A quantum kinetic approach for modeling a two-band resonant tunneling diode

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1 Abstract

We present a mathematical study of a two-band quantum kinetic transport model. The multiband model, derived in the "kp" formalism, is designed to describe the dynamics in semiconductor devices when interband conduction-valence transition cannot be neglected. The Wigner formulation consists of a four-by-four system, containing two effective mass Wigner equations (one for the electron in conduction band and one for the valence band) coupled by pseudo-differential operators arising from the electric field in the semiconductor. Existence and uniqueness of a solution to the initial value problem are proved in a L^2-setting for sufficiently regular electric potentials. An extension of the single band splitting-scheme algorithm is presented to solve the one-dimensional system for a bounded domain. Finally, we show some numerical result concerning the simulation of an interband resonant diode.

Key words: Multiband transport; Wigner formulation; interband resonant diode.

2 Introduction

Recently much attention has been paid to quantum transport models. In particular, multiband transport is a topic of growing interest among physicists and applied mathematicians studying semiconductor devices of nanometric size. Indeed, quantum effects cannot be neglected when the size of the electronic device becomes comparable to the electron wavelength, as in new generation devices. For this reason, quantum modeling becomes a crucial aspect in nanoelectronics research in perspective of analog and digital applications. Resonant interband tunneling diodes (RITD) are examples of semiconductor devices of great importance in the nanotechnology for high-speed and miniaturized systems. Such diodes exhibit a band diagram structure with a band alignment, so that there is a small region where the valence band edge lies above the conduction band (valence quantum well). Therefore, the tunnel effect is the main mechanism of the charge carriers dynamics.

In electronics, the most popular model capable to describe the interaction of two bands is based on the Kane Hamiltonian (Kane, 1956). By means of a perturbative approach and an averaging procedure, the effect of the periodic lattice potential is taken into account by some phenomenological parameters, such as the energy-band gap and the coupling coefficient (Kane momentum) between the two bands.

The two-band Kane system is studied from the mathematical point of view in (Borgioli, Frosali, and Zweifel, 2003), where the well-posedness of the corresponding Wigner system is analyzed. In (Kefi, 2003), instead, an existence and uniqueness result for a coupled Kane-Poisson system is proved directly at the Schrödinger level. Also hydrodynamic models based on the Kane Hamiltonian can be found in the literature, e.g. (Alì and Frosali, 2005).

More recently, a new Schrödinger-like multiband model has been introduced that seems particularly suitable to deal with quantum transport in high-field interband resonant diodes. Such a multiband quantum model arises from the Bloch envelope theory (Kane, 1956; Modugno and Morandi, 2005).

In this paper we shall consider the two-band envelope function model in the Wigner function formulation. This approach is justified because the Wigner formalism can be applied to quantum statistical ensembles like a gas of electrons in a semiconductor device, e.g.. In addition, the Wigner formulation gives a mathematical system in a quasi-kinetic form.

In section 2 we briefly resume the multiband envelope function model (MEF model) in the two-band case. Then we apply the well-known Wigner formalism to the Schrödinger-like system. In section 3 and 4 we obtain some preliminary results concerning the mathematical properties of the problem and in section 5 we study the well-posedness of the Wigner system, using operator perturbation theory and the Stone's theorem. In section 6 we present an extension of the splitting scheme algorithm to implement our problem and we simulate a simple interband resonant diode. In the Appendix we give some remarks.

3 A two-band envelope function system

In this section we recall the multiband envelope function model, introduced recently by Modugno and Morandi, in the case of only two-bands. For the derivation of the model in the framework of the Bloch theory, the reader can refer to (Morandi and

Modugno, 2005).

Let $\psi_c(x,t)$ be the conduction band envelope function and $\psi_v(x,t)$ be the valence band envelope function. The multi-band envelope function model in the two-band time-dependent case reads as follows:

$$\begin{cases} i\hbar\dfrac{\partial\psi_c}{\partial t} &= -\dfrac{\hbar^2}{2m_c^*}\Delta\psi_c + (V_c+V)\psi_c - \dfrac{\hbar^2}{m}\dfrac{P\cdot\nabla V}{E_g}\psi_v\,, \\[2ex] i\hbar\dfrac{\partial\psi_v}{\partial t} &= \dfrac{\hbar^2}{2m_v^*}\Delta\psi_v + (V_v+V)\psi_v - \dfrac{\hbar^2}{m}\dfrac{P\cdot\nabla V}{E_g}\psi_c\,. \end{cases} \tag{3.1}$$

Here, i is the imaginary unit, $\hbar$ is the reduced Planck constant, m_c^* and m_v^* are the effective mass of the electron in the conduction and valence band respectively, and m is the bare mass of the carrier. Further, V_c and V_v are the minimum and the maximum of the conduction and the valence band energy, respectively. The external potential V depends on the layer composition and takes into account the electrostatic potential. In this way, the model allows us to treat a generic heterostructure where the edges of the bands can depend on the space coordinate while their difference, which is called energy gap E_g, remains constant. The coupling coefficient P represents the momentum operator matrix element between the Bloch functions related respectively to the minimum of the conduction band energy and the maximum of the valence band energy.

In this paper we will perform a one-dimensional analysis of this model. It is convenient to write system (3.1) more concisely as

$$i\hbar\frac{\partial\psi}{\partial t} = \mathcal{H}\psi \tag{3.2}$$

where the envelope function vector ψ is the couple $\psi_c\,,\,\psi_v$ and the Hamiltonian $\mathcal{H}$ is given by

$$\mathcal{H} = \begin{pmatrix} -\chi_c\dfrac{\hbar^2}{2m_c^*}\Delta + V_c + V & -\dfrac{\hbar^2}{m}\dfrac{P\cdot\nabla V}{E_g} \\[2ex] -\dfrac{\hbar^2}{m}\dfrac{P\cdot\nabla V}{E_g} & -\chi_v\dfrac{\hbar^2}{2m_v^*}\Delta + V_v + V \end{pmatrix}$$

with

$$\chi_i = \begin{cases} 1\,, & i=c\,, \\ -1\,, & i=v\,. \end{cases}$$

4 Wigner formulation

In this section we apply the Wigner formalism to the MEF model. Following the Wigner function approach (Frensley, 1990; Wigner, 1932), the MEF system takes the shape of an integro-differential equation for distribution-like functions.

