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A QUANTUM-TRANSPORT MODEL FOR SEMICONDUCTORS : THE WIGNER-POISSON PROBLEM ON A BOUNDED BRILLOUIN ZONE (*)

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Abstract. — *We analyse a quantum-mechanical model for the transport of electrons in semiconductors. The model consists of the quantum Liouville (Wigner) equation posed on the bounded Brillouin zone corresponding to the semiconductor crystal lattice, with a self-consistent potential determined by a Poisson equation. A global existence and uniqueness proof for this model is the main result of the paper.*

Résumé. — *Nous présentons et analysons un modèle quantique de transport des électrons dans un semiconducteur. Le modèle est constitué de l'équation de Liouville quantique (ou équation de Wigner), posée sur un domaine borné en vitesse correspondant à la zone de Brillouin du semiconducteur, couplée à un potentiel déterminé par une équation de Poisson. Dans cet article, nous prouvons l'existence globale et l'unicité des solutions pour ce modèle.*

1. THE MODEL

This paper is concerned with the mathematical analysis of a model for the quantum transport of electrons in a semiconductor. The model relies on the Wigner (or quantum Liouville) equation as presented in [6, 7, 9, 10]. The velocity variable is assumed to belong to a bounded set corresponding to the first Brillouin zone of the semiconductor.

Let us first review the classical transport model for a (d-dimensional, $d = 1$, 2 or 3) semiconductor. The electrical potential is the sum of a periodic, very rapidly oscillating potential due to the ions of the crystal lattice, and a slowly varying nonperiodic potential which arises from the doping profile, from externally applied potentials and from mobile charges.

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In the quasi-classical formalism it is assumed that the wavelength of the oscillating potential is short enough so that electrons can be considered as moving along classical trajectories associated with the Hamiltonian

$$H(x, k) = \varepsilon(k) + q\psi(x, t) \tag{1.1}$$

where k is the wave vector of the electron, $\varepsilon(k)$ its (kinetic) energy given by the band diagram of the semiconductor, and ψ the smoothly varying potential contribution. q denotes the elementary charge. In classical mechanics the energy-momentum-relationship is quadratic

$$\varepsilon(k) = \frac{\hbar^2 k^2}{2m}, \tag{1.2}$$

where m denotes the electron mass and $\hbar$ the Planck constant normalized by 2π.

Defining the velocity as

$$v(k) = 1/\hbar \, \nabla_k \varepsilon(k), \tag{1.3}$$

the evolution of the distribution function $f = f(x, k, t)$ of the electrons in the phase-space (x, k) is governed by the classical Liouville equation

$$\frac{\partial f}{\partial t} + v(k) \cdot \nabla_x f - \frac{q}{\hbar} \nabla_x \psi \cdot \nabla_k f = 0, \tag{1.4}$$

where the chosen time scale is assumed to be much shorter than the mean time between two collisions with defects of the crystal lattice.

At this level, quantum mechanics and the periodic oscillating potential modify the classical picture in two ways. Firstly, the wave vector k does not vary in the whole space R^d, but only in the first Brillouin zone B_z, which is the fundamental domain of the reciprocal lattice $\hat{L}_c$ associated with the crystal lattice $L_c = \left\{ \sum_{i=1}^{d} \alpha_i a_c^i \,\middle|\, \alpha_i \in \mathbb{Z} \right\}$, where $a_c^1, \ldots, a_c^d \in R^a$ are the basic lattice vectors (see [5]). Secondly, (1.2) does not hold anymore, the energy-momentum relationship is more complicated. Note that any quantity of interest, such as the energy and the velocity, is a periodic function of k over B_z. A mathematical analysis of this semi-classical formalism can be found in [4]. Moreover, in many applications the potential ψ has locally large gradients which induce important quantum effects such as tunnelling through barriers or generation of discrete states inside potential wells, although these gradients are moderate compared to the gradients of the lattice periodic potential. More precisely, the wavelength of the periodic potential is the interatomic distance in the crystal lattice ($\approx 10^{-10}$ m), whereas the width of the potential barrier at a typical heterojunction is approximately 5×10^{-8} m. A variation of the potential energy of the order of several 0.1 Volts can be expected over this distance. Such a variation leads to quantum effects, but it is still small compared to the variation of the crystal lattice potential.

