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Convergence of the Von-Neumann equation towards the Quantum Boltzmann equation in a deterministic framework.

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Abstract. *We prove the convergence of a periodic Von-Neumann equation with a damping term towards the Quantum Boltzmann equation, when the perturbing potential is deterministic.*

Convergence de l'équation de Von-Neumann vers l'équation de Boltzmann Quantique dans un cadre déterministe

Résumé. *Nous démontrons la convergence d'une équation de Von-Neumann périodique avec terme d'amortissement vers l'équation de Boltzmann Quantique, lorsque le potentiel perturbateur est déterministe.*

Version française abrégée -

Dans cette note, nous nous intéressons à la dynamique quantique d'un électron sur le Tore de période L, $(\mathbb{R}/2\pi L\mathbb{Z})^3$, sous la double influence d'un potentiel perturbateur V et d'un paramètre d'amortissement $\alpha > 0$. Nous considérons en effet l'équation de Von-Neumann mise à l'échelle,

$$i\frac{\alpha^2}{(2\pi L)^3}\partial_t\tilde{\rho}(t,x,y) = [-\Delta_x + \alpha\lambda_0 V(x), \tilde{\rho}] + \alpha F(\tilde{\rho})(t,x,y) \ . \tag{1}$$

Ici, $\tilde{\rho}$ est la matrice densité de l'électron, x et y parcourent le Tore, et λ_0 est un paramètre fixe, indépendant de L et α. Le terme αF ($\alpha > 0$) dans (1) décrit un amortissement exponentiel de la partie "non-diagonale" de $\tilde{\rho}$. Nous prouvons que, lorsque $L \to \infty$ puis $\alpha \to 0$, l'équation (1) converge vers une équation de Boltzmann linéaire homogène avec une section efficace satisfaisant la "règle d'or de Fermi", connue sous le nom d'équation de Boltzmann quantique (voir (15)). Plus précisément, la section efficace obtenue satisfait la règle d'or de Fermi à l'ordre le plus bas (en V), et nous en calculons le développement à tous les ordres (Théorème 4 ci-dessous). En particulier, nos résultats établissent la convergence d'une dynamique irréversible et non-Markovienne vers une dynamique irréversible et Markovienne. Nous renvoyons à la section suivante ainsi qu'à [CD] pour des résultats et des références plus complets.

English version -

In this note, we are interested in the quantum dynamics of an electron on the Torus $(\mathbb{R}/2\pi L\mathbb{Z})^3$ with period L, under both influences of a perturbing potential V and of a small damping parameter α. In the limit where the period L goes to infinity and the damping parameter α goes to zero, we show that the limiting dynamics is described by a linear homogeneous Boltzmann equation with a quantum cross-section given by the "Fermi Golden Rule", the so-called Quantum Boltzmann equation (See (15)). More precisely, we prove that the cross-section has a leading order term (in V) satisfying the Fermi Golden Rule, and we compute its full expansion to all orders (Theorem 4). Our results describe in particular the convergence of an irreversible and non-Markovian dynamics towards an irreversible and Markovian dynamics (Markovian limit). We mention also that the method presented here can be adapted in the case of an electron in a box of size L with Dirichlet or Neumann boundary conditions.

The convergence of the linear Von-Neumann equation $i\partial_t\tilde{\rho} = [-\Delta + V, \tilde{\rho}]$ towards the linear Quantum Boltzmann equation was first introduced in a formal way in [Pa], [KL], [Ku], [VH]. Later, the convergence of these models was proved, amongst others, in [Sp], [La], [HLW], [EPT], [EY] when the perturbing potential is stochastic, and the convergence holds in expectation. In particular, the above mentionned authors show in the celebrated "Van-Hove limit" $i\varepsilon^2\partial_t\tilde{\rho} = [-\Delta+\varepsilon V, \tilde{\rho}]$ $(\varepsilon \to 0)$ that some reversible and non-Markovian models converge towards irreversible and Markovian Boltzmann equations, and the limiting Boltzmann equation is not necessarily homogeneous.

