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Wigner Series and (Semi)classical Limits with Periodic Potentials

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Abstract

We present a rigorous derivation of the semiclassical Liouville equation for electrons which move in a crystal lattice (without the influence of an external field). The approach is based on carrying out the semiclassical limit in the band - structure Wignerequation. The semiclassical macroscopic densities are also obtained as limits of the corresponding quantum quantities.

Key words. Energy bands, Bloch-electrons, One-band approximation, Wannierfunctions, Wigner-Weyl transform, Wignerfunction, Husimifunction, semiclassical limit, Vlasov equation, semiconductor device modelling

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1 Introduction

When conduction electrons move in a solid, then quantum effects of the ions located at the crystal lattice points have to be taken into account in the equations of motion. On a fully quantum mechanical level of description (see e.g [1]) this is done by incorporating a lattice-periodic potential V (generated by the lattice ions) in the (effective one-particle) Hamilton-operator for a conduction electron

$$H = -\frac{\hbar^2}{2m}\Delta_x + V, \quad x \in \mathbb{R}^3. \tag{1.1}$$

Here m denotes the mass of the electron and $\hbar$ the Planck constant.

The electron wave function ψ then satisfies the IVP for the Schrödinger equation

$$i\hbar\psi_t = H\psi, \quad x \in \mathbb{R}^3, t > 0 \tag{1.2}$$

$$\psi(t=0)=\psi_I, \quad x \in \mathbb{R}^3$$

with the quantum position density

$$n(x,t)=|\psi(x,t)|^2. \tag{1.3}$$

Note that in this paper no exterior (non-periodic) field influences the motion of the considered particle and we also do not take into account the Coulomb interaction among electrons . Usually, the initial state ψ_I is not known exactly and, thus, corresponding statistical mixtures (so called mixed states) with given occupation probabilities for the set of possible states have to be considered.

It is well known that the Hamilton operator (1.1) with the lattice periodic potential V induces a direct sum decomposition of the space of states $L^2(\mathbb{R}^3)$ corresponding to the eigenspaces of the Floquet - eigenvalues of H (see e.g. [11], [4]). These eigenvalues $\{E_m\}_{m\in \mathbb{N}}$, called 'energy bands' in solid state physics, are periodic functions of the wave-vector k defined in the Brillouin zone B of the crystal lattice.

On a semi-classical level of description, the Schrödinger equation is usually replaced by the semiclassical Liouville equation for the phase space (i.e. position-wave vector space) density $w=w(x,k,t)$. When no exterior field is present and when the electron is known to 'move in the m-th band' (i.e. the states of the statistical mixture belong to the m-th Floquet eigenspace) then the semiclassical Liouville equation reads

$$\frac{\partial w}{\partial t}+\frac{1}{\hbar}\nabla_k E_m(k)\cdot\nabla_x w=0, \quad x\in\mathbb{R}^3,\ k\in B \tag{1.4}$$

subject to a periodic boundary condition in k and an initial condition

$$w(t=0)=w_I, \quad x\in\mathbb{R}^3,\ k\in B. \tag{1.5}$$

The position density n and the current density J are computed as

$$n(x,t)=\frac{1}{4\pi^3}\int_B w\,dk, \quad J(x,t)=\frac{1}{4\pi^3}\int_B \frac{1}{\hbar}\nabla_k E_m w\,dk \tag{1.6}$$

and the electron energy density

$$\epsilon(t,x)=\frac{1}{4\pi^3}\int_B E_m(k)w\,dk. \tag{1.7}$$

In the physical literature (e.g. [1]) the equations of motion

$$\dot{x}=\frac{1}{\hbar}\nabla_k E_m(k)\,, \tag{1.8}$$

$$\hbar\dot{k}=0\,, \tag{1.9}$$

which correspond to the semiclassical Liouville equation (1.4) are usually derived by tracking the motion of wavepackets of the Schrödinger equation (1.2). This stationary phase method does, however, not lead to a rigorous justification of the semiclassical Liouville equation and of the semiclassical moments.

A rigorous derivation of the semiclassical transport equation (1.4), (1.5) was given by P. Gerard in [10]. His very elegant approach is based on microlocal analysis of pseudodifferential operators. For a bounded sequence in L^2 he constructs "the semiclassical measure" which describes the oscillations of the sequence. He proves that the measure associated to the sequence of solutions of (1.2) satisfies (1.4), (1.5). In fact, it can be shown (cf. [6]) that the semiclassical measure is nothing but the limit of the Wignertransform of the density matrix corresponding to (1.2). This approach does, however, not provide immediate information on the macroscopic densities and seems to run into difficulties when an exterior nonperiodic potential is present in the Hamilton operator. In this paper we shall rigorously derive the semiclassical approximations by a completely different approach based entirely on kinetic equations (cp. [6] and [7] for the vacuum case). Using the above mentioned eigenspace decomposition of the space of states we shall reformulate the IVP for the Schrödinger equation as a denumerable system of Wigner-type equations. The basis for this reformulation lies in the appropriate definition of a Wigner-type function for each band. These Band-Wignerfunctions are defined in analogy (i.e. using Fourierseries instead of Fouriertransform) to the non-crystal 'whole space case' (which is presented e.g. in [2], [12], [13]) and have similar properties as the semiclassical distribution functions (solutions of the semiclassical Liouville equations). In particular they allow the calculation of the macroscopic densities in analogy to the semiclassical k- space moments (1.6), (1.7).

