VLSI DESIGN
1999, Vol. 9, No. 4, pp. 315–323
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Semi-classical Limit in a Semiconductor Superlattice

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(Received 13 August 1997; In final form 1 December 1998)

In this paper, we perform a mathematical study of a semiconductor superlattice. Since the thickness of the layers is very small, quantization plays an important role. The modelling is therefore given by a Schrödinger equation with a periodic potential. The scaled lattice thickness is denoted by a small parameter ε which is of the same order of magnitude as the Planck constant. When this parameter tends to zero, *i.e.*, the semi-classical limit, we obtain classical transport of the charge carriers described by a Vlasov equation.

Keywords: Semiconductor, superlattice, quantum transport, Schrödinger equation, semi-classical limit

1. INTRODUCTION

Superlattices technology represent a modern technology used also in the design of semiconductors. In order to gain insight in the complex physical behaviour of these devices it is sometimes necessary to have very precise models which give a description on the atomic level. In this work we start with such a fundamental model that takes in account the quantum effects and investigate its semi-classical approximation in a mathematically rigorous way.

A superlattice can be described as material which consists of a stack of layers, those will be of two kinds: a layer A and a layer B as it is shown on Figure 1.

This is the model of Si/Ge, GaAs/AlAs or InAsSb/InSb superlattices for instance.

In the first part of this paper, we give a quantum description of such superlattices describing structures which are periodic in one direction x_1 but whose properties vary slowly in other directions x_2, x_3. This means that in this model we regard layers which have a slowly varying doping profile.

The motion of a charged particle in a stratified medium can be described by the Schrödinger equation:

$$i\hbar\frac{\partial\Psi}{\partial T} = -\frac{\hbar^2}{2m}\Delta_X\Psi(X,T) + qV(X)\Psi(X,T) \qquad (1.1)$$
$$X = (X_1, X_2, X_3) \in \mathbb{R}^3,\ T \in \mathbb{R}$$

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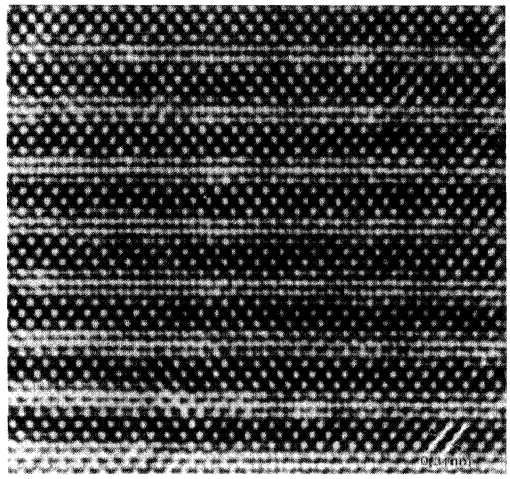

FIGURE 1 Compositional and structural characterization of a Si/Ge superlattice and heterostructures by high resolution transmission electron microscopy.

where $\hbar$ is the Planck constant, q the charge of the particle and m its mass. In our "stratified medium" the crystal is periodic with period λ in the direction X_1 such that the potential V verifies:

$$V(X_1 + \lambda\gamma, X_2, X_3) = V(X_1, X_2, X_3), \quad \gamma \in \mathbb{Z}. \tag{1.2}$$

We will also assume that the potential is bounded, *i.e.*,

$$V \in L^\infty(\mathbb{R}^3) \tag{1.3}$$

Let us define the quantum scale:

- λ is the length of the period of the medium in the direction X_1
- τ is its time unit such that we have (*e.g.* [10])

$$\tau = \frac{m\lambda^2}{h}$$

Now if we denote by L and T_0 the macroscopic length of the crystal, we can define a scaled potential by:

$$qV(X) = \frac{m\lambda^2}{\tau^2} v\left(\frac{X_1}{\lambda}, \frac{X_2}{L}, \frac{X_3}{L}\right) \tag{1.4}$$

Let us introduce new variables x, t, ε:

$$x = \frac{X}{L}, \quad t = \frac{T}{T_0}, \quad \varepsilon = \frac{\lambda}{L}$$

We now scale the wave function.

We recall that Ψ has to be normalized in such a way that:

$$\int_{\mathbb{R}^3} |\Psi(X, T)|^2 dX = 1.$$

So we put:

$$\psi(x, t) = L^{3/2}\Psi(Lx, T_0 t) \tag{1.5}$$

We remark that ψ is also normalized.