Thus, it is desirable to derive a model which accounts for these quantum effects but which keeps a simplified description of the crystal lattice potential as in the quasi-classical formalism.

This goal can be achieved by considering the Schrödinger equation or, equivalently, at the level of the kinetic theory, the Wigner equation with a quantum Hamiltonian given by (1.1). In order to simplify the description, we still assume the quadratic energy-wave vector relationship (1.2) with

$$v(k) = \frac{\hbar k}{m} \tag{1.5}$$

but restricted to wave vectors k belonging to the Brillouin zone B_z. We shall consider all functions of k (such as the distribution function $f(x, k, t)$) as restrictions to B_z of periodic functions on $\mathbb{R}_k^d$ with period $\hat{L}_c$. In this context, any function $\phi = \phi(k)$ in $L^2(B_z)$ can be expanded into a Fourier series:

$$\phi(k) = \sum_{\eta_c \in L_c} \hat{\phi}(\eta_c)\, e^{ik \cdot \eta_c}, \quad k \in B_z \tag{1.6a}$$

$$\hat{\phi}(\eta_c) = \frac{1}{|B_z|} \int_{B_z} \phi(k)\, e^{-ik \cdot \eta_c}\, dk, \quad \eta_c \in L_c \tag{1.6b}$$

where $|B_z|$ stands for the Lebesgue measure of B_z and $\hat{\phi} \in l^2(L_c)$ holds.

The Wigner equation is a quantum equivalent of the classical transport equation (1.4). It governs the evolution of the (not necessarily nonnegative) quantum (quasi) distribution function of the electrons (see [6, 7, 9] for physical details):

$$\frac{\partial f}{\partial t} + \frac{\hbar k}{m} \cdot \nabla_x f - \frac{q}{\hbar} \theta_w[\psi] f = 0, \quad x \in R_x^d, \quad k \in B_z, \quad t > 0, \tag{1.7a}$$

where the operator $\theta_w[\psi]$ is given by its Fourier-coefficients:

$$(\widehat{\theta_w[\psi] f})(x, \eta_c, t) = \tag{1.7b}$$
$$= i\left[\psi\left(x + \frac{\eta_c}{2}, t\right) - \psi\left(x - \frac{\eta_c}{2}, t\right)\right] f(x, \eta_c, t), \; x \in R_x^d, \; \eta_c \in L_c, \; t > 0.$$

For a derivation of the Wigner equation (1.7) from the Schrödinger equation with the quantum Hamiltonian (1.1) we refer to [10, 11]. Here we only mention that this derivation is based on a limiting procedure, in which the normalized spacing of the direct lattice L_c tends to zero.

A more classical form of (1.6) is obtained by introducing the velocity variable (1.5). Then, setting

$$B = \frac{\hbar}{m} B_z , \quad L = \frac{m}{\hbar} L_c , \quad \eta = \frac{m}{\hbar} \eta_c ,$$

we define a (quasi) distribution function $f = f(x, v, t)$, periodic in $v \in B$, with Fourier-indices $\hat{f}(x, \eta, t)$:

(1.8a) $$f(x, v, t) = \sum_{\eta \in L} \hat{f}(x, \eta, t)\, e^{iv \cdot \eta} , \quad v \in B$$

(1.8b) $$\hat{f}(x, \eta, t) = \frac{1}{|B|} \int_B f(x, v, t)\, e^{-iv \cdot \eta}\, dv , \quad \eta \in L$$

(1.8c) $$L = \left\{ \sum_{i=1}^{d} \alpha_i\, a^i \,\middle|\, \alpha_i \in \mathbb{Z} \right\} ,$$

where $a^i = \frac{m}{\hbar} a_c^i$, $1 \leq i \leq d$, are the basic vectors of the scaled lattice L. f solves the scaled equation (1.7), which reads :

