

An analysis of a quantum kinetic two-band model with inflow boundary conditions

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In the last decade, the interest in multi-band quantum models has grown due to the introduction of diodes, such as Resonant Interband Tunneling Diode (RITD, cf. [3] and the Refs. therein), that are built on the quantum effect of tunneling of electrons between conduction and valence bands. Such models describe the evolution in time of pure states of a quantum system in terms of couples of envelope functions Ψ_c, Ψ_v , which can be considered as wave-functions relative to conduction and valence bands, respectively. The dynamics of transport in and between the two bands is modelled via two-band Hamiltonians. Quantum multi-band models differentiate according to the choice of envelope functions and thus of Hamiltonians: we name, e.g., Kane, [4], and Morandi-Modugno, [8], models.

The (quantum) kinetic formulation of multi-band models is obtained by applying Wigner formalism to envelope-function models, namely by Wigner-transforming component-wise envelope-function density matrices ρ_{ij} , given by $\rho_{ij}(x, x') = \Psi_i(x) \bar{\Psi}_j(x')$. Thus, we consider 2×2 matrices of Wigner functions (Wigner matrices)

$$w_{ij}(x, v) = (\mathcal{W} \rho_{ij})(x, v), \quad i, j \in \{c, v\}.$$

Observe that the self-adjointness of density operators implies the Hermiticity of Wigner matrices for any fixed (x, v) :

$$\rho_{ij}(x, x') = \overline{\rho_{ji}(x', x)} \implies w_{ij}(x, v) = \overline{w_{ji}(x, v)}.$$

The evolution equation for Wigner matrices in the case of Kane model has been studied from a mathematical point of view in [2]. The Wigner matrix describing thermal equilibrium of Kane model has been obtained in [1].

The evolution equation for the Wigner matrix in the case of M-M model [8] is

$$\begin{aligned} (\partial_t + v \cdot \nabla_x + i\Theta[V_{cc}]) w_{cc} &= \Theta[F_-]w_{cv} - \Theta[F_+]w_{vc} \\ (\partial_t - i\Delta_x + iv^2 + i\Theta[V_{cv}]) w_{cv} &= \Theta[F_-]w_{cc} - \Theta[F_+]w_{vv} \\ (\partial_t + i\Delta_x - iv^2 + i\Theta[V_{vc}]) w_{vc} &= -\Theta[F_+]w_{cc} + \Theta[F_-]w_{vv} \\ (\partial_t - v \cdot \nabla_x + i\Theta[V_{vv}]) w_{vv} &= -\Theta[F_+]w_{cv} + \Theta[F_-]w_{vc}, \end{aligned} \tag{0.1}$$

cf. [3] for the dimensional version, here we put physical constants equal to one. We define

$$\begin{aligned} V_{ij}(x, \xi) &= (E_i + V)(x + \xi/2) - (E_j + V)(x - \xi/2), \quad i, j \in \{c, v\}, \\ F_{\pm}(x, \xi) &= (\nabla V \cdot P)(x \pm \xi/2), \end{aligned}$$

with $E_{c,v}$ minimum and maximum of conduction and valence bands, respectively, V potential, P given coupling vector and $\Theta[\cdot]$ the pseudo-differential operator defined by, in the d -dimensional case,

$$(\Theta[\phi]f)(x, p) = (2\pi)^{-d} \int_{\mathbb{R}^{2d}} e^{-i(v-v')\cdot\xi} \phi(x, \xi) f(x, v') d\xi dv'.$$

Since P and, consequently, F_{\pm} are purely imaginary, the following relations hold:

$$\overline{\Theta[F_{\pm}]w_{ij}} = -\Theta[F_{\mp}]w_{ji}, \quad i, j \in \{c, v\}.$$

The system (1) with unknown $w_{ij} = w_{ij}(x, v, t)$, $(x, v) \in \mathbb{R}^2$, $t > 0$, $i, j \in \{c, v\}$ has been studied in [3], in case of a (bounded) external potential V and an existence and uniqueness result has been assessed in L^2 -setting.