Let us choose T_0 and L such that:

$$\frac{\hbar}{T_0} \cdot \frac{\tau^2}{m\lambda^2} = \varepsilon \quad \text{and} \quad \frac{\hbar^2}{2mL^2} \cdot \frac{\tau^2}{m\lambda^2} = \frac{\varepsilon^2}{2} \tag{1.6}$$

With this scaling Eq. (1.1) becomes:

$$i\varepsilon\partial_t\psi = -\frac{\varepsilon^2}{2}\Delta_x\psi(x, t) + v\left(\frac{x_1}{\varepsilon}, x_2, x_3\right)\psi(x, t) \qquad x \in \mathbb{R}^3, \ t \in \mathbb{R} \tag{1.7}$$

We want to study rigorously the semi-classical limit of 1.7 when ε goes to zero. In particular we are concerned with the limit behavior of the density:

$$n_\varepsilon(x, t) = |\psi(x, t)|^2 \tag{1.8}$$

Semi-classical limits of Schrödinger operators have been intensively studied. In the case of perturbed periodic potential we refer to [2]. In this works the limit behaviour of the Schrödinger operator is given. Our purpose is to study the limit behaviour of the particle dynamics. This problem has been already been investigated in the case of: – v periodic [8, 6]– $v \in C^1$ [4, 7, 6]– $v + u$ with v periodic and u a small perturbation [9, 1]. The result in the periodic case is that the limit concentration is given by the sum of the concentrations $n_p(x, t)$ $p = 1, \ldots, \infty$

corresponding to the eigenvalue problems *e.g.* [8].

$$\begin{aligned}-\frac{\varepsilon^2}{2}\frac{d^2}{dx_1^2}\psi_p(x_1,k_1)+v\left(\frac{x_1}{\varepsilon}\right)\psi_p(x_1,k_1)\\ =E_p(k)\psi_p(x_1,k_1)\psi_p(x_1+\varepsilon\gamma,k_1)\\ =\mathrm{e}^{i\psi k_1\gamma}\psi_p(x_1,k_1)\end{aligned}$$

and the concentration are given by:

$$n_p(x,t)=\int_{\mathbb{R}^3}f_p(x,k_1,t)\ dk_1$$

where the non negative distribution f_p solves the transport equations.

$$\partial_t f_p(x,k_1,t)+\partial_{k_1}E_P(k_1)\cdot\partial_{x_1}f_p(x,k_1,t)=0.$$

In this work the main tools are the Wigner transform of wave functions and the Bloch decomposition of Schrödinger operators.

The Bloch decomposition *e.g.* [12, 4, 11] is the projection of wave functions on generalized eigenspaces, the Floquet spaces. In our framework they depend on x_2, x_3. To each eigenspace $V_p(x_2,x_3)$ corresponds an energy band $E_p(k_1,x_2,x_3)$ and the projector $\Pi_p(x_2,x_3)$. The main difficulty is that the projectors $\Pi_p(x_2,x_3)$ do not commute with $(-\varepsilon^2/2)\Delta_{x_2,x_3}$.

We overcome this difficulty by using asymptotic expansions of Wigner transforms given in [6].

In the following of this paper, we will make the assumption that the energy Bands don't cross. In fact it is possible to choose the eigenvectors of the Bloch decomposition such that the energy Bands do not cross. Such an choice can always been done for a Bloch decomposition in one dimension, which is the case here, but it has been proved that it is false in higher dimensions (*e.g.* [5, 3]).

The result is that the distribution function solves the transport equation:

$$\begin{aligned}\frac{\partial}{\partial t}f_p(x,k,t)=\begin{pmatrix}\partial_{k_1}E_p(k_1,x_2,x_3)\\ k_2\\ k_3\end{pmatrix}\cdot\nabla_x f_p(x,k,t)\\ +\nabla_{x_2,x_3}E_p(k_1,x_2,x_3)\cdot\nabla_{k_2,k_3}f_p(x,k,t)\end{aligned}\tag{1.9}$$

and the limit concentration n is given by:

$$n(x,t)=\sum_p\int_{[-\pi,\pi]\times\mathbb{R}^2}f_p(x,k,t)\frac{dk_1}{2\pi}\ dk_2\ dk_3\tag{1.10}$$

We remark in Eq. (1.9) that the band velocity in the first variable

$$\partial_{k_1}E_p\,(k_1,x_2,x_3)$$

depends on the two parameters x_2, x_3 and that in the other variable the velocity corresponds to free transport.

This paper is organized as follows: In the next section we introduce the Bloch decomposition of the wave operators but only in the x_1-direction and examine the x_2, x_3 dependence of the projectors and the energy bands. Then we derive a Wigner equation by using Wigner series in the direction x_1 and Wigner transforms in the directions x_2, x_3. In the last section we pass to the semi-classical limit and give the main results.

The main results concerning Bloch waves are used in [2, 4, 6] and those concerning Wigner transforms and series in [7, 4, 6].

In this paper we will assume that the initial data is ε-ocillating; more precisely we assume:

$$\text{for } |\alpha|\leq\ 4\quad\int_{\mathbb{R}^3}|D^\alpha\psi_I(x)|^2dx\leq\frac{C}{\varepsilon^{2|\alpha|}}\quad\alpha\in\mathbb{N}^3\tag{1.11}$$

Remark 1.1 As in [6], this assumption can be weaken to the usual condition of ε-ocillation of [4].

