ON THE DERIVATION OF A QUANTUM BOLTZMAN EQUATION FROM THE PERIODIC VON-NEUMANN EQUATION

F. CASTELLA
C.N.R.S. et I.R.M.A.R.
Universit de Rennes 1 - Campus de Beaulieu
35042 - Rennes Cedex - France
e-mail: castella@maths.univ-rennes1.fr

Mod. Math. An. Num., Vol. 33, N. 2, p. 329-349 (1999)

Résumé. Nous présentons l'équation de Boltzmann des semi-conducteurs, qui est irréversible en temps, et indiquons qu'elle peut être dérivée heuristiquement par une limite en temps grand et potentiel perturbateur petit dans l'équation de Von-Neumann (réversible). Puis nous calculons rigoureusement cette asymptotique dans le cas de l'équation de Von-Neumann sur le Tore. Nous montrons que le modèle limite ainsi obtenu ne coïncide pas avec le modèle physique attendu. Il s'agit d'une équation de type Boltzmann, mais avec un effet de mémoire en temps, de sorte qu'elle apparaît réversible dans le temps. Nous commentons ce point, et proposons une description plus complète des propriétés de l'équation limite.

Abstract. We present the semi-conductor Boltzmann equation, which is time-reversible, and indicate that it can be formally derived by considering the large time and small perturbing potential limit in the Von-Neumann equation (time-reversible). We then rigorously compute the corresponding asymptotics in the case of the Von-Neumann equation on the Torus. We show that the limiting equation we obtain does not coincide with the physically realistic model. The former is indeed an equation of Boltzmann type, yet with memory in time, so that it appears to be time-reversible. We comment on this point, and further describe the properties of the limiting equation.

Key-words. Quantum Boltzmann equation, Von-Neumann equation, Fermi Golden Rule, time-irreversibility, memory effects, weak-coupling limit.

1 Introduction.

In the theory of semi-conductors, many transport phenomena can not be correctly described in the mere framework of the standard kinetic equations, like the Vlasov, Vlasov-Poisson, Vlasov-Maxwell, or Vlasov-Boltzmann equations. In many applications, one needs to write down transport equations which take into account purely quantum phenomena. Examples or considerations of this kind can be found for instance in the books [Markowich-Ringhoffer-Schmeiser90], [Zwanzig66], or in the papers [Lions-Paul93], [Nier95,96].

One famous example of a purely quantum transport equation is the Boltzmann equation of semi-conductors, derived in the late fifties by Kubo [Kubo58], as well as Kohn and Luttinger [Kohn-Luttinger57,58].

Formally, the Boltzmann equation of semi-conductors, also called quantum Boltzmann equation (See (1.2)-(1.5)), describes the limiting dynamics of an electron in a Hamiltonian of the type "Free Hamiltonian+ perturbation", for "large" values of time and "small" values of the perturbation. In this framework, the perturbation can represent a large class of phenomena, such as the interaction of an electron with some impurities in a box (or in a periodic cristal), the interaction of an electron with phonons, or other scattering events, and we refer to [Markowich-Schmeiser97], [Majorana-Marano97], [Majorana93], [Mustieles90], or [BenAbdallah-Degond96]. Also, the free Hamiltonian H_0 can take fairly general values, and the case $H_0 = -\Delta$ is not prescribed.

In the simplest case of an electron interacting with some impurities, described through a perturbing potential V, the formalism of Quantum Mechanics leads to write down the Von-Neumann equation on the density matrix ρ associated with the electron. It reads,

$$i\partial_t \rho = [H_0 + V_e + V, \rho] \ , \tag{1.1}$$

where H_0 is the free Hamiltonian, V_e denotes the electric potential, with associated electric field E_e, and $[\cdot, \cdot]$ denotes the commutator.

When dealing whith the large-time/small-perturbing-potential asymptotics in (1.1), the general method of [Kohn-Luttinger57,58], [Kubo58], leads to transform ρ into a function $f(t, k)$ which depends on the time $t \in \mathbb{R}$ and on the "impulse" $k \in \mathbb{R}^3$. The vector k corresponds to the different (degenerated) energy levels of the electron, and the function $f(t, k)$ represents the probability for finding the electron in the energy level k, at time t. Also, for physical reasons, the function f is expected to satisfy the semi-conductor Boltzmann equation, which is a linear transport equation of Boltzmann type, namely,

$$\partial_t f(t, k) + E_e.\nabla_k f = Q(f) \ , \tag{1.2}$$

and equation (1.1) should converge in some sense towards (1.2) in the abovementionned asymptotics. Here, the field E_e is assumed constant (in space) to simplify the presentation. The expression $Q(f)$ in (1.2) describes the transitions of the electron between the different energy levels due to the perturbation, and it has the standard form of a Boltzmann integral kernel,

$$Q(f) = \int_{k'} B(k, k')[f(t, k') - f(t, k)] \, dk' \ . \tag{1.3}$$

This integral involves a purely quantum cross-section B, and in some sense these transitions can be interpreted as "collisions" between the electron and the perturbing potential V. Also, the expression $E_e.\nabla_k f$ in (1.2) describes the transport of the particles due to the electric field E_e, as it is standard in kinetic equations.

To be more precise, starting from (1.1), the quantum cross-section B should satisfy (See, e.g., [Kohn-Luttinger57,58]),

$$B(k, k') = W(k, k') \ \delta(\varepsilon_k - \varepsilon_{k'}) \ , \tag{1.4}$$

with the Fermi-Golden-Rule,

$$W(k,k') = 2\pi \mid \int_{x,y} \psi_k(x)\, V(x-y)\, \psi^*_{k'}(y)\, dx\, dy \mid^2. \tag{1.5}$$

In (1.4)-(1.5), the δ denotes the Dirac measure, the ψ_k's and ε_k's are the eigenfunctions and eigen-energies of the free Hamiltonian H_0. Also, in (1.4), the Dirac measure indicates that the collision operator Q acts on the energy-shell $\varepsilon_k = \varepsilon_{k'}$. In other terms, only eigenstates ψ_k and $\psi_{k'}$ having the same energy (degenerated eigenstates) can interact *via* Q. Finally, one recognizes in (1.5) the celebrated Fermi Golden Rule (See [CohenTannoudji-Diu-Laloë73]), which gives the transition rate between two eigenstates ψ_k, $\psi_{k'}$ in terms of the perturbing potential V.

More complete references on the physical derivation of (1.2) by means of (1.1) can be found in [Castella97], and we would like to quote the references [Calecki97], as well as the books [Barker82], [Kreuzer83], [Luttinger68], [Prigogine62], [Zwanzig66].

Before coming to the description of our results, we emphasize here some important features of the limiting equation (1.2), in comparison to (1.1):

a) equation (1.2)-(1.5) is time-irreversible, which is a fact of paramount importance: this shows indeed how the microscopic dynamics (the Von-Neumann equation (1.1), which is time-reversible) generates an irreversible dynamics in the macroscopic scale. This kind of considerations is very general in statistical physics.

b) equation (1.2) is local in time. In other words, the collisional process as described in equation (1.3) is Markovian. This is obviously not the case in the original model (1.1) (see sections 3, 4 below for precise statements).

c) equation (1.2) decouples the influence of the electric field and the effect of the perturbation, where the latter generates "collisions", or transitions between the different energy levels.

Needless to say, the points a,b,c above give rise to important mathematical difficulties when one wants to derive the quantum Boltzmann equation (1.2) from the Von-Neumann equation (1.1).

Now, the purpose of the present paper is to study the *rigorous* large-time/small-perturbation asymptotics of the Von-Neumann equation *on the Torus*: in section 2, we start from the Von-Neumann equation in a three-dimensional periodic box $\mathbb{T}^3 = [-\pi;\pi]^3$, with a vanishing electric field ($E_e = 0$ in (1.1)), and perform the natural scaling $V \to \lambda V$, $t \to t/\lambda$, where λ is some (small) parameter, as it is suggested by the physics. We perform the limit $\lambda \to 0$ in section 3. We give in this way a rigorous derivation of an equation *similar* to (1.2). Nevertheless, our limit *does not* coincide with the physically realistic equation (1.2). Indeed, our scaling leads to a model which is non-local in time,

contrary to (1.2), namely,

$$\begin{cases} \partial_t f(t,k) = \int_0^t Q(s,f)ds \ , \\ \text{with} \ , \forall s \in \mathbb{R} \ , \ \ Q(s,f) = \int_{k'} B(s,k,k')[f(s,k') - f(s,k)] \ dk' \ . \end{cases} \tag{1.6}$$

(See Theorem 1 and 2). Also, our model (1.6) appears to be time-reversible, contrary to (1.2) (Theorem 6). On the more, the scaling presented here is the only non-trivial scaling when starting from the Von-Neumann equation on the Torus as we do here.

This paper shows therefore that the periodic Von-Neumann equation can by no means converge towards the physically realistic Quantum Boltzmann equation (1.2). This is due to the fact that the periodic case studied here is highly non-generic, and we mention in this respect that the author proved recently (see [Castella-Degond99] and [Castella01]) that the correct Boltzmann equation (1.2) can be recovered from the (damped) Von-Neumann equation on a periodic box $[-L;L]^3$ when we *first* perform the infinite-volume limit $L \to \infty$. This first limit cancels indeed effects due to the periodicity. Thus, the present paper together with [Castella01] (see also [Castella-Degond99]) show how the convergence towards the Quantum-Boltzmann Equation (1.2) is deeply linked, amongst others, to the infinite volume limit. From the physical point of view, we would like to mention that the possibility of getting a non-Markovian Boltzmann equation by means of the Von-Neumann equation (1.1) in the limit $V \to 0$, $t \to \infty$, as we do here, was already pointed out in [Zwanzig66] (See also [Jancel69]), so that the lack of Markovianity of the limiting equation (1.6) derived in the present paper is somewhat not surprising (See section 4).