To this aim, we introduce the density matrix

$$\rho = \begin{pmatrix} \rho_{cc} & \rho_{cv} \\ \rho_{vc} & \rho_{vv} \end{pmatrix} \tag{4.3}$$

with

$$\rho_{ij}(r,s) = \overline{\psi_i}(r)\psi_j(s), \quad i,j = c, v\,,$$

where the overbar means complex conjugate, and $\rho_{ij}(r,s) = \overline{\rho}_{ji}(r,s)$.

Now we formally differentiate the density matrix elements with respect to time t and we obtain for $i,j = c,v$,

$$\begin{aligned} i\hbar \frac{\partial \rho_{ij}}{\partial t} &= \frac{\hbar^2}{2m^*}\left(\chi_i \frac{\partial^2}{\partial r^2} - \chi_j \frac{\partial^2}{\partial s^2}\right)\rho_{ij} - \left(\frac{\chi_i - \chi_j}{2}\right) E_g\, \rho_{ij} - [V(r) - V(s)]\, \rho_{ij} \\ &\quad + \frac{\hbar^2 P}{m E_g}\frac{\mathrm{d}V}{\mathrm{d}r}\,\rho_{\bar{i}j} - \frac{\hbar^2 P}{m E_g}\frac{\mathrm{d}V}{\mathrm{d}s}\,\rho_{i\bar{j}}\,. \end{aligned} \tag{4.4}$$

Hereafter we will write $\bar{c} = v, \bar{v} = c$, and we will suppose that the conduction and valence electrons have the same effective mass, that is $m^* = m_c^* = m_v^*$.

Now we perform the following change of variables in the previous set of four coupled equations for the density matrix elements

$$\begin{cases} r &= x + \dfrac{\hbar}{2m^*}\eta\,, \\ s &= x - \dfrac{\hbar}{2m^*}\eta\,. \end{cases} \tag{4.5}$$

Putting $u_{ij}(x,\eta) = \rho_{ij}(r,s)$, we define the Wigner functions w_{ij} by inverse Fourier transform, that is

$$w_{ij}(x,v,t) = \mathcal{F}_v^{-1} u_{ij} = \frac{1}{2\pi}\int_{-\infty}^{\infty} \rho_{ij}\left(x + \frac{\hbar}{2m^*}\eta, x - \frac{\hbar}{2m^*}\eta\right) e^{i\,v\eta}\,\mathrm{d}\eta\,.$$

For the reader's convenience, we recall that the inverse Fourier transform with respect the v variable

$$\mathcal{F}_v^{-1} g(v) = \frac{1}{2\pi}\int_{-\infty}^{\infty} g(\eta) e^{i\,v\eta}\,\mathrm{d}\eta$$

satisfies the following property

$$\mathcal{F}_v^{-1}\left(\frac{\partial g}{\partial \eta}\right) = -iv\mathcal{F}^{-1}(g)\,.$$

Noting that

$$\frac{\hbar^2}{2m^*}\left(\chi_i \frac{\partial^2}{\partial r^2} - \chi_j \frac{\partial^2}{\partial s^2}\right) = \begin{cases} \chi_i\,\hbar \dfrac{\partial^2}{\partial x \partial \eta}\,, & i = j \\ \chi_i \left(\dfrac{\hbar^2}{4m^*}\dfrac{\partial^2}{\partial x^2} + m^* \dfrac{\partial^2}{\partial \eta^2}\right)\,, & i \neq j \end{cases}$$

by Fourier inverse transform we obtain

$$\mathcal{F}_v^{-1}\left[\frac{\hbar^2}{2m^*}\left(\chi_i\frac{\partial^2}{\partial r^2}-\chi_j\frac{\partial^2}{\partial s^2}\right)\rho_{ij}\right]$$
$$= -i\hbar\left(\frac{\chi_i+\chi_j}{2}\right)v\frac{\partial w_{ij}}{\partial x}+\left(\frac{\chi_i-\chi_j}{2}\right)\left(\frac{\hbar^2}{4m^*}\frac{\partial^2 w_{ij}}{\partial x^2}-m^*v^2 w_{ij}\right).$$

Moreover, for $i,j=c,v$, we have

$$\begin{aligned}
\mathcal{F}_v^{-1}\left[(V(r)-V(s))\rho_{ij}\right] &= \hbar\,\theta[V]w_{ij}\ ,\\
\mathcal{F}_v^{-1}\left[\frac{\hbar^2 P}{mE_g}\frac{\mathrm{d}V}{\mathrm{d}r}\rho_{ij}\right] &= \frac{P\hbar^2}{mE_g}\mathcal{O}^+[V]w_{ij}\ ,\\
\mathcal{F}_v^{-1}\left[-\frac{\hbar^2 P}{mE_g}\frac{\mathrm{d}V}{\mathrm{d}s}\rho_{ij}\right] &= -\frac{P\hbar^2}{mE_g}\mathcal{O}^-[V]w_{ij}\ ,
\end{aligned}$$

where we have defined

$$\mathcal{F}_v\left(\theta[V]f\right)(x,\eta)=\frac{1}{\hbar}\left(\delta V\mathcal{F}_v f\right)(x,\eta)\,, \tag{4.6}$$

$$\delta V(x,\eta)=V\left(x+\frac{\hbar}{2m^*}\eta\right)-V\left(x-\frac{\hbar}{2m^*}\eta\right), \tag{4.7}$$

or more explicitly

$$\theta[V]f=\frac{1}{2\pi}\int_{\mathbb{R}_\eta}\int_{\mathbb{R}_{v'}}\frac{V\left(x+\frac{\hbar}{2m^*}\eta\right)-V\left(x-\frac{\hbar}{2m^*}\eta\right)}{\hbar}f(x,v')\,e^{i(v-v')\eta}\ \mathrm{d}v'\,\mathrm{d}\eta \tag{4.8}$$

and

$$\mathcal{O}^{\pm}[V]f=\frac{1}{2\pi}\int_{\mathbb{R}_\eta}\int_{\mathbb{R}_{v'}}\frac{\mathrm{d}V}{\mathrm{d}x}\left(x\pm\frac{\hbar}{2m^*}\eta\right)f(x,v')\,e^{i(v-v')\eta}\ \mathrm{d}v'\,\mathrm{d}\eta\,. \tag{4.9}$$

