it is not always positive.

The Wigner function does not violate the uncertainty principle. However the uncertainty principle does impose restrictions on the Wigner function. This can be seen easily in the case of a system in a pure state where

$$\hat{\rho} = |\psi\rangle\langle\psi| \tag{3.10}$$

From Schwarz's inequality and using 3.10 in 3.8 we get

$$|f(q,k)|^2 \leq \left[\int dv |\psi(q - v/2)|^2 \right] \left[\int dv |\psi(q + v/2)|^2 \right] \tag{3.11}$$

Since the wave functions are normalized, $|f(q,k)| \leq 2$. Also, as defined, $f(q,k)$ is normalized to unity. Therefore, the support of the Wigner function must be $\Delta_q \Delta_k \geq 1/2$, a reflection of the uncertainty principle (Groot & Suttorp, 1972). Therefore functions of the form $\delta(q)\delta(k)$ which imply that the system is in state (q,k) are not permitted. Whereas in classical mechanics, a point in phase-space describes a state of the system, in quantum mechanics it cannot. Hillery et al. (1984) discuss other properties that the Wigner function must satisfy.

3.2 Equation of motion of the Wigner function

The equation that describes the time evolution of the Wigner function is obtained by considering the time dependence of the average of an observable in the density matrix formulation:

$$\langle b(t) \rangle = Tr[\hat{b}\hat{\rho}(t)] \tag{3.12}$$

The time dependence of the density matrix is given by the von Neumann equation

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{\imath}{\hbar}\left[\hat{H}, \hat{\rho}\right] \equiv L\hat{\rho} \tag{3.13}$$

where L is the Liouville superoperator. Taking the Weyl transform of the von Neumann equation results in the equation of motion for the Wigner function. The Weyl transform of the commutator is

$$\left[\hat{H}, \hat{\rho}\right] \leftrightarrow 2\imath \sin\left\{\frac{1}{2}\left(\frac{\partial^{(h)}}{\partial q}\frac{\partial^{(f)}}{\partial k} - \frac{\partial^{(f)}}{\partial k}\frac{\partial^{(h)}}{\partial q}\right)\right\} H(q,k) f(q,k) \tag{3.14}$$

where the superscripts on the partial derivatives indicate the function on which they act. H is the Weyl transform of $\hat{H}$ and f is the Weyl transform of $\hat{\rho}$. Here, the Weyl transform is not the same as the corresponding classical function, the Poisson bracket. In the limit $\hbar \to 0$, however, only the first term in the series expansion of the sine function will survive and we get the Poisson bracket.

Using 3.14, the equation of motion of the Wigner function is

$$\frac{\partial f}{\partial t} = \frac{2}{\hbar}\sin\left\{\frac{1}{2}\left(\frac{\partial^{(h)}}{\partial q}\frac{\partial^{(f)}}{\partial k} - \frac{\partial^{(f)}}{\partial k}\frac{\partial^{(h)}}{\partial q}\right)\right\}H(q,k)f(q,k) \tag{3.15}$$

In this form the equation is of limited use because of the presence of the higher order derivatives in the expansion of the sine function. However, it is useful in obtaining the classical limit. In the limit $\hbar \to 0$, and assuming $H(q,p) = v(q) + p^2/m^*(q)$, we obtain the classical equation:

$$\frac{\partial f}{\partial t} = -\frac{p}{m^*(q)}\frac{\partial f}{\partial q} + \left[\frac{\partial v(q)}{\partial q} + \frac{p^2}{2}\frac{\partial}{\partial q}\frac{1}{m^*(q)}\right]\frac{\partial f}{\partial p} \tag{3.16}$$

regardless of how rapidly the potential or the band structure changes in position and momentum. Also, if all derivatives of order higher than that appearing in Eq. 3.16 vanish, there are no quantum corrections even if the limit $\hbar \to 0$ is not taken. In the presence of a rapidly varying potential $v(q)$, or abrupt changes in bandstructure across heterointerfaces, the following identity is extremely useful in incorporating quantum corrections to all orders (Buot & Jensen, 1990):