Here, we shall consider instead the case of a one-dimensional, bounded, spatial domain and we shall assign *physical*, time-dependent ‘‘inflow’’ boundary conditions (b.c.) to the unknowns $w_{ij} = w_{ij}(x, v, t)$, $x \in [0, 1]$, $v \in \mathbb{R}$, $t > 0$, $i, j \in \{c, v\}$. Moreover, $V = (V_{\text{ext}} + U)(x, t)$, with U satisfying for all t , Poisson equation with homogeneous b.c.

$$(0.2) \quad -\partial_x^2 U(x, t) = n(x, t), \quad x \in (0, 1), \quad U(0, t) = U(1, t) = 0.$$

In the multi-band case we shall define the position (particle) density n as

$$n(x, t) := n_{cc}(x, t) + n_{vv}(x, t) = \int_{\mathbb{R}} (w_{cc} + w_{vv})(x, v, t) dv,$$

namely, as the sum of the position densities n_{cc}, n_{vv} relative to electrons in conduction and valence bands, respectively. For *physical*, ‘‘inflow’’ b.c. we mean that we shall assign functions $\gamma_{c,v}(0, v, t)$, $v > 0$, $t > 0$ and $\gamma_{c,v}(1, v, t)$, $v < 0$, $t > 0$ as boundary values for w_{ii} , $i = c, v$, precisely,

$$(0.3) \quad \begin{aligned} w_{ii}(0, v, t) &= \gamma_i(0, v, t), \quad v > 0, t > 0, \\ w_{ii}(1, v, t) &= \gamma_i(1, v, t), \quad v < 0, t > 0, \end{aligned}$$

while we shall assign homogeneous b.c. to w_{ij} , $i \neq j$. With this choice of b.c. we intend to model the most common case in real device simulation, of an incoming beam of electrons in conduction and/or in valence band in a semiconductor heterostructure (cf. the profile of the assigned potential V_{ext}), and to describe intraband and interband transport of electrons, taking into account the reciprocal repulsion of electrons via the self-consistent potential U . Observe that we can modify the b.c. of the potential U according to the applied bias.

The forthcoming study of system (0.1), (0.2), with b.c. (0.3) and initial data $w_{ij}^0(x, v) = w_{ij}(x, v, 0)$, $(x, v) \in \mathbb{R}^2$, $i, j \in \{c, v\}$, is the analytical counterpart of the numerical simulation in [3] and the natural extension to the multi-band case of the analyses of the Wigner-Poisson system performed in [6,7]. Analogously to [6,7], the difficulty is two-fold: on one hand, the ‘‘affine’’ domain of the operators in (0.1), due to the choice of non-homogeneous b.c. (0.3), on the other, the definition of the position density, starting from L^2 -Wigner functions ([5]) and the regularity of Poisson potential U . Thus, first of all, we shall deal with a *linear* (i.e., with unknowns satisfying homogeneous b.c.) version of

problem (0.1),(0.2),(0.3) with a source term suitably added to take into account affine b.c. The latter difficulty is typically solved by working in a v -weighted L^2 -space. In the one-dimensional case, it's well-known ([7], e.g.) that $w_{ii}(t), vw_{ii}(t) \in L^2([0, 1] \times \mathbb{R}, dx, dv; \mathbb{R})$ is enough to ensure $n_{ii}(t) \in L^2([0, 1], dx; \mathbb{R})$ and thus $U(t) \in W^{1,\infty}([0, 1])$ with $U''(t) \in L^2([0, 1], dx)$. This is enough for the operators $\Theta[\cdot]$ to be well-defined and to constitute a locally-Lipschitz perturbation of the remaining (unbounded) operators. The latter ones, when defined on linear domains, generate semigroup. Then, we can state an existence and uniqueness result for the linear version of (0.1),(0.2),(0.3) with source term, via a Banach fixed-point argument, in the space $X^4 := (L^2([0, 1] \times \mathbb{R}, (1 + v^2)dx dv; \mathbb{R}))^4$ and finally recover the solution of the originary (affine) problem. More precisely,

Theorem

Let $u_{ii}^0 \in \mathcal{D}_1 := \{u \in X \mid vu_x \in X, u(0, v) = 0, \forall v > 0, u(1, v) = 0, \forall v < 0\}$ and $u_{ij}^0 \in \mathcal{D}_2 := \{u \in X \mid u_{xx}, v^2u \in X, u(0, v) = u(1, v) = 0, \forall v \in \mathbb{R}\}$. Let $V_{\text{ext}} \in \mathcal{C}([0, +\infty); W^{1,\infty}([0, 1]))$ and $\gamma_{c,v} \in L^1_{\text{loc}}([0, +\infty); L^2(\times \mathbb{R}, (1 + v^2) dv; \mathbb{R}))$ be admissible inflow data. Then there exists a unique, global-in-time, classical and real-valued solution $\{w_{ij} \mid i, j \in \{c, v\}\}$ of the system (0.1),(0.2),(0.3).

We remark that, at difference with [6], the extension to the three-dimensional case is not straightforward, due to terms $\Theta[F_{\pm}]$, which require more regularity than the solution of Poisson problem has.

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