After an inverse Fourier transform, Eq. (4.4) gives

$$\frac{\partial w_{ij}}{\partial t}=-\left(\frac{\chi_i+\chi_j}{2}\right)v\frac{\partial w_{ij}}{\partial x}-i\left(\frac{\chi_i-\chi_j}{2}\right)\left[\frac{\hbar}{4m^*}\frac{\partial^2 w_{ij}}{\partial x^2}-\frac{1}{\hbar}\left(E_g+m^*v^2\right)w_{ij}\right]+$$
$$+i\theta[V]w_{ij}-i\frac{P\hbar}{mE_g}\mathcal{O}^+[V]w_{\bar{i}j}+i\frac{P\hbar}{mE_g}\mathcal{O}^-[V]w_{i\bar{j}}\,.$$

In conclusion the Wigner formulation of system (3.1) takes the following form

$$\begin{cases} \dfrac{\partial w_{cc}}{\partial t} &= -v\dfrac{\partial w_{cc}}{\partial x} + i\theta[V]w_{cc} - i\dfrac{P\hbar}{mE_g}\mathcal{O}^+[V]w_{vc} + i\dfrac{P\hbar}{mE_g}\mathcal{O}^-[V]w_{cv} \\ \dfrac{\partial w_{cv}}{\partial t} &= -i\dfrac{\hbar}{4m^*}\dfrac{\partial^2 w_{cv}}{\partial x^2} + \dfrac{i}{\hbar}\left(E_g + m^* v^2\right) w_{cv} + i\theta[V]w_{cv} \\ & \qquad - i\dfrac{P\hbar}{mE_g}\mathcal{O}^+[V]w_{vv} + i\dfrac{P\hbar}{mE_g}\mathcal{O}^-[V]w_{cc} \\ \dfrac{\partial w_{vc}}{\partial t} &= i\dfrac{\hbar}{4m^*}\dfrac{\partial^2 w_{vc}}{\partial x^2} - \dfrac{i}{\hbar}\left(E_g + m^* v^2\right) w_{vc} + i\theta[V]w_{vc} \\ & \qquad - i\dfrac{P\hbar}{mE_g}\mathcal{O}^+[V]w_{cc} + i\dfrac{P\hbar}{mE_g}\mathcal{O}^-[V]w_{vv} \\ \dfrac{\partial w_{vv}}{\partial t} &= v\dfrac{\partial w_{vv}}{\partial x} + i\theta[V]w_{vv} - i\dfrac{P\hbar}{mE_g}\mathcal{O}^+[V]w_{cv} + i\dfrac{P\hbar}{mE_g}\mathcal{O}^-[V]w_{vc} \end{cases} \tag{4.10}$$

with the previously defined operators $\theta[V]$ and $\mathcal{O}^{\pm}[V]$.

5 Some preliminary results

In this section we give some preliminary results on the operators appearing in the system (4.10).

Let us consider the Hilbert space $\mathbf{L}^2(\mathbb{R}_x \times \mathbb{R}_v;\, \mathrm{d}x\,\mathrm{d}v)$ of complex valued functions with the usual inner product and norm. We recall that

$$\mathbf{L}^2(\mathbb{R}_x \times \mathbb{R}_v; \mathrm{d}x\,\mathrm{d}v) = \mathbf{L}^2(\mathbb{R}_x; \mathrm{d}x) \otimes \mathbf{L}^2(\mathbb{R}_v; \mathrm{d}v)$$

is the $\mathbf{L}^2$-space with respect to the product measure $\mathrm{d}x \otimes \mathrm{d}y$, ($\otimes$ denotes the tensor product) (Reed and Simon, 1972).

Let us consider the Fourier unitary map $\mathcal{F}_x$ of the space $\mathbf{L}^2(\mathbb{R}_x; \mathrm{d}x)$ onto $\mathbf{L}^2(\mathbb{R}_\mu;\, \mathrm{d}\mu)$. We may extend such map $\mathcal{F}_x$ to $\mathcal{F}_x \otimes I_v$ as a map from the space $\mathbf{L}^2(\mathbb{R}_x \times \mathbb{R}_v;\, \mathrm{d}x\,\mathrm{d}v)$ onto $\mathbf{L}^2(\mathbb{R}_\mu \times \mathbb{R}_v;\, \mathrm{d}\mu\,\mathrm{d}v)$. I_v is the identity operator on $\mathbf{L}^2(\mathbb{R}_v; \mathrm{d}v)$.

Lemma 5.1 *The operator* $T_s f = v\frac{\partial}{\partial x} f$ *with domain* $D_{T_s} = \left\{ f \in \boldsymbol{L}^2(\mathbb{R}_x \times \mathbb{R}_v;\, dx\, dv) : v\frac{\partial}{\partial x} f \in \boldsymbol{L}^2(\mathbb{R}_x \times \mathbb{R}_v;\, dx\, dv) \right\}$ *is self-adjoint on* $\boldsymbol{L}^2(\mathbb{R}_x \times \mathbb{R}_v;\, dx\, dv)$.

Proof. Let us consider the operator $\mathcal{F}_x \otimes \mathcal{I}$ as an extended Fourier unitary map of the space $\mathbf{L}^2(\mathbb{R}_x \times \mathbb{R}_v;\, \mathrm{d}x\,\mathrm{d}v)$ onto $\mathbf{L}^2(\mathbb{R}_\mu \times \mathbb{R}_v;\, \mathrm{d}\mu\,\mathrm{d}v)$. In fact by using Fubini's theorem

$$\|f\|_{\mathbf{L}^2(\mathbb{R}_x \times \mathbb{R}_v; \mathrm{d}x\mathrm{d}v)} = \int_{\mathbb{R}_v} \left(\int_{\mathbb{R}_x} |f|^2 \,\mathrm{d}x \right) \mathrm{d}v = \int_{\mathbb{R}_v} \left(\int_{\mathbb{R}_\mu} |\mathcal{F}_x f|^2 \,\mathrm{d}\mu \right) \mathrm{d}v = \|\mathcal{F}_x f\|_{\mathbf{L}^2(\mathbb{R}_\mu \times \mathbb{R}_v; \mathrm{d}\mu \mathrm{d}v)}.$$

Accordingly, D_{T_s} is isomorphic to $D'_{T_s} = \left\{ f \in \mathbf{L}^2(\mathbb{R}_\mu \times \mathbb{R}_v;\, \mathrm{d}\mu\,\mathrm{d}v) : v\mu f \in \mathbf{L}^2(\mathbb{R}_\mu \times \mathbb{R}_v;\, \mathrm{d}\mu\,\mathrm{d}v) \right\}$ and the proof reduces to show that the multiplication operator $T_s f = v\mu f$ with domain D'_{T_s} is a self-adjoint operator. This follows directly from Prop.1 Chapter VIII of (Reed and Simon, 1972). ∎