We are interested here in a situation where the potential V is periodic and deterministic. This framework was already considered by one of the authors [Ca] when the size of the period is fixed and equal to one. In this case, it was proved in [Ca] that the Von-Neumann equation $i\varepsilon\partial_t\tilde{\rho} = [-\Delta + \varepsilon V, \tilde{\rho}]$ converges towards a linear, Boltzmann-like equation, which *does not* (and *can not*) coincide with the equation (15) predicted by the physics, since it remains reversible and non-Markovian. In this spirit, we consider here a Von-Neumann equation with large period L. Nevertheless, our model is from the very beginning time-irreversible, due to the small parameter α. It reads, in compact form (See (3)),

$$i\frac{\alpha^2}{(2\pi L)^3}\partial_t\tilde{\rho}(t,x,y) = [-\Delta_x + \alpha\lambda_0 V(x), \tilde{\rho}] + \alpha F(\tilde{\rho})(t,x,y) \ , \tag{2}$$

where $\tilde{\rho}$ is the density matrix of the electron, the variables x and y belong to the Torus $(\mathbb{R}/2\pi L\mathbb{Z})^3$, and the parameter λ_0 is fixed independently of α and L. The term αF describes an exponential damping of the "non-diagonal" part of $\tilde{\rho}$ (See, e.g., [Bo]). We are interested in the successive (and non-commuting) limits $L \to +\infty$, then $\alpha \to 0$ in (2). Note that time is rescaled like α^{-2} with respect to α, while the potential V is rescaled like α: this corresponds to a Van-Hove limit. Note also that time is rescaled like L^3 with respect to L, and this corresponds to a Boltzmann-Grad limit since the density of obstacles is like L^{-3} in our case.

Let $\rho(t,n,p)$ $(n, p \in \mathbb{Z}^3)$ be the discrete Fourier transform of $\tilde{\rho}$, which we split into its diagonal part $\rho_d(t,n) := \rho(t,n,n)$ and its non-diagonal part $\rho_{nd}(t,n,p) := \rho(t,n,p)\mathbf{1}(n \neq p)$. The system

(2) reads then more explicitely,

$$\text{(3)}\quad \frac{\alpha^2}{(2\pi L)^3}\partial_t \rho_{nd}(t,n,p) = +i\frac{n^2-p^2}{L^2}\rho_{nd}(t,n,p) + \frac{i\alpha\lambda_0}{(2\pi L)^3}\widehat{V}(\frac{p-n}{L})[\rho_d(t,p)-\rho_d(t,n)]$$
$$+\frac{i\alpha\lambda_0}{(2\pi L)^3}\sum_k \big[\widehat{V}(\frac{k-n}{L})\rho_{nd}(t,k,p) - \widehat{V}(\frac{p-k}{L})\rho_{nd}(t,n,k)\big] - \alpha\rho_{nd}(t,n,p)\ ,$$

$$\text{(4)}\quad \frac{\alpha^2}{(2\pi L)^3}\partial_t \rho_d(t,n) = +\frac{i\alpha\lambda_0}{(2\pi L)^3}\sum_k [\widehat{V}(\frac{k-n}{L})\rho_{nd}(t,k,n) - \widehat{V}(\frac{n-k}{L})\rho_{nd}(t,n,k)\ ]\ .$$

Here, $\widehat{V}(\mathbf{n})$ ($\mathbf{n} \in \mathbb{R}^3$) represents the usual Fourier transform of the profile of the perturbing potential which is supported in the elementary cell $[0; 2\pi L]^3$. We assume $\widehat{V}$ is very smooth (in the Schwartz class $\mathcal{S}$). Also, we restrict ourselves to purely diagonal initial data, with the following normalization in L,

$$\text{(5)}\qquad \rho_{nd}(t,n,p)\big|_{t=0} = 0\ ,\qquad \rho_d(t,n)\big|_{t=0} = (2\pi L)^{-3}\rho_d^0(\frac{n}{L})\ .$$

Here, $\rho_d^0(\mathbf{n})$ ($\mathbf{n} \in \mathbb{R}^3$) is a given function in $\mathcal{S}(\mathbb{R}^3_{\mathbf{n}})$. We adopt the following convention: bold letters ($\mathbf{n},\ \mathbf{k} \in \mathbb{R}^3$) represent continuous variables, whereas standard letters ($n,\ k \in \mathbb{Z}^3$) represent discrete variables. The symbol $\mathcal{R}$ represents the real part of a complex number. Our results are the following.