Since the energy of the system reads

$$E(t)=\frac{\varepsilon^2}{2}\int_{\mathbb{R}^3}|\nabla\psi|^2dx+\int V\left(\frac{x_1}{\varepsilon},x_2,x_3\right)|\psi|^2$$

this implies that

$$\int_{\mathbb{R}^3}|\nabla\psi(x,t)|^2dx\leq\frac{C}{\varepsilon^2}\tag{1.12}$$

2. BLOCH DECOMPOSITION

In this section we will recall classical results about Bloch decomposition. But here we only make one-dimensional (x_1) Bloch decomposition and then analyse the regularity of the eigenvalues and of the projectors w.r.t. x_2 and x_3. We want to "diagonalize" the Hamiltonian

$$H\psi = -\frac{\varepsilon^2}{2}\cdot\frac{\partial^2\psi}{\partial x_1^2} + V\left(\frac{x_1}{\varepsilon}, x_2, x_3\right)\psi \tag{2.1}$$

If we consider the microscopic scale (*e.g.* [10, 1]) in the first variable,

$$\psi_1(y_1, x_2, x_3) = \varepsilon^{1/2}\psi_2(\varepsilon y_1, x_2, x_3)$$

As in [10, 4] or [6, 1], we expand the function $\psi_1 \in L^2(\mathbb{R}^3)$ into the Block waves

$$\phi(y_1, x_2, x_3, k) = \sum_{\gamma\in\mathbb{Z}} \psi_1(y_1 - \gamma, x_2, x_3)\mathrm{e}^{ik_1\gamma}, \qquad k \in \mathbb{R} \tag{2.2}$$

Properties of the Bloch Waves

Property 2.1

$$\Psi_1(y_1, x_2, x_3) = \int_{-\pi}^{\pi} \phi(y_1, x_2, x_3, k_1)\frac{dk_1}{2\pi}, \tag{2.3}$$

$$\|\phi\|_{L^2\left([0,1]\times\mathbb{R}^2\times[-\pi,\pi]\right)} = \|\psi_1\|_{L^2(\mathbb{R}^3)} \tag{2.4}$$

Property 2.2 ψ is k-periodic *i.e.*,

$$\phi(y_1 + \gamma, x_2, x_3, k_1) = \mathrm{e}^{ik_1\gamma}\phi(y_1, x_2, x_3, k_1) \tag{2.5}$$

Let H be the Hamiltonian defined on

$$D(H) = \left\{\psi \in L^2(\mathbb{R}^3),\ \frac{\partial^2}{\partial y_1^2}\psi \in L^2(\mathbb{R}^3)\right\}$$

Property 2.3 If H_{k_1} is the Hamiltonian which acts on k-periodic functions *i.e.*,

$$\begin{aligned} D(H_{k_1}) &= \Big\{\phi(y_1, x_2, x_3, k_1) \in L^2([0,1]\times\mathbb{R}^2\times[-\pi,\pi]), \\ &\quad \frac{\partial^2}{\partial y_1^2}\phi(y_1, x_2, x_3, k_1) \in L^2([0,1] \\ &\quad \times\mathbb{R}^2\times[-\pi,\pi])\Big\} \end{aligned}$$

and

$$\phi(y_1 - \gamma, x_2, x_3, k_1) = \mathrm{e}^{ik_1\gamma}\phi(y_1, x_2, x_3, k_1)$$

then *e.g.* [12, 11] H_{k_1} is a compact operator and diagonalizable. Moreover

$$H\psi = \int_{-\pi}^{\pi} H_{k_1}\phi(., k_1)\frac{dk_1}{2\pi} \tag{2.6}$$

where ϕ is given by 2.2. Let us denote by $E_1(k_1, x_2, x_3), \ldots, E_p(k_1, x_2, x_3), \ldots$ the eigenvalues on H_{k_1},

$$\begin{aligned} E_1(k_1, x_2, x_3) &\le E_2(k_1, x_2, x_3) \\ &\le \cdots \le E_p(k_1, x_2, x_3) \le \cdots \end{aligned}$$

and by $\phi_p(., k_1) = \phi_p(y_1, x_2, x_3, k_1)$ the associated eigenvectors. Then we have

THEOREM 2.1 *cf.* [11, 12] *There is a choice of the eigenvector family* $\{\phi_p(., k_1)\}$ *such that it is an Hilbert Basis of* $L^2(\mathbb{R}^3)$ *and such that the functions*

$$k_1 \mapsto \phi_p(y_1, ., k_1)\overline{\phi_p}(z_1, ., k_1)$$

are all analytical. The $\phi_p(., k_1)$ *are* k_1*-periodic and* $\phi_p \in L^2([0,1]\times\mathbb{R}^2\times[-\pi,\pi])$.

