Numerical and Analytical Applications of Multiband Transport in Semiconductors

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Abstract. A multiband transport model for electron transport in semiconductors, based on the Wigner-function approach and allowing for energy bands of arbitrary shape, is presented and applied to two simple examples: a comparison of exact and free streaming solutions of the Wigner equation in non-parabolic regime and an interband transition in an infinite homogeneous medium.

INTRODUCTION

Significant progress in understanding the transport properties of electronic devices, such as the Resonant Tunneling Diode (RTD) and others, has been made by introducing the use of phase space concepts. The most important model, based on a phase-space description, is the Wigner-function approach [1], which has been applied, in particular, to the calculation of the I-V curves of the RTD [2]. This model, however, considers only conduction band electrons together with the parabolic band approximation, so that the evolution equation for the Wigner function becomes the evolution equation for semiclassical particles with an effective mass.

For the description of those devices in which interband transitions or non-parabolicity effects are important, the single-band, effective mass approximation is no longer satisfactory. A correctly defined Wigner function for these phenomena should include the populations of all bands involved in the transport processes and the evolution equation that governs the time dependence of the Wigner function should take into account possible non-parabolicity effects.

The formulation of a general multi-band transport model, allowing for energy bands of any shape, is underway and some preliminary results have recently been presented [3, 4]. In this model, a multi-band Wigner function f has been introduced by using the Bloch-state representation of the density matrix. As a result, f can be written as a sum,

$$f(x,p) = \sum_{mn} f_{mn}(x,p), \tag{1}$$

where the functions f_{mn} are obtained from the Wigner function f by the action of the integral operators $\mathcal{P}_{mn}$,

$$f_{mn}(x,p) = \mathcal{P}_{mn} f(x,p) = \frac{1}{2\pi\hbar} \int\int dx'dp' W_{mn}(x,p,x',p') f(x',p'), \tag{2}$$

with $W_{mn}(x,p,x',p')$ an integral kernel defined entirely in terms of Bloch states. The operators $\mathcal{P}_{mn}$ are projection operators, and the f_{mn}'s are the projections of the Wigner function onto the Floquet subspaces of the energy bands. The evolution equations that govern the time dependence of the Wigner function and of its band projections in time, with or without external fields, have also been derived.

In this work, after recalling the main results of the multi-band transport model, we present two simple applications: (i) we investigate non-parabolicity corrections to the free-streaming transport properties, by comparing the results of the exact model with those obtained with the parabolic band approximation in absence of external fields; (ii) we illustrate the time evolution of the Wigner function during an elementary interband transition in a homogeneous infinite medium, induced by the action of a constant external field (a simplified situation is considered, with only two energy bands, each of them treated within the effective mass approximation).

MULTI-BAND WIGNER FUNCTION AND EVOLUTION EQUATIONS

Equations (1) and (2), which show the partition of the Wigner function into the Floquet spaces of the energy bands, can be derived by using the Bloch-state representation of the density matrix. If ρ is the single particle density operator, the corresponding density matrix in the space representation is given by $\rho(r,s) =< r|\rho|s >$ and the Wigner function is defined by

$$f(x,p) = \int d\eta < x + \frac{\eta}{2}|\rho|x - \frac{\eta}{2} > e^{-ip\eta/\hbar}. \tag{3}$$

The evolution equation for the Wigner function, called the Wigner equation, follows from the Liouville-von Neumann evolution equation for the density matrix and differs from the classical Boltzmann equation in the form of the acceleration term, which is given by a pseudodifferential operator in place of the standard differential operator of the Boltzmann equation:

$$\frac{\partial f}{\partial t} + \frac{p}{m}\frac{\partial f}{\partial x} - \frac{i}{\hbar}\Theta(\delta V)f = 0, \tag{4}$$

where the pseudodifferential operator $\Theta(\delta V)$ is defined by

$$(\Theta(\delta V)f)(x,p) = \int d\eta \delta V(x,\eta)\widehat{f}(x,\eta)e^{-ip\eta/\hbar}, \tag{5}$$

with symbol $\delta V(x,\eta) = V(x+\eta/2) - V(x-\eta/2)$, and

$$\widehat{f}(x,\eta) = \frac{1}{2\pi\hbar}\int dp f(x,p)e^{ip\eta/\hbar}$$

is the Fourier transform of the Wigner function with respect to the momentum variable.