$$\begin{aligned}
&\sin\left\{\frac{1}{2}\left(\frac{\partial^{(h)}}{\partial q}\frac{\partial^{(f)}}{\partial k} - \frac{\partial^{(f)}}{\partial k}\frac{\partial^{(h)}}{\partial q}\right)\right\}H(q,k)f(q,k) \\
\equiv\ &\frac{-\imath}{8\pi^2}\int dk'\,dq'\,dv\,dr\,e^{-\imath[(k-k')r + (q-q')v]}f(q',k') \\
&\times\left[H(q'+\frac{r}{2},k'-\frac{v}{2}) - H(q'-\frac{r}{2},k'+\frac{v}{2})\right]
\end{aligned} \tag{3.17}$$

We assume that only the momentum in a direction parallel to the electron current is important, and the degrees of freedom associated with the perpendicular momenta can be integrated out of the problem. This is valid only if the Wigner function for these momenta are not coupled to the Wigner function for the parallel momenta. A magnetic field couples the Wigner function in both momentum directions. Electron-phonon collisions also have a similar effect. Also, to be able to integrate out the perpendicular momenta, it is necessary that any variations in the bandstructure occur only in one direction in momentum, a highly unphysical situation. While extending Eq. 3.17 to two

dimensions in momentum (assuming radial symmetry in plane perpendicular to current flow) is straightforward, the numerical evaluation of the Wigner function in three dimensions, $f(q, k_\perp, k_\parallel)$, is intractable.

Dissipation in the Wigner formulation of quantum transport has been most commonly treated using the relaxation time approach

$$\left.\frac{\partial f}{\partial t}\right| = \frac{1}{\tau_f}\left(\frac{n(q)}{n^{eq}(q)} f^{eq}(q,k) - f(q,k)\right) \tag{3.18}$$

where f^{eq} is the equilibrium distribution function and τ_f is the characteristic time that governs the relaxation of the distribution function. $n(q)$ is the electron density and $n^{eq}(q)$ is the equilibrium electron density. The relaxation time model used here represents collisions in which the scattering rate out of the phase space point (q,k) is proportional to $f(q,k)$. The scattering rate into (q,k) is proportional to the local electron concentration $n(q)$ and the equilibrium distribution $f^{eq}(q,k)$.

3.2.1 Parabolic energy band

To relate this work to the results of Tsuchiya et al. (1991) and Miller and Neikirk (1991), we first consider a parabolic bandstructure with spatially varying effective-mass:

$$H(q,k) = \frac{\hbar^2 k^2}{2m^*(q)} + v(q) \tag{3.19}$$

$v(q)$ includes, in addition to the heterostructure band-offsets, the self-consistent Hartree potential. The Hartree potential can be obtained from Poisson's equation for the charge distribution in the device. Substituting in the integral form we get the equation of motion for the Wigner function in flux-conservative form:

$$\begin{aligned}\frac{\partial f}{\partial t} &= -\frac{\hbar}{\pi}\int dk'\, k' \frac{\partial}{\partial q}\left[f(q,k')\mathcal{M}^e(q,k-k')\right] \\ &\quad -\frac{\hbar}{4\pi}\int dk'\, \frac{\partial^2}{\partial q^2}\left[f(q,k')\mathcal{M}^o(q,k-k')\right]\end{aligned}$$

$$+\frac{\hbar}{\pi}\int dk'\,k'^2 f(q,k')\mathcal{M}^o(q,k-k')$$
$$+\frac{2}{\pi\hbar}\int dk'\,f(q,k')\mathcal{V}(q,k-k') \tag{3.20}$$

where

$$\mathcal{M}^e(q,k)=\int dr\,\frac{\cos 2k(q-r)}{m^*(r)}$$
$$\mathcal{M}^o(q,k)=\int dr\,\frac{\sin 2k(q-r)}{m^*(r)}$$
$$\mathcal{V}(q,k)=\int dr\,v(r)\sin 2k(q-r) \tag{3.21}$$