Remark. We want to stress that the previous operator is not self-adjoint in the space $D_1 = \mathbf{H}^1(\mathbb{R}_x) \otimes \mathbf{L}^2(\mathbb{R}_v; (1+v^2)\,\mathrm{d}v)$. By the definition of the previous Sobolev space, it is indeed easy to show that D_1 via Fourier transform is isomorphic to

$$D_1' = \mathbf{L}^2(\mathbb{R}_\mu; (1+\mu^2)\,\mathrm{d}\mu) \otimes \mathbf{L}^2(\mathbb{R}_v; (1+v^2)\,\mathrm{d}v)\,.$$

According to (Reed and Simon, 1972) this space is equivalent to

$$D_1'' = \mathbf{L}^2(\mathbb{R}_v \times \mathbb{R}_\mu; (1+v^2)(1+\mu^2)\,\mathrm{d}\mu\,\mathrm{d}v)\,.$$

On the other hand, D_{T_s} is mapped onto

$$\begin{aligned} D_{T_s}' &= \left\{ f \in \mathbf{L}^2(\mathbb{R}_\mu \times \mathbb{R}_v;\, \mathrm{d}\mu\,\mathrm{d}v) : v\mu f \in \mathbf{L}^2(\mathbb{R}_\mu \times \mathbb{R}_v;\, \mathrm{d}\mu\,\mathrm{d}v) \right\} \\ &= \mathbf{L}^2\left(\mathbb{R}_\mu \times \mathbb{R}_v; (1+\mu^2 v^2)\,\mathrm{d}\mu\,\mathrm{d}v\right)\,. \end{aligned}$$

We have that $D_1'' \subset\subset D_{T_s}'$, hence the T operator cannot be self-adjoint in D_1''. It is easy to see that D_1'' is strictly contained in D_{T_s}'. It is sufficient to find a function $f \in \mathbf{L}^2$ so that $\mu v f \in \mathbf{L}^2$, but $\mu f, v f \notin \mathbf{L}^2$, for instance taking f in a such way that

$$|f|^2 = \frac{1}{(1+\mu^2)(1+v^2)(1+\mu^2 v^2)}\,.$$

Lemma 5.2 *The operator* $T_d f = \left(\dfrac{\partial^2}{\partial x^2} + v^2\right) f$ *with domain* $D_{T_d} = \Big\{ f \in \boldsymbol{L}^2\,(\mathbb{R}_\mu \times \mathbb{R}_v;\, d\mu\, dv) \colon \left(\frac{\partial^2}{\partial x^2} + v^2\right) f \in \boldsymbol{L}^2\,(\mathbb{R}_\mu \times \mathbb{R}_v;\, d\mu\, dv) \Big\}$ *is self-adjoint on* $\boldsymbol{L}^2\,(\mathbb{R}_\mu \times \mathbb{R}_v;\, d\mu\, dv)$.

Proof. Also this lemma follows immediately from Prop. 1 Chapter VIII (Reed and Simon, 1972). ■

As before, we remark that the domain of T_d does not coincide with $D_2 = \mathbf{H}^2\,(\mathbb{R}_x;\, \mathrm{d}x) \otimes \mathbf{L}^2\left(\mathbb{R}_v; (1+v^2)^2\,\mathrm{d}v\right)$.
In fact D_2 is isomorphic to $D_2' = \mathbf{L}^2\left(\mathbb{R}_\mu; (1+\mu^2)^2\,\mathrm{d}\mu\right) \otimes \mathbf{L}^2\left(\mathbb{R}_v; (1+v^2)^2\,\mathrm{d}v\right)$ and thus to $D_2'' = \mathbf{L}^2\left(\mathbb{R}_\mu \times \mathbb{R}_v; (1+\mu^2)^2(1+v^2)^2\,\mathrm{d}\mu\,\mathrm{d}v\right)$. On the other hand D_{T_d} is isomorphic to $D_{T_d}' = \mathbf{L}^2\left(\mathbb{R}_\mu \times \mathbb{R}_v; (1+\mu^2+v^2)^2\,\mathrm{d}\mu\,\mathrm{d}v\right)$; D_{T_d}' and D_2'' are different spaces since their metrics are not equivalent.

6 Mathematical formulation and well-posedness of the problem

Let us consider the Hilbert space $\mathbf{H} = \mathbf{L}^2\left(\mathbb{R}_x \times \mathbb{R}_v;\, \mathrm{d}x\,\mathrm{d}v\,; \mathbb{C}^4\right)$ equipped with the scalar product

$$(f,g)_{\mathbf{H}} = \int_{\mathbb{R}_x \times \mathbb{R}_v} < f(x,v), g(x,v) > \mathrm{d}x\,\mathrm{d}v\,, \qquad \|f\|_{\mathbf{H}} = \sum_{i=1}^{4} \|f_i\|_{\mathbf{L}^2(\mathbb{R}_x \times \mathbb{R}_v;\, \mathrm{d}x\,\mathrm{d}v)},$$

where $f = (f_1, f_2, f_3, f_4)$ and $<,>$ is the usual scalar product in $\mathbb{C}^4$

$$< f, g >= f^T \overline{g} = \sum_i^4 f_i \overline{g}_i \,,$$

(we use the apex T to denote the transposed vector). Let us introduce the following 4×4 matrix operators defined as

$$\mathcal{T} = \text{ diag}\left[iv\frac{\partial}{\partial x}, -\frac{\hbar}{4m^*}\frac{\partial^2}{\partial x^2} + \frac{1}{\hbar}\left(E_g + m^* v^2\right) \,, \frac{\hbar}{4m^*}\frac{\partial^2}{\partial x^2} - \frac{1}{\hbar}\left(E_g + m^* v^2\right), -iv\frac{\partial}{\partial x}\right] \,,$$

$$\mathcal{B} = \mathcal{I}\,\theta[V] \,,$$

$$\mathcal{O} = \frac{P\hbar}{m_0 E_g}\begin{pmatrix} 0 & \mathcal{O}^-[V] & -\mathcal{O}^+[V] & 0 \\ \mathcal{O}^-[V] & 0 & 0 & -\mathcal{O}^+[V] \\ -\mathcal{O}^+[V] & 0 & 0 & \mathcal{O}^-[V] \\ 0 & -\mathcal{O}^+[V] & \mathcal{O}^-[V] & 0 \end{pmatrix} \,.$$

$\mathcal{I}$ is the identity operator in $\mathbf{H}$. Then we can rewrite system (4.10) in the Schrödinger-like form

$$\frac{\partial w}{\partial t} = i(\mathcal{T} + \mathcal{B} + \mathcal{O})w$$

where $w = (w_{cc}, w_{cv}, w_{vc}, w_{vv})^T$.