Let $\{|mk>\}$ be the Bloch states and

$$< x|mk > \equiv \Psi_m(x,k) = e^{ikx}u_{mk}(x) \tag{6}$$

the Bloch functions of an infinite homogeneous semiconductor crystal with lattice period a. Here, $m \in \mathbf{N}$ is the band index, $k \in B$ is the crystal momentum and B is the Brillouin zone. Also, let $\epsilon_1(k)$, $\epsilon_2(k)$, ..., $\epsilon_{m-1}(k)$, $\epsilon_m(k)$, ..., be the energy bands. The energy bands are real periodic functions of k, with period $2\pi/a$, and as such they can be expanded in Fourier series,

$$\epsilon_m(k) = \sum_{\mu\in L}\widehat{\epsilon}_m(\mu)e^{ik\mu}, \tag{7}$$

where L is the crystal lattice and $\widehat{\epsilon}^*_m(\mu) = \widehat{\epsilon}_m(-\mu)$ from the reality condition.

By introducing the elements of the density operator in the Bloch-state representation, $\rho_{mn}(k,k') =< mk|\rho|nk' >$, and the coefficients

$$\Phi_{mn}(k,k',x,p) = \int d\eta < x + \frac{\eta}{2}|mk >< nk'|x - \frac{\eta}{2} > e^{-ip\eta/\hbar}, \tag{8}$$

the integral kernel W_{mn} that appears in (2) can be written as

$$W_{mn}(x,p,x',p') = \int_{B^2} dkdk'\Phi_{mn}(k,k',x,p)\Phi^*_{mn}(k,k',x',p'), \tag{9}$$

The coefficients Φ_{mn} are similar to the ones introduced in [5, 6].

The macroscopic quantities such as particle density, current and energy, are likewise expressed as a sum of Floquet terms. It can be shown that only the diagonal terms contribute to the total number of particles, that is

$$\int\int dx dp f(x,p) = \sum_m \int\int dx dp f_{mm}(x,p).$$

The time evolution of the Wigner function is determined by the periodic potential of the crystal and by the possible presence of an external potential $V(x)$. The evolution equation is given by

$$i\hbar\frac{\partial f}{\partial t}(x,p,t) = \sum_{mn} i\hbar\frac{\partial f_{mn}}{\partial t}(x,p,t) = \sum_{mn} i\hbar\left(\frac{\partial f_{mn}}{\partial t}\right)_0 (x,p,t) + \sum_{mn} i\hbar\left(\frac{\partial f_{mn}}{\partial t}\right)_V (x,p,t),$$

where $(\partial/\partial t)_0$ denotes the time evolution due to the periodic potential and $(\partial/\partial t)_V$ the time evolution due to the external potential. By using the Liouville-von Neumann equation for the time evolution of the density matrix, it can be shown that [3, 4]

$$i\hbar\left(\frac{\partial f_{mn}}{\partial t}\right)_0 (x,p,t) = \sum_{\mu\in L}\left[\widehat{\epsilon}_m(\mu) f_{mn}(x+\frac{\mu}{2},p,t) - \widehat{\epsilon}_n(\mu) f_{mn}(x-\frac{\mu}{2},p,t)\right] e^{ip\mu/\hbar} \tag{10}$$

and that

$$i\hbar\left(\frac{\partial f_{mn}}{\partial t}\right)_V (x,p,t) = \int\int dx' d\eta \widehat{W}_{mn}(x,p,x',-\eta)\delta V(x',\eta)\widehat{f}(x',\eta,t), \tag{11}$$

where

$$\widehat{W}_{mn}(x,p,x',\eta) = \frac{1}{2\pi\hbar}\int dp' W_{mn}(x,p,x',p') e^{ip'\eta/\hbar}$$

is the Fourier transform of $W_{mn}(x,p,x',p')$ with respect to p'. It is well known that, in the parabolic-band approximation, equation (10) reduces to the freestreaming transport equation. For a parabolic band $\epsilon(k)$ having a minimum at $k = k_*$, the evolution equation for the Wigner function f in absence of external fields is

$$\frac{\partial f}{\partial t} + \frac{p-\hbar k_*}{m_*}\frac{\partial f}{\partial x} = 0, \tag{12}$$

where $m_* = \hbar^2\left(\partial^2\epsilon/\partial k^2\right)^{-1}_{k=k_*}$ is the effective mass.