DEFINITION 2.2 Let us define now the Wannier functions:

$$\psi_p(y_1, x_2, x_3) = \int_{-\pi}^{\pi} \phi_p(y_1, x_2, x_3, k_1)\frac{dk_1}{2\pi} \tag{2.7}$$

These functions are associated to the Bloch waves $\phi_p(., k_1)$. They also verify the Property 2.1 and the following properties.

Property 2.4

$$\phi_p(.,x_2,x_3,k_1) = \sum_{\gamma\in\mathbb{Z}} \psi_p(\cdot-\gamma,x_2,x_3)\ \mathrm{e}^{ik_1.\gamma}\ ie$$

and $\psi_p(.-\gamma,x_2,x_3)$ are the Fourier coefficients of $\phi_p(.,x_2,x_3,k_1)$.

Property 2.5

$$\int_{\mathbb{R}^3} |\psi_p(y_1,x_2,x_3)|^2 dy_1 dx_2 dx_3 = 1$$

and

$$\int_{\mathbb{R}} \psi_p(y_1,x_2,x_3)\ \overline{\psi_p}\ (y_1-\gamma,x_2,x_3)\ dy_1 = 0 \quad \gamma\neq 0$$

Definition 2.3 Let us define the Floquet subspaces by

$$\begin{aligned} V_p(x_2,\ x_3) = \Big\{ &\psi\in L^2(\mathbb{R}^3),\ \psi(y_1,x_2,x_3) \\ &= \int_{-\pi}^{\pi} \alpha_p(k_1,x_2,x_3) \\ &\qquad \phi_p(y_1,x_2,x_3,k_1)\frac{dk}{2\pi}, \\ &\qquad \alpha_p\in L^2\big([-\pi,\pi]\times\mathbb{R}^2\big)\Big\} \end{aligned} \tag{2.8}$$

where the ϕ_p are the Bloch waves associated to H_{k_1}.

Theorem 2.4 *cf.* [11, 12]

$$L^2(\mathbb{R}^3) = \bigoplus_p V_p(x_2,x_3), \quad x_2,x_3\in\mathbb{R}$$

Let $\hat{E}_p(\gamma,x_2,x_3), \gamma\in\Gamma$, be the Fourier coefficient of $E_p(k_1,x_2,x_3)$. We also have $V_p(x_2,x_3)\in D(H)$ and

$$H(\psi) = \sum_{\gamma\in\mathbb{Z}} \hat{E}_p(\gamma,x_2,x_3)\psi(y_1+\gamma,x_2,x_3), \qquad \psi\in V_p(x_2,x_3);$$

moreover we have $H(\psi)\in V_p(x_2,x_3)$.

For the proof of Theorem 2.4 we refer to [10, 11, 8, 6].

Remark 2.5 The function $E_p(.,x_2,x_3)$ is even. Therefore its Fourier coefficients satisfy

$$\hat{E}_p(\gamma,x_2,x_3) = \hat{E}_p(-\gamma,x_2,x_3)\in\mathbb{R}$$

Remark 2.6 The equation

$$H_k\phi_P(y_1,x_2,x_3,k_1) = E_p(k_1,x_2,x_3)\phi_P(y_1,x_2,x_3,k_1) \tag{2.9}$$

implies (by derivating in direction x_2, multiplying by $\overline{\phi_p}$ and integrating in y_1) that

$$\begin{aligned} &\frac{\partial}{\partial x_2} E_p(k_1,x_2,x_3) \\ &\quad = \int_{\mathbb{R}} \frac{\partial}{\partial x_2} V(y_1,x_2,x_3)|\phi_p(y_1,x_2,x_3,k_1)|^2 dy_1 \end{aligned} \tag{2.10}$$

Let us denote by $\Pi_p(x_2,x_3)$ the projectors from $L^2(\mathbb{R}^3)$ on $V_p(x_2,x_3)$. Let us define the operator

$$\begin{aligned} G_k &= -\frac{1}{2}\left(\frac{\partial}{\partial y_1}+ik_1\right)^2\cdot + V(y_1,x_2,x_3). \\ &= \mathrm{e}^{ik_1.y_1} H_k\big(\mathrm{e}^{-ik_1.}.\big), \\ DG_k &= \big\{\psi\in H^2(\mathbb{R}^3), \psi(y_1+\gamma,\ x_2,\ x_3) \\ &\quad = \psi(y), \quad \gamma\in\Gamma\big\}. \end{aligned}$$