(1.9a) $$\frac{\partial f}{\partial t} + v \,.\, \nabla_x f - q\theta[\psi] f = 0$$

with $x \in R^d$, $v \in B$ and $t > 0$, where

(1.9b) $$\widehat{(\theta[\psi] f)}(x, \eta, t) = = \frac{i}{\hbar} \left[\psi\left(x + \frac{\hbar\eta}{2m}, t\right) - \psi\left(x - \frac{\hbar\eta}{2m}, t\right) \right] \hat{f}(x, \eta, t) , \quad \eta \in L .$$

Equivalently, we have the following representation for the operator $\theta[\psi]$:

(1.10) $$(\theta[\psi] f)(x, v, t) = \frac{i}{|B|} \sum_{\eta \in L} \left[\frac{\psi\left(x + \frac{\hbar\eta}{2m}, t\right) - \psi\left(x - \frac{\hbar\eta}{2m}, t\right)}{\hbar} \right] \times \int_B f(x, v', t)\, e^{i(v - v') \cdot \eta}\, dv ,$$

with $v \in B$.

We assume that the semiconductor occupies the bounded convex domain $\Omega \subseteq \mathbb{R}^d$. As usual in semiconductor simulation we determine the self-consistent potential ψ from the Poisson-equation (Coulomb force) :

(1.11a) $$\Delta\psi = q/\varepsilon\,(n - C(x)) , \quad x \in \Omega , \quad t > 0$$

where $\varepsilon > 0$ is the permittivity constant of the semiconductor, $C = C(x)$ the doping profile (fixed charges) which determines the device under consideration, and n the electron density :

$$n(x, t) \int_B f(x, v, t)\, dv \,. \tag{1.11b}$$

The externally applied potential ψ_D determines a Dirichlet boundary condition for (1.11) (a) :

$$\psi = \psi_D \,, \quad x \in \partial\Omega \,. \tag{1.11c}$$

Alternatively (and even more realistically), mixed Neumann-Dirichlet boundary conditions modelling insulating segments (homogeneous Neumann conditions) and contact segments (inhomogeneous Dirichlet conditions) could be employed.

The quantum transport equation (1.9) then is also restricted to $x \in \Omega$ and Dirichlet boundary conditions are applied at the inflow segments

$$f = f_D \,, \; x \in \partial\Omega \,, \; v \in B \,, \; v \,.\, r \;\, (x) < 0 \,, \; t > 0 \tag{1.12}$$

where $r = r(x)$ denotes the outward unit normal vector of $\partial\Omega$ at x.

Also, an initial distribution is prescribed

$$f(t = 0) = f_I \,, \quad x \in \Omega \,, \quad v \in B \,. \tag{1.13}$$

Note that the equation (1.9) requires ψ to be defined on all of $\mathbb{R}_x^d$. Thus the solution of the Poisson equation (1.11) has to be extended from Ω to $\mathbb{R}_x^d$. At this point, it is not clear what the physically most reasonable way to extend the potential is. For our purposes the precise form of the extension is not important.

In Section 2 we prove a global existence and uniqueness result for the coupled Wigner-Poisson problem on the bounded Brillouin zone.

The existence proof presented below is based on the fact that the Wigner equation provides an immediate L^2-bound on the distribution function f. We remark that this is the only L^p-estimate carrying over from the family of L^p-estimates $(1 \leqslant p \leqslant \infty)$, which hold in the semiclassical case. The boundedness of the Brillouin zone B_z then allows for an L^2-estimate on the density n. In the whole space case there is a major problem in defining the density in a proper function space since an L^1-estimate of the distribution function f is not available. Also, the boundedness of B_z allows us to use either a recently obtained result on the compactness of the velocity averages of f (see [3]) or a constructive method for proving existence of a solution. In this paper we choose the first approach. The second can be deduced by extending the uniqueness proof given below.

In the presented scaling, the limit $\hbar \to 0$ is not relevant. Indeed, in the wave-vector formulation (1.7) the semiclassical equation (1.4) still contains $\hbar$, which is clearly incompatible with a limiting procedure $\hbar \to 0$. On the other hand, in the velocity formulation (1.9), the scaled Brillouin zone B expands to the entire space when $\hbar$ tends to 0. This leads to the same mathematical problems as mentioned above since no uniform a priori estimate on the density is available. The relevant limiting procedure is associated with the normalized spacing of the direct lattice. It is — together with the appropriate scaling — presented and analysed in [10, 11].