Before ending this introduction, we would like to quote the works of F. Nier [Nier95 and 96], where an equation *similar* to (1.2) is rigorously derived, using very different arguments than those of the present article. Indeed, the articles [Nier95,96] heavily relie on arguments from the Semiclassical Analysis ($\hbar \to 0$) and from the Scattering Theory. More precisely, it is shown in [Nier96] that the Schrödinger equation,

$$i\hbar\partial_t\psi(t,x) = -\frac{\hbar^2}{2}\Delta\psi + V(x)\psi + \sum_{j\in\mathbb{Z}} U(\frac{x-x_j}{\hbar})\psi \ , \tag{1.7}$$

"converges" in the one dimensional case $x \in \mathbb{R}$ towards,

$$\partial_t f(t,x,v) + v\cdot\partial_x f - \partial_x V\cdot\partial_v f = \sum_j \delta(x-x_j)Q_j(f)(t,x_j,v) \ , \tag{1.8}$$

as $\hbar \to 0$, where the collision kernels Q_j, describing the collisions with each center x_j, act on the energy-shell $v^2 = (v')^2$, and are Markovian. Nevertheless, the model (1.8) appears to be time-reversible, contrary to (1.2).

Also, we would like to quote [Spohn77], [Ho-Landau-Wilkins93], [Erdös-Yau98], [Esposito-Pulvirenti-Teta98]. In all these references, the Schrödinger equation with a random potential is shown to converge towards a time-irreversible,

Markovian, Boltzmann equation, under different appropriate scalings. In particular, in [Spohn77], [Ho-Landau-Wilkins93], rigorous results are given concerning the celebrated "Van Hove limit" (See [VanHove55,57,62], [VanKampen81]), also called the "weak coupling limit". Here the potential is scaled by λ ($V \to \lambda V$), λ tends to zero, and t goes to infinity with $\lambda^2 t = \tau$ being fixed. However, in these models, the assumption of a stochastic potential allows to compute averaged quantities which behave quite differently from the deterministic quantities involved in [Nier95, 96], or in the present paper. We refer to section 4 for more considerations in this direction.

Finally, we mention [Markowich-Schmeiser97], [Majorana-Marano97], [Mustieles90], for the mathematical analysis of the semiconductor Boltzmann equations like (1.2), as well as for various related problems. More references to related topics can be found in [Castella97].

This paper is organized as follows: In sections 2 and 3, we rescale (1.1) using a small parameter $\lambda > 0$, and we perform the rigorous limiting procedure $\lambda \to 0$. We recover a quantum Boltzmann equation like (1.6) in the limit. Section 4 is therefore devoted to some physical and mathematical comments on the models (1.6) (the rigorous limit obtained in the present paper) and on (1.2) (the physically realistic model). We prove in section 5 several properties of our model (1.6), and we prove in particular that it satisfies the natural maximum principle: if the initial data is non-negative, then the corresponding solution remains non-negative for all times, and this important property makes (1.6) a "reasonable" kinetic model. We prove also in section 5 that the model (1.6) is time-reversible.

The main results of this paper are Theorems 1, 2, 5, 6.

2 A rescaled Von-Neumann equation.

We consider the following rescaled Von-Neumann equation on the Torus $\mathbb{T}^3 = \mathbb{R}^3/(2\pi\mathbb{Z})^3$,

$$\left\{ \begin{array}{l} i\lambda\partial_t\hat{\rho}_\lambda(t) = [\dfrac{-\Delta}{2} + \lambda V \ , \ \hat{\rho}^\lambda(t)] \ , \\ \hat{\rho}(t=0) = \exp(\dfrac{+\Delta_x}{2})/Tr(\exp(\dfrac{+\Delta_x}{2})) \ , \end{array} \right. \tag{2.1}$$

or, in other words:

$$\left\{ \begin{array}{l} i\lambda\partial_t\hat{\rho}_\lambda(t,x,y) = \dfrac{-\Delta_x + \Delta_y}{2}\hat{\rho}_\lambda(t,x,y) + \lambda(V(x) - V(y))\hat{\rho}_\lambda(t,x,y) \ , \\ \hat{\rho}(t=0,x,y) = \displaystyle\sum_{n\in\mathbb{Z}^3} e^{-n^2/2}e^{-in(x-y)} \times \left[(2\pi)^3 \sum_{n\in\mathbb{Z}^3} e^{-n^2/2}\right]^{-1} \ , \end{array} \right. \tag{2.2}$$

and $\hat{\rho}_\lambda(t,x,y) \in L^2(\mathbb{T}^3_x \times \mathbb{T}^3_y)$ is called the density matrix of the system. Here $\lambda > 0$ is a small parameter.

The initial data that we choose here corresponds to a system which is initially at the thermodynamical equilibrium for the free Hamiltonian $-\Delta_x/2$. This important assumption is suggested by the physics, and we refer to [Calecki97],

or also [VanKampen81]. We will consider in fact a generalization of this initial data below, and we refer to the equations (2.8)-(2.9).

On the other hand, the scaling (2.1)-(2.2) corresponds to the Von-Neuman equation for large times (change of variables $t \to t/\lambda$), and for a small perturbation (the potential is λV). Again, this agrees with the usual physical derivation of (1.2), as briefly explained in the introduction. Moreover, it is in fact the only non-trivial scaling for which the limit $\lambda \to 0$ is not obvious, as it is clear from the computations below (See the proof of Theorem 1).

Finally, we choose here to consider the Von-Neumann equation in a periodic box (i.e. we impose periodic boundary conditions in (2.1)) since it agrees with the Born-Von Karmann approximation [CohenTannoudji-Diu-Laloë73] in the limit where the size of the box is great.

We now write down equation (2.2) in the basis of the eigenfunctions e^{inx}. In other words, we now perform a Fourier transform on (2.2), and obtain therefore an equation on the coefficients,

$$\rho^\lambda(t,n,p) =< e^{inx}|\hat{\rho}^\lambda(t)|e^{ipx} > \quad (= \int_{x,y\in\mathbb{T}^3} \hat{\rho}^\lambda(t,x,y)\; e^{iny}e^{-ipx}\; dx\; dy\;) \; . \tag{2.3}$$

We shall need at this level the following fundamental assumptions for $\hat{V}(n) = \mathcal{F}V(n) = \int_{\mathbb{T}^3} V(x)e^{inx}dx$,

$$\hat{V}(n) \in l^1_n \quad (= l^1(\mathbb{Z}^3_n)) \; , \tag{2.4}$$

$$\hat{V}(-n) = \hat{V}(n)^* \;\; , \;\; \forall n \in \mathbb{Z}^3 \quad (\; V \text{ is real }). \tag{2.5}$$

Now equations (2.2)-(2.3) give, for $(n,p) \in \mathbb{Z}^6$,

$$\forall\; (n,p) \in \mathbb{Z}^6 \; , \;\; i\lambda\partial_t\rho^\lambda(t,n,p) = \frac{n^2-p^2}{2}\rho^\lambda(t,n,p) + \tag{2.6}$$
$$\lambda \sum_{k\in\mathbb{Z}^3} [\hat{V}(k)\rho^\lambda(t,n-k,p) - \hat{V}(-k)\rho^\lambda(t,n,p-k)\;] \; ,$$

The initial data satisfies on the other hand, according to (2.1),

$$\rho^\lambda(t=0,n,p) = Cte\; e^{-n^2}\; \chi(n=p) \; . \tag{2.7}$$

($\chi(n=p) = 1$ iff $n = p$).

Before describing the limiting procedure, we first consider slightly more general initial data than (2.7) above (initial thermodynamical equilibrium).

We shall consider indeed two sets of assumptions. The first set (See (2.8)-(2.9)) will be used in an essential way in order to perform the limit $\lambda \to 0$. The second set (See (2.11)) is more related to physical considerations, and it plays no particular role in the mere limiting procedure. The second set of assumptions is discussed in detail in section 5 below.

To be more precise, we *first* generalize the assumption of initial thermodynamical equilibrium (2.7), and we will consider an initial data satisfying the following conditions. The diagonal part satisfies, as $\lambda \to 0$,

$$\left\{ \begin{array}{l} \rho^\lambda(t=0,n,n) \in l^2(\mathbb{Z}^3_n) \; , \\ \rho^\lambda(t=0,n,n) \to \rho(t=0,n,n) \quad \text{in } l^2(\mathbb{Z}^3_n) \; , \end{array} \right. \tag{2.8}$$

and the non-diagonal part satisfies,

$$\rho^\lambda(t=0,n,p)\ \chi(n\neq p)\to 0 \quad \text{in}\ \ l^2_{n,p}=l^2(\mathbb{Z}^3_n\times\mathbb{Z}^3_p)\ . \tag{2.9}$$

In fact, one of the main ideas leading from the Von-Neumann equation (1.1) to the Quantum Boltzmann equation (1.2) in the physical literature (see, e.g., [Kohn-Luttinger57,58]), is the following: for a physical system which is initially at thermodynamical equilibrium, the density matrix is purely diagonal at time $t=0$. Therefore, one naturally considers (at least formally) the non-diagonal part of the density matrix as a higher order perturbation of the diagonal part, for *all* values of time. One recovers in this way a closed equation relating the diagonal elements $\rho(t,n,n)$ only, at least in the higher order approximation, and this leads formally to (1.2). The mathematical assumptions (2.8), (2.9) are therefore very natural.

In a *second* step, we now observe that the density matrix $\hat\rho^\lambda(t=0,x,y)$ (which we identify with its kernel) has to be a hermitian, positive, and trace class operator on the Hilbert space $L^2(\mathbb{T}^3_x)$. This property is implied by the usual formalism of Quantum Mechanics, and we refer for instance to [CohenTannoudji-Diu-Laloe73], [Lions-Paul93]. Again, this point will play no particular role in performing the limit $\lambda\to 0$, and we will discuss the consequences of this property in detail in section 5 below. Nevertheless, it is equivalent to,

$$\left\{\begin{array}{l}
\hat\rho^\lambda(t=0,x,y)\in L^2(\mathbb{T}^3_x\times\mathbb{T}^3_y)\ ,\\
\hat\rho^\lambda(t=0,x,y)=\hat\rho^\lambda(t=0,y,x)^* \quad \text{(hermiticity)}\ \ ,\\
\forall\phi(x)\in L^2(\mathbb{T}^3_x)\ ,\ \displaystyle\int_{x,y\in\mathbb{T}^3}\phi(y)\ \hat\rho^\lambda(t=0,x,y)\ \phi(x)^*\ \geq 0\\
\qquad\qquad\qquad\qquad\qquad\qquad \text{(positivity)}\ \ ,\\
\int_{x\in\mathbb{T}^3}\ \hat\rho^\lambda(t=0,x,x)<\infty \quad \text{(trace class)}\ \ ,
\end{array}\right. \tag{2.10}$$

and we refer to [Lions-Paul93] for a detailed discussion of this equivalence.