Writing the equation of motion in a flux conservative form is essential in the subsequent development of a discrete numerical model. The result of Miller and Neikirk (1991) is based on the discrete Weyl transform and can be obtained by discretizing the following equation of motion

$$\begin{aligned}\frac{\partial f}{\partial t} &= -\frac{\hbar k}{\pi}\int dk' M^e(q,k-k')\frac{\partial f(q,k')}{\partial q}\\ &\quad -\frac{\hbar}{4\pi}\int dk'\,M^o(q,k-k')\frac{\partial^2 f(q,k')}{\partial q^2}\\ &\quad +\frac{\hbar k^2}{\pi}\int dk' f(q,k')\mathcal{M}^o(q,k-k')\\ &\quad +\frac{2}{\pi\hbar}\int dk'\,f(q,k')\mathcal{V}(q,k-k')\end{aligned} \tag{3.22}$$

which is obtained by using instead of Eq. 3.17, the following flux non-conserving form

$$\begin{aligned}&\sin\left\{\frac{1}{2}\left(\frac{\partial^{(h)}}{\partial q}\frac{\partial^{(f)}}{\partial k}-\frac{\partial^{(f)}}{\partial k}\frac{\partial^{(h)}}{\partial q}\right)\right\}H(q,k)f(q,k)\\ \equiv\ &\frac{-\imath}{8\pi^2}\int dk'\,dq'\,dv\,dr\,e^{-\imath[(k-k')r+(q-q')v]}f(q',k')\\ &\qquad\times\left[H(q+\frac{r}{2},k-\frac{v}{2})-H(q-\frac{r}{2},k+\frac{v}{2})\right]\end{aligned} \tag{3.23}$$

Expanding the derivatives in q in Eq. 3.20 and using the fact that $\mathcal{M}'^e(q,k)=2k\mathcal{M}^o$ and $\mathcal{M}'^o(q,k)=-2k\mathcal{M}^e(q,k)$, it is easy to show that Eqs. 3.22 and 3.20

are identical. However, the corresponding discrete models are very different in nature. Both equations satisfy current continuity in the continuum. However, discretizing Eq. 3.22 yields a numerical model that does not satisfy current continuity.

A simpler example to illustrate the point is to compare

$$\frac{\partial n}{\partial t} = \frac{\partial vn}{\partial z}$$

with

$$\frac{\partial n}{\partial t} = v\frac{\partial n}{\partial z} + n\frac{\partial v}{\partial z}$$

which are identical (n is a density and v a z-dependent velocity) in the continuum. However the first form leads to a flux conserving discrete model, while the second does not.

Equation 3.20 is not the same as that obtained by Tsuchiya et al. (1991). In that work, the Fourier transform was applied to the von Neumann equation with the explicit quantum mechanical Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m^*(z)}\frac{\partial}{\partial z} + v(z) \tag{3.24}$$

already in place. The Hamiltonian Eq. 3.24 does not lead to the equation of motion of the Wigner function Eq. 3.20 because it is inconsistent with the Weyl correspondence rule. It is instructive to determine the quantum-mechanical Hamiltonian by inverting the Weyl transform. Using the Weyl transform pair (Groot & Suttorp, 1972):

$$f(p)p^2 \Longleftrightarrow \frac{1}{4}\left[f(\hat{q})\hat{p}^2 + 2\hat{p}f(\hat{q})\hat{p} + \hat{p}^2 f(\hat{q})\right] \tag{3.25}$$

the Hamiltonian in position representation is:

$$\hat{H} = -\frac{\hbar^2}{8}\left[\frac{1}{m^*(z)}\frac{\partial^2}{\partial x^2} + 2\frac{\partial}{\partial z}\frac{1}{m^*(z)}\frac{\partial}{\partial z} + \frac{\partial^2}{\partial z^2}\frac{1}{m^*(z)}\right] + v(z) \tag{3.26}$$