Theorem 6.1 *The operator $\mathcal{T}$ with domain $D_{\mathcal{T}} = D_{T_s} \oplus D^2_{T_d} \oplus D_{T_s}$ is self-adjoint on $\mathbf{H}$.*

Proof. The theorem follows directly from lemmas (5.1) and (5.2), and from the definition of the Hilbert space $\mathbf{H}$. ■

We observe that the operator $\mathcal{B}$ is symmetric, and bounded in $\mathbf{H}$, since the pseudo-differential operator $\theta[V]$ is a symmetric bounded operator in $\mathbf{L}^2\,(\mathbb{R}_x \times \mathbb{R}_v;\, \mathrm{d}x\, \mathrm{d}v)$.

Theorem 6.2 *The operator $\mathcal{O}$ is symmetric, and bounded on $\mathbf{H}$.*

Proof. First let us write the operator $\mathcal{O}^{\pm}[V]$ as follows

$$\mathcal{O}^{\pm}[V]f = \mathcal{F}_v^{-1}\left[\frac{\mathrm{d}V}{\mathrm{d}x}(x \pm \epsilon\eta)\mathcal{F}_v f\right] \qquad \text{with} \quad \epsilon = \frac{\hbar}{2m^*} \,. \tag{6.11}$$

Hence, it is convenient to apply the Fourier transform with respect to the variable v to the operator $\mathcal{O}$. Here we use the symbol $\mathcal{F}$ as Fourier transform on $\mathbf{H}$ and we denote $\mathcal{F}_v f$ by $\hat{f}$. Then we obtain

$$\mathcal{F}_v\left(\mathcal{O}f\right) = \mathbf{O}\mathcal{F}_v f$$
$$= \frac{P\hbar}{m_0 E_g}\begin{pmatrix} 0 & \frac{\mathrm{d}V}{\mathrm{d}x}(x-\epsilon\eta) & -\frac{\mathrm{d}V}{\mathrm{d}x}(x+\epsilon\eta) & 0 \\ \frac{\mathrm{d}V}{\mathrm{d}x}(x-\epsilon\eta) & 0 & 0 & -\frac{\mathrm{d}V}{\mathrm{d}x}(x+\epsilon\eta) \\ -\frac{\mathrm{d}V}{\mathrm{d}x}(x+\epsilon\eta) & 0 & 0 & \frac{\mathrm{d}V}{\mathrm{d}x}(x-\epsilon\eta) \\ 0 & -\frac{\mathrm{d}V}{\mathrm{d}x}(x+\epsilon\eta) & \frac{\mathrm{d}V}{\mathrm{d}x}(x-\epsilon\eta) & 0 \end{pmatrix}\begin{pmatrix} \hat{f}_{cc} \\ \hat{f}_{cv} \\ \hat{f}_{vc} \\ \hat{f}_{vv} \end{pmatrix}.$$

It is easy to see that the matrix operator $\mathbf{O}$ of components $\mathbf{O}_{ij}$, defined above, satisfies the following relations:

$$\begin{aligned}(\mathcal{O}f, g)_{\mathbf{H}} &= (\mathcal{F}_v^{-1}\mathbf{O}\mathcal{F}_v f, g)_{\mathbf{H}} = (\mathbf{O}\mathcal{F}_v f, \mathcal{F}_v g)_{\mathbf{L}^2(\mathbb{R}_x\times\mathbb{R}_\eta;\,\mathrm{d}x\,\mathrm{d}\eta)} \\ &= \sum_{i,j}(\mathbf{O}_{ij}\hat{f}_i, \hat{g}_j)_{\mathbf{L}^2(\mathbb{R}_x\times\mathbb{R}_\eta;\,\mathrm{d}x\,\mathrm{d}\eta)} = \sum_{i,j}(\hat{f}_i, \overline{\mathbf{O}}_{ij}\hat{g}_j)_{\mathbf{L}^2(\mathbb{R}_x\times\mathbb{R}_\eta;\,\mathrm{d}x\,\mathrm{d}\eta)} = (f, \mathcal{O}g)_{\mathbf{H}}\end{aligned}$$

where we used that $\mathbf{O}_{ij}$ is a symmetric matrix and $\mathcal{F}_v$ is a unitary operator. Noting that

$$\begin{aligned}\left\|\mathcal{O}^{\pm}[V]f\right\|_{\mathbf{L}^2(\mathbb{R}_x\times\mathbb{R}_v;\,\mathrm{d}x\,\mathrm{d}v)} &= \left\|\frac{\mathrm{d}V}{\mathrm{d}x}\left(x\pm\epsilon\eta\right)\hat{f}\right\|_{\mathbf{L}^2(\mathbb{R}_x\times\mathbb{R}_\eta;\,\mathrm{d}x\,\mathrm{d}\eta)} \\ &\le \left\|\frac{\mathrm{d}V}{\mathrm{d}x}\right\|_{\mathbf{L}^\infty(\mathbb{R}_x;\,\mathrm{d}x)}\|f\|_{\mathbf{L}^2(\mathbb{R}_x\times\mathbb{R}_v;\,\mathrm{d}x\,\mathrm{d}v)},\end{aligned}$$

we have

$$\|\mathcal{O}f\|_{\mathbf{H}} = \sum_i\Big\|\sum_j\mathbf{O}_{ij}\hat{f}_j\Big\|_{\mathbf{L}^2(\mathbb{R}_x\times\mathbb{R}_\eta;\,\mathrm{d}x\,\mathrm{d}\eta)} \le 8\left\|\frac{\mathrm{d}V}{\mathrm{d}x}\right\|_{\mathbf{L}^\infty(\mathbb{R}_x;\,\mathrm{d}x)}\|f\|_{\mathbf{H}}\,.$$

This proves our thesis. ∎

The previous estimates suggested us to require some regularity assumption on the potential V in order to prove the following existence theorem. We denote by $W^{1,\infty}$ the usual Sobolev spaces.