Now if we Fourier transform (2.10), we get the following informations on the coefficients $\rho^\lambda(t=0,n,p)$,

$$\left\{\begin{array}{l}
\rho^\lambda(t=0,n,p)\in l^2(\mathbb{Z}^3_n\times\mathbb{Z}^3_p)\ ,\\
\rho^\lambda(t=0,n,p)=\rho^\lambda(t=0,p,n)^* \quad \text{(hermiticity)}\ \ ,\\
\forall\phi(n)\in l^2(\mathbb{Z}^3_n)\ ,\ \displaystyle\sum_{n,p\in\mathbb{Z}^3}\phi(p)\ \rho^\lambda(t=0,n,p)\ \phi(n)^*\ \geq 0\\
\qquad\qquad\qquad\qquad\qquad\qquad \text{(positivity)}\ \ ,\\
\sum_{n\in\mathbb{Z}^3}\ \rho^\lambda(t=0,n,n)<\infty \quad \text{(trace class)}\ \ .
\end{array}\right. \tag{2.11}$$

We would like to quote that the assumption $\rho^\lambda(t=0,n,p)\in l^2_{n,p}$ appears already in (2.8)-(2.9), so that the first point in (2.11) could also be removed.

We emphasize also that we choose here to work in an l^2 framework, which is the natural physical setting when considering the Von-Neumann equation. But the limiting procedure as described below (Theorems 1 and 2) would work, without any modification, in an l^s framework for any $1\leq s\leq\infty$

3 Taking the limit $\lambda \to 0$.

In this section we study the convergence of the solution $\rho^\lambda(t,n,p)$ to the Von-Neumann equation (2.6) as $\lambda \to 0$, under the smallness assumption on the non-diagonal part of $\rho^\lambda(t,n,p)$ (2.8)-(2.9).

More precisely, we show here how one can recover a closed equation of Boltzmann type (3.11) (see also (3.13)) involving only the diagonal coefficients $f(t,n)$, the limit of $\rho^\lambda(t,n,n)$ as $\lambda \to 0$. We show also that the limit $\rho(t,n,p)$ of $\rho^\lambda(t,n,p)$ as $\lambda \to 0$ (for $n \neq p$) is supported on the set $n^2 = p^2$, which indicates that the transitions can only occur between two eigenstates having the *same* energy (degenerated eigenstates).

We now come to the details.

With the assumptions (2.4), (2.8), (2.9), it is straightforward that, for any $\lambda > 0$, there exists a unique global solution $\rho^\lambda(t,n,p)$ to (2.6),

$$\rho^\lambda(t,n,p) \in C^1_t(l^2_{n,p}) = C^1(\mathbb{R}_t; l^2(\mathbb{Z}^3_n \times \mathbb{Z}^3_p)) \; . \tag{3.1}$$

Now, following the usual derivation of (1.2) ([Calecki97]), we decompose the sequence $\rho^\lambda(t,n,p)$ into its diagonal and non-diagonal parts, at each time t, and we define,

$$f^\lambda(t,n,p) = \rho^\lambda(t,n,n)\; \chi(n=p) \quad \in C^1_t(l^2_{n,p}) \; , \tag{3.2}$$

$$g^\lambda(t,n,p) = \rho^\lambda(t,n,p)\; \chi(n\neq p) \; \in C^1_t(l^2_{n,p}) \; . \tag{3.3}$$

We emphasize the fact that we will identify in what follows the sequence $f^\lambda(t,n,p) \in l^2_{n,p}$ with a sequence $f^\lambda(t,n)$ depending on a single variable.

We readily observe that the sequence g^λ is complex valued, while the sequence f^λ is real valued (we will even prove in section 5 below that it takes only non-negative values). Indeed, since the initial data $\rho^\lambda(t=0,n,p)$ is hermitian (2.11) and because of the property $\hat{V}(-n) = \hat{V}(n)^*$ (Cf (2.5)), it is straightforward to check that,

$$\forall\; (t,n,p) \; , \quad \rho^\lambda(t,n,p) = \rho^\lambda(t,p,n)^* \; , \tag{3.4}$$

so that,

$$f^\lambda(t,n) \in \mathbb{R} \; , \tag{3.5}$$

$$g^\lambda(t,n,p) = g^\lambda(t,p,n)^* \; . \tag{3.6}$$

We are now ready to perform the limit $\lambda \to 0$ in (2.6). For that purpose, we introduce here two operators which play a central role in the sequel.

Definition and Lemma 1. *We define the following operators acting on the functions $u(t,n,p) \in C^0_t(l^2_{n,p})$:*

a) Let T be given by,

$$(Tu)(t,n,p) = -i \sum_{k\in\mathbb{Z}^3} \left[\hat{V}(k)\; u(t,n-k,p) - \hat{V}(-k)\; u(t,n,p-k) \; \right] . \tag{3.7}$$

Then T acts continuously on $C^0_t(l^2_{n,p})$, and it satisfies the estimate,

$$\|Tu\|_{l^2_{n,p}}(t) \leq 2\|\hat{V}\|_{l^1_n}\|u\|_{l^2_{n,p}}(t) \; . \tag{3.8}$$

b) Let K be given by,

$$(Ku)(t,n,p) = -i\int_0^t \chi[n^2=p^2] \sum_{k\in\mathbb{Z}^3-\{0\}} [\hat{V}(k)\; u(s,n-k,p) - \\ -\hat{V}(-k)\; u(s,n,p-k)]\; ds \; . \tag{3.9}$$

Then K acts continuously on $C^0_t(l^2_{n,p})$. More precisely, the following estimate holds true for all values of $l \in \mathbb{N}^*$,

$$\|K^l u\|_{l^2_{n,p}} \leq \frac{(2|t|\|\hat{V}\|_{l^1_n})^{l-1}}{(l-1)!} \sup_{s\in[-|t|,|t|]} \|u(s)\|_{l^2_{n,p}} \; . \tag{3.10}$$

In particular, the operator $(Id-K)^{-1} = \sum_{l\in\mathbb{N}} K^l$ is well defined and continuous on $C^0_t(l^2_{n,p})$ (here and in the sequel, we write Id = identity).

The operator T appears explicitely in the right-hand side of (2.6), and that is the reason why we introduce it here. Also, the operator K appears in a natural way when one wants to take the limit $\lambda \to 0$ in (2.6). This operator allows to describe the transitions of an electron between the different eigenstates (See Theorems 1 and 2).

Proof. The point a) is obvious. In order to prove b), we first write, thanks to (3.8) and from the definition of K,

$$\|Ku\|_{l^2_{n,p}} \leq 2|t|\|\hat{V}\|_{l^1_n} \sup_{s\in[-|t|,|t|]} \|u(s)\|_{l^2_{n,p}} \; .$$

Reiterating this estimate, we get (3.10). ■

With these notations and preliminary results, we now show the following,

Theorem 1. (Convergence as $\lambda \to 0$).
Let $\rho^\lambda(t=0,n,p)$ satisfy (2.8), (2.9), (2.11). Let $\rho^\lambda(t,n,p)$ be the unique solution to (2.6) with initial data $\rho^\lambda(t=0,n,p)$. Then, the diagonal part $f^\lambda(t,n)$ of ρ^λ (See (3.2)) converges in the space $C^1_t(l^2_n)$ towards $f(t,n) \in \mathbb{R}$, the solution to,

$$\begin{aligned} \partial_t f(t,n) &= [\sum_{l\geq 1} T\; K^l f](t,n,n) \\ &= [T(Id-K)^{-1}Kf](t,n,n) \; , \end{aligned} \tag{3.11}$$

with initial data $f(t=0,n) = \rho(t=0,n,n)$.

On the other hand, the non-diagonal part $g^\lambda(t,n,p)$ of $\rho^\lambda(t,n,p)$ (See (3.3)) converges in the space $C^0_t(l^2_{n,p})$ towards g given by,

$$\begin{aligned} g(t,n,p) &= [\sum_{l\geq 1} K^l f](t,n,p) \\ &= [(Id-K)^{-1}Kf](t,n,p)\ . \end{aligned} \tag{3.12}$$

The sequence $g(t,n,p)$ is supported on the set $n^2=p^2$, and it satisfies the hermiticity property, $g(t,n,p)=g(t,p,n)^*$.

Theorem 2. (Description of the limiting equation).
For each $l\in\mathbb{N}^*$, the term $[TK^lf](t,n,n)$ appearing in the series on the right-hand side of (3.11) is given by the following explicit formula,

$$\begin{aligned} [TK^lf](t,n,n) = &- i^{l+1}\int_0^t ds\ \frac{(t-s)^{l-1}}{(l-1)!}\times \\ &\times\sum(-1)^{\varepsilon_1+\cdots+\varepsilon_l}\ \hat V(k_1)\cdot\hat V(k_2)\ldots\hat V(k_l)\cdot\hat V^*(k_1+\cdots+k_l)\times \\ &\times\big[f(s,n+(1-\varepsilon_1)k_1+\cdots+(1-\varepsilon_l)k_l)-f(s,n-\varepsilon_1k_1-\cdots-\varepsilon_lk_l)\big]\ , \end{aligned} \tag{3.13}$$

where the sum $\sum\ldots$ is extended to all $(k_1,\ldots,k_l)\in(\mathbb{Z}^3)^l$, and $(\varepsilon_1,\ldots,\varepsilon_l)\in\{0,1\}^l$ such that,

$$\left\{\begin{array}{l} k_1\neq 0\ ,\ \ k_2\neq 0\ ,\ \ldots\ ,\ \ k_l\neq 0\ , \\ (n-\varepsilon_1k_1)^2=(n+(1-\varepsilon_1)k_1)^2\ , \\ (n-\varepsilon_1k_1-\varepsilon_2k_2)^2=(n+(1-\varepsilon_1)k_1+(1-\varepsilon_2)k_2)^2\ , \\ \ldots \\ (n-\varepsilon_1k_1-\cdots-\varepsilon_lk_l)^2=(n+(1-\varepsilon_1)k_1+\cdots+(1-\varepsilon_l)k_l)^2\ . \end{array}\right. \tag{3.14}$$

Remark. It is clear from Theorems 1 and 2 that the limiting equation (3.11) is a linear Boltzmann equation with memory in time.