The semiclassical Liouville equation (1.4) (1.5) is then obtained by introducing an appropriate scaling (analogously to the one used in [10]), which assumes that the period of the potential V is 'of order $\hbar$' (after appropriate scaling) and by carrying out the limit $\hbar \to 0$. The convergence of the quantum position-, current- and momentum-densities can then be concluded from the convergence properties of the Band-Wignerfunctions (plus some additional compactness).

We remark that this approach (just as the one of P. Gerard) is not limited to a one-band approximation. Initial wave-functions which belong to the direct sum of arbitary many eigenspaces are admissible.

As already mentioned, this paper only deals with the case of a periodic potential in the Hamilton equation. Most of the proofs are skipped here, we refer to [8] for a detailed analysis.

2 Preliminaries: Schrödinger Operators with Periodic Potentials

Let $a_{(1)}, a_{(2)}, a_{(3)}$ be a basis of $\mathbb{R}^3$. Then we define the crystal lattice by

$$L = \{a_{(1)}j_1 + a_{(2)}j_2 + a_{(3)}j_3 \,|\, j_1, j_2, j_3 \in \mathbb{Z}\} \tag{2.1}$$

The dual basis vectors $a^{(1)}, a^{(2)}, a^{(3)}$ are determined by the equation

$$a_{(\ell)}a^{(m)} = 2\pi\, \delta_{\ell m} \quad ; \ell, m = 1,2,3 \tag{2.2}$$

and the dual lattice L^* ('reciprocal lattice') reads

$$L^* = \{a^{(1)}j_1 + a^{(2)}j_2 + a^{(3)}j_3 \,|\, j_1, j_2, j_3 \in \mathbb{Z}\}. \tag{2.3}$$

The basic period cell of the lattice L is denoted by

$$C := \{\sum_{i=1}^{3} t_i a_{(i)} \,|\, 0 \le t_1, t_2, t_3 < 1\} \tag{2.4}$$

and, as usual ([1], [11]), the Brillouin zone B is the Wigner - Seitz cell of the dual lattice L^* :

(2.5) $$B := \{k \in \mathbb{R}^3_k \mid k \text{ is closer to zero than to any other point of } L^*\}$$

Note that

(2.6) $$|C|\,|B| = (2\pi)^3$$

holds, where $|.|$ denotes here the volume. For the following let $V = V(x)$ be a real-valued potential on $\mathbb{R}^3$ with the properties

(A1) (i) $\quad V \in L^\infty(\mathbb{R}^3)$
(A1) (ii) $\quad V$ *is* L *– periodic, i.e.* $V(x+\mu) = V(x)$ *on* $\mathbb{R}^3 \quad \forall \mu \in L$.

For $\alpha \in (0, \alpha_0]$, $\alpha_0 > 0$ fixed, we define the Hamiltonian

(2.7) $$H^\alpha := -\frac{\alpha^2}{2}\Delta_x + V(\frac{x}{\alpha})$$

which we will regard both on $L^2(C)$ and on $L^2(\mathbb{R}^3)$. Obviously, H^α is obtained from H^1 by the rescaling of the position variable $x \to \frac{x}{\alpha}$, where α is the scaled Planck constant. For $k \in \overline{B}$ we define the operator $H^1(k)$ as H^1 with the periodicity conditions :

(2.8) $$\psi(x+\mu) = e^{i\mu\cdot k}\psi(x), \quad x \in \mathbb{R}^3,\ \mu \in L$$

(2.9) $$\frac{\partial\psi}{\partial x_\ell}(x+\mu) = e^{i\mu\cdot k}\frac{\partial\psi}{\partial x_\ell}(x), \quad x \in \mathbb{R}^3, \mu \in L,\ \ell = 1,2,3$$

It is well known [11] that each $H^1(k)$ has a complete set of eigenfunctions $\psi = \Psi_m(x,k), m \in \mathbb{N}$, (orthonormed in $L^2(C)$) with eigenvalues $E_1(k) \le E_2(k) \le E_3(k) \le \cdots \le E_{m-1}(k) \le E_m(k) \le \cdots$ (counted with multiplicities). For every fixed $m \in \mathbb{N}$ the function $E_m = E_m(k)$ is continuous on $\overline{B}$ and the eigenfunctions can be chosen measurably in $k \in B$. Also $E_m(k) \overset{m\to\infty}{\longrightarrow} \infty$ uniformly for $k \in \overline{B}$.

The set

(2.10) $$\{E_m(k) | k \in B\} \subseteq \mathbb{R},$$

is called the m-th (energy) - band of H^1 and the eigenfunction Ψ_m is called the $m-th$ Bloch-function. Note that Ψ_m can be written as the product of a plane wave and a lattice periodic function.