The full time evolution of the Floquet projection f_{mn} of the Wigner function, due both to the periodic potential of the crystal lattice and to the external potential, is obtained by adding the two contributions of equation (10) and equation (11):

$$\begin{aligned} i\hbar\frac{\partial f_{mn}}{\partial t} &= \\ &= \sum_{\mu\in L}\left[\widehat{\epsilon}_m(\mu) f_{mn}(x+\frac{\mu}{2},p,t) - \widehat{\epsilon}_n(\mu) f_{mn}(x-\frac{\mu}{2},p,t)\right] e^{ip\mu/\hbar} + \\ &+ \int\int dx' d\eta \widehat{W}_{mn}(x,p,x',-\eta)\delta V(x',\eta)\hat{f}(x',\eta,t). \end{aligned} \tag{13}$$

Equation (13) gives the full time evolution of each component of the Wigner function, in presence of an external field and in the absence of collisions.

EXAMPLES AND APPLICATIONS

Freestreaming evolution

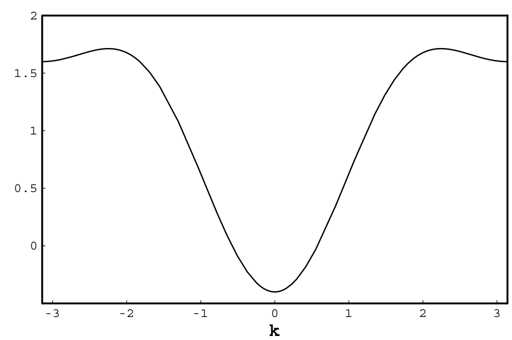

Figure 1: Band profile $\epsilon(k) = 1 - \cos k + 0.4 \cos 2k$, $-\pi \leq k \leq \pi$ (dimensionless units).

In this section, we shall discuss the parabolic band approximation by comparing the solution of equation (10) with the solution of the corresponding free-streaming equation (12) in a simple case. For the comparison, we use dimensionless variables: the space variable x is measured in units of a, the momentum p in units of $\hbar/a$, time t in units of $ma^2/\hbar$ and the crystal momentum k in units of $1/a$. In the dimensionless variables, equation (10) for a single band becomes

$$i\hbar \frac{\partial f}{\partial t}(x,p,t) = \sum_{\mu \in L} \hat{\epsilon}(\mu) \left[f(x + \frac{\mu}{2}, p, t) - f(x - \frac{\mu}{2}, p, t) \right] e^{ip\mu/\hbar} \tag{14}$$

and the free-streaming equation (12) becomes

$$\frac{\partial f}{\partial t} + p \frac{\partial f}{\partial x} = 0.$$

Also, we have chosen $\epsilon(k) = 1 - \cos k + 0.4 \cos 2k$, $-\pi \leq k \leq \pi$ (thus $k_* = 0$), for the band profile, which is shown in Figure 1, and which has a parabolicity region that covers about one half of the Brillouin zone. Note that, with these dimensionless quantities, the phase-space momentum p and the crystal momentum k, though different variables, are measured in the same units. We have followed the time evolution of an initial Gaussian shaped Wigner function in phase space, according to the exact equation and according to the free-streaming approximation. The initial Wigner function corresponds to a pure state characterized by the wave function

$$\Psi(x) = e^{-\alpha(x-x_0)^2} e^{-ik_0(x-x_0)},$$

where x_0 is the initial average position, k_0 the initial average momentum and α the initial momentum spread. The density matrix is given by $\rho(x,x') = \Psi(x)\Psi^*(x')$ and the Wigner function that results is

$$f(x,p,0) = \sqrt{\frac{2\pi}{\alpha}} e^{-2\alpha(x-x_0)^2 - (p-k_0)^2/(2\alpha)}.$$

We have performed the comparison for two different values of the momentum spread, $\alpha = 0.02$ and $\alpha = 0.2$. The former corresponds to a narrow (in momentum) wave packet, whose time evolution is not affected by the states near the edges of the band, where non-parabolicity effects are important. The latter, instead, corresponds to a broad wave packet, for which we expect that non-parabolicity effects are important from the very early evolution. Equation (14) can be solved explicitely by using Fourier Transforms in space. If $\widehat{f}_k$ is the $k-$th Fourier component of f with respect to x, it is easy to see that

$$\widehat{f}_k(p,t) = \widehat{f}_k(p,0)e^{i\gamma_k(p)t} \tag{15}$$

where

$$\gamma_k(p) = 2i\sum_{\mu}\widehat{\epsilon}(\mu)\sin\frac{k\mu}{2}e^{ip\mu/\hbar}.$$