2. EXISTENCE AND UNIQUENESS

Let us collect the model equations first :

(2.1a) $\quad \dfrac{\partial f}{\partial t} + v \cdot \nabla_x f - q\theta[\psi] f = 0 , \quad x \in \Omega , \quad v \in B , \quad t > 0$

(2.1b) $\quad f(x, v, t = 0) = f_I(x, v) , \quad x \in \Omega , \quad v \in B$

(2.1c) $\quad f(x, v, t) = f_D(x, v, t) , \ x \in \partial\Omega , \ v \in B , \ v \cdot r\ (x) < 0 , \ t > 0$

(2.1d) $\quad \Delta\phi = q/\varepsilon(n - C(x)) , \quad x \in \Omega , \quad t > 0$

(2.1e) $\quad n(x, t) = \displaystyle\int_B f(x, v, t)\, dv , \quad x \in \Omega , \quad t > 0$

(2.1f) $\quad \phi(x, t) = \psi_D(x, t) , \quad x \in \partial\Omega , \quad t > 0$

(2.1g) $\quad \psi = E\phi .$

The operator $\theta[\psi]$ is given by (1.9b), (1.10). E denotes a linear extension operator.

For the following analysis we use the assumptions :

(A1) $\Omega \subseteq \mathbb{R}_x^d$ is a convex bounded domain, $\partial\Omega$ is C^2; $B \subseteq \mathbb{R}_v^d$ is a bounded fundamental domain point symmetric to the origin, $1 \leqslant d \leqslant 3$

(A2) $f_I \in L^2(\Omega \times B)$

(A3) $f_D \in L^2_{\mathrm{loc}}([0, \infty) \to L^2(\Gamma_-))$,

$$\Gamma_- := \{(x, v) \mid x \in \partial\Omega, v \in B, v \cdot r\ (x) < 0\} .$$

We assume that f_D can be extended to a function $f_D \in L^2_{\mathrm{loc}}([0, \infty) \to L^2(\Omega \times B))$ such that :

$$\frac{\partial f_D}{\partial t} + v \cdot \nabla_x f_D \in L^2_{\mathrm{loc}}([0, \infty) \to L^2(\Omega \times B)) .$$

(A4) $C \in L^2(\Omega)$

(A5) $\psi_D \in L^{\infty}_{\mathrm{loc}}([0, \infty) \to H^2(\Omega))$

(A6) $E : C(\bar{\Omega}) \to L^{\infty}(\mathbb{R}^d_x)$ is continuous ; $E\phi|_{\bar{\Omega}} = \phi|_{\bar{\Omega}}$,

$$E\phi|_{R^d_x - \bar{\Omega}} \in C(\mathbb{R}^d_x - \bar{\Omega}) \quad \text{for all} \quad \phi \in C(\bar{\Omega}),$$

(A7) f_I, f_D, ψ_D, C realvalued.

At first we decouple the problem (2.1) and prove a priori estimates.

LEMMA 2.1 : *Let* (A1)-(A3), (A6), (A7) *hold. Then, for any given realvalued* $\phi \in L^{\infty}((0, T) \to C(\bar{\Omega}))$, *the problem* (2.1*a*, *b*, *c*, *g*) *has a unique realvalued mild solution* $f \in C([0, T] \to L^2(\Omega \times B))$, *which satisfies*

$$(2.2) \quad |f(t)|^2_{L^2(\Omega \times B)} \leq |f_I|^2_{L^2(\Omega \times B)} + \\ + \int_0^t \int_{\Gamma^-} \int |v \,.\, r(x)|\, |f_D(x, v, \tau)|^2 \, ds \, dv \, d\tau$$

for $t \in [0, T]$.

Remark : ds denotes the surface element on $\partial\Omega$.