We now set

(2.11) $$\Psi^\alpha_m(x,k) := \alpha^{-\frac{3}{2}}\Psi_m(\frac{x}{\alpha}, k) \quad , x \in \mathbb{R}^3, k \in B.$$

The scaling argument mentioned above implies

(2.12) $$H^\alpha\Psi^\alpha_m(.,k) = E_m(k)\Psi^\alpha_m(.,k)$$

(2.13) $$\Psi^\alpha_m(x+\alpha\mu, k) = e^{i\mu\cdot k}\Psi^\alpha_m(x,k), \quad x \in \mathbb{R}^3,\ \mu \in L$$

(2.14) $$\frac{\partial\Psi^\alpha_m}{\partial x_\ell}(x+\alpha\mu, k) = e^{i\mu\cdot k}\frac{\partial\Psi^\alpha_m}{\partial x_\ell}(x,k), \quad x \in \mathbb{R}^3,\ \mu \in L,\ \ell = 1,2,3$$

Obviously , the set $\{\ \Psi^\alpha_m(.,k)\ \}$ is orthonormed in $L^2(\alpha C)$.

The following decomposition Theorem is obtained from [11], Theorem XIII.98, by rescaling $x \to \frac{x}{\alpha}$.

Theorem 2.1 *For $\psi \in L^2(\mathbb{R}^3)$ set*

$$\tilde{\psi}^\alpha(k,m) := \int_{\mathbb{R}^3} \psi(x)\overline{\Psi}^\alpha_m(x,k)\,dx \quad ,k \in B,\ m \in \mathbb{N} \tag{2.15}$$

Then the following statements hold :

(*i*) $\psi(x) = \frac{1}{|B|}\sum_{m=1}^{\infty}\int_B \tilde{\psi}^\alpha(k,m)\Psi^\alpha_m(x,k)\,dk, \quad x \in \mathbb{R}^3$

(*ii*) $\|\psi\|^2_{L^2(\mathbb{R}^3)} = \frac{1}{|B|}\sum_{m=1}^{\infty}\int_B |\tilde{\psi}^\alpha(k,m)|^2 dk$

(*iii*) $\widetilde{H^\alpha\psi}(k,m) = E_m(k)\tilde{\psi}^\alpha(k,m), \quad k \in B,\ m \in \mathbb{N}$

(*iv*) *The mapping* $\tilde{}$ $: L^2(\mathbb{R}^3) \to \bigoplus_m L^2(B)$ *is one-to-one and onto.*

(*v*) *Let* $\psi_1, \psi_2 \in L^2(\mathbb{R}^3)$. *Then the Plancherel formula*

$$\int_{\mathbb{R}^3} \psi_1(x)\overline{\psi_2}(x)\,dx = \frac{1}{|B|}\sum_{m\in\mathbb{N}}\int_B \tilde{\psi}^\alpha_1(k,m)\overline{\tilde{\psi}^\alpha_2}(k,m)dk \tag{2.16}$$

holds .

Here $\bigoplus_m$ H denotes the denumerable direct sum of the Hilbertspace H and "$^-$" denotes complex conjugation.

The subspace

$$S^\alpha_m := \left\{\frac{1}{|B|}\int_B \sigma(k)\Psi^\alpha_m(x,k)\,dk \quad | \quad \sigma \in L^2(B)\right\} \tag{2.17}$$

of $L^2(\mathbb{R}^3)$ which is invariant under the action of H^α (cf. Theorem 2.1 (iii)), is called the m-th band space. Obviously $S^\alpha_{m_1}$ and $S^\alpha_{m_2}$ are orthogonal for $m_1 \neq m_2$.

The action of the Hamiltonian in the subspaces is described in :

Lemma 2.1 *Let* $\psi \in S^\alpha_m$. *Then*

$$(H^\alpha\psi)(x) = \sum_{\mu\in L} \mathcal{E}_m(\mu)\psi(x+\alpha\mu) \tag{2.18}$$

where $\mathcal{E}_m(\mu)$ *are the Fouriercoefficients of* $E_m(k)$ *:*

$$E_m(k) = \sum_{\mu\in L} \mathcal{E}_m(\mu)e^{ik\cdot\mu}. \tag{2.19}$$

3 The Quantum Band - Problem

We now consider the Schrödinger equations

$$(3.1)\qquad i\alpha\frac{\partial}{\partial t}\psi^{\alpha}_{\ell m} = -\frac{\alpha^2}{2}\Delta\psi^{\alpha}_{\ell m} + V(\frac{x}{\alpha})\psi^{\alpha}_{\ell m}, \quad x \in I\!R^3,\ t > 0$$

$$(3.2)\qquad \psi^{\alpha}_{\ell m}(x, t=0) = \omega^{\alpha}_{\ell m}(x), \quad x \in I\!R^3$$

for $\ell, m \in I\!N$, where we prepare the initial data $\omega^{\alpha}_{\ell m}$ as follows :

Let $\tilde{\omega}^{\alpha}_{\ell m}(.,m) \in L^2(B), \ell$ and $m \in I\!N$, be a double sequence (m...'band-index', l...'mixed state index') with the property