We now come to the proof of Theorems 1 and 2.

Proof of Theorem 1. We start from (2.6), and we begin by writing the corresponding equations on g^λ and f^λ, according to the decomposition (3.2)-(3.3). We have,

$$\begin{aligned} \lambda\partial_t g^\lambda(t,n,p) &= -i\frac{n^2-p^2}{2}g^\lambda(t,n,p)+ \\ &\quad +\lambda(Tf^\lambda)(t,n,p)+\lambda(Tg^\lambda)(t,n,p)\ , \end{aligned} \tag{3.15}$$

$$\partial_t f^\lambda(t,n)=(Tg^\lambda)(t,n,n)\ , \tag{3.16}$$

with initial data $g^\lambda(t=0,n,p)=o(1)$ in $l^2_{n,p}$, and $f^\lambda(t=0,n)=\rho^\lambda(t=0,n,n)\to\rho(t=0,n,n)$ in $l^2_{n,p}$.

The useful point to notice is that the right-hand side of (3.16) involves the function g^λ *only*, thanks to the equality,

$$(Tf^\lambda)(t,n,n) = \hat{V}(n-p)\,[f(t,p) - f(t,n)]|_{n=p} = 0\ . \tag{3.17}$$

This is the key observation that allows to get a *closed* equation on the diagonal coefficients f^λ in the limit $\lambda \to 0$, as described in Theorem 1.

We now solve separately equations (3.15) et (3.16). At first, Duhamel's formula gives in (3.15),

$$g^\lambda(t,n,p) = \exp[-i\frac{n^2-p^2}{2\lambda}t]\ g^\lambda(t=0,n,p) + iK_\lambda[f^\lambda + g^\lambda]\ , \tag{3.18}$$

with the operator K_λ given by,

$$(K_\lambda u)(t,n,p) = -i\ \chi[n \neq p]\ \int_0^t \exp[-i\frac{n^2-p^2}{2\lambda}(t-s)]\ (Tu)(s,n,p)\ ds\ , \tag{3.19}$$

for $u \in C^0_t(l^2_{n,p})$. We will prove below that K_λ converges towards K (See (3.25)).

Now we rewrite equation (3.18) in the form,

$$g^\lambda = K_\lambda f^\lambda + K_\lambda g^\lambda + \exp(-i\frac{n^2-p^2}{2\lambda}t)g^\lambda(t=0,n,p)\ . \tag{3.20}$$

It is clear that the estimate (3.10) applies to K_λ as well as K (the $e^{i\cdots}$ factor in (3.19) has modulus one), so that we have the following estimate, uniform with respect to λ, for all $l \in \mathbb{N}^*$,

$$\|(K_\lambda)^l u\|_{l^2_{n,p}} \leq \frac{(2|t|\|\hat{V}\|_{l^1_n})^{l-1}}{(l-1)!} \sup_{s\in[-|t|,|t|]} \|u(s)\|_{l^2_{n,p}}\ . \tag{3.21}$$

In particular, the operators K_λ and $(Id - K_\lambda)^{-1}$ are well defined and uniformly continuous with respect to λ on $C^0_t(l^2_{n,p})$. With this observation, (3.20) gives, thanks to the assumption $g^\lambda(t=0) = o(1)$ in $l^2_{n,p}$,

$$g^\lambda = (Id - K_\lambda)^{-1}K_\lambda f^\lambda + o(1)\ \text{ in } C^0_t(l^2_{n,p})\ . \tag{3.22}$$

Therefore, g^λ is now an explicit function of f^λ, and inserting (3.22) into (3.16) gives the following equation on f^λ,

$$\partial_t f^\lambda(t,n) = T(Id - K_\lambda)^{-1}K_\lambda f^\lambda + o(1)\ \text{ in } C^0_t(l^2_{n,p})\ . \tag{3.23}$$

As desired, we now have a *closed* equation on f^λ (up to an $o(1)$).

On the other hand, the Gronwall Lemma in equations (3.22) and (3.23) readily gives the following uniform bounds,

$$\left\{ \begin{array}{l} g^\lambda\ \text{ is uniformly bounded in } C^0_t(l^2_{n,p})\ , \\ f^\lambda\ \text{ is uniformly bounded in } C^1_t(l^2_{n,p})\ . \end{array} \right. \tag{3.24}$$

We prove below the following estimate,

$$\|K_\lambda u - Ku\|_{l^2_{n,p}}(t) \ \ \leq \ \ C\ \lambda\ \|u(s,n,p)\|_{C^1_s(l^2_{n,p})}\ , \tag{3.25}$$

for all $u \in C^1_t(l^2_{n,p})$. This estimate shows that $K_\lambda u$ converges to Ku in $C^0_t(l^2_{n,p})$, uniformly with respect to the norm of u in $C^1_t(l^2_{n,p})$. Obviously, this estimate, together with (3.24), allows to pass to the limit in (3.22)-(3.23) and to get (3.11)-(3.12).

It remains to prove (3.25). We first observe, using (3.7),

$$(K_\lambda u)(t,n,p) = -i\ \chi[n \neq p] \int_0^t e^{-i\frac{n^2-p^2}{2\lambda}(t-s)}(Tu)(s,n,p)\ ds$$
$$= -i \int_0^t e^{-i\frac{n^2-p^2}{2\lambda}(t-s)} \sum_{k\neq 0} \left[\hat{V}(k)u(s,n-k,p) - \hat{V}(-k)u(s,n,p-k)\right] ds\ . \tag{3.26}$$

We let $v(t,n,p) = \sum_{k\neq 0} \dots$, and observe in an obvious way that $v \in C^1_t(l^2_{n,p})$, with $\|v\|_{C^1_t(l^2_{n,p})} \leq C\ \|u\|_{C^1_t(l^2_{n,p})}$. Therefore, we estimate using an integration by parts,

$$|K_\lambda u - Ku|(t,n,p) = \Big|\ \int_0^t e^{-i\frac{n^2-p^2}{2\lambda}(t-s)}\ v(s,n,p)\ ds - \int_0^t \chi(n^2=p^2)\ v(s,n,p)\ ds\ \Big|$$

$$\begin{aligned}
&= \Big|\ \int_0^t e^{-i\frac{n^2-p^2}{2\lambda}(t-s)}\ \chi(n^2\neq p^2)\ v(s,n,p)\ ds\ \Big| \\
&= \Big|\frac{2i\lambda}{n^2-p^2}\chi(n^2\neq p^2)\ \Big[\exp(-i\frac{n^2-p^2}{2\lambda}t)v(0,n,p) - v(t,n,p) - \\
&\qquad - \int_0^t\ e^{-i\frac{n^2-p^2}{2\lambda}(t-s)}\ \partial_s v(s,n,p)\ ds\Big]\ \Big| \\
&\leq\ C\ \lambda\ \|v\|_{C^1_t(l^2_{n,p})}\ , \\
&\qquad (\text{ because}(n^2-p^2)\chi[n^2\neq p^2] \geq 1)
\end{aligned}$$

from which (3.25) follows, and the proof of (3.11)-(3.12) is complete.

It remains to observe that the solution f to (3.11) is in fact real valued. A first possibility is given by the observation that f^λ itself is real-valued, and we conclude by taking the limit $\lambda \to 0$. One might worry that this first method does not indicate which simple algebraic properties of the operator K implie that f remains real-valued for all values of time. Therefore, we also mention that f^* satisfies the same equation (3.11) than f with the same initial data, which gives the result using the uniqueness of the solution. To observe this, one has to make a repeated use of the property $\hat{V}(-n) = \hat{V}(n)^*$, and of the corresponding symmetries for the operator K. This point of view has the advantage that it makes a precise use of all the symmetries of the problem, and in particular it explains the central role of the coefficient $-i$ in the definition of the operator K (Cf (3.9)). The fact that g is hermitian is obtained in the same manner. We do not give details on this point, and we refer to section 5 (See Theorem 5) for detailed calculations in this spirit. ■

Proof of Theorem 2. We have,

$$(Ku)(t,n,p) = -i\int_0^t \chi[n^2=p^2]\,[\sum_{k\neq 0}\hat V(k)\,u(s,n-k,p) - \\ -\hat V(-k)\,u(s,n,p-k)]\,ds\,.$$

In order to simplify the presentation, we introduce here the two operators A and B, given by the following formulae,

$$(Au)(t,n,p) = \int_0^t u(s,n,p)\,ds\,,$$
$$(Bu)(t,n,p) = -i\,\chi[n^2=p^2]\sum_{k\neq 0}[\hat V(k)\,u(t,n-k,p) - \hat V(-k)\,u(t,n,p-k)]\,.$$

It is clear from these definitions that the operator K admits the decomposition $K=AB=BA$ (A and B obviously commute).