which was discussed in the previous chapter. It is easily verified that the Hamiltonian is Hermitian as it must be. Since the definition of the Wigner function is associated with the Weyl correspondence rule, Eq. 3.26 must be used to obtain the correct equation of motion in a parabolic energy band in the presence of non-uniform effective-mass. The Hamiltonian Eq. 3.26 leads to the following von Neumann equation in position representation:

$$\begin{aligned}\frac{\partial \rho}{\partial t} &= \frac{\imath\hbar}{8}\left[\left(\frac{1}{m^*(z)}\frac{\partial^2}{\partial z^2} - \frac{1}{m^*(z')}\frac{\partial^2}{\partial z'^2}\right) + 2\left(\frac{\partial}{\partial z}\frac{1}{m^*(z)}\frac{\partial}{\partial z} - \frac{\partial}{\partial z'}\frac{1}{m^*(z')}\frac{\partial}{\partial z'}\right)\right. \\ &\quad \left. + \left(\frac{\partial^2}{\partial z^2}\frac{1}{m^*(z)} - \frac{\partial^2}{\partial z'^2}\frac{1}{m^*(z')}\right) - \frac{8}{\hbar^2}\left[v(z) - v(z')\right]\right]\rho(z, z') \qquad (3.27)\end{aligned}$$

Although more tedious than using Eq. 3.17, it is straightforward to show that the procedure of (Tsuchiya et al., 1991) applied to Eq. 3.27 will lead to the equation of motion Eq. 3.20.

While the "minimal Hermitian" Hamiltonian does lead to the equation of motion presented by Tsuchiya et al. (1991), it is written in a very awkward form that does not lend itself to elegant, and more importantly, accurate discretization. The discrete model derived by Tsuchiya et al. (1991) suffers from severe problems. Their work suggests that as the effective mass in the barrier increases, the peak current increases. From the discussion in Section 2.2.2, this result is unphysical. The error may be due to improper discretization. In Appendix A, we show how their equation can be manipulated to yield a form that lends itself to an accurate and aesthetically pleasing numerical model. Further, this exercise also serves the purpose of highlighting the differences between their model and the one presented in this work.

3.2.2 General energy band

Equation 3.20 describes quantum transport in a model heterostructure device where the bandstructure everywhere is parabolic. In real devices, however, the deviation from parabolicity is significant. The band structure in the , $-X$

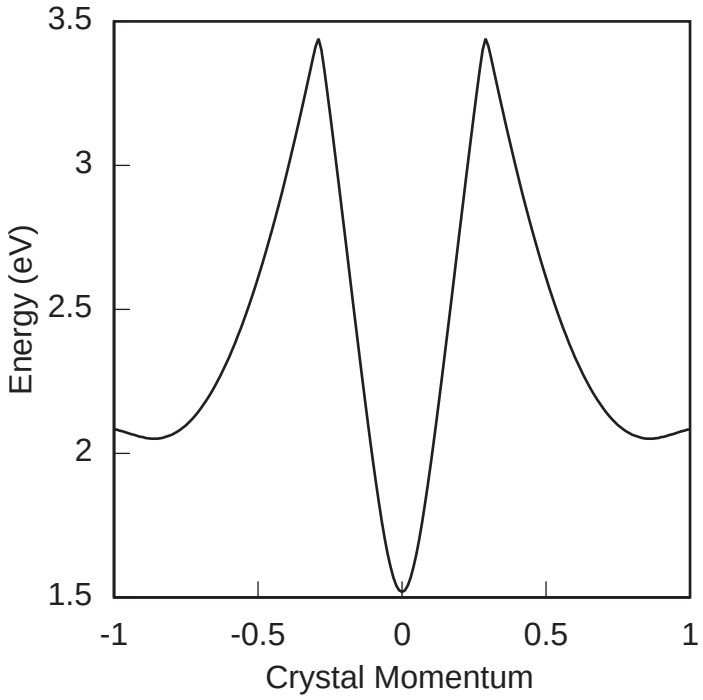

Figure 3.1: , $-X$ pseudopotential bandstructure in GaAs (calculated by V. Chandramouli).