Proof : Since the transport operator $Au := -v \,.\, \nabla_x u$, $D(A) := \{u \in L^2(\Omega \times B) \mid v \,.\, \nabla_x u \in L^2(\Omega \times B),\ u = 0 \text{ on } \Gamma_-\}$ generates a semigroup of contractions on $L^2(\Omega \times B)$ (see [2, p. 1087, theorem 2]) and since (1.10) implies

$$(2.3a) \qquad |\theta[\psi](t)|_{L^2(\Omega \times B) \to L^2(\Omega \times B)} \leq 2/\hbar\, |\psi(t)|_{L^{\infty}(\mathbb{R}^d_x)}$$

we conclude (after subtracting off f_D) by proceeding as in [3, p. 77] that (2.1*a*, *b*, *c*) has a unique mild solution $f \in C([0, T) \to L^2(\Omega \times B))$. Clearly, the mild solution is also a distributional solution of (2.1*a*). Since $f_t + v \,.\, \nabla_x f = q\theta[\psi] f \in L^{\infty}((0, T) \to L^2(\Omega \times B))$, the trace of f at $\Gamma_- {}_x (0, T)$ exists and equals f_D (this follows from a time-dependent version of [1, theorem 3]). Obviously, the trace of f at $t = 0$ equals f_I.

We multiply (2.1*a*) by $\bar{f}$, apply the Green's formula in [2, p. 1090], take real parts and immediately obtain (2.2) by using

$$(2.3b) \quad \int_B \bar{f}\theta[\psi] f \, dv = \\ = \frac{i}{|B|} \sum_{\eta \in L} \left[\frac{\psi\left(x + \frac{\hbar}{2m}\eta, t\right) - \psi\left(x - \frac{\hbar}{2m}\eta, t\right)}{\hbar} \right]_{|\hat{f}(x, \eta, t)|^2} \in i\mathbb{R}$$

($\theta[\psi]$ is skew-symmetric). We conclude as in [6] that $\theta[\psi]$ maps realvalued functions into realvalued functions. ∎

Conversely, for given $f \in L^{\infty}((0, T) \to L^2(\Omega \times B))$, we conclude from (2.1*e*) :

$$|n(t)|_{L^2(\Omega)} \leq \sqrt{|B|}\, |f(t)|_{L^2(\Omega \times B)} . \tag{2.4a}$$

Since the solution ϕ of (2.1*d*, *f*) satisfies

$$|\phi(t)|_{H^2(\Omega)} \leq K(|n(t)|_{L^2(\Omega)} + |\psi_D(t)|_{H^2(\Omega)} + |C|_{L^2(\Omega)}) , \tag{2.4b}$$

we conclude from the Sobolev imbedding Theorem ($1 \leq d \leq 3!$) and from (A6) :

$$|\psi(t)|_{L^{\infty}(\mathbb{R}_x^d)} \leq K(|f(t)|_{L^2(\Omega \times B)} + |\psi_D(t)|_{H^2(\Omega)} + |C|_{L^2(\Omega)}) . \tag{2.5}$$

We denote by K generic, not necessarily equal constants.

Now we proceed to prove the main result of this paper.

THEOREM 2.1 : *Let the assumptions* (A1)-(A7) *hold. Then the problem* (2.1) *has a unique mild solution* $(f, \phi) \in C([0, \infty) \to L^2(\Omega \times B)) \times L^{\infty}_{\text{loc}}([0, \infty) \to H^2(\Omega))$.

Proof : We consider the following iteration $\phi^{l-1} \to \phi^l$, $l \geq 1$. Given $\phi^{l-1} \in L^{\infty}((0, T) \to C(\bar{\Omega}))$, $T > 0$, we solve

$$\frac{\partial f^l}{\partial t} + v \cdot \nabla_x f^l - q\theta[\psi^{l-1}] f^l = 0 , \quad x \in \Omega , \quad v \in B , \quad t \in (0, T) \tag{2.6a}$$

$$f^l(t = 0) = f_I , \quad x \in \Omega , \quad v \in B \tag{2.6b}$$

$$f^l = f_D , \quad (x, v) \in \Gamma_- , \quad t \in (0, T) \tag{2.6c}$$

$$\psi^{l-1} = E\phi^{l-1} \tag{2.6d}$$

and

$$\Delta\phi^l = q/\varepsilon(n^l - C(x)) , \quad x \in \Omega , \quad t \in (0, T) \tag{2.7a}$$

$$n^l = \int_B f^l \, dv , \quad x \in \Omega , \quad t \in (0, T) \tag{2.7b}$$

$$\phi^l = \psi_D , \quad x \in \partial\Omega , \quad t \in (0, T) . \tag{2.7c}$$

We choose $\phi^0 = 0$.