Hence,

$$TK^l = A^lTB^l\,, \tag{3.27}$$

(T and A commute), so that the identity,

$$(A^lu)(t,n,p) = \int_0^t \frac{(t-s)^{l-1}}{(l-1)!}u(s,n,p)\,ds\,,$$

gives the factor $(t-s)^{l-1}/(l-1)!$ in Theorem 2. On the other hand, we easily get the following equality, using the commutation properties of T and B,

$$(TBu)(t,n,p) = -i\sum_{k\neq 0}[\chi[(n-k)^2=p^2]\,\hat V(k)\,(Tu)(t,n-k,p) - \\ -\chi[n^2=(p-k)^2]\,\hat V(-k)\,(Tu)(t,n,p-k)]\,. \tag{3.28}$$

We can therefore reiterate formula (3.28) in order to compute the explicit value of TB^lu in terms of Tu in (3.27). We obtain,

$$[TB^lu](t,n,p) = i^l\sum(-1)^{\varepsilon_1+\cdots+\varepsilon_l}\,\hat V(k_1)\cdot\hat V(k_2)\ldots\hat V(k_l)\times \\ \times(Tu)(s,n-\varepsilon_1k_1-\cdots-\varepsilon_lk_l,p+(1-\varepsilon_1)k_1+\cdots+(1-\varepsilon_l)k_l)\,, \tag{3.29}$$

where the sum $\sum\ldots$ is as in Theorem 2. Using now the obvious identity,

$$[Tf](t,n,p) = -i\,\hat V(n-p)\,[f(t,p)-f(t,n)]\,,$$

in (3.27) and (3.29), gives Theorem 2. ■

4 Some comments on the limiting equation.

Now it seems interesting to comment on the result obtained in the previous section. We have proved that the solution f^λ to (2.6) converges to f, where f solves (3.11). On the other hand, the physical derivation as briefly described

in the introduction leads to write down the following Boltzmann equation (see (1.2)-(1.5) - here, $E_e = 0$, $\psi_n(x) = e^{inx}$, $n \in \mathbb{Z}^3$),

$$\partial_t f(t,n) = 2\pi \sum_{k\in\mathbb{Z}^3} |\hat{V}(n-k)|^2 \, \chi[n^2 = k^2] \, [f(t,k) - f(t,n)] \, . \tag{4.1}$$

In order to compare the two models, we write down the explicit value of the first two terms in the series appearing on the right-hand side of (3.11):

$$\partial_t f(t,n) \quad = \quad [TKf](t,n) + [TK^2 f](t,n) + \dots \, .$$

It is indeed clear from Theorem 2 that this series involves at each order $l \in \mathbb{N}$ a collisional operator describing the transitions between the eigenstates $n - \varepsilon_1 k_1 - \cdots - \varepsilon_l k_l$ and $n + (1-\varepsilon_1)k_1 + \cdots + (1-\varepsilon_l)k_l$ of the electron. Moreover, these eigenstates should have the same energy, thanks to the equality $(n - \varepsilon_1 k_1 - \cdots - \varepsilon_l k_l)^2 = (n + (1-\varepsilon_1)k_1 + \cdots + (1-\varepsilon_l)k_l)^2$ (Cf Theorem 2). Therefore, we want to compare the sum of collisional operators in (3.11) with the single collisional operator appearing in the physically realistic equation (4.1).

The first collisional term (corresponding to $l = 1$) on the right-hand side of (3.11) is,

$$[TKf](t,n) = \int_0^t \sum_{k\neq 0} \chi[n^2 = (n-k)^2] \, |\hat{V}(k)|^2 \, [f(s,n-k) - f(s,n)] \, ds \, , \tag{4.2}$$

and the second term ($l = 2$) is,

$$[TK^2 f](t,n) = i \int_0^t (t-s) \sum_{k,\, k' \neq 0} [\, b_1 + b_2 + b_3 + b_4 \,](s,n,k,k') \, ds \, , \tag{4.3}$$

where b_1 describes the transition between the eigenstates n and $n - k - k'$,

$$\begin{aligned} b_1(s,n,k,k') = \chi[(n-k')^2 = n^2] \, \chi[(n-k-k')^2 = n^2] \, \hat{V}(k) \, \hat{V}(k') \times \\ \times \hat{V}(-k-k') \, [f(s,n) - f(s,n-k-k')] \, . \end{aligned}$$

The terms $b_2, \dots, b_4$ are of the same kind.

Therefore, in the collisional operators themselves (that is, if we forget about the integrals in time and concentrate on the sums in the k, n, ... , variables), we observe that the scaling that we present here allows to describe the transitions of the electrons between the different eigenstates, due to the perturbing potential V. Moreover, the first term $[TKf](t,n)$ appearing in (3.11) is exactly the right-hand side of the physical equation (4.1), up to the 2π factor. Therefore, if we concentrate on the higher order term (in V) of the collisional operator on the right-hand side of (3.11), the transitions are described according to the Fermi Golden Rule (1.5), up to the 2π factor.

Now the main drawback of equation (3.11) is clearly its non-local nature (in time). In other words, (3.11) describes a non-Markovian collisional process, contrary to what is expected. Moreover, it is proved in section 5 that the

memory terms are also precisely responsible for the time-reversibility of equation (3.11) (See Theorem 6) contrary to the time-irreversibility of the physical model (4.1).

Besides, it is proved in [Spohn77], [Ho-Landau-Wilkins93] (See also [Esposito-Pulvirenti-Teta98], [Erdös-Yau98]) that the Schrödinger equation with a random potential $V = \lambda V_0$, converges in the weak coupling limit $\lambda \to 0$, $t \to \infty$, $\lambda^2 t = \tau$ being fixed, towards a linear, Markovian, irreversible, Boltzmann equation like (4.1). Also, it is proved in [Castella01] that the "damped" Von-Neumann equation on the periodic box $[-L, L]^3$ converges equally towards a linear, Markovian, irreversible, Boltzmann equation like (4.1) in the infinite volume limit $L \to \infty$ and for a small "damping". (We refer to the articles quoted for precise statements). It is therefore natural to look at the connections between these previous results and the present model.

In fact, it is clear from the mathematical point of view that the weak coupling limit with a random potential has deep differences in structure from the present deterministic approach. One of the key ingredients in [Spohn77], [Ho-Landau-Wilkins93] (it is also very transparent in [Erdös-Yau98]) is a fine study of the order of growth or decay (in λ) of iterated kernels like K_λ above (see (3.19)), in cases where the variables n, p,..., become continuous. In these works, both the fact that the variables n, p,..., vary in the whole space $\mathbb{R}^3$, and the stochastic nature of the equations (which allows to consider *averages* over the possible events), lead to gain powers of the λ variable in many places. This phenomenon is of paramount importance, since it can not hold in the present deterministic, and discrete, case. In particular, we would like to emphasize that the proof of our Theorem 1 relies essentially on a simple application of the Riemann-Lebesgue Lemma (See (3.25)).

In the same vein, the convergence result established in [Castella01] heavily relies on two ingredients: due to a systematic use of oscillatory integrals, the fact that the variables n, p, ... , become continuous in the infinite volume limit is a key argument in the above mentionned paper. In other words, the infinite volume limit allows to cancel effects which are specific to the periodic case, like the non-Markovianity appearing in the limiting equation of the present paper. Also, in [Castella01], since the potential V is chosen deterministic, the time-irreversibility of the limiting Boltzmann equation appears as a consequence of the damping that the author introduces in the original Von-Neumann equation.

These differences are the reasons why we are led both to a different scaling ($t \to t/\lambda$ instead of $t \to t/\lambda^2$), and to a different (non-Markovian) limit in the present paper. All these considerations indicate that, in order to recover a Markovian, irreversible limit in a deterministic framework, one should (at least) avoid the highly non-generic case of the periodic Von-Neumann equation with given (deterministic) potential V (for example we could look at the case of a disordered ditribution of obstacles in the whole space $\mathbb{R}^3$). This last point clearly agrees, amongst others, with the Born-Von Karmann approximation, according to which periodic boundary conditions make sense in the limit of a "large" periodic box.

On the more, Zwanzig already pointed out in a similar context that one can

derive an equation of Boltzmann type still containing memory effects, and we refer to [Zwanzig66] (See also [Jancel69]) for a physical discussion of this point. Roughly speaking, the Markovianity of the limiting model appears in these references as a consequence of certain physical assumptions (the weak coulping limit *and* the Markov approximation for the heat bath), and it is a general feature that the Markovianity of the quantum Boltzmann equation always derives from additional assumptions in the physical literature. We refer in particular to the celebrated Random Phase Approximation [VanKampen81]. (See also [Caldeira-Leggett83], [Castella-Erdös-Frommlet-Markowich99] for considerations about the origin of Markovianity in the context of Fokker-Planck equations.)

Before ending this section, we would like to mention an analogous problem in classical mechanics: it is well-known that a random distribution of scatterers gives a linear transport equation in the Boltzmann-Grad limit, while it was proved in [Bourgain-Golse-Wennberg98] that a deterministic, periodic distribution does not yield such a transport equation in the same limit.

All these observations indicate that the lack of Markovianity of (3.11) in the quantum framework considered here, is somewhat not unexpected.

5 The limiting equation is reversible and preserves the positive cone.

In this section, we are interested in the following natural question: let the initial data $f(t=0,n)$ in (3.11) be non-negative, is it possible to prove that, for all $t \geq 0$, the function $f(t,n)$ remains non-negative ($f(t,n) \geq 0$)? In other words, can one show that a natural maximum principle holds for the Boltzmann equation (3.11) obtained in the previous section ?

We prove here that such a maximum principle holds indeed (Cf. Theorem 5 below). This point relies on a specific factorization Theorem (Cf Theorem 5) which allows to decompose at each time t the solution $f(t,n)$ to (3.11) as,

$$f(t,n) = \sum_{m \in \mathbb{N}} \mu_m |\phi_m(t,n)|^2 \, , \tag{5.1}$$

for some complex-valued functions $\phi_m(t,n) \in C^1_t(l^2_n)$ and some weights $\mu_m \geq 0$. The functions $\phi_m(t,n)$ are obtained by passing to the limit in a rescaled Schrödinger equation which is naturally associated to (2.6) (Cf Theorems 4 and 5 below). This factorization result implies that (3.11) is time reversible (Theorem 6).

In fact, before proving that the solution $f(t,n)$ to (3.11) remains non-negative, we will first prove that the coefficients $\rho^\lambda(t,n,n)$ themselves (where ρ^λ is the solution to (2.6)) remain non-negative (before we take the limit $\lambda \to 0$).

At this level, assumption (2.11) plays a crucial role. We recall that, according to (2.11), the initial data $\rho^\lambda(t=0)$ in (2.6) has to be hermitian, positive, and trace class, and this point has not been really exploited in the previous section.