Theorem 6.3 *For all $V \in W^{1,\infty}$ and initial datum $w^0 \in \mathbf{H}$, system (4.10) admits a unique solution $w \in \mathbf{H}$.*

Proof. By the perturbation theorem, we have that $\mathcal{T}+\mathcal{B}+\mathcal{O}$ is a self-adjoint operator. Thus, by Stone's theorem, it generates the unitary group $e^{i(\mathcal{T}+\mathcal{B}+\mathcal{O})t}$ in $\mathbf{H}$. Hence our theorem is proved. ∎

We would like to remark that, even if the previous analysis was performed in the complex Hilbert space $\mathbf{L}^2(\mathbb{R}_x\times\mathbb{R}_v;\,\mathrm{d}x\,\mathrm{d}v)$, physical considerations suggest to restrict to a more suitable domain. In fact, since it is well-known that the single-band Wigner function is a real function, a proper extension of the Wigner formalism to multiband framework requires that also the quantities w_{cc} and w_{vv} have to be real functions. In this way, when E_g goes to infinity (in the single-band limit), it is immediate to verify that system (3.1) decouples, recovering the correct single-band dynamics. This is what we expect from the physical point of view. Furthermore consistence with the definition of ρ_{cv} and ρ_{vc} suggests that also w_{cv} and w_{vc} are to be conjugate functions one another. To this aim, we choose as initial datum for the system (3.1) a function w^0 so that w^0_{cc} and w^0_{vv} are real functions and $w^0_{cv} = \overline{w^0_{vc}}$ holds. In appendix we show that the previous properties are preserved for all times: this allow us to solve the system (4.10) only for the non vanishing components of w, becoming

$$\begin{cases} \dfrac{\partial w_{cc}}{\partial t} = -v\dfrac{\partial w_{cc}}{\partial x} + i\theta[V]w_{cc} - 2\dfrac{P\hbar}{mE_g}\ \mathrm{Im}\ \left\{\mathcal{O}^-[V]w_{cv}\right\} \\ \dfrac{\partial w_{vv}}{\partial t} = v\dfrac{\partial w_{vv}}{\partial x} + i\theta[V]w_{vv} + 2\dfrac{P\hbar}{mE_g}\ \mathrm{Im}\ \left\{\mathcal{O}^+[V]w_{cv}\right\} \\ \dfrac{\partial w_{cv}}{\partial t} = -i\dfrac{\hbar}{4m^*}\dfrac{\partial^2 w_{cv}}{\partial x^2} + \dfrac{i}{\hbar}\left(E_g + m^* v^2\right) w_{cv} + i\theta[V]w_{cv} \\ \qquad\qquad - i\dfrac{P\hbar}{mE_g}\mathcal{O}^+[V]w_{vv} + i\dfrac{P\hbar}{mE_g}\mathcal{O}^-[V]w_{cc} \end{cases} \tag{6.12}$$

written for the real functions w_{cc}, w_{vv} and for the complex one w_{cv}.

In [7] we present an extension of this work, where the system, coupled with the Poisson equation, is studied in a bounded spatial domain with inflow boundary conditions.

7 Numerical simulation

In this section we present a numerical scheme to solve our problem by applying the algorithm to a simple interband resonant diode.

The $1D$ numerical scheme used to get an approximate solution of (4.10) is an extension of the splitting-scheme algorithm implemented in the one-band case, see e.g. (Arnold and Ringhofer, 1996; Demeio, 2003). In this spirit, we propose the following approximation of the evolution group

$$e^{i(\mathcal{T}+\mathcal{B}+\mathcal{O})t} \simeq \left[e^{i\mathcal{T}\frac{t}{2N}}\, e^{i\mathcal{B}\frac{t}{N}}\, e^{i\mathcal{T}\frac{t}{2N}}\, e^{i\mathcal{O}\frac{t}{N}}\right]^N \tag{7.13}$$

with N sufficiently large. Here we indicate with $e^{i\mathcal{T}t}, e^{i\mathcal{B}t}, e^{i\mathcal{O}t}$ the free-streaming, vertical shift and tunneling operators, respectively; each one of them solves a simplified differential or pseudo-differential problem. More explicitly, if w^n denotes the approximate solution at the time step $t = n\Delta_t$, (7.13) means that the subsequent evolution problems can be solved successively

$$
Free - streaming \quad \begin{cases} \dfrac{\partial f}{\partial t} & = & i\mathcal{T} f, \quad t_n \leq t \leq t_n + \Delta_t \\ f(t_n) & = & w^n \\ w^{n+\frac{1}{3}} & = & f(t_n + \Delta_t) \end{cases} , \tag{7.14}
$$

$$
Vertical - shift \quad \begin{cases} \dfrac{\partial f}{\partial t} & = & i\mathcal{B} f, \quad t_n \leq t \leq t_n + \Delta_t \\ f(t_n) & = & w^{n+\frac{1}{3}} \\ w^{n+\frac{2}{3}} & = & f(t_n + \Delta_t) \end{cases} , \tag{7.15}
$$

$$
Tunneling \quad \begin{cases} \dfrac{\partial f}{\partial t} & = & i\mathcal{O} f, \quad t_n \leq t \leq t_n + \Delta_t \ , \\ f(t_n) & = & w^{n+\frac{2}{3}} \\ w^{n+1} & = & f(t_n + \Delta_t) \end{cases} . \tag{7.16}
$$

The analysis of problems (7.14) and (7.15) can be performed in $\mathbb{R}_x \times \mathbb{R}_v$. In particular, for (7.14) we have that the explicit solutions are

$$
w_{ii}^{n+\frac{1}{3}}(x, v) = w_{ii}^{n}(x - v\Delta_t, v)\,, \quad i = c, v \tag{7.17}
$$

while for w_{cv}, we use the Fourier transform with respect to x, and we get

$$
\left(\mathcal{F}_x w_{cv}^{n+\frac{1}{3}}\right)(\mu, v) = \left(\mathcal{F}_x w_{cv}^{n}\right)(\mu, v) e^{\frac{i}{\hbar}\ \ E_g + \frac{\hbar^2}{4m^*}\mu^2 + m^* v^2\ \ \Delta_t}\,. \tag{7.18}
$$