Therefore the projectors $\Pi_p(k_1,x_2,x_3)$, $P_p(k_1,x_2,x_3)$ on the eigenspace corresponding to $E_p(k_1,x_2,x_3)$ for the operator H_k, G_k can be defined by

$$\begin{aligned} &P_p(k_1,x_2,x_3) \\ &\quad = \frac{1}{2i\pi}\int_{|\zeta|=r} (G_k - E_p,(k_1,x_2,x_3)-\zeta)^{-1} d\zeta \\ &\quad \Pi_p(k_1,x_2,x_3) = \mathrm{e}^{ik_1.y_1} P_p(k_1,x_2,x_3)(\mathrm{e}^{ik_1.}.) \end{aligned} \tag{2.11}$$

Remark 2.7 The functions $E_p(.,x_2,x_3)$, $P_p(.,x_2,x_3)$ and $\Pi_p(.,x_2,x_3)$ are analytical since we suppose

that the energy bands $E_p(., x_2, x_3)$ never cross for every $p \geq 0$.

Remark 2.8 Of course we have for $\psi \in L^2(\mathbb{R}^3)$

$$\Pi_p(x_2, x_3)\psi = \int_{-\pi}^{\pi} \Pi_p(k_1, x_2, x_3)\phi_p(k_1, x_2, x_3)\frac{dk_1}{2\pi}$$

where ϕ_p is the Bloch wave associated to ψ and Eq. (2.9) implies that Π_p commutes with H. More exactly we have

$$\begin{aligned} H\,\Pi_p\psi(y_1, x_2, x_3) &= \Pi_p H\psi(y_1, x_2, x_3) \\ &= \sum_{\gamma\in\mathbb{Z}} \hat{E}_p(\gamma, x_2, x_3) \\ &\quad \Pi_p\psi(y_1 + \gamma, x_2, x_3) \end{aligned} \tag{2.12}$$

Returning to the microscopic variable $y_1 = (x_1/\varepsilon)$ Eq. (2.12) becomes

$$\begin{aligned} \left[-\frac{\varepsilon^2}{2}\cdot\frac{\partial^2}{\partial x_1^2} + V\left(\frac{x_1}{\varepsilon}, x_2, x_3\right)\right]\Pi_p\psi(x_1, x_2, x_3) \\ = \sum_{\gamma\in\mathbb{Z}} \hat{E}_p(\gamma, x_2, x_3) \\ \Pi_p\psi(x_1 + \varepsilon\gamma, x_2, x_3) \end{aligned} \tag{2.13}$$

which is a "diagonalisation" of H defined in (2.1).

We now turn back to Eq. (1.7), by taking the projection of (1.7) on V_p we get

$$i\varepsilon\partial_t\Pi_P\psi = H\,\Pi_p\psi - \frac{\varepsilon^2}{2}\Pi_p(\Delta_{x_2,x_3}\psi) \tag{2.14}$$

where H is the Hamiltonian defined in (2.1) and $\Delta_{x_2,\,x_3} = (\partial^2/\partial x_2^2) + (\partial^2/\partial x_3^2)$ is the Laplacian in both variable x_2 and x_3.

3. WIGNER TRANSFORMS

In this paper since we have periodicity in the direction x_1, we will associate Wigner series in the direction x_1, and classical Wigner transforms in the direction x_2, x_3.

For a couple of functions $\psi, \varphi \in L^2(\mathbb{R}^3)$, let us define

$$\begin{aligned} W^\varepsilon(\psi, \varphi)(x, k) \\ = \frac{1}{2\pi}\int_{\mathbb{R}^2}\sum_{\gamma\in\mathbb{Z}} \psi\left(x_1 - \frac{\varepsilon\gamma}{2}, x_2 - \frac{\varepsilon z_2}{2}, x_3 - \frac{\varepsilon z_3}{2}\right). \\ \overline{\varphi}\left(x_1 + \frac{\varepsilon\gamma}{2}, x_2 + \frac{\varepsilon z_2}{2}, x_3 + \frac{\varepsilon z_3}{2}\right) \\ \times\, e^{ik_1.\gamma} e^{i(k_2 z_2 + k_3 z_3)} dz_2 dz_3. \end{aligned} \tag{3.1}$$

We define as in [7, 8, 10] an algebra of test functions by

$$\begin{aligned} \mathcal{A} = \Big\{ w = w(x, k) = \frac{1}{(2\pi)^3} \\ \sum_{\gamma\in\mathbb{Z}} e^{ik_1\cdot\gamma}\int_{\mathbb{R}^2} \hat{w}^{k_2,k_3}(x, \gamma, \eta_2, \eta_3) e^{i(k_2\cdot\eta_2 + k_3\cdot\eta_3)} d\eta_2 d\eta_3; \\ \hat{w} \in l^1\Big(\mathbb{Z}\ ;\ L^1(d\eta_2 \times \eta_3\ ;\ \mathcal{C}^0(\mathbb{R}^3_x))\Big)\Big\} \end{aligned} \tag{3.2}$$