From (2.2) we conclude :

$$|f^l|_{L^{\infty}((0, T) \to L^2(\Omega \times B))} \leq K(f_I, f_D, T) , \quad l \in N_0 \tag{2.8}$$

and, thus, from (2.4) :

$$(2.9) \qquad |\phi^l|_{L^\infty((0,T)\to C(\bar\Omega))} \leq K(f_I, f_D, C, \psi_D, T)\,, \quad l \in N_0\,.$$

Also, by the Plancherel formula

$$(2.10) \quad |\theta[\psi^{l-1}]f^l|_{L^2(\Omega\times B\times(0,T))} \leq$$

$$\leq \frac{2}{\hbar}\,|\psi^{l-1}|_{L^\infty(\mathbb{R}^d_x\times(0,T))}\,|f^l|_{L^2(\Omega\times B\times(0,T))}$$

$$\leq K(f_I, f_D, C, \psi_D, \hbar, T)\,, \quad l \in N\,.$$

From (2.6*a*) we conclude

$$(2.11) \qquad \left|\frac{\partial f^l}{\partial t} + v\,.\,\nabla_x f^l\right|_{L^2(\Omega\times B\times(0,T))} \leq K\,, \quad l \in N_0\,.$$

Thus, by a result of [3, theorem 4], we obtain

$$(2.12) \qquad |n^l|_{H^{1/2}((0,T)\times\Omega)} \leq K\,, \quad l \in N_0\,.$$

Since the bounds (2.8), (2.12) are independent of l, we conclude by eventually restricting to a subsequence (which we denote as the sequence) :

$$(2.13a) \qquad f^l \overset{l\to\infty}{\to} \quad \text{in} \quad L^2(\Omega\times B\times(0,T)) \quad \text{weakly}$$

$$(2.13b) \qquad n^l \overset{l\to\infty}{\to} n = \int_B f\,dv \quad \text{in} \quad L^2(\Omega\times(0,T))\,.$$

From (2.7*a*, *c*) we obtain

$$(2.13c) \qquad \phi^l \overset{l\to\infty}{\to} \phi \quad \text{in} \quad L^2((0,T)\to H^2(\Omega)) \quad \text{and in} \quad L^2((0,T)\to C(\bar\Omega))\,,$$

where ϕ satisfies the Poisson equation :

$$(2.14a) \qquad \Delta\phi = q/\varepsilon(n - C(x))\,, \quad x\in\Omega\,, \quad t\in(0,T)$$

$$(2.14b) \qquad \phi = \psi_D\,, \quad x\in\partial\Omega\,, \quad t\in(0,T)\,.$$

Note that $f \in L^\infty((0,T)\to L^2(\Omega\times B))$, $\phi\in L^\infty((0,T)\to C(\bar\Omega))$.

We now take a realvalued testfunction $g\in C_0^\infty(\Omega\times B\times(0,T))$. Since f^l is a mild solution of (2.6), it is also a weak solution :

$$(2.15) \quad \int f^l(g_t + v\,.\,\nabla_x g)\,dx\,dv\,dt + q\int g\theta[\psi^{l-1}]f^l\,dx\,dv\,dt = 0$$

where the integration is performed over $\Omega \times B \times (0, T)$. By Plancherel's formula we have

$$(2.16) \quad \int g\theta[\psi^{l-1}] f^l \, dx \, dv \, dt = \frac{i}{|B|} \int_0^T \int_\Omega \times \sum_{\eta \in L} \left[\frac{\psi^{l-1}\left(x + \frac{\hbar}{2m}\eta, t\right) - \psi^{l-1}\left(x - \frac{\hbar}{2m}\eta, t\right)}{\hbar} \right] \times \hat{f}^l(x, \eta, t) \overline{\hat{g}(x, \eta, t)} \, dx \, dt .$$