First point: A closed equation on ρ_d before any scaling limit. Following the explicit computations already made in [Ca] (See [Zw] for an abstract result in this direction), we show that for any given L and α, the diagonal part ρ_d satisfies the following non-Markovian Boltzmann equation,

Theorem 1 *Let $\rho_d(t,n)$, $\rho_{nd}(t,n,p)$ be the (unique) solutions to (3)-(4) with initial data as in (5). Then, for all $t \geq 0$, $\rho_d(t,n)$ satisfies,*

$$\text{(6)}\qquad \partial_t \rho_d(t,n) = \sum_{l=1}^{+\infty} \lambda_0^{l+1}\ \alpha^{l-1}\ (Q_l^{L,\alpha}\rho_d)(t,n)\ ,$$

and for each $l \in \mathbb{N}$, the linear collision operator $Q_l^{L,\alpha}$ is given by,

$$\text{(7)}\quad \begin{aligned} &(Q_l^{L,\alpha}\rho_d)(t,n) = (2\pi L)^{-3l}\ (-2\mathcal{R}) \sum_{\varepsilon_1,\cdots,\varepsilon_l}\ \sum_{k_1,\cdots,k_l} \int_{u_1,\cdots,u_l} (-1)^{\tilde{\varepsilon}_1+\cdots+\tilde{\varepsilon}_l} \times \\ &\times \exp\big(i\ \frac{(n+\varepsilon_1 k_1)^2-(n-\tilde{\varepsilon}_1 k_1)^2}{L^2}\ u_1 - \alpha u_1\big) \times\cdots\times \\ &\times \exp\big(i\ \frac{(n+\varepsilon_1 k_1+\cdots+\varepsilon_l k_l)^2-(n-\tilde{\varepsilon}_1 k_1-\cdots-\tilde{\varepsilon}_l k_l)^2}{L^2}\ u_l - \alpha u_l\big) \times \\ &\times \big[i\widehat{V}(\frac{k_1}{L})\big]\ \big[i\widehat{V}(\frac{k_2}{L})\big]\cdots\big[i\widehat{V}(\frac{k_l}{L})\big]\ \Big[i\widehat{V}^*(\frac{k_1+k_2+\cdots k_l}{L})\Big] \times \\ &\times \rho_d(t-\alpha^2\ (2\pi L)^{-3}(u_1+u_2+\cdots+u_l), n+\varepsilon_1 k_1+\varepsilon_2 k_2+\cdots+\varepsilon_l k_l)\ . \end{aligned}$$

In (7), the sums $\sum_{\varepsilon_1,\cdots,\varepsilon_l}$, $\sum_{k_1,\cdots,k_l}$ *carry over the variables,*

$$(8)\qquad \begin{array}{l} (\varepsilon_1\ ,\ \varepsilon_2\ ,\ \cdots\ ,\ \varepsilon_l\ )\ \in \{0,1\}^l\ , \qquad \textit{with:}\quad \forall\, j\ ,\ \tilde{\varepsilon}_j = (1-\varepsilon_j)\ , \\ (k_1\ ,\ k_2\ ,\ \cdots\ ,\ k_l)\ \in (\mathbb{Z}^3)^l\ ,\ \ k_1 \neq 0\ ,\ \ k_1+k_2 \neq 0\ ,\ \cdots\ ,\ \ k_1+k_2+\cdots k_l \neq 0\ , \end{array}$$

and the integrals $\displaystyle\int_{u_1,\cdots,u_l}$ *carry over the variables,*

$$(9)\qquad \left\{ \begin{array}{l} 0 \leq u_1 \leq (2\pi L)^3\alpha^{-2}t\ , \\ 0 \leq u_2 \leq (2\pi L)^3\alpha^{-2}t - u_1\ , \\ \cdots\ , \\ 0 \leq u_l \leq (2\pi L)^3\alpha^{-2}t - u_1 - \cdots - u_{l-1}\ . \end{array} \right.$$