Indeed, the Theorems we prove in this section all relie more or less on the following fundamental argument:

Let $\rho^\lambda(t=0,n,p) \in l^2_{n,p}$ be hermitian, positive, and trace class as in (2.11). We consider from now on $\rho^\lambda(t=0,n,p)$ as a compact, hermitian and trace class operator on l^2_n. This operator associates with a given function $\phi(n) \in l^2_n$ the function,

$$(\rho^\lambda(t=0)\cdot\phi)(n) := \sum_{p\in\mathbb{Z}^3} \rho^\lambda(t=0,n,p)\ \phi(p)\ . \tag{5.2}$$

The standard theory of compact operators allows then to factorize $\rho^\lambda(t=0)$ under the form,

$$\rho^\lambda(t=0,n,p) = \sum_{m\in\mathbb{N}} \mu^\lambda_m\ \psi^\lambda_m(t=0,n)\ \psi^\lambda_m(t=0,p)^*\ , \tag{5.3}$$

where the weights μ^λ_m $(m\in\mathbb{N})$ are the eigenvalues of the operator $\rho^\lambda(t=0)$ (defined by (5.2)), and the family $\psi^\lambda_m(t=0,n)$ $(m\in\mathbb{N})$ is an orthonormal basis of l^2_n, the $\psi^\lambda_m(t=0)$ being the eigenvectors of $\rho^\lambda(t=0)$.

Once $\rho^\lambda(t=0)$ is decomposed as in (5.3), it is clear from this formula that $\rho^\lambda(t=0)$ is hermitian. The fact that $\rho^\lambda(t=0)$ is positive and trace class translates into,

$$\begin{cases} \forall\ m\in\mathbb{N}\ ,\ \ \mu^\lambda_m \geq 0\ , \\ \sum_{m\in\mathbb{N}} \mu^\lambda_m < \infty\ . \end{cases} \tag{5.4}$$

We are now ready to give the Theorems of this section.

Theorem 3. *Let $\rho^\lambda(t=0,n,p) \in l^2_{n,p}$ be hermitian, positive, and trace class as in (2.11). We consider its natural factorization as in (5.3)-(5.4). Let $\rho^\lambda(t,n,p)$ be the solution to (2.6) with initial data $\rho^\lambda(t=0)$. Let also $\psi^\lambda_m(t,n) \in C^1_t(l^2_n)$ be the unique solution to the following rescaled Schrödinger equation,*

$$i\lambda\partial_t\psi^\lambda_m(t,n) = \frac{n^2}{2}\psi^\lambda_m(t,n) + \lambda\ \sum_{k\in\mathbb{Z}^3} \hat{V}(k)\ \psi^\lambda_m(t,n-k)\ , \tag{5.5}$$

with initial data $\psi^\lambda_m(t=0,n)$. Then, we have the following identity,

$$\forall\ t\in\mathbb{R}\ ,\ \ \rho^\lambda(t,n,p) = \sum_{m\in\mathbb{N}} \mu^\lambda_m\psi^\lambda_m(t,n)\ \psi^\lambda_m(t,p)^*\ . \tag{5.6}$$

In particular, the operator $\rho^\lambda(t,n,p)$ remains hermitian, positive and trace class for all values of time.

We also have the following Theorem describing the limit $\lambda\to 0$ in (5.5),

Theorem 4. *Let $\psi^\lambda(t=0,n) \in l^2_n$. Let $\psi^\lambda(t,n) \in C^1_t(l^2_n)$ be the unique solution to (5.5) with initial data $\psi^\lambda(t=0,n)$. Assume $\psi^\lambda(t=0,n) \to \psi(t=$*

$0, n)$ *in* l^2_n . *Let also* $\phi^\lambda(t,n) = \exp(i\frac{n^2}{2\lambda}t)\ \psi^\lambda(t,n)$. *Then, we have the following convergence,*

$$\phi^\lambda(t,n) \to \phi(t,n) \quad in \ \ C^0_t(l^2_n)\ ,$$

where $\phi(t,n)$ *satisfies,*

$$\left\{ \begin{array}{l} \partial_t \phi(t,n) = -i \sum_{k\in\mathbb{Z}^3} \hat{V}(k)\ \chi(n^2 = (n-k)^2)\ \phi(t,n-k)\ , \\ \phi(t=0,n) = \psi(t=0,n)\ . \end{array} \right. \tag{5.7}$$

In the spirit of the factorization formula (5.6) which holds for all $\lambda > 0$, we state the following factorization theorem in the case $\lambda = 0$. We would like to emphasize the fact that, while formula (5.6) above (case $\lambda > 0$) is standard, formula (5.8) (case $\lambda = 0$) below is quite surprising. In particular, a proof of this latter identity by means of direct computations is far from obvious, as it is clear from the proof given below.

Theorem 5. *With the notations and assumptions of Theorem 1, let* $\rho(t = 0, n, p) \in l^2_{n,p}$ *be given by*

$$\rho(t=0,n,p) = f(t=0,n)\ \chi(n=p)\ .$$

We define, as in (5.3)-(5.4), the natural factorization of $\rho(t=0)$,

$$\rho(t=0,n,p) = \sum_{m\in\mathbb{N}} \mu_m \psi_m(t=0,n)\ \psi_m(t=0,p)^*\ ,$$

where $\mu_m \geq 0$, $\mu_m \in l^1_m$, $\psi_m(t=0,n) \in l^2_n$, *and the functions* $\psi_m(t=0,n)$ *form an orthonormal basis of* l^2_n. *Let* $\phi_m(t,n) \in C^1_t(l^2_n)$ *be the unique solution to (5.7) with initial data* $\psi_m(t=0,n)$. *Then, we have the following factorization formula,*

$$\left\{ \begin{array}{l} f(t,n) = \sum_{m\in\mathbb{N}} \mu_m\ |\phi_m(t,n)|^2\ , \\ g(t,n,p) = \big[\sum_{m\in\mathbb{N}} \mu_m\ \phi_m(t,n)\ \phi_m(t,p)^*\big]\ \chi(n\neq p)\ . \end{array} \right. \tag{5.8}$$

In particular, we have,

$$\left\{ \begin{array}{l} f(t,n) \geq 0 \quad \textit{(maximum principle)}\ , \\ g(t,n,p) = g(t,p,n)^*\ . \end{array} \right. \tag{5.9}$$

Theorem 5 indicates that a natural density matrix $\rho(t)$ is associated with the solution $f(t,n)$ to (3.11), namely,

$$\rho(t,n,p) = \sum_{m\in\mathbb{N}} \mu_m \phi_m(t,n) \phi^*_m(t,p)\ , \tag{5.10}$$

and it is clear from Theorems 1 and 5 that the knowledge of the function f allows to reconstruct the full matrix ρ (ρ does not contain more information than f).

Using this, the theorem below states the time-reversibility of the equation (3.11),

Theorem 6. *With the notations and assumptions of Theorem 5, we define the density matrix $\rho(t,n,p)$ by (5.10). Then, for any non-linear function F, we have,*

$$Tr(F[\rho(t)]) = Tr(F[\rho(t=0)]) = \sum_{m\in\mathbb{N}} F(\mu_m) \ .$$

In particular, the entropy $S(t) = Tr[\rho(t)\ln\rho(t)]$ of the solution to the system (3.11)-(3.12), is constant with respect to time.

The rest of this section is devoted to the proof of these Theorems.

Proof of Theorem 3. The proof is standard, and it relies on the following simple observation: if $\psi^\lambda_m(t,n)$ satisfies the Schrödinger equation (5.5), then the function $\sum_{m\in\mathbb{N}} \mu^\lambda_m \ \psi^\lambda_m(t,n) \ \psi^\lambda_m(t,p)^*$ automatically satisfies the Von-Neumann equation (2.6), with the same initial data. We conclude by using uniqueness. ■

Proof of Theorem 4. The proof follows essentially the same arguments as the proof of Theorem 1 above (See section 3).

We observe indeed that the function $\phi^\lambda(t,n) = \exp(i\frac{n^2}{2\lambda}t)\ \psi^\lambda(t,n)$ belongs to $C^1_t(l^2_n)$, and it satisfies the following equation,

$$\partial_t\phi^\lambda(t,n) = -i\sum_{k\in\mathbb{Z}^3} \hat{V}(k)\ \exp(i\frac{n^2-(n-k)^2}{2\lambda}t)\phi^\lambda(t,n-k) \ . \tag{5.11}$$

Integrating (5.11) with respect to time gives therefore,

$$\phi^\lambda(t,n) = \psi^\lambda(t=0,n) - i\sum_{k\in\mathbb{Z}^3}\int_0^t \hat{V}(k)\ \exp(i\frac{n^2-(n-k)^2}{2\lambda}s)\phi^\lambda(s,n-k)\ ds \ ,$$

which implies the estimate,

$$\|\phi^\lambda\|_{l^2_n}(t) \leq \|\hat{V}\|_{l^1_n}\int_0^t \|\phi^\lambda\|_{l^2_n}(s)\ ds \ , \tag{5.12}$$

so that ϕ^λ is uniformly bounded in $C^1_t(l^2_n)$.

On the other hand, and as in (3.25), we easily prove the following estimate, which holds for all $u(t,n) \in C^1_t(l^2_n)$,

$$\|\sum_{k\in\mathbb{Z}^3}\int_0^t \hat{V}(k)\ [\exp(i\frac{n^2-(n-k)^2}{2\lambda}s) - \chi[n^2=(n-k)^2]]\phi^\lambda(s,n-k)\ ds\|_{l^2_n} =$$

$$\begin{aligned} &= \|\sum_{k\in\mathbb{Z}^3}\int_0^t e^{i\frac{n^2-(n-k)^2}{2\lambda}s}\ \chi(n^2\neq(n-k)^2)\ u(s,n-k)\ ds\|_{l^2_n} \\ &\leq C\ \lambda\ \|u\|_{C^1_t(l^2_n)} \ , \end{aligned} \tag{5.13}$$

thanks to an integration by parts. From this, we easily deduce Theorem 4. ■

Proof of Theorem 5. We can prove in fact Theorem 5 using two different methods.