From (2.13c) and (A6) we conclude $\psi^l \overset{l \to \infty}{\to} \psi$ in $L^2((0, T) \to L^\infty(\mathbb{R}_x^d))$, ψ continuous in $\bar{\Omega}$ and in $\mathbb{R}_x^d - \bar{\Omega}$. Since $\hat{f}^l \overset{l \to \infty}{\to} \hat{f}$ in $l^2(L \to L^2(\Omega \times (0, T)))$ weakly we obtain :

$$(2.17) \quad \int g\theta[\psi^{l-1}] f^l \, dx \, dv \, dt \overset{l \to \infty}{\to} \frac{i}{|B|} \int_0^T \int_\Omega \times \sum_{\eta \in L} \left[\frac{\psi\left(x + \frac{\hbar}{2m}\eta, t\right) - \psi\left(x - \frac{\hbar}{2m}\eta, t\right)}{\hbar} \right] \hat{f}(x, \eta, t) \overline{\hat{g}(x, \eta, t)} \, dx \, dt$$
$$= \int g\theta[\psi] f \, dx \, dv \, dt = - \int f\theta[\psi] g \, dx \, dv \, dt .$$

From (2.15), (2.17) we conclude :

$$(2.18) \quad \int f(g_t + v \cdot \nabla_x f - q\theta[\psi] g) \, dx \, dv \, dt = 0 , \quad \forall g \in C_0^\infty(\Omega \times B \times (0, T)) .$$

i.e. f is a weak solution of (2.1a) for $t \in (0, T)$.

To prove that f satisfies the initial and boundary conditions we now take $g \in C_0^\infty(\bar{\Omega} \times B \times [0, T))$ with $g = 0$ on $\Gamma_+ \times [0, T]$, where $\Gamma_+ := \{(x, v) \in \partial\Omega \times B \mid v \cdot r(x) > 0\}$, multiply (2.6$a$) by g and integrate by parts :

$$(2.19) \quad \int f^l(g_t + v \cdot \nabla_x g) \, dx \, dv \, dt + q \int g\theta[\psi^{l-1}] f \, dx \, dv \, dt + \int f_I \, g(x, v, t = 0) \, dx \, dv + \int_0^T \int_{\Gamma_-} |v \cdot r(x)| \, f_D \, g \, ds \, dv \, dt = 0$$

(see the Green's formula [2, p. 1090]).

By employing the same argument as above we obtain for $l \to \infty$:

$$(2.20)\quad \int f(g_t + v \cdot \nabla_x g)\, dx\, dv\, dt + q \int g\theta[\psi] f\, dx\, dv\, dt + \\ + \int f_I\, g(x, v, t = 0)\, dx\, dv + \int_0^T \int_{\Gamma_-} |v \cdot r(x)|\, f_D\, g\, ds\, dv\, dt = 0 .$$

Since $f \in Y = \{h \mid h, h_t + v \cdot \nabla_x h \in L^2(\Omega \times B \times (0, T))\}$ the « reverse integration by parts » can be performed (this follows from a time dependent version of the Green's formula [2, p. 1088, formula (2.20)]) :

$$(2.21)\quad \int (f_t + v \cdot \nabla_x f)\, g\, dx\, dv\, dt - q \int g\theta[\psi] f\, dx\, dv\, dt \\ + \int (f_I - f(x, v, t = 0))\, g(x, v, t = 0)\, dx\, dv \\ + \int_0^T \int_{\Gamma_-} |v \cdot r(x)|\, (f_D - f(x, v, t))\, g(x, v, t)\, dx\, dv\, dt = 0.$$

Since f solves (2.1*a*) for $t \in (0, T)$ we conclude $f = f_I$ for $t = 0$ and $f = f_D$ on $\Gamma_- \times (0, T)$.