The main features of the comparison are shown in Figures 2, 3 and 4. Figure 2 refers to the case with

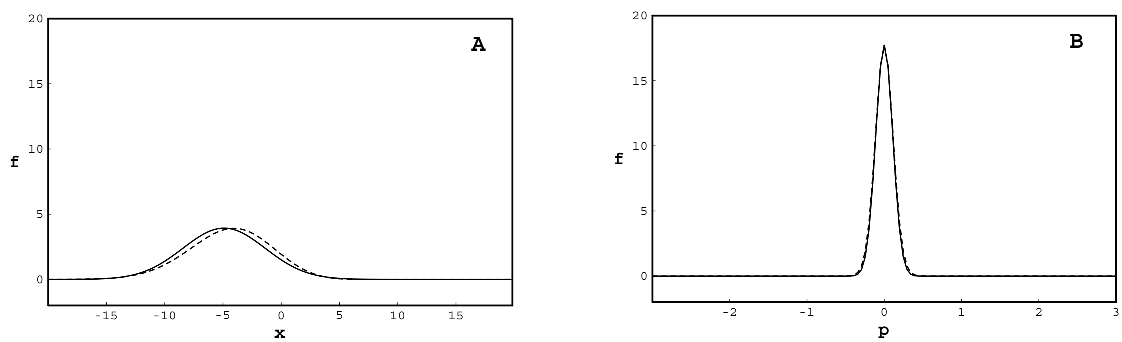

Figure 2: $f(x,p)$ as a function of x, $0 \leq x \leq 20$ for $p = 0.5$ (A) and $f(x,p)$ as a function of p, $-\pi \leq p \leq \pi$, for $x = 0$ (B), for $\alpha = 0.02$ and $t = 20$; exact solution from equation (15) (dashed line), free-streaming approximation from equation (12) (solid line). Dimensionless variables as defined in the text.

$\alpha = 0.02$, Figures 3 and 4 to the case with $\alpha = 0.2$. Figures 2 and 4 show $f(x,p)$ as a function of x for $p = 0.5$ (A) and as a function of p for $x = 0$ (B) at $t = 20$ (in our dimensionless units). The dashed lines represent the exact solution and the solid lines represent the free-streaming approximation. Figure 3 shows $f(x,p)$ as a function of x and p at $t = 20$.

These figures confirm that the free-streaming approximation gives an accurate description of the evolution of a wave packet having a narrow momentum spread, such that only momentum states belonging to the parabolicity region of the band contribute to the Wigner function. The effects of non-parabolicity become important for the evolution of a wave packet having a wide momentum spread, and they result in oscillations and bending of the Wigner function in phase space (see Figure 3), that cannot be properly described by the free-streaming approximation.

A homogeneous two-band model with external field

As a second example, we consider a simple, space-homogeneous, two-band model whith a constant external field. In a two-band model the Wigner function and its evolution equation are given by equations (1) and (13) respectively, where now $m = 0,1$ and $n = 0,1$. It can be seen easily from equation (2) that $f_{01} = f_{10}^*$, while f_{00} and f_{11} are real. In the absence of spatial gradients, the time evolution of the Wigner function is determined by the external field only (see equation (10) or equation (12)). Also, in the presence of a constant external field, the pseudodifferential operator (5) reduces to the classical differential operator of the Boltzmann equation, so that the evolution equation for the Wigner function (4) is given by

$$\frac{\partial f}{\partial t}(p,t) - E\frac{\partial f}{\partial p}(p,t) = 0, \tag{16}$$

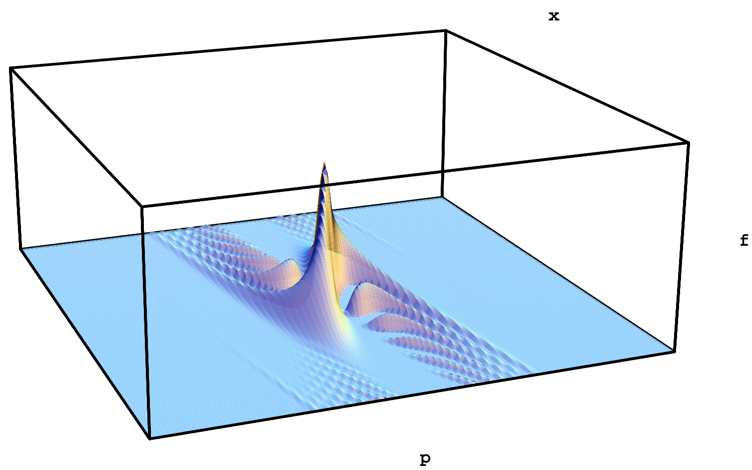

Figure 3: $f(x,p)$ for $\alpha = 0.2$ at $t = 20$, $0 \le x \le 20$, $-\pi \le p \le \pi$.