$\mathcal{A}$ is equipped with its natural norm:

$$\begin{aligned} \|w\|_{\mathcal{A}} = \sum_{\gamma\in\mathbb{Z}} \| \ \|\hat{w}^{k_1,k_2}(., \gamma, \eta_2, \eta_3) \\ \|_{L^\infty(\mathbb{R}^3)}\|_{L^1(d\eta_2\times d\eta_3)} \end{aligned}$$

Let us recall a theorem from [7, 10, 6]:

THEOREM 3.1 *Let (ψ^ε) be a bounded family of $L^2(\mathbb{R}^3)$; then the family $(W^\varepsilon) = W^\varepsilon(\psi^\varepsilon, \psi^\varepsilon)$ is bounded in $\mathcal{A}'$. The accumulation points in $\mathcal{A}'$ weak $-*$ when $\varepsilon \to 0$ are bounded non negative measures.*

$$W^\varepsilon \to f \quad in \quad \mathcal{A}' weak - *.$$

Moreover we have

$$\begin{aligned} |\psi^\varepsilon|^2 \to \int_{[-\pi,\pi]\times\mathbb{R}^2} f(., k)\frac{dk}{2\pi} \\ in\ \mathcal{C}^{0'}(\mathbb{R}^3) weak - * \end{aligned}$$

if (ψ^ε) is ε-oscillatory for the variable x_2, x_3.

Let us now mention a property which will be very useful in the following of this paper. This is an

expansion of Wigner transform with a pseudo differential operator $p(x, \varepsilon D)$.

DEFINITION 3.2 Let us consider a symbol

$$p(x,\xi) \in \mathcal{S}(\mathbb{R}^m_x \times \mathbb{R}^m_\xi)$$

then for $f \in \mathcal{S}'(\mathbb{R})^m$

$$P(x,\varepsilon D)f(x) = \frac{1}{(2\pi)^m}\int_{\mathbb{R}^m\times\mathbb{R}^m} p(x,\varepsilon\xi)f(y)\mathrm{e}^{i(x-y)\cdot\xi}d\xi dy \tag{3.3}$$

DEFINITION 3.3 The Weyl operator associated to the symbol $p(x,\xi)$ is defined by

$$P^W(x,\varepsilon D)f(x) = \frac{1}{(2\pi)^m}\int_{\mathbb{R}^m\times\mathbb{R}^m} p\left(\frac{x+y}{2},\varepsilon\xi\right)f(y)\mathrm{e}^{i(x-y)\cdot\xi}d\xi dy \tag{3.4}$$

DEFINITION 3.4 If the notation $\{p,q\}$ denotes the Poisson bracket of $p = p(x,\varepsilon)$ and $q = q(x,\xi)$ defined by

Remark 3.5 We can weaken the regularity of p if we take a more regular function f.

$$\{p,q\}\ (x,\xi) = \nabla_\xi p(x,\xi)\cdot\nabla_x q(x,\xi) - \nabla_x p(x,\xi)\cdot\nabla_\xi q(x,\xi) \tag{3.5}$$

DEFINITION 3.6 Classical Wigner transform expansion with a pseudo differential operator. The classical Wigner transform of $(f,g)\in L^2(\mathbb{R})^m$ is defined by

$$w_\varepsilon(f,g) = \frac{1}{2\pi^m}\int_{\mathbb{R}^m} f\left(x-\frac{\varepsilon z}{2}\right)\overline{g}\left(x+\frac{\varepsilon z}{2}\right)\mathrm{e}^{i\xi.z}dz \tag{3.6}$$

Property 3.6 Let $p \in \mathcal{C}^\infty(\mathbb{R}^m\times\mathbb{R}^m)$ satisfy for some $M \geq 0$:

$$\forall\alpha \in (\mathbb{N}^m\times\mathbb{N}^m) : |\partial^\alpha_{x,\xi}\ p(x,\xi)| \leq C_\alpha(1+|\xi|)^M.$$

If f and y lie in a bounded set of $L^2(\mathbb{R})^m$, we have the expansion

$$w_\varepsilon(P^W(x,\varepsilon D)f,g) = pw_\varepsilon(f,g) + \frac{\varepsilon}{2i}\{p(x,\xi),\ w_\varepsilon(f,g)\} + \varepsilon^2 r_\varepsilon \tag{3.7}$$

where r_ε is bounded in $\mathcal{S}'(\mathbb{R}^m\times\mathbb{R}^m)$ uniformly w.r.t. ε.
This property is proved in [6].