To prove uniqueness, let $(f_1, \psi_1)(f_2, \psi_2)$ be two solutions of (2.1). Then $e := f_2 - f_1$ solves

$$(2.22a)\quad e_t + v \cdot \nabla_x e - q\theta[\psi_2]\, e = q\theta[\psi_2 - \psi_1]\, f_1$$

$$(2.22b)\quad e(t = 0) = 0$$

$$(2.22c)\quad e = 0 \quad \text{on} \quad \Gamma_- \times (0, T) .$$

Since (2.3*b*) implies $\operatorname{Re}\left(\int_B f\theta[\psi]\, f\, dv\right) = 0$ for realvalued f, we obtain by multiplying (2.22*a*) by e and integrating by parts :

$$(2.23)\quad |e(t)|^2_{L^2(\Omega \times B)} \leqslant q \int_0^t \int_\Omega \int_B e\theta[\psi_2 - \psi_1]\, f_1\, dv\, dx\, d\tau .$$

We estimate (2.23) by using (2.3*a*) :

$$(2.24)\quad |e(t)|^2_{L^2(\Omega \times B)} \leqslant \\ \leqslant \frac{2q}{\hbar} \int_0^t |e(s)|_{L^2(\Omega \times B)}\, |\psi_2(s) - \psi_1(s)|_{L^\infty(R_x^d)}\, |f_1(s)|_{L^2(\Omega \times B)}\, ds .$$

We have

$$(2.25)\quad \Delta(\phi_2 - \phi_1) = q/\varepsilon(n_2 - n_1), \quad \phi_2 - \phi_1 = 0 \text{ on } \partial\Omega$$

and $\psi_1 = E\phi_1$, $\psi_2 = E\phi_2$. Thus, by proceeding as in (2.4), (2.5) we have

$$|\psi_2 - \psi_1|_{L^\infty(R_x^d)} \leq K_1 |\phi_2 - \phi_1|_{C(\bar{\Omega})} \leq K_2 |n_2 - n_1|_{L^2(\Omega)} \leq K_3 |e|_{L^2(\Omega \times B)} \tag{2.26}$$

and, thus

$$|e(t)|^2_{L^2(\Omega \times B)} \leq \frac{2q}{\hbar} K_3 |f_1|_{L^\infty((0,T) \to L^2(\Omega \times B))} \int_0^t |e(s)|^2_{L^2(\Omega \times B)} ds \tag{2.27}$$

follows. Gronwall's inequality gives $e(t) = 0$ for $t \in (0, T)$.

Clearly, the weak solution f of (2.1*a*, *b*, *c*) is also the mild solution and the asserted regularity on f, ϕ follows.

This concludes the proof of the Theorem. ■

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REFERENCES

[1] M. Cessenat, *Théorèmes de Trace pour des Espaces des Fonctions de la Neutronique*. C.R. Acad. Sc. Paris, tome 300, série I, n° 3, 1985.

[2] R. Dautray and J. L. Lions, *Analyse Mathématique et Calcul Numérique pour les Sciences et les Techniques*. Tome 3, Masson, Paris, 1985.

[3] F. Golse, P. L. Lions, B. Perthame and R. Sentis, *Regularity of the Moments of the Solution of a Transport Equation*. J. Funct. Anal. 88, pp. 110-125, 1988.

[4] J. C. Guillot, J. Ralston and E. Trubowitz, *Semi-Classical Asymptotics in Solid State Physics*. Communications in Math. Phys., vol. 116, n° 3, pp. 401-415, 1988.

[5] C. Kittel, *Introduction to Solid States Physics*, J. Wiley and Sons, New York, 1968.

[6] P. A. Markowich and C. Ringhofer, *An Analysis of the Quantum Liouville Equation*. To appear in ZAMM, 1988.

[7] P. A. Markowich, *On the Equivalence of the Schrödinger and the Quantum Liouville Equations*. To appear in Math. Meth. In the Appl. Sci., 1988.

[8] A. PAZY, *Semigroups of Linear Operators and Applications to Partial Differential Equations*. Springer Verlag, New York-Berlin-Heidelberg-Tokyo, 1983.

[9] V. I. TATARSKII, *The Wigner Representation of Quantum Mechanics*. Sov. Phys. Usp., vol. 26, n° 4, pp. 311-327, 1983.

[10] A. ARNOLD, P. DEGOND, P. A. MARKOWICH and H. STEINRÜCK, *The Wigner-Poisson Equation in a Crystal,* to appear in : Applied Mathematics Letters, 1989.

[11] P. DEGOND, P. A. MARKOWICH and H. STEINRÜCK, *A Mathematical Derivation of the Wigner-Poisson Problem on a bounded Brillouin Zone from the Schrödinger Equation,* manuscript.