(A2) (*i*) $\frac{1}{|B|}\int\limits_B \tilde{\omega}^{\alpha}_{\ell_1}(k,m)\overline{\tilde{\omega}^{\alpha}_{\ell_2}}(k,m)\,dk = \delta_{\ell_1\ell_2} \quad \forall m, \ell_1, \ell_2 \in I\!N$

(A2) (*ii*) *Set* $\omega^{\alpha}_{\ell m}(x) = \frac{1}{|B|}\int\limits_B \tilde{\omega}^{\alpha}_{\ell}(k,m)\Psi^{\alpha}_{m}(x,k)dk$

Obviously the function $\omega^{\alpha}_{\ell m}$ lies in the m-th band space S^{α}_{m}.

From Theorem 2.1 we conclude

$$(3.3)\qquad \int\limits_{I\!R^3} \omega^{\alpha}_{\ell_1 m_1}\overline{\omega^{\alpha}}_{\ell_2 m_2}dx = \delta_{\ell_1\ell_2}\delta_{m_1 m_2} \quad \forall\,\ell_1,\ \ell_2, m_1, m_2 \in I\!N$$

The sequence $\omega^{\alpha}_{\ell m}$ of initial data is orthonormed in $L^2(I\!R^3)$ and therefore the solutions $\psi^{\alpha}_{\ell m}(.,t)$ remain orthonormed for all times $t > 0$. Moreover $\psi^{\alpha}_{\ell m}(.,t) \in S^{\alpha}_{m}$ for all $t > 0$ follows from Theorem 2.1 (iii). Also this Theorem implies the existence of functions $\tilde{\psi}^{\alpha}_{\ell}(.,m,t) \in L^2(B)$ with the properties

$$(3.4)\qquad \psi^{\alpha}_{\ell m}(x,t) = \frac{1}{|B|}\int\limits_B \tilde{\psi}^{\alpha}_{\ell}(k,m,t)\Psi^{\alpha}_{m}(x,k)\,dk, \quad x \in I\!R^3, t > 0$$

$$(3.5)\qquad \tilde{\psi}^{\alpha}_{\ell}(k,m,t) = \int\limits_{I\!R^3} \psi^{\alpha}_{\ell m}(x,t)\overline{\Psi^{\alpha}_{m}}(x,k)\,dx, \quad k \in B, t > 0$$

$$(3.6)\qquad \frac{1}{|B|}\int\limits_B \tilde{\psi}^{\alpha}_{\ell_1}(k,m,t)\overline{\tilde{\psi}^{\alpha}_{\ell_2}}(k,m,t)\,dk = \delta_{\ell_1\ell_2} \quad \forall m, \ell_1, \ell_2 \in I\!N, t > 0$$

From Lemma 2.1 we conclude that the IVP for $\psi^{\alpha}_{\ell m}$ can be written as

$$(3.7)\qquad i\alpha\frac{\partial}{\partial t}\psi^{\alpha}_{\ell m}\psi^{\alpha}_{\ell m} = \sum_{\mu\in L}\mathcal{E}_m(\mu)\psi^{\alpha}_{\ell m}(x+\alpha\mu, t), \quad x \in I\!R^3, t > 0$$

$$(3.8)\qquad \psi^{\alpha}_{\ell m}(x, t=0) = \omega^{\alpha}_{\ell m}(x),\ x \in I\!R^3.$$

For the definition of the mixed state densities we prescribe a sequence of α - dependent occupation probabilities $\lambda^{\alpha}_{\ell m}$ of the sequence of states $\omega^{\alpha}_{\ell m}$. We shall use the following assumptions (cp. [7])

(A3) (*i*) $\lambda^{\alpha}_{\ell m} \geq 0 \quad \forall \ell, m \in I\!N$

(A3) (*ii*) $\sum_{m=1}^{\infty}\sum_{\ell=1}^{\infty}\lambda_{\ell m}^{\alpha}\leq D$, where D is independent of $\alpha\in(0,\alpha_0]$.

Note that the same superscript α denotes both the α -dependence due to the scaling and the α- dependence stemming from the initial data.

We now define the m-th band mixed state position density.

$$n_m^{\alpha}(x,t):=\sum_{\ell=1}^{\infty}\lambda_{\ell m}^{\alpha}|\psi_{\ell m}^{\alpha}(x,t)|^2 \tag{3.9}$$

and the total charge density :

$$n^{\alpha}(x,t):=\sum_{m=1}^{\infty}n_m^{\alpha}(x,t). \tag{3.10}$$

Then the total charge is bounded uniformly in α :

$$\int_{\mathbb{R}^3}n^{\alpha}(x,t)\,dx \quad\equiv\quad \sum_{m=1}^{\infty}\sum_{\ell=1}^{\infty}\lambda_{\ell m}^{\alpha}\leq \quad D. \tag{3.11}$$