THEOREM 3.7 *Let $p \in \mathcal{C}^\infty(\mathbb{R}^2\times\mathbb{R}^2)$ satisfy for some $M \geq 0$,*

$$\forall\alpha \in (\mathbb{N}^2\times\mathbb{N}^2) : \left|\partial^\alpha_{x_2,x_3,k_2,k_3}p(x_2,x_3,k_2,k_3)\right| < C_\alpha(1+|\xi|)^M \tag{3.8}$$

Then as ϕ and φ lie in a bounded set of $L^2(\mathbb{R}^3)$ we have the expansion

$$W^\varepsilon(P^W(x_2,x_3,\varepsilon D_{2,3})\psi,\varphi) = p(x_2,x_3,k_2,k_3)W^\varepsilon(\psi,\varphi) + \frac{\varepsilon}{2i}\{p(x_2,x_3,k_2,k_3),W^\varepsilon(\psi,\varphi)\} + \varepsilon^2 R_\varepsilon \tag{3.9}$$

where R_ε is bounded in $\mathcal{S}'(\mathbb{R})^6$ uniformly w.r.t. ε

THEOREM 3.8 *Let $a \in \mathcal{C}^0(\mathbb{R}^2{}_{x_2,x_3},\mathcal{C}^1(\mathbb{R}_{k_1}))$ 1-periodic with respect to k_1. Then as ψ and φ lie in a bounded set of $L^2(\mathbb{R})^3$ we have the expansion*

$$\begin{aligned} W^\varepsilon(a(\varepsilon D_1,x_2,x_3)\psi,\varphi) &= (a(D_1,x_2,x_3)W^\varepsilon(\psi,\varphi) \\ &\quad - \frac{\varepsilon}{2i}\nabla_{x_2,x_3}a(k_1,x_2,x_3)\cdot\nabla_{k_2,k_3}W^\varepsilon(\psi,\varphi) \\ &\quad + \frac{\varepsilon}{2i}\nabla_{k_1}a(k_1,x_2,x_3)\cdot\nabla_{x_1}W^\varepsilon(\psi,\ \varphi) + \varepsilon^2 T_\varepsilon. \end{aligned} \tag{3.10}$$

in $\mathcal{S}'$ with T_ε bounded in $\mathcal{S}'(\mathbb{R}^6)$ uniformly w.r.t. ε.

The proof of Theorem (3.7) and Theorem (3.8) is almost the same as in [6]: we make a Taylor expansion of the Fourier transform of the Wigner function and we get the desired result.

4. COMMUTATOR ESTIMATES

Let ψ_ε be a bounded family of functions in $L^2(\mathbb{R})^3$ satisfying Eq. (1.7). $\Pi_p\psi$ satisfies Eq. (2.14) with $\Pi_p\psi_{I\varepsilon} = \psi_{I\varepsilon} \in V_p$. In order to pass to the limit $\varepsilon \to 0$, let us rewrite Eq. (2.14) in an other way:

$$i\varepsilon\partial_t\Pi_p\psi = iE_p(\varepsilon D_1, x_2, x_3)\Pi_p\psi - \frac{\varepsilon^2}{2}\Delta_{x_2,x_3}\Pi_p\psi + \frac{\varepsilon^2}{2}[\Delta_{x_2,x_3};\ \Pi_p]\psi \tag{4.1}$$

where $[\Delta_{x_2,x_3};\ \Pi_p]$ is a commutator defined by

$$[\Delta_{x_2,x_3};\ \Pi_p]\psi = \Delta_{x_2,x_3}\Pi_p\psi - \Pi_p\Delta_{x_2,x_3}\psi \tag{4.2}$$

PROPOSITION 4.1

$$\frac{1}{\varepsilon}\big(W^\varepsilon([\Delta_{x_2,x_3};\Pi_p]\psi, \Pi_p\psi) - W^\varepsilon(\Pi_p\psi, [\Delta_{x_2,x_3};\Pi_p\psi])\big) \to 0 \quad \text{in } L^\infty(0,T;\mathcal{S}'(\mathbb{R}^6))$$

follows from these very useful lemmas

LEMMA 4.1 *Let $\psi_p^\varepsilon \in V_p^\varepsilon, \psi_q^\varepsilon \in V_q^\varepsilon$ be two bounded sequences in $L^2(\mathbb{R}^3)$ satisfying the equations*

$$H\psi_p^\varepsilon = E_p(\varepsilon D_1, x_2, x_3)\psi_p^\varepsilon \tag{4.3}$$

$$H\psi_q^\varepsilon = E_q(\varepsilon D_1, x_2, x_3)\psi_q^\varepsilon \tag{4.4}$$

where H is the Hamiltonian defined in Eq. (2.1). We have

$$W^\varepsilon(\psi_p^\varepsilon, \psi_q^\varepsilon) = \frac{\varepsilon^2}{E_p - E_q} div_{x_1} W^\varepsilon(\partial_{x_1}\psi_p^\varepsilon, \psi_q^\varepsilon) + \varepsilon^2\|\psi_p^\varepsilon\|_{L^2}\|\psi_q^\varepsilon\|_{L^2}R^\varepsilon$$

$$= \frac{\varepsilon}{(E_p - E_q)^2} div_{x_1} W^\varepsilon\left(\partial_{x_1}V\left(\frac{x_1}{\varepsilon}, x_2, x_3\right)\psi_p^\varepsilon, \psi_q^\varepsilon\right) + \varepsilon^2\|\psi_p^\varepsilon\|_{L^2}\|\psi_q^\varepsilon\|_{L^2}R^\varepsilon$$

where R^ε is uniformly bounded in $\mathcal{S}'(\mathbb{R}^6)$ with respect to $\varepsilon, \psi_p^\varepsilon$ and ψ_q^ε.