In particular, when $l=1$, the first collision operator $Q_1^{L,\alpha}$ is,

$$(10)\quad \begin{aligned} (Q_1^{L,\alpha}\rho_d)(t,n) \;=\;& 2\,(2\pi L)^{-3}\int_{u=0}^{(2\pi L)^3\alpha^{-2}t}\sum_{k\neq 0}\cos\big(\frac{n^2-k^2}{L^2}u\big)\exp(-\alpha u)\ \times \\ & \times|\widehat{V}|^2\big(\frac{n-k}{L}\big)\ [\rho_d(t-\alpha^2(2\pi L)^{-3}u,k)-\rho_d(t-\alpha^2(2\pi L)^{-3}u,n)]\ du\ . \end{aligned}$$

Second point: loss of memory as $L\to+\infty$. In the limit $L\to\infty$, the non-Markovian Boltzmann equations (6)-(7) converges towards the following Markovian equation,

Theorem 2 *Let $\rho_d(t,n)$ be the solution to (6)-(7). We define the distribution $f^{L,\alpha}$, depending on L and α,*

$$(11)\qquad f^{L,\alpha}(t,\mathbf{n}) := \sum_{k\in\mathbb{Z}^3}\rho_d(t,k)\ \delta(\mathbf{n}-\frac{k}{L})\ .$$

Assume also that λ_0 is small enough, independently of L and α. Then, as $L\to\infty$, the distribution $f^{L,\alpha}(t,\mathbf{n})$ converges in $C^\infty(\mathbb{R}_t,\mathcal{S}'_{\mathbf{n}}-w*)$ towards $f^\alpha(t,\mathbf{n})$, the solution to,

$$(12)\qquad \partial_t f^\alpha(t,\mathbf{n}) = \sum_{l=1}^{+\infty}\lambda_0^{l+1}\alpha^{l-1}\ (Q_l^\alpha f^\alpha)(t,\mathbf{n})\ ,\qquad f^\alpha(t=0,\mathbf{n}) = (2\pi)^{-3}\rho_d^0(\mathbf{n})\ ,$$

and the collision operators Q_l^α are given by,

$$(13)\qquad \begin{array}{l} (Q_l^\alpha f^\alpha)(t,\mathbf{n}) = (2\pi)^{-3l}(-2\mathcal{R})\displaystyle\sum_{\varepsilon_1,\cdots,\varepsilon_l}\int_{\mathbf{k}_1,\cdots,\mathbf{k}_l}\int_{u_1=0}^{+\infty}\int_{u_2=0}^{+\infty}\cdots\int_{u_l=0}^{+\infty}(-1)^{\tilde{\varepsilon}_1+\cdots+\tilde{\varepsilon}_l}\times \\ \quad\times\exp\big(i[(\mathbf{n}+\varepsilon_1\mathbf{k}_1)^2-(\mathbf{n}-\tilde{\varepsilon}_1\mathbf{k}_1)^2]u_1-\alpha u_1\big)\times\cdots\times \\ \quad\times\exp\big(i[(\mathbf{n}+\varepsilon_1\mathbf{k}_1+\cdots+\varepsilon_l\mathbf{k}_l)^2-(\mathbf{n}-\tilde{\varepsilon}_1\mathbf{k}_1-\cdots\tilde{\varepsilon}_l\mathbf{k}_l)^2]u_l-\alpha u_l\big)\times \\ \quad\times[i\widehat{V}(\mathbf{k}_1)]\cdots[i\widehat{V}(\mathbf{k}_l)]\times[i\widehat{V}^*(\mathbf{k}_1+\cdots+\mathbf{k}_l)]\times f^\alpha(t,\mathbf{n}+\varepsilon_1\mathbf{k}_1+\cdots+\varepsilon_l\mathbf{k}_l)\ . \end{array}$$