which shows that the Wigner function evolves according to a streaming law in momentum space and is given by $f(p,t) = f(p + Et, 0)$ with $f(p,0)$ the initial condition. Here, all the variables are dimensionless and measured in the units indicated in the previous Section, and E is the electric field measured in units of $\hbar^2/(ma^3)$.

In this homogeneous example, the energy bands are irrelevant to the dynamics of the Wigner function, whose evolution is determined entirely by the external field. Once the Wigner function is given as a function of time, however, we can calculate the Floquet projections and see how the total Wigner function is partitioned among the Floquet subspaces.

The projections f_{mn} of the Wigner function on the Floquet subspaces are obtained from equation (2) by using the definitions (8) and (9). In order to calculate the functions $f_{mn}(p)$, the explicit expressions of the Bloch functions are needed. In this simple two-band model, we approximate the Bloch functions with lattice-periodic plane waves:

$$\Psi_{0k}(x) = < x|0k >= \frac{1}{\sqrt{2\pi}} e^{ikx} \tag{17}$$

$$\Psi_{1k}(x) = < x|1k >= \frac{1}{\sqrt{2\pi}} (H(k)e^{-iKx} + H(-k)e^{iKx})e^{ikx}. \tag{18}$$

with H the Heavyside function and $K = 2\pi$ (in dimensionless units). After some calculations, it can be shown that, for a homogeneous Wigner function $f(x,p) = f(p)$, the band projections $f_{mn}(p)$ are given by:

$$f_{00}(p) = H\left(\frac{K}{2} - |p|\right) f(p) \tag{19}$$

$$Re(f_{01})(p) = 0 \tag{20}$$

$$f_{11}(p) = \left[H\left(p+K\right) H\left(-p - \frac{K}{2}\right) + H\left(p + \frac{K}{2}\right) H\left(K - p\right)\right] f(p). \tag{21}$$

These expressions show that, according to the model developed here, the projection f_{00} of the Wigner function onto the $m = 0$, $n = 0$ Floquet subspace is non-zero only inside the first Brillouin zone and is zero outside, while the projection f_{11} onto the $m = 1$, $n = 1$ subspace is zero in the first zone and non-zero in the second zone. We study an electron population initially characterized by a wave function belonging to the band $m = 0$. In the representation in which the density matrix is diagonal, we have

$$\rho(x,x') = \int \Psi_{0k}(x)\Psi^*_{0k}(x')w(k)dk \tag{22}$$

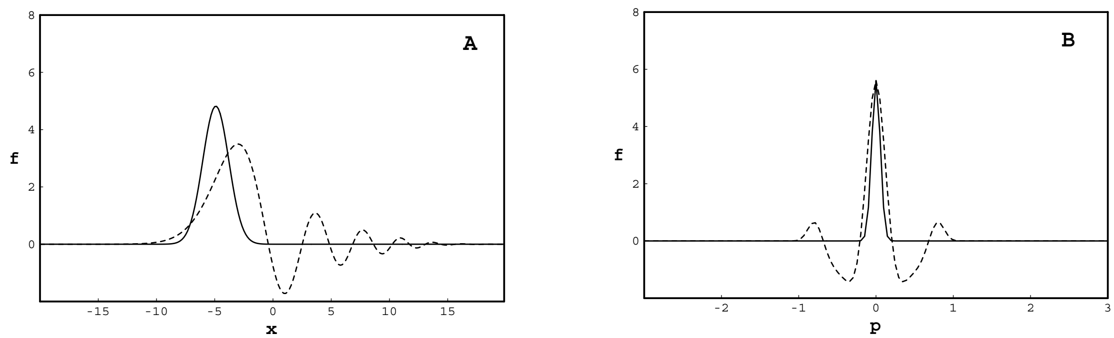

Figure 4: $f(x,p)$ as a function of x, $0 \leq x \leq 20$ for $p = 0.5$ (A) and $f(x,p)$ as a function of p, $-\pi \leq p \leq \pi$, for $x = 0$ (B), for $\alpha = 0.2$ and $t = 20$; exact solution from (15) (dashed line), free-streaming approximation from equation (12) (solid line). Dimensionless variables as defined in the text.