LEMMA 4.2 *Let ψ^ε be a function such that ψ^ε, $H^\varepsilon\psi$ are bounded sequences in L^2, then*

$$\|\Pi_p\psi\|_{L^2} \le \frac{C}{p^2}.$$

Of course this implies

$$\int_{\mathbb{R}^3} n_p\, dx \le \frac{C}{cp^4} \tag{4.5}$$

Therefore the sequence $\Sigma_p n_p$ is uniformly convergent w.r.t. ε.

Proof of Proposition (4.1) In the following, we will note with a prime′ a derivation w.r.t. the variable x_2 or x_3 and define $\psi_p = \Pi_p\psi$. We have

$$\Pi_p\varepsilon^2\psi'' = \varepsilon^2\psi_p'' + \sum_{q\neq p}(\psi_q'' - \Pi_q(\varepsilon^2\psi''))$$

Therefore we have

$$W^\varepsilon(\Pi_p\varepsilon^2\psi'', \psi_p) = W^\varepsilon(\varepsilon^2\psi_p'', \psi_p) + \sum_{q\neq p}\big(W^\varepsilon(\psi_q'', \psi_p) - W^\varepsilon(\Pi_q(\varepsilon^2\psi''), \psi_p)\big)$$

Since the series $\Sigma_{q\neq p}\Pi_q\psi$ and $\Sigma_{q\neq p}\Pi_q\varepsilon^2\psi''$ converge uniformly by Lemma (4.2) see also [6, 8], we only have to verify that for every fixed q, the terms with different indices converge to zero in $\mathcal{S}'(\mathbb{R}^6)$. By a little computation using Lemma (4.1) and the

asymptotic expansion of Theorem (3.7), we have

$$\begin{aligned} &W^{\varepsilon}(\psi_q'', \psi_p) - W^{\varepsilon}(\Pi_q(\varepsilon^2\psi''), \psi_p) \\ &= \varepsilon \mathrm{div}_{x_1}\left[W^{\varepsilon}\left(\partial_{x_1} V\left(\frac{x_1}{\varepsilon}, x_2, x_3\right)\right.\right. \\ &\quad \left.\left. \times (2\varepsilon\Pi_q'\varepsilon\psi' + \varepsilon^2\Pi_q''\psi, \psi_p)\right)\right] + O(\varepsilon^2) \\ &= O(\varepsilon^2) \end{aligned}$$

We are done.

5. SEMI-CLASSICAL LIMIT

We now compute the semi-classical limit *i.e.*, $\varepsilon \to 0$ of the Wigner equation.

THEOREM 5.1 *As $\varepsilon \to 0$, if for some subsequence $W_I^{\varepsilon} \to f_{pI}$ in $\mathcal{A}'$-weak*, then we have $W^{\varepsilon} \to f_p$ in $C^0(0, T, \mathcal{S}'(\mathbb{R})^6)$*
where $f_p \geq 0$ verifies the Vlasov equation:

$$\partial_t f_p = \{\mathcal{E}_p, f_p\} \tag{5.1}$$

$$f_p(0, x, k) = f_{pI}(x, k). \tag{5.2}$$

where

$$\mathcal{E}_p(k, x_2, x_3) = E_p(k_1, x_2, x_3) + \frac{|k_2|^2}{2} + \frac{|k_3|^2}{2}$$

and $n^{\varepsilon}(t, x) \to n(t, x)$ in $C(0, T, C^{0'}(\mathbb{R}^3) - weak*)-$ weak where*:

$$n(x, t) = \sum_p \int_{[-\pi,\pi]\times\mathbb{R}^2} f_p(x, k, t)\frac{dk}{2\pi}.$$

Remark 5.2 In extended form the Eq. (5.1) reads

$$\begin{aligned} \partial_t f_p = &\begin{pmatrix} \partial_{k_1} E_p(k_1, x_2, x_3) \\ k_2 \\ k_3 \end{pmatrix} . \nabla_x f_p\ (t, x, k) \\ &- \nabla_{x_2,x_3} E_p(t, x, k) . \nabla_{k_2,k_3} f_p(t, x, k) \end{aligned} \tag{5.3}$$

The proof of Theorem (5.1) follows immediately from proposition (4.1) by using the asymptotic expansions from Theorems (3.7) and (3.8) applied to Eq. (4.1).

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