Here, the variables $\varepsilon_1, \cdots, \varepsilon_l$ *are as in (8), and the variables* $\mathbf{k}_1, \cdots, \mathbf{k}_l$ *carry over the full space* $\mathbb{R}^3$*. Also, the first collision operator* Q_1^α *in (13) has the more explicit value,*

(14)

$$(Q_1^\alpha f^\alpha)(t,\mathbf{n}) = 2\lambda_0^2 \int_{\mathbf{k}\in\mathbb{R}^3} \int_{u=0}^{+\infty} e^{-\alpha u} \cos\left([\mathbf{n}^2 - \mathbf{k}^2]u\right) |\widehat{V}(\mathbf{n}-\mathbf{k})|^2 \left[f^\alpha(t,\mathbf{k}) - f^\alpha(t,\mathbf{n})\right] \frac{d\mathbf{k}}{(2\pi)^3} .$$

Third point: the limit $\alpha \to 0$**.** As $\alpha \to 0$, we recover the convergence towards the desired Quantum Boltzmann equation, as described in the following two theorems,

Theorem 3 *(Limit as* $\alpha \to 0$*).*
Let $f^\alpha(t,\mathbf{n}) \in C^\infty(\mathbb{R}_t, \mathcal{S}_\mathbf{n})$ *be the solution to (12)-(13). Then, as* α *tends to* 0*,* $f^\alpha(t,\mathbf{n})$ *converges in* $C^\infty(\mathbb{R}_t, \mathcal{S}'_\mathbf{n} - w*)$ *towards* g*, the solution to the Quantum Boltzmann equation, with a quantum cross section satisfying the Fermi Golden Rule,*

$$\left\{ \begin{array}{l} g(t=0,\mathbf{n}) = (2\pi)^{-3} \rho_d^0(n) , \\ \partial_t g(t,\mathbf{n}) = 2\pi\lambda_0^2 \displaystyle\int_\mathbf{k} \delta(\mathbf{n}^2 - \mathbf{k}^2)\, |\widehat{V}(\mathbf{n}-\mathbf{k})|^2 \left[g(t,\mathbf{k}) - g(t,\mathbf{n})\right] \frac{d\mathbf{k}}{(2\pi)^3} . \end{array} \right. \tag{15}$$

Theorem 4 *(Precise asymptotics as* $\alpha \to 0$*).*
Under the assumptions of Theorem 3, let $g^\alpha(t,\mathbf{n})$ *be the solution to the system (17)-(18) below. Then,* f^α *is asymptotic to* g^α *as* $\alpha \to 0$ *in the following sense: for all* α *and* λ_0 *,* f^α *and* g^α *are analytic in* λ_0*, with values in* $C_t^\infty(\mathcal{S}'_\mathbf{n} - w*)$*,*

$$f^\alpha(t,\mathbf{n}) = \sum_{j=0}^{+\infty} \lambda_0^{j+2} \alpha^j f_j^\alpha(t,\mathbf{n}) , \qquad g^\alpha(t,\mathbf{n}) = \sum_{j=0}^{+\infty} \lambda_0^{j+2} \alpha^j g_j(t,\mathbf{n}) , \tag{16}$$

and we have the following term-by-term asymptotics: $\qquad \forall j ,\quad f_j^\alpha(t,\mathbf{n}) \to_{\alpha\to 0} g_j(t,\mathbf{n})$.
Here, the function g^α *satifies,*

$$\partial_t g^\alpha(t,\mathbf{n}) = \sum_{l=1}^{+\infty} \lambda_0^{l+1}\, \alpha^{l-1} (Q_l g^\alpha)(t,\mathbf{n}) , \quad g^\alpha(t=0,n) = (2\pi)^{-3} \rho_d^0(n) , \tag{17}$$