with $w(k)$ a statistical distribution. We have chosen $w(k) = \exp[-(k/\Delta k)^2]$ with $\Delta k = 0.1$. The corresponding Wigner function f is spatially homogeneous and is given by

$$f(p, t = 0) = H\left(\frac{K}{2} - |p|\right) w(p) .$$

At the initial time $t = 0$ we then have $f(p, 0) = f_{00}(p)$, which is shown in Figure 5A. Figures 5B, 5C and 5D show the time evolution of the Wigner function for an electric field $E = 0.4$ at $t = 1$, $t = 1.2$ and $t = 1.4$, respectively. The sequence shows how the Wigner function, which initially occupies only the lower band, moves towards higher energies and occupies the higher band. As the distribution moves rigidly towards higher momenta, it starts crossing the boundary of the Brillouin zone in momentum space. The portion of the Wigner function which has exited the Brillouin zone is taken up by the projection of f onto the next energy band subspace. While the Wigner momentum variable p ranges over the whole real line, the different portions of the p space correspond to the Floquet projections of f onto the band subspaces. We emphasize, however, that this behaviour is a consequence of using the lattice-periodic plane waves (17)-(18) for our Bloch functions and is to be regarded only as a tool for clarifying the concepts; the application of this model to a real situation will modify the general picture described above.

ACKNOWLEDGEMENTS

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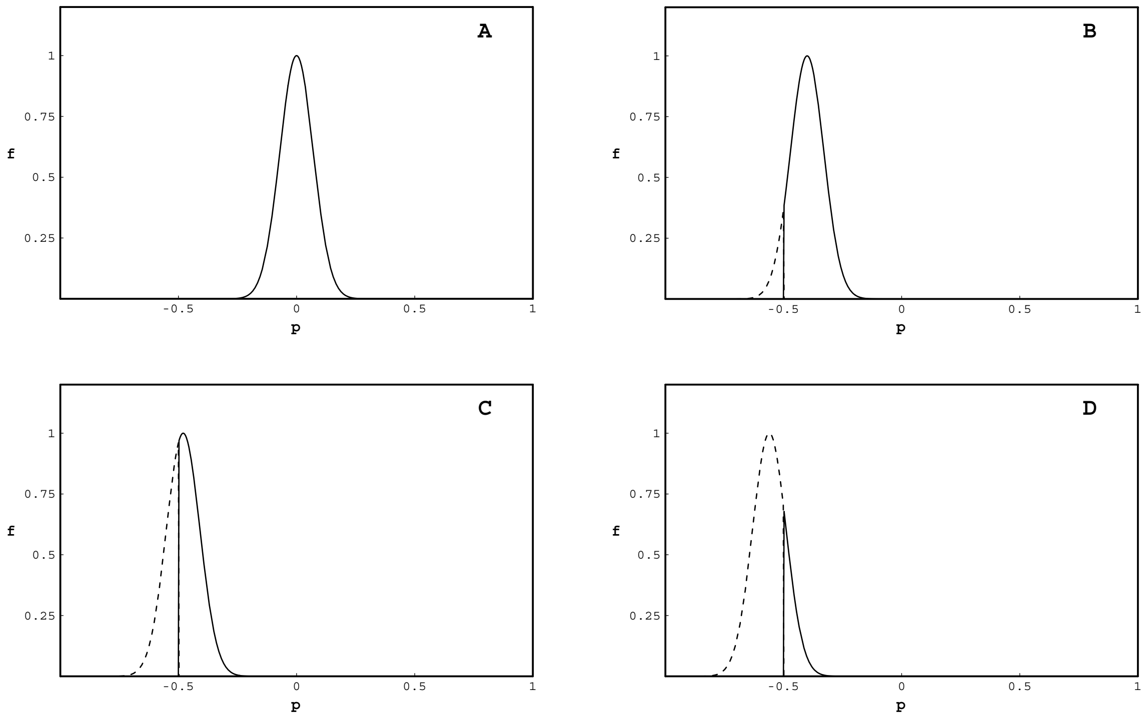

Figure 5: $f_{00}(p)$ (solid line) and $f_{11}(p)$ (dashed line) as functions of p, $-K/(2\pi) \leq p \leq K/(2\pi)$ for $E = 0.4$ and $t = 0$ (A), $t = 1$ (B), $t = 1.2$ (C) and $t = 1.4$ (D).

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