(we used (3.6), (A3)(ii)).
Since the usually defined current densities are extremely impractical in calculations where the band structure is involved, we make use of the arbitrariness of their definition (based on the macroscopic conservation law). The following definition of the current densities is convenient for the band-structure set-up.
Let " ^ " denote the Fourier-transform of a function with respect to x :

$$\hat{f}(\xi)=\frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}f(x)e^{-i\xi\cdot x}\,dx,\qquad f(x)=\int_{\mathbb{R}^3}\hat{f}(\xi)e^{i\xi\cdot x}\,d\xi.$$

We remark that in the sequel we shall not distinguish between a function in $L^2(B)$ and its L^*- periodic extension to $L^2_{loc}(\mathbb{R}^3_k)$, except that we denote the argument by k and ξ, resp.
We now define the m-th band current density J by its Fourier-transform :

$$\hat{J}_m^{\alpha}(\xi,t):=\sum_{\ell=1}^{\infty}\lambda_{\ell m}^{\alpha}\int_{\mathbb{R}^3_\omega}\int_0^1\nabla_k E_m(\alpha\omega+(s-1)\alpha\xi)\,ds\,\hat{\psi}_{\ell m}^{\alpha}(\omega,t)\overline{\hat{\psi}}_{\ell m}^{\alpha}(\omega-\xi,t)\,dw \tag{3.12}$$

and the total current density

$$J^{\alpha}(x,t):=\sum_{m=1}^{\infty}J_m^{\alpha}(x,t). \tag{3.13}$$

Our definition of J_m^{α} is motivated by the macroscopic conservation law and relies on the regularity of the energy bands. Indeed we have :

Lemma 3.1 *:*

(*i*) $\|\hat{J}_m^{\alpha}(.,t)\|_{L^{\infty}(\mathbb{R}^3_\xi)}\leq\frac{1}{(2\pi)^3}\|\nabla E_m\|_{L^{\infty}(B)}\sum_{\ell=1}^{\infty}\lambda_{\ell m}^{\alpha}\quad\forall t\geq 0,$

(*ii*) $\frac{\partial}{\partial t}n_m^{\alpha}+div J_m^{\alpha}=0$ *holds in* $D'(\mathbb{R}^3_x\times(0,\infty))$.

Other important quantities are the m-th band energy density

$$\epsilon_m^\alpha(x,t) := Re\,(\sum_{\ell=1}^{\infty} \lambda_{\ell m}^\alpha \overline{\psi_{\ell m}^\alpha}(x,t)(H^\alpha \psi_{\ell m}^\alpha)(x,t)) \tag{3.14}$$

and the m-th band energy

$$\varepsilon_m^\alpha(t) := \sum_{\ell=1}^{\infty} \lambda_{\ell m}^\alpha \int_{\mathbb{R}^3} \overline{\psi_{\ell m}^\alpha}(x,t)(H^\alpha \psi_{\ell m}^\alpha)(x,t)\, dx \quad . \tag{3.15}$$

Application of Lemma 2.1 and Theorem 2.1 give the equivalent representation :

$$\varepsilon_m^\alpha(t) = \frac{1}{|B|} \sum_{\ell=1}^{\infty} \lambda_{\ell m}^\alpha \int_B E_m(k) |\tilde{\psi}_\ell^\alpha(k,m,t)|^2\, dk. \tag{3.16}$$

Since ε_m^α is a constant of the motion we obtain

$$\varepsilon_m^\alpha(t) \equiv \frac{1}{|B|} \sum_{\ell=1}^{\infty} \lambda_{\ell m}^\alpha \int_B E_m(k) |\tilde{\omega}_\ell^\alpha(k,m)|^2 dk \quad \forall t > 0 \tag{3.17}$$

The total energy is defined in the obvious way

$$\varepsilon^\alpha(t) := \sum_{m=1}^{\infty} \varepsilon_m^\alpha(t) \tag{3.18}$$

and we have

$$\varepsilon^\alpha(t) \equiv \frac{1}{|B|} \sum_{m=1}^{\infty} \sum_{\ell=1}^{\infty} \lambda_{\ell m}^\alpha \int_B E_m(k) |\tilde{\omega}_\ell^\alpha(k,m)|^2\, dk \quad \forall t > 0 \quad . \tag{3.19}$$

4 Band - Wignerfunctions

We set up the density matrix for the m-th band

$$z_m^\alpha(r,s,t) = \sum_{\ell=1}^{\infty} \lambda_{\ell m}^\alpha \overline{\psi}_{\ell m}^\alpha(r,t) \psi_{\ell m}^\alpha(s,t), \quad r,s \in \mathbb{R}^3,\, t > 0 \tag{4.1}$$

and define the m-th "Band-Wignerfunction" w_m^α by the coordinate transformation

$$r = x + \frac{\alpha}{2}\mu \quad , \; s = x - \frac{\alpha}{2}\mu \tag{4.2}$$

restricting μ to the lattice L and by successive 'discrete' Fouriertransformation :

$$w_m^\alpha(x,k,t) \;:=\; \sum_{\mu \in L} z_m^\alpha(x + \frac{\alpha}{2}\mu, x - \frac{\alpha}{2}\mu, t) e^{ik\cdot\mu}, \; x \in \mathbb{R}^3\,, k \in B. \tag{4.3}$$

A discussion of this definition of a "Wignerfunction" in the general context of phase-space formulations of quantum mechanics is given in [9].