direction, shown in Fig. 3.1, can be expanded into its Fourier components:

$$\mathcal{E}(k) = \sum_{n=1}^{\infty} \frac{4\hbar^2}{n^2 m_n^* a^2} \left[1 - \cos(\frac{nka}{2})\right] \quad |k| \leq \tfrac{2\pi}{a} \tag{3.28}$$

where $a = 5.6533$Å in GaAs and the Brillouin zone is $|k| \leq 2\pi/a$. The Fourier coefficients $1/m_n^*$ are shown in Fig. 3.2. The significance of the Fourier components of the energy band has been discussed in the previous chapter in relation to the effective-mass equation. Expanded as a Fourier series it is easy to formulate the tight-binding problem on a discrete lattice that results in the assumed energy band. Here, the advantage of using a Fourier expansion of the bandstructure is that it leads to a consistent numerical quantum transport model (Gullapalli & Neikirk, 1994), as will be described in the next chapter. In the , $-X$ energy band, the equation of motion for the Wigner function is

$$\frac{\partial f}{\partial t} = -\sum_{n=1}^{\infty} \frac{4\hbar}{n^2 \pi a^2}$$

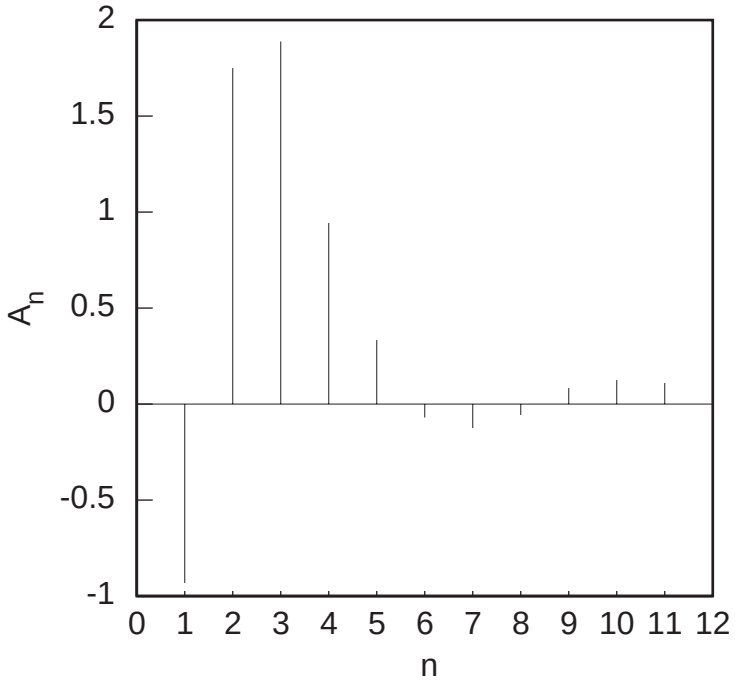

Figure 3.2: Fourier components of the , $-X$ bandstructure in GaAs. $A_n = 4\hbar^2/m_n^* a^2 n^2$.