The first method uses the limiting procedure $\lambda \to 0$. For that purpose, we observe the following identity, thanks to Theorem 3,

$$f^\lambda(t,n) = \sum_{m\in\mathbb{N}} \mu_m |\psi_m^\lambda(t,n)|^2 = \sum_{m\in\mathbb{N}} \mu_m |\phi_m^\lambda(t,n)|^2 \ , \tag{5.14}$$

where the weights μ_m, $\psi_m(t=0,n)$ are defined as in the statement of Theorem 5, $\psi_m^\lambda(t,n)$ satisfies the Schrödinger equation (5.5) (Cf Theorem 3), and $\phi_m^\lambda(t,n) = \exp(i\frac{n^2}{2\lambda}t)\ \psi_m^\lambda(t,n)$, as in Theorem 4. This identity is exactly formula (5.6) in Theorem 3.

Taking the limit on both sides of (5.14), and using the convergence results of Theorems 1 and 4, gives the result. The same method applies for the function g^λ.

The drawback of this first method is that it only uses the case $\lambda > 0$ to prove a result at the level $\lambda = 0$, and never the limiting equation (3.11). This is unsatisfactory for our purpose. This is the reason why we do not give the details.

Our second method makes the algebraic properties of the quantum Boltzmann equation (3.11) more transparent. We define, using the notations of Theorem 4,

$$\left\{ \begin{array}{l} \tilde{f}(t,n) = \sum_{m\in\mathbb{N}} \mu_m |\phi(t,n)|^2 \ , \\ \tilde{g}(t,n,p) = [\sum_{m\in\mathbb{N}} \mu_m \phi(t,n)\ \phi(t,p)^*]\chi(n\neq p) \ , \end{array} \right. \tag{5.15}$$

and we now aim at proving the identities $\tilde{f} = f$, $\tilde{g} = g$. This is achieved by observing that $\tilde{f}$, $\tilde{g}$ on the one hand, and f, g on the other hand, satisfy the same differential equations with the same initial data.

First, it is clear from the definitions that we have $\tilde{f}(t=0) = f(t=0)$, and $\tilde{g}(t=0) = g(t=0)$ $(= 0)$.

Our second step is therefore to find a simple differential system satisfied by $f(t)$, $g(t)$. For that purpose, we need do perform some computations on these functions. Indeed, using the equations satisfied by f and g (Theorem 1), and using also the definition of the operators T and K in Lemma 1, we readily obtain,

$$\left\{ \begin{array}{l} \partial_t f(t,n) = [\sum_{l\geq 1} TK^l f](t,n,n) \ , \\ g(t,n,p) = [\sum_{l\geq 1} K^l f](t,n,p) \ , \end{array} \right.$$

so that,

$$\left\{ \begin{array}{l} \partial_t f(t,n) = [Tg](t,n,n) \ , \\ g(t,n,p) = [Kf](t,n,p) + [Kg](t,n,p) \ . \end{array} \right. \tag{5.16}$$

On the other hand, it is clear from the definition of g and of the operator K (Cf Lemma 1 and Theorem 1) that the sequence $g(t,n,p)$ (for fixed values of

time) is entirely supported on the set $n^2 = p^2$, which implies that $g = \chi[n^2 = p^2]g$. We obtain in this way,

$$[Kg](t,n,p) = -i\chi[n^2=p^2]\int_{s=0}^{t} ds \sum_{k\neq 0} \hat{V}(k)\, g(s,n-k,p) - \hat{V}(-k)\, g(s,n,p-k)$$

$$\begin{aligned} &= -i\int_{s=0}^{t} \sum_{k\in\mathbb{Z}^3} [\hat{V}(k)\, \chi[n^2=(n-k)^2]\, g(s,n-k,p) - \\ &\qquad -\hat{V}(-k)\, \chi[p^2=(p-k)^2]\, g(s,n,p-k)]\, ds \\ &\quad (\text{ because the contribution when } k=0 \text{ vanishes,} \\ &\qquad \text{and thanks to the property on the support of } g\ ) \\ &:= [K^* g](t,n,p)\ , \end{aligned} \tag{5.17}$$

where formula (5.17) serves as the definition of the operator K^*.

We obtain also in the same way,

$[Tg](t,n,n) =$

$$\begin{aligned} &= -i \sum_{k\in\mathbb{Z}^3} \hat{V}(k)\, g(t,n-k,n) - \hat{V}(-k)\, g(t,n,n-k) \\ &= -i \sum_{k\in\mathbb{Z}^3} \chi[n^2=(n-k)^2][\hat{V}(k)\, g(t,n-k,n) - \hat{V}(-k)\, g(t,n,n-k)] \\ &:= [T^* g](t,n,n)\ , \end{aligned} \tag{5.18}$$

where formula (5.18) serves as the definition of the operator T^*.

Using (5.17) and (5.18), (5.16) gives therefore,

$$\left\{ \begin{array}{l} \partial_t f(t,n) = [T^* g](t,n,n)\ , \\ g(t,n,p) = [Kf](t,n,p) + [K^* g](t,n,p)\ , \end{array} \right. \tag{5.19}$$

which is the simple differential system for f and g.

We now establish that the functions $\tilde{f}$, $\tilde{g}$ satisfy the same system (5.19). We first write, thanks to (5.7),

$$\begin{aligned} \partial_t \tilde{f}(t,n) &= \partial_t \sum_{m\in\mathbb{N}} \mu_m |\phi(t,n)|^2 \\ &= \sum_{m\in\mathbb{N}} \mu_m [(\partial_t \phi_m)(t,n)\phi(t,n)^* + \phi(t,n)(\partial_t\phi_m)(t,n)^*] \\ &= -i \sum_{k\in\mathbb{Z}^3} \hat{V}(k)\, \chi(n^2=(n-k)^2)\, [\sum_{m\in\mathbb{N}} \mu_m \phi_m(n-k)\phi_m(n)^*] - \\ &\qquad -\hat{V}(-k)\, \chi(n^2=(n-k)^2)\, [\sum_{m\in\mathbb{N}} \mu_m \phi_m(n)\phi_m(n-k)^*] \\ &= -i \sum_{k\in\mathbb{Z}^3} [\hat{V}(k)\, \chi(n^2=(n-k)^2)\, \tilde{g}(n-k,n) - \\ &\qquad -\hat{V}(-k)\, \chi(n^2=(n-k)^2)\, \tilde{g}(n,n-k)]\ . \end{aligned}$$

This last equality uses the definition of $\tilde{g}$ and the fact that the contribution vanishes when $k=0$. Thus, by (5.18),

$$\partial_t \tilde{f}(t,n) = [T^* \tilde{g}](t,n,n)\ . \tag{5.20}$$

Then we have, using the same computations,

$$
\begin{aligned}
\partial_t \tilde{g}(t,n,p) &= -i \sum_{k\in\mathbb{Z}^3} \hat{V}(k)\ \chi[n^2=(n-k)^2]\ [\sum_{m\in\mathbb{N}} \mu_m \phi_m(n-k)\phi_m(p)^*] - \\
&\qquad -\hat{V}(-k)\ \chi[p^2=(p-k)^2]\ [\sum_{m\in\mathbb{N}} \mu_m \phi_m(n)\phi_m(p-k)^*] \\
&= -i\chi[n^2=p^2]\ \hat{V}(n-p)\ [\tilde{f}(t,p)-\tilde{f}(t,n)] - \\
&\qquad -i \sum_{k\in\mathbb{Z}^3} \hat{V}(k)\ \chi[n^2=(n-k)^2]\ \tilde{g}(t,n-k,p) - \\
&\qquad -\hat{V}(-k)\ \chi[p^2=(p-k)^2]\ \tilde{g}(t,n,p-k)\ .
\end{aligned}
\tag{5.21}
$$

The last identity is obtained by considering separately the cases $n-k=p$ and $p-k=n$ in the sum over the k variable.

Integrating (5.21) between 0 and t, using the initial data $\tilde{g}(t=0)=0$, and inserting the definition of K, K^*, we obtain,

$$
\tilde{g}(t,n,p) = [K\tilde{f}](t,n,p) + [K^*\tilde{g}](t,n,p)\ . \tag{5.22}
$$

This, together with (5.19) and (5.20), proves that $\tilde{f}=f$, and $\tilde{g}=g$, and the proof of Theorem 5 is complete. ■

Proof of Theorem 6. Using the notations of Theorem 5, let $\rho(t,n,p) = \sum_{m\in\mathbb{N}} \mu_m \phi_m(t,n)\phi_m^*(t,p)$. Also, given the initial value $\phi_m(t=0,n)\in l^2_n$, we define the functions $\psi^\lambda_m(t,n)\in C^0_t(l^2_n)$ and $\phi^\lambda_m(t,n)=\exp[in^2t/2\lambda]\psi^\lambda_m(t,n)\in C^0_t(l^2_n)$ according to the notations of Theorems 3 and 4.

With these notations, it is clear that the density matrix,

$$
\rho^\lambda(t,n,p) = \sum_{m\in\mathbb{N}} \mu_m \psi^\lambda_m(t,n)\psi^{\lambda\,*}_m(t,p) \tag{5.23}
$$

is the unique solution to the rescaled Von-Neumann equation (2.6) with initial data $\rho^\lambda(t=0,n,p)=\rho(t=0,n,p)$ $(=f(t=0,n)\ \chi[n=p])$. In particular, the entropy of the system before letting $\lambda\to 0$ is,

$$
S^\lambda(t) \;=\; Tr[\rho^\lambda(t)\ln\rho^\lambda(t)].
$$

Now writing,

$$
\rho^\lambda(t,n,p) = \sum_{m\in\mathbb{N}} \mu_m \exp[-i\frac{n^2-p^2}{2\lambda}t]\phi^\lambda_m(t,n)\phi^{\lambda\,*}_m(t,p)\ ,
$$

we obtain, in view of Theorems 3,4 and 5, that ρ^λ converges in $C^0_t(l^2_{n,p})$ towards the density matrix $\rho(t,n,p)$. Indeed, Theorem 4 ensures that the terms $\rho^\lambda(t,n,p)$ for which $n^2=p^2$ have the correct behaviour, and another use of the Riemann-Lebesgue Lemma ensures that the part of ρ^λ for which $n^2\neq p^2$ tends strongly to 0. In fact this convergence clearly holds in $C^0_t(\mathcal{L}^1_+(l^2_n))$, where $\mathcal{L}^1_+(l^2_n)$ denotes the subspace of $l^2_{n,p}$ consisting of Hilbert-Schmidt, positive, and trace

class operators acting on l^2_n. Therefore, the entropy of the system (3.11)-(3.12) as λ vanishes has to be defined as,

$$S(t) = Tr[\rho(t) \ln \rho(t)] \ . \tag{5.24}$$

It remains to compute this quantity.