The initial m-th Band-Wignerfunction $w^{\alpha}_{I,m}(x,k)$ is defined by replacing $\psi^{\alpha}_{\ell m}(.,t)$ by the initial wave functions $\omega^{\alpha}_{\ell m}(.)$ in (4.1) , i.e. $w^{\alpha}_{I,m} = w^{\alpha}_{m}(t=0)$.

For the following analysis we define the space of test-functions on $I\!R^3_x \times B$:

$$\mathcal{B} := \{\varphi(x,k) = \sum_{\mu\in L} \check{\varphi}(x,\mu)e^{i\mu\cdot k} | \check{\varphi} \in l^1(L; C_0(I\!R^3_x))\}$$

(in analogy to the analysis of the whole space case in [6]). It is an easy exercise to show that $\mathcal{B}$ is a separable Banachalgebra. We equip $\mathcal{B}$ with the norm

$$\|\varphi\| := |B| \sum_{\mu\in L} \|\check{\varphi}(.,\mu)\|_{L^\infty(I\!R^3_x)}$$

and we easily obtain

Proposition 4.1

$$\|w^{\alpha}_{m}(t)\|_{\mathcal{B}^*} \quad \leq \quad \sum_{l=1}^{\infty} \lambda^{\alpha}_{lm} \quad \leq \quad D \qquad \forall m \in I\!N, \quad \forall t \geq 0.$$

A somewhat better bound, i.e. an L^2 -estimate, on the Band-Wignerfunctions can be obtained by also assuming

(A4) $\qquad \frac{1}{\alpha^3}\sum_{m=1}^{\infty}\sum_{l=1}^{\infty}(\lambda^{\alpha}_{lm})^2 \quad \leq \quad D \quad ,\quad$ where D is independent of $\alpha \in (0,\alpha_0]$.

Then as in [7] for the whole space case we have

Lemma 4.1 *Let* (A1) - (A4) *hold. Then*

$$(4.4) \qquad \|w^{\alpha}_{m}(t)\|^2_{L^2(I\!R^3\times B)} \quad \leq \quad K(1+\|E_m\|^2_{L^\infty(B)})\frac{1}{\alpha^3}\sum_{\ell=1}^{\infty}(\lambda^{\alpha}_{lm})^2 \quad \leq \quad K$$

$$(4.5) \qquad \sum_{m=1}^{\infty} \frac{1}{1+\|E_m\|^2_{L^\infty(B)}} \|w^{\alpha}_{m}(t)\|^2_{L^2(I\!R^3\times B)} \quad \leq \quad K.$$

It is well known that the 'full space' Wignertransform of an arbitrary positive definite density matrix is not non-negative everywhere. However, an appropriate averaging of the Wignerfunction over sufficently large phase space regions smoothes out those oscillations which are due to the uncertainty principle and gives a non-negative function (see [2], [13], [12], [6], [7]). We shall now discuss the band-analogue of this so called Husimi-transformation (cp. also [3], [5] and references given in [5]).

Lemma 4.2 *Set*

$$(4.6) \qquad F^{\alpha}(k) := \sum_{\mu\in L} e^{-\frac{\alpha}{8}|\mu|^2 + ik\cdot\mu}, \quad k \in B$$

$$(4.7) \qquad G^{\alpha}(x) := \frac{1}{(2\pi\alpha)^{\frac{3}{2}}} exp(-\frac{|x|^2}{2\alpha}), \quad x \in I\!R^3$$

and define the m-th band Husimi - function by

$$(4.8) \qquad w^{\alpha}_{m,H} := (w^{\alpha}_{m} *_k F^{\alpha}) *_x G^{\alpha}.$$

Then $w^{\alpha}_{m,H} = w^{\alpha}_{m,H}(x,k,t)$ *is non-negative almost everywhere on* $I\!R^3 \times B \times (0,\infty)$.

The most important consequence of Lemma 4.2 lies in the fact that weak limits of Band-Wignerfunctions are non-negative :

Lemma 4.3 *Let $w_{I,m}, w_m$ be accumulation points of $w^\alpha_{I,m}$ and, resp., w^α_m in the $\mathcal{B}^* -$ weak$*$ - weak and, resp., $L^\infty((0,\infty);\mathcal{B}^*)-$ weak $*$ topologies. Then*

$$w_{I,m} \geq 0 \quad on\ \mathbb{R}^3 \times B, \quad w_m \geq 0 \quad on\ \mathbb{R}^3 \times B \times (0,\infty), \tag{4.9}$$

in the sense of measures.