$$\times \left[\int_{BZ} dk' \, \sin\left(\frac{nk'a}{2}\right) \left[f\left(q + \frac{na}{4}, k'\right) \mathcal{M}_n^e \left(q + \frac{na}{4}, k - k'\right) \right.\right.$$
$$\left. - f\left(q - \frac{na}{4}, k'\right) \mathcal{M}_n^e \left(q - \frac{na}{2}, k - k'\right) \right]$$
$$+ \int_{BZ} dk' \, \cos\left(\frac{nk'a}{2}\right) \left[f\left(q + \frac{na}{4}, k'\right) \mathcal{M}_n^o \left(q + \frac{na}{4}, k - k'\right) \right.$$
$$\left. \left. + \, f\left(q - \frac{na}{4}, k'\right) \mathcal{M}_n^o \left(q - \frac{na}{4}, k - k'\right) \right] \right.$$
$$\left. - \, 2 \int_{BZ} dk' \, f(q, k') \mathcal{M}_n^o(q, k - k') \right]$$
$$+ \frac{2}{\pi\hbar} \int_{BZ} dk' \, f(q, k') \mathcal{V}(q, k - k') \tag{3.29}$$

where

$$\mathcal{M}_n^e(q, k) = \int dr \, \frac{\cos 2k(q - r)}{m_n^*(r)}$$
$$\mathcal{M}_n^o(q, k) = \int dr \, \frac{\sin 2k(q - r)}{m_n^*(r)}$$
$$\mathcal{V}(q, k) = \int dr \, v(r) \sin 2k(q - r) \tag{3.30}$$

While the bandstructure is based on the tight-binding approach on a finite-difference mesh with spacing $a/2$, the equation of motion for the Wigner function must be solved on a mesh with spacing $a/4$. In the following discussion we refer to the Wigner lattice as the lattice on which the Wigner equation is solved. It is important to remember that the Wigner lattice is twice as dense as the lattice on which the effective-mass equation is solved. In the numerical model to be developed in the next chapter, this also assures that the periodicity of the Wigner function coincides with that of the bandstructure.

The fact that the Brillouin zone is not specified by the Wigner lattice constant Δ, but by twice the Wigner lattice constant 2Δ, has not been appreciated in the past. This is due to the fact that past treatment has been based on parabolic energy bands which are not consistent with a discrete lattice. This confusion led Miller (1994) to conclude that the Wigner function midway between the mesh points were also important. This is unnecessary,

and the confusion is elegantly resolved using the tight-binding energy band, that is consistent with a discrete lattice, instead of using the parabolic band.

To incorporate multi-band effects into the Wigner transport equation, it is necessary to start with the multi-band Hamiltonian. A general consideration of the problem has been presented by Miller (1994) where the single band approximation is justified for the heterostructures studied in this work. In any case, numerical simulations have not proceeded beyond the single-band effective-mass approximation, even including the full , $-X$ energy band being computationally intractable.

, *valley transport*

Since the number of Fourier coefficients required to represent the bandstructure is large (~ 10), Eq. 3.29 is highly nonlocal in position. This is in addition to the highly nonlocal coupling in momentum due to $\mathcal{V}$. Available computational resources permit the inclusion of only the nearest and second-nearest-neighbor coupling in position. If transport is principally in the , valley, the bandstructure is reasonably well described by the $n = 4$ component alone. The bandstructure in the , valley is thus approximated:

$$\mathcal{E}(k) = \frac{\hbar^2}{4m^*a^2}\left[1 - \cos\left(2ka\right)\right] \quad |k| < \tfrac{\pi}{2a} \tag{3.31}$$

where $m^* = m^*_{GaAs}$. In the given region of the Brillouin zone, the fit is better than the parabolic relation and is shown in Fig. 3.3. In this work we assume that the relevant portion of the bandstructure in AlAs is also the , valley. The heterostructure device is thus assumed to be described by

$$H(q,k) = \frac{\hbar^2}{4m^*(q)a^2}\left[1 - \cos\left(2ka\right)\right] + v(q) \tag{3.32}$$

where, for convenience the lattice constant a is assumed to be the same for AlAs and GaAs. The following equation of motion is obtained:

$$\frac{\partial f}{\partial t} \;=\; -\frac{\hbar}{4\pi a^2}\int_{BZ} dk' \,\sin\left(2k'a\right)\left[f(q+a,k')\mathcal{M}^e(q+a,k-k')\right.$$