where the collision operators Q_l *are given by,*

$$\begin{array}{l} (Q_l g^\alpha)(t,\mathbf{n}) = (2\pi)^{-3l}\, (-2\mathcal{R}) \displaystyle\sum_{\varepsilon_1,\cdots,\varepsilon_l} \int_{\mathbf{k}_1,\cdots,\mathbf{k}_l} \int_{u_1=0}^{+\infty} \cdots \int_{u_l=0}^{+\infty} (-1)^{\tilde{\varepsilon}_1+\cdots+\tilde{\varepsilon}_l} \times \\ \times \exp\left(i[(\mathbf{n}+\varepsilon_1\mathbf{k}_1)^2 - (\mathbf{n}-\tilde{\varepsilon}_1\mathbf{k}_1)^2]u_1\right) \times \cdots \times \\ \times \exp\left(i[(\mathbf{n}+\varepsilon_1\mathbf{k}_1+\cdots+\varepsilon_l\mathbf{k}_l)^2 - (n-\tilde{\varepsilon}_1\mathbf{k}_1 - \cdots \tilde{\varepsilon}_l\mathbf{k}_l)^2]u_l\right) \times \\ \times [i\widehat{V}(\mathbf{k}_1)] \cdots [i\widehat{V}(\mathbf{k}_l)] \times [i\widehat{V}^*(\mathbf{k}_1+\cdots+\mathbf{k}_l)] \times g^\alpha(t,\mathbf{n}+\varepsilon_1\mathbf{k}_1+\cdots+\varepsilon_l\mathbf{k}_l) . \end{array} \tag{18}$$

Moreover, the variables $\varepsilon_1, \cdots, \varepsilon_l$*, and* $\mathbf{k}_1, \cdots, \mathbf{k}_l$ *are as in Theorem 2. Obviously, the first collision operator in (18) is given through,*

$$(Q_1 g^\alpha)(t,\mathbf{n}) = 2\pi\lambda_0^2 \int_\mathbf{k} \delta(\mathbf{n}^2 - \mathbf{k}^2)\, |\widehat{V}(\mathbf{n}-\mathbf{k})|^2 \left[g^\alpha(t,\mathbf{k}) - g^\alpha(t,\mathbf{n})\right] \frac{d\mathbf{k}}{(2\pi)^3} . \tag{19}$$

Fourth point. The key-lemma of our work, which allows in particular to give a rigorous meaning to the oscillating integrals involved in (18), reads as follows,

Lemma 1 *(Oscillating integrals with quadratic phases).*
Let $\psi(\mathbf{n}, \mathbf{k}_1, \mathbf{k}_2, \cdots, \mathbf{k}_l) \in \mathcal{S}(\mathbb{R}^{3(l+1)})$. Then, for any choice of the parameters $\varepsilon_1, \cdots, \varepsilon_l$ as in Theorem 2, the following oscillating integrals are well defined,

$$\begin{aligned} I_l(\psi) \quad := \quad & \int_{u_1=0}^{+\infty} \cdots \int_{u_l=0}^{+\infty} \int_{(\mathbf{n},\mathbf{k}_1,\cdots,\mathbf{k}_l)\in\mathbb{R}^{3(l+1)}} \exp\left(i \left[(\mathbf{n}+\varepsilon_1\mathbf{k}_1)^2 - (\mathbf{n}-\tilde{\varepsilon}_1\mathbf{k}_1)^2\right] u_1\right) \times \\ & \times \cdots \times \exp\left(i \left[(\mathbf{n}+\varepsilon_1\mathbf{k}_1+\cdots+\varepsilon_l\mathbf{k}_l)^2 - (\mathbf{n}-\tilde{\varepsilon}_1\mathbf{k}_1-\cdots-\tilde{\varepsilon}_l\mathbf{k}_l)^2\right] u_l\right) \times \\ & \times \psi(\mathbf{n},\mathbf{k}_1,\cdots,\mathbf{k}_l)\, d\mathbf{n}\, d\mathbf{k}_1 \cdots d\mathbf{k}_l\, du_1 \cdots du_l \,. \end{aligned}$$

These integrals converge absolutely in the variables $u_1, \cdots, u_l$, and we have the bound,

$$|I_l(\psi)| \leq C_0^l \|\psi\|_{\mathcal{S}} \,,$$

for some universal constant C_0, $\|.\|_{\mathcal{S}}$ being the usual distance in $\mathcal{S}$.

The interested reader can find more references, a detailed discussion of the model, as well as the proofs in [CD].

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