We now derive an evolution equation for w^α_m :

Lemma 4.4 *The m-th Band-Wignerfunction w^α_m solves the initial value problem:*

$$\frac{\partial}{\partial t} w^\alpha_m(x,k,t) + i \sum_{\mu \in L} \mathcal{E}_m(\mu) e^{ik\cdot\mu} \frac{w^\alpha_m(x+\frac{\alpha}{2}\mu,k,t) - w^\alpha_m(x-\frac{\alpha}{2},k,t)}{\alpha} = 0 \tag{4.10}$$

$$for\ x \in \mathbb{R}^3,\ k \in B,\ t > 0$$

$$w^\alpha_m(x,k,t=0) = w^\alpha_{I,m}(x,k)\,, \quad x \in \mathbb{R}^3, k \in B \tag{4.11}$$

$$w^\alpha_m \text{ is periodic in } k. \tag{4.12}$$

The proof is a simple computation using the definitions (4.1), (4.3), the Schrödinger equation (3.1), (3.2) and the representation (2.18), (2.19) of the Hamilton operator acting on S^α_m.

It is the k -moments which give the Band-Wignerfunctions a physical meaning. From the definition (4.3) and from the Fourier inversion formula we obtain the zeroth order k - moment

$$\frac{1}{|B|} \int_B w^\alpha_m(x,k,t)\,dk = n^\alpha_m(x,t) \tag{4.13}$$

and, thus, for the total density

$$\sum_{m=1}^{\infty} \frac{1}{|B|} \int_B w^\alpha_m(x,k,t)\,dk = n^\alpha(x,t). \tag{4.14}$$

The representation of the m-th band current density J^α_m (defined by its Fourier-transform (3.12)) is not completely straightforward. We obtain

Lemma 4.5 *The representation*

$$J^\alpha_m(x,t) = \frac{i}{|B|} \sum_{\mu \in L} \mu \mathcal{E}_m(\mu) \frac{1}{2} \int_{-1}^{1} \int_B e^{ik\cdot\mu} w^\alpha_m(x + \frac{\alpha\mu s}{2}, k, t)\,dk\,ds \tag{4.15}$$

holds.

The m-th band energy density is related to the Band-Wignerfunction as follows (cf.(3.16))

$$\epsilon_m^\alpha(x,t) := Re\,(\sum_{\mu\in L} \mathcal{E}_m(\mu)\hat{w}_m^\alpha(x+\alpha\mu,\mu,t)\,) \tag{4.16}$$

The computation of the m-th band energy gives

$$\varepsilon_m^\alpha(t) = \frac{1}{|B|}\int_{\mathbb{R}_x^3}\int_B E_m(k)w_m^\alpha(x,\,k,\,t)\,dk\,dx \tag{4.17}$$

and for the total energy

$$\varepsilon^\alpha(t) = \sum_{m=1}^\infty \frac{1}{|B|}\int_{\mathbb{R}_x^3}\int_B E_m(k)w_m^\alpha(x,\,k,\,t)\,dk\,dx. \tag{4.18}$$

5 The Semiclassical Limit $\alpha \to 0$

The scaling which leads to the Hamilton operator (2.7) is based on the assumption that the characteristic periodicity length of the lattice potential is of the same order of magnitude as the appropriety scaled planck constant . Hence the usual classical limit is combined with a homogenization limit. In this section we show that this semi-classical limit $\alpha \to 0$ gives the free-streaming semiclassical Liouville-equations.
As before we employ the assumption (A1) (on the lattice potential V), (A2) (on the initial wave function) and (A3) (on the occupation probabilities of the initial states).

It is a well known property of the energy bands E_m that there exists a closed set $F_m \subseteq \overline{B}$ of measure zero, such that the periodic extension of E_m to $\mathbb{R}_k^3$ is an analytic function in $\mathbb{R}_k^3 - \bigcup_{\sigma\in L^*}(F_m+\sigma)$. The sets F_m are analytic manifolds of dimension ≤ 2 and the sets $\overline{B} - F_m$ have a finite (m -dependent) number of topological components. We refer to [14] for details. Using this we prove in [8] :

Theorem 5.1 *Let* (A1), (A2), (A3) *hold and let* $\alpha \in (0,\alpha_0]$ *be a sequence with limit zero. Then there exist subsequences of* $\{w_m^\alpha\}_{m\in\mathbb{N}}, \{w_{I,m}^\alpha\}_{m\in\mathbb{N}}$ *(denoted by the same symbol) such that*

$$w_{I,m}^\alpha \overset{\alpha\to 0}{\longrightarrow} w_{I,m} \geq 0 \quad in \quad \mathcal{B}^*\,weak\,*\,,\,\forall m \in \mathbb{N} \tag{5.1}$$

$$w_m^\alpha \overset{\alpha\to 0}{\longrightarrow} w_m \geq 0 \quad in \quad L^\infty((0,\infty);\mathcal{B}^*)\ weak\,*,\ \forall m \in \mathbb{N} \tag{5.2}$$