Similarly, for Eq. (7.15) we obtain by Fourier transform with respect to v,

$$
\left(\mathcal{F}_v w_{ij}^{n+\frac{2}{3}}\right)(x, \eta) = \left(\mathcal{F}_v w_{ij}^{n+\frac{1}{3}}\right)(x, \eta) e^{\frac{i}{\hbar}\delta V(x,\eta)\Delta_t}\,, \quad i, j = c, v\,, \tag{7.19}
$$

with δV defined in (4.7). Finally, by writing the operator $\mathcal{O}$ in the Fourier space as in Eq. (6.11), we get the following explicit solution of Eq. (7.16)

$$
\left(\mathcal{F}_v w^{n+1}\right)(x, \eta) = \left(\mathcal{F}_v w^{n+\frac{2}{3}}\right)(x, \eta) e^{i\mathbf{O}(x,\eta)\Delta_t}\,. \tag{7.20}
$$

For each temporal step Δ_t, the previous equations are numerically implemented into a discretized domain. To this aim, we reduce our initial unbounded domain to $\Omega = [0, L] \times [-V_M, V_M]$. Further, for consistence with the whole space analysis performed, we assume that Ω is an open domain. Accordingly, we assign the following inflow boundary condition in $x = 0, x = L$ (Markowich, Ringhofer and Schmeiser, 1990)

$$
\begin{cases} w(0, v, t) = \tilde{w}(v) \quad \text{for } v > 0 \\ \\ w(L, v, t) = \tilde{w}(v) \quad \text{for } v < 0 \end{cases} \tag{7.21}
$$

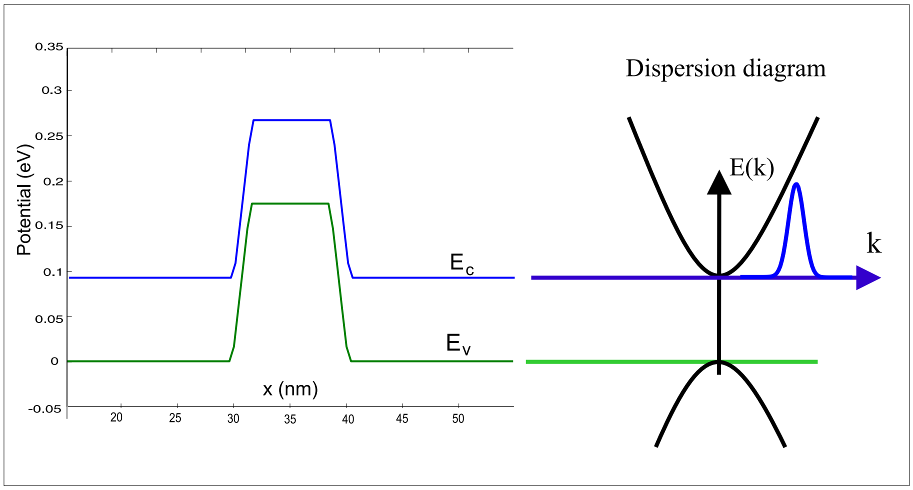

Figure 1: R.h.s.: Simulated heterostructure profile of the RITD. The widths of the layers are chosen: 5.00 nm for the quantum well, 3.00 nm for the barriers. L.h.s.: We show the dispersion diagram of the semiconductor and the quasi-momentum distribution function of the injected electron in the diode.

where $\tilde{w}(v)$ is a given function. Moreover, we require that $w(x, \pm V_M, t) = 0$. Let us introduce a $N \times 2M$ uniform mesh

$$\begin{cases} x_j = j\Delta_x & , \quad j = 1 \dots N \,, \\ v_k = k\Delta_v & , \quad k = 1 \dots 2M \,, \\ \eta_{k'} = k' \dfrac{2\pi}{V_M} & , \quad k' = -M \dots M \,, \end{cases}$$

and a matrix of three elements vector (with two real and one complex components)

$$\mathbf{w}^n_{jk} = (w^n_{cc}(x_j, v_k), w^n_{vv}(x_j, v_k), w^n_{cv}(x_j, v_k))^T \ .$$

The solutions (7.17)-(7.18)-(7.19)-(7.20) are approximated by $\mathbf{w}^n_{jk}$ in the following way: for (7.17) we use a spline interpolation scheme, (Demeio, 2003), which takes into account the inflow boundary conditions (7.21), while (7.18), (7.19) are directly implemented by FFT (Fast Fourier Transform) algorithms. Finally for (7.20) we define a matrix $\mathbf{O}_{jk'} = \mathbf{O}(x_j, \eta_{k'})$ and we use a Caylay scheme to approximate the exponential term (Frensley, 1990). A more detailed numerical analysis and comparison with other algorithms will be subject of a future work.

As an application of the model (4.10), we consider a simple interband resonant diode (see fig.1) consisting of two homogeneous regions separated by a potential barrier and realizing a single quantum well in the valence band.

As initial datum $w(x, v, 0)$ we choose a vanishing function, and for boundary

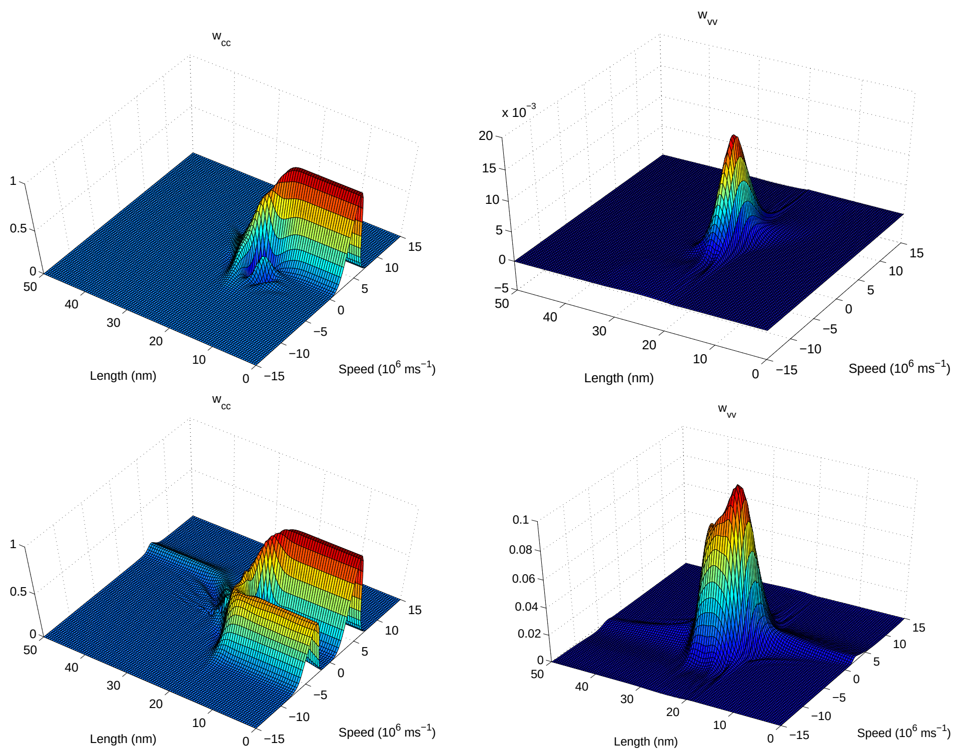

Figure 2: Computed Wigner functions w_{cc} (left-hand side) and w_{vv} (right-hand side) for $t = 10^{-14}\ s$ (top) and $t = 10^{-13}\ s$ (bottom).