It is clear from the definition of $\phi_m(t = 0, n)$ that we have the following orthogonality property initially,

$$\sum_{n \in \mathbb{Z}^3} \phi_m(t = 0, n) \phi^*_{m'}(t = 0, n) = \chi(m = m') \ . \tag{5.25}$$

Now, using equation (5.7), we easily see that the orthogonality in l^2_n of the ϕ_m's is preserved through time evolution, since we have, using $\hat{V}^*(k) = \hat{V}(-k)$,

$$\partial_t \sum_{n \in \mathbb{Z}^3} \phi_m(t, n) \phi^*_{m'}(t, n) = 0 \ .$$

Hence in the decomposition, $\rho(t, n, p) = \sum_{m \in \mathbb{N}} \mu_m \phi_m(t, n) \phi^*_m(t, p)$, the ϕ_m's are eigenvectors of the operator ρ (See 5.2) forming an orthonormal basis of l^2_n, and the μ_m's are the eigenvalues of ρ. Hence, for any non-linear function F, we have,

$$F(\rho) = \sum_{m \in \mathbb{N}} F(\mu_m) \phi_m(t, n) \phi^*_{m'}(t, n) \ ,$$

as an operator acting on l^2, and we get,

$$Tr(F(\rho(t))) = \sum_{m \in \mathbb{N}} F(\mu_m) = Tr(F(\rho(t = 0))) \ .$$

In particular, the time-reversibility is proved. ■

Acknowledgements. The author would like to thank Prof. M. Pulvirenti for his fruitful comments, leading to a substantial improvement of the present paper. Also, the author expresses his gratitude to Prof. D. Calecki for numerous discussions on the topic of "master equations".

Finally, the author would like to thank Prof. B. Perthame for pointing out to his attention the topic of the Quantum Boltzmann equation.

This work has been supported by the program on Charged Particle Kinetics at the Erwin Schrödinger Institute (Vienna-Austria), and by the TMR network "Asymptotic methods in kinetic theory" , number ERB FMBX CT97 0157.

Note added in Proof: We would like to mention the following fact. Equation (3.11) reads $\partial_t f = \sum_l TK^l f$. If we only keep track of the leading order term (in V) in this equation, we obtain:

$$\partial_t f \approx TKf \ ,$$

with TK given by (3.13) or more explicitely (4.2). Up to differentiating this last equation once in the time variable, we observe that $f(t)$ has an oscillating

behaviour in this simplified case. This is typical for the discrete-spectrum case, and this phenomenon is known under the name of Rabi oscillations. We refer to the book "Processus d'interaction entre photons et atomes" ("Savoirs actuels", Intereditions/Editions du CNRS, 1988) by C. Cohen-Tannoudji, J. Dupont-Roc, and G. Grynberg.

This observation partly explains the lack of reversibility of our limiting model (3.11) (with the full expansion on the r.h.s). Our Theorem 6 says indeed essentially that the lack of reversibility, which obviously holds for the simplified model above, also holds for the fully expanded model (3.11). On the other hand, the present paper also indicates that, unfortunately, there is no natural rescaling in time and potential (rescaling t like t/ε^α for some $\alpha > 0$ and V like εV) leading from the fully expanded model (3.11) to the truncated model above. Indeed, the only non-trivial rescaling corresponds to $\alpha = 1$, and it leaves (3.11) invariant. In some sense, this means that the 'right' cross-section in the present (naive) case is rather the cross-section given by the full expansion (3.11) than its leading order term given in (4.2).

REFERENCES

[Barker82] J.R. Barker, *Fundamental aspects of Quantum Transport*, in **Handbook on Semiconductors**, Vol. 2, T.S. Moss ed., North-Holland (1982).

[BenAbdallah-Degond96] N. Ben Abdallah, P. Degond, *On a hierarchy of macroscopic models for semi-conductors*, J. Math. Phys., Vol. 37, N. 7, p. 3306-3333 (1996).

[Bourgain-Golse-Wennberg98] J. Bourgain, F. Golse, B. Wennberg, *On the distribution of free path lengths for the periodic Lorentz gas*, Comm. Math. Phys., Vol. 190, p. 491-508 (1998).

[Caldeira-Leggett83] A.O. Caldeira, A.J. Leggett, *Path Integral Approach to Brownian Motion*, Physica A, Vol. 121, pp. 587-616 (1983).

[Calecki97] D. Calecki, Lecture, University Paris 6 (1997).

[Castella97] F. Castella, PhD Thesis, University Paris VI (1997).

[Castella01] F. Castella, *From the Von-Neumann equation to the Quantum Boltzmann equation in a deterministic framework*, to appear in J. Stat. Phys. (2001).

[Castella-Degond99] F. Castella, P. Degond, *Convergence de l'équation de Von-Neumann vers l'équation de Boltzmann Quantique dans un cadre déterministe*, C. R. Acad. Sci., t. 329, sér. I, pp. 231-236 (1999).

[Castella-Erdös-Frommlet-Markowich99] F. Castella, L. Erdös, F. Frommlet,

P.A. Markowich, *Fokker-Planck equations as scaling limits of reversible quantum systems*, J. Statist. Phys., Vol. 100, N. 3-4, pp. 543-601 (2000).

[CohenTannoudji-Diu-Laloë73] C. Cohen-Tannoudji, B. Diu, F. Laloë, **Mécanique Quantique**, I et II, Enseignement des Sciences, Vol. 16, Hermann (1973).

[Erdös-Yau98] L. Erdös, H.T. Yau, *Linear Boltzmann equation as scaling limit of quantum Lorentz gas*, Comm. Pure Appl. Math., Vol. 53, N. 6, pp. 667-735 (2000).

[Esposito-Pulvirenti-Teta98] R. Esposito, M. Pulvirenti, A. Teta, *The Boltzmann Equation for a one-dimensional Quantum Lorentz gas*, Preprint (1998).

[Ho-Landau-Wilkins93] T.G. Ho, L.J. Landau, A.J. Wilkins, *On the weak coupling limit for a Fermi gas in a random potential*, Rev. Math. Phys., Vol. 5, N. 2, p. 209-298 (1993).

[Jancel69] R. Jancel, **Foundations of Classical and Quantum Statistical Mechanics**, Pergamon, Braunschweig (1969).

[Kohn-Luttinger57] W. Kohn, J.M. Luttinger, Phys. Rev., Vol. 108, p. 590 (1957).

[Kohn-Luttinger58] W. Kohn, J.M. Luttinger, Phys. Rev., Vol. 109, p. 1892 (1958).

[Kreuzer83] H.J. Kreuzer, **Nonequilibrium thermodynamics and its statistical foundations**, Oxford Science Publications, Monographs on Physics and Chemistry of Materials (1983).

[Kubo58] R. Kubo, J. Phys. Soc. Jap., Vol. 12 (1958).

[Lions-Paul93] P.L.Lions, T.Paul, *Sur les mesures de Wigner*, Revista Matematica ibero americana, Vol.9, n.3, 553-618 (1993).

[Luttinger68] J.M. Luttinger, **Mathematical Methods in Solid State and Superfluid Theory**, Oliver and Boyd eds., p. 157 (1968).

[Majorana-Marano97] A. Majorana, S.A. Marano, *Space homogeneous solutions to the Cauchy problem for the semi-conductor Boltzmann equation*, SIAM J. Math. Anal., Vol. 28, N. 6, p. 1294-1308 (1997).

[Markowich-Ringhoffer-Schmeiser90] P.A. Markowich, C. Ringhoffer, C. Schmeiser, **Semiconductor equations**, Springer-Verlag, Wien (1990).

[Markowich-Schmeiser97] P.A. Markowich, C. Schmeiser, *The drift-diffusion*

limit for electron-phonon interaction in semiconductors, Math. Mod. Meth. Appl. Sci., Vol. 7, N. 5, 707-729 (1997).

[Mustieles90] F.J. Mustieles, Global existence of solutions for the non-linear Boltzmann equation of semiconductors physics, Rev. Mat. Iberoam., Vol. 6, p. 43-59 (1990).

[Nier95] F. Nier, *Asymptotic Analysis of a scaled Wigner equation and Quantum Scattering*, Transp. Theor. Stat. Phys., Vol. 24, N. 4 et 5, p. 591-629 (1995).

[Nier96] F. Nier, *A semi-classical picture of quantum scattering*, Ann. Sci. Ec. Norm. Sup., 4. Sér., t. 29, p. 149-183 (1996).

[Prigogine62] I. Prigogine, **Non-Equilibrium Statistical Mechanics**, Interscience, New-York (1962).

[Spohn77] H. Spohn, *Derivation of the transport equation for electrons moving through random impurities*, J. Stat. Phys., Vol. 17, N. 6, p. 385-412 (1997).

[Van Hove55] L. Van Hove, Physica, Vol. 21 p. 517 (1955).

[Van Hove57] L. Van Hove, Physica, Vol. 23 p. 441 (1957).

[Van Hove62] L. Van Hove, in **Fundamental Problems in Statistical Mechanics**, E.G.D. Cohen ed., p. 157 (1962).

[Van Kampen81] N.G. Van Kampen, **Stochastic processes in physics and chemistry**, Lecture Notes in Mathematics, Vol. 888, North-Holland (1981).

[Zwanzig66] R. Zwanzig, **Quantum Statistical Mechanics**, P.H.E. Meijer ed., Gordon and Breach, New-York (1966).