The limits $w_m = w_m(x,k,t)$ *are the unique solutions in* $D'_{per}(\mathbb{R}_x^3 \times (\overline{B}-F_m)\times[0,\infty))$ *of the IVP's*

$$\frac{\partial}{\partial t}w_m + \nabla_k E_m(k)\cdot\nabla_x w_m = 0\,, \tag{5.3}$$

$$w_m(t=0) = w_{I,m}\,, \tag{5.4}$$

$$w_m \text{ is } L^* - \text{periodic in } k \tag{5.5}$$

Also, the m-th band position densities satisfy (for the considered subsequence):

$$n_m^\alpha \overset{\alpha\to 0}{\longrightarrow} n_m := \frac{1}{|B|}\int_B w_m(.,k,.)\,dk \quad in\, L^\infty((0,\infty);C_0(\mathbb{R}_x^3)^*)\,weak\,*, \quad \forall m \in \mathbb{N} \tag{5.6}$$

Note that the unique solution of (5.3) - (5.5) reads

$$(5.7)\quad w_m(x,k,t) = w_{I,m}(x - \nabla_k E_m(k)t, k); \quad x \in \mathbb{R}^3_x\ , k \in \mathbb{R}^3_k - \bigcup_{\sigma \in L^*} (F_m + \sigma), \quad t > 0.$$

Clearly, if the whole sequence of initial data $w^\alpha_{I,m}$ converges to w^α_m, then the whole sequence of Wignerfunctions w^α_m converges to the measure w_m given by (5.7) , i.e. to the unique solution of the free streaming m-th band semiclassical Liouville equation.

However, we remark that taking out the zero- Lebesgue-measure-set F_m may have importance since the measures $w_{I,m}(x,.)$ may be supported in F_m. No assertion is made on the evolution of this part of the initial measure $w_{I,m}$.

A stronger result can be proven if the assumption (A4) on the occupation probabilities is added. Then the limiting Wigner-measure is an L^2-function and, thus, absolutely continous with respect to the Lebesgue measure. Taking out the set F_m then is of no importance anymore.

For the setting of L^2 -convergence for an arbitrary number of occupied energy bands we define the Hilbert space $\mathcal{H}$ of sequences $\{f_m\}_{m\in\mathbb{N}}$ with values in $L^2(\mathbb{R}^3_x \times B)$ equipped with the scalar product

$$(\{f_m\}, \{g_m\}_{m\in\mathbb{N}})_{\mathcal{H}} \quad := \quad \sum_{m=1}^{\infty} \frac{1}{1 + \|E_m\|^2_{L^\infty(B)}} (f_m, g_m)_{L^2(\mathbb{R}^3_x \times B)}$$

Theorem 5.2 *Let the assumptions* (A1) - (A4) *hold and let* $\alpha \in (0, \alpha_0]$ *be a sequence with limit 0. Then there exist subsequences of* $\{w^\alpha_{I,m}\}_{m\in\mathbb{N}}, \{w^\alpha_m\}_{m\in\mathbb{N}}$ *(denoted by the same symbol) such that*

$$(5.8)\qquad \{w^\alpha_{I,m}\}_{m\in\mathbb{N}} \stackrel{\alpha\to 0}{\longrightarrow} \{w_{I,m}\}_{m\in\mathbb{N}} \quad in \quad \mathcal{H}\, weakly$$

$$(5.9)\qquad \{w^\alpha_m\}_{m\in\mathbb{N}} \stackrel{\alpha\to 0}{\longrightarrow} \{w_m\}_{m\in\mathbb{N}} \quad in \quad L^\infty((0,\infty);\mathcal{H})\ weak\ *$$

The limits $w_{I,m}$ *and* w_I *are nonnegative a.e on* $\mathbb{R}^3_x \times B$ *and, resp. ,* $\mathbb{R}^3_x \times B \times (0,\infty)$*. The functions* w_m *are the unique solutions in* $D'_{per}(\mathbb{R}^3_x \times \overline{B} \times [0,\infty))$ *of the IVP* (5.3) - (5.5)*. Also, the m -th band position and current densities satisfy*

$$(5.10)\qquad n^\alpha_m \stackrel{\alpha\to 0}{\longrightarrow} n_m := \frac{1}{|B|}\int_B w_m(k)\, dk \quad in\ L^\infty((0,\infty); L^2(\mathbb{R}^3_x)) \quad weak\ *$$

$$(5.11)\qquad J^\alpha_m \stackrel{\alpha\to 0}{\longrightarrow} J_m := \frac{1}{|B|}\int_B \nabla_k E_m(k) w_m\, dk \quad in\ L^\infty((0,\infty); L^2(\mathbb{R}^3_x)) \quad weak\ *$$

for all $m \in \mathbb{N}$ *(and for the considered subsequence). Also the macroscopic conservation laws*

$$(5.12)\qquad \frac{\partial}{\partial t} n_m + div J_m = 0 \quad in \quad D'(\mathbb{R}^3_x \times (0,\infty)) \quad m \in \mathbb{N}$$

hold.

The energy density $\epsilon_m(x,t)$ *converges, too :*

$$(5.13)\qquad \epsilon^\alpha_m \stackrel{\alpha\to 0}{\longrightarrow} \epsilon_m = \frac{1}{|B|}\int_B E_m(k) w_m(x,k,t)\, dk \quad in\ L^\infty((0,\infty); L^2(\mathbb{R}^3_x)) \quad weak\ *$$

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