condition the function

$$\begin{cases} \tilde{w}_{cc}(v) = e^{-\frac{m^*(v-v_0)^2}{\delta_v}} \quad , \quad \text{for } v > 0 \quad , \\ \\ \tilde{w}_{ij}(v) = 0 \qquad\qquad\quad , \quad \text{otherwise} \quad , i,j = c,v \ , \end{cases} \tag{7.22}$$

which describes a flux of conduction electrons injected into the diode with a positive mean momentum and gaussian dispersion (see Rhs of fig.1). In our simulation, we used the following parameters: $E_g = E_c - E_v = 0.16\ eV$, $m^* = 0.023\ m_0$, $P = 5 \cdot 10^9\ m^{-1}$, $v_0 = 5 \cdot 10^6\ ms^{-1}$, $\delta_v = 10^{-22}\ J$. In fig.2 we plot the solution $\mathbf{w}_{jk}$ computed for $t_1 = 10^{-14}\ s$, $t_2 = 10^{-13}\ s$.

The results of the simulation can be interpreted as follows. w_{cc} describes the motion of the electron ensemble in conduction band. It shows that the conduction electron beam is (mainly) reflected back by the potential barrier. Besides, the gradient of the potential couples conduction electrons with valence ones. Since the central region realizes a single quantum well in valence band, the w_{vv} component (representing the part of the electrons in valence band) grows, giving rise to the electric charge accumulation inside the well. Finally, we can note that it appears a non-vanishing flux of electrons travelling outside the $x = L$ side of the diode. This is possible due to the tunneling (from the valence band to the conduction band) of the electrons stored inside the valence well. The initial datum guarantees that the resonant states in the valence well are unexcited for $t = 0$, avoiding any initial correlation between conduction and valence electrons.

8 Appendix

Let $w_0 = \left(w^0_{cc}, w^0_{cv}, w^0_{vc}, w^0_{vv}\right)^T$ belong to $\mathbf{H'}$, where $\mathbf{H'} = \left\{f \in \mathbf{H} | f_{cc} = \overline{f_{cc}}, f_{vv} = \overline{f_{vv}}, f_{cv} = \overline{f_{vc}}\right\}$, and let w be the unique solution of (4.10) with initial datum w_0, then $w \in \mathbf{H'}$. In details, we take the imaginary part of the first and fourth equations and we write the equations for the quantities $w_{cv} - \overline{w_{vc}}$ and $w_{vc} - \overline{w_{cv}}$, then we get the following closed system

$$\begin{cases} \dfrac{\partial w^I_{cc}}{\partial t} = -v \dfrac{\partial w^I_{cc}}{\partial x} + i\theta[V] w^I_{cc} - \dfrac{i}{2} \dfrac{P\hbar}{mE_g} \mathcal{O}^+[V] \left(w_{vc} - \overline{w_{cv}}\right) \\ \qquad\qquad + \dfrac{i}{2} \dfrac{P\hbar}{mE_g} \mathcal{O}^-[V] \left(w_{cv} - \overline{w_{vc}}\right) \\ \dfrac{\partial w^I_{vv}}{\partial t} = v \dfrac{\partial w^I_{vv}}{\partial x} + i\theta[V] w^I_{vv} - \dfrac{i}{2} \dfrac{P\hbar}{mE_g} \mathcal{O}^+[V] \left(w_{cv} - \overline{w_{vc}}\right) \\ \qquad\qquad + \dfrac{i}{2} \dfrac{P\hbar}{mE_g} \mathcal{O}^-[V] \left(w_{vc} - \overline{w_{cv}}\right) \\ \dfrac{\partial (w_{cv} - \overline{w_{vc}})}{\partial t} = -i \dfrac{\hbar}{4m^*} \dfrac{\partial^2 \left(w_{cv} - \overline{w_{vc}}\right)}{\partial x^2} + \dfrac{i}{\hbar} \left(E_g + m^* v^2\right) \left(w_{cv} - \overline{w_{vc}}\right) \\ \quad + i\theta[V] \left(w_{cv} - \overline{w_{vc}}\right) - i \dfrac{P\hbar}{mE_g} \mathcal{O}^+[V] \left(w_{vv} - \overline{w_{vv}}\right) + i \dfrac{P\hbar}{mE_g} \mathcal{O}^-[V] \left(w_{cc} - \overline{w_{cc}}\right) \\ \dfrac{\partial (w_{vc} - \overline{w_{cv}})}{\partial t} = i \dfrac{\hbar}{4m^*} \dfrac{\partial^2 \left(w_{vc} - \overline{w_{cv}}\right)}{\partial x^2} - \dfrac{i}{\hbar} \left(E_g + m^* v^2\right) \left(w_{vc} - \overline{w_{cv}}\right) \\ \quad + i\theta[V] \left(w_{vc} - \overline{w_{cv}}\right) - i \dfrac{P\hbar}{mE_g} \mathcal{O}^+[V] \left(w_{cc} - \overline{w_{cc}}\right) + i \dfrac{P\hbar}{mE_g} \mathcal{O}^-[V] \left(w_{vv} - \overline{w_{vv}}\right) \end{cases}$$

Here we denoted the imaginary part of w_{cc} and w_{vv} by w^I_{cc} and w^I_{vv}, respectively, and we used $\overline{\theta[V] f} = -\theta(\overline{f})$, $\overline{\mathcal{O}^{\pm}[V] f} = \mathcal{O}^{\mp}(\overline{f})$ and the fact that $i\theta(f^I)$ is a real valued operator (see e.g. (Markowich and Ringhofer, 1989)).

The analysis carried out in Section 6 allows us to state that the previous system admits a unique solution. Hence, if the initial datum is the zero-function, the solution remains identically zero for all times.

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