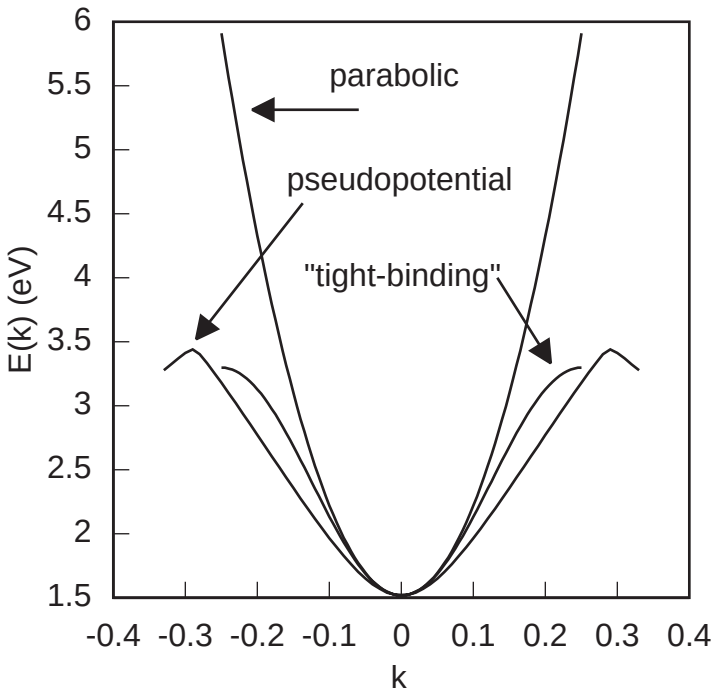

Figure 3.3: A comparison of the parabolic and tight-binding energy bands with the pseudo-potential energy band in the , $-X$ direction. The crystal momentum k is in units of $2\pi/a$ where a is the lattice constant of GaAs.

$$
\begin{aligned}
&\qquad\qquad - f(q-a,k')\mathcal{M}^e(q-a,k-k')] \\
&- \frac{\hbar}{4\pi a^2}\int_{BZ} dk'\,\cos(2k'a)\,[f(q+a,k')\mathcal{M}^o(q+a,k-k') \\
&\qquad\qquad + f(q-a,k')\mathcal{M}^o(q-a,k-k')] \\
&+ \frac{\hbar}{2\pi a^2}\int_{BZ} dk'\, f(q,k')\mathcal{M}^o(q,k-k') \\
&+ \frac{2}{\pi\hbar}\int_{BZ} dk'\, f(q,k')\mathcal{V}(q,k-k') \qquad (3.33)
\end{aligned}
$$

In the limit $a \to 0$ we get a parabolic energy band and Eq. 3.33 reduces to Eq. 3.20. Since the energy band in Eq. 3.32 is based on the discrete Schrödinger equation in the finite-difference basis, it is not surprising that the resulting transport equation is also discrete in q, the evolution of $f(q)$ depending only on the nearest neighbors $f(q+a)$ and $f(q-a)$.

3.3 Summary

It has been shown that the Weyl transform allows quantum mechanical averages to be calculated as in semiclassical transport, the Wigner function taking the place of the distribution function. The equation of motion of the Wigner function has been derived by considering the Weyl transform of the von Neumann equation of motion and a relaxation time model was used to obtain a quantum kinetic equation. The appeal of the Wigner formulation is its similarity to the more familiar Boltzmann transport equation. This similarity is of importance in the study of the transition from quantum to classical behavior. Also, the similarity in forms may lead to a generalization of powerful methods already developed for the solution of the Boltzmann equation.

The equation of motion of the Wigner function in a parabolic energy band, that is consistent with the Weyl transform and also satisfies current continuity, has been discussed. The incorporation of spatially varying band structure has also been discussed. Another issue addressed in this chapter is that the band structure in real semiconductors is far from being a parabola that

extends to infinite energy. Expanding the bandstructure into its Fourier series allows its incorporation into the Wigner transport equation in a consistent manner.