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From the Von-Neumann Equation to the Quantum Boltzmann Equation in a Deterministic Framework

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In this paper, we investigate the rigorous convergence of the Density Matrix Equation (or Quantum Liouville Equation) towards the Quantum Boltzmann Equation (or Pauli Master Equation). We start from the Density Matrix Equation posed on a cubic box of size L with periodic boundary conditions, describing the quantum motion of a particle in the box subject to an external potential V. The physics motivates the introduction of a damping term acting on the off-diagonal part of the density matrix, with a characteristic damping time α^{-1}. Then, the convergence can be proved by letting *successively* L tend to infinity and α to zero. The proof relies heavily on a lemma which allows to control some oscillatory integrals posed in large dimensional spaces. The present paper improves a previous announcement [CD].

KEY WORDS: Density matrix; Liouville equation; Pauli Master Equation; time-dependent scattering theory; Fermi's Golden Rule; oscillatory integrals in large dimensions.

1. INTRODUCTION

1.1. Introduction

In this paper we are interested in the quantum dynamics of an electron in a given *periodic* distribution of obstacles in d dimensions of space ($d \geqslant 3$, we will actually restrict ourselves with the case $d = 3$). More exactly the

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electron is assumed to evolve on a Torus, and the present dynamics is naturally described by a periodic Von-Neumann equation. In our model, the size of the period is measured by the large scaling parameter L, and each elementary cell contains one obstacle occupying a volume of the order $O(1)$. We consider the asymptotic dynamics as $L \to \infty$. In order to obtain a non-trivial limiting dynamics, one has to rescale time as well, and to look at the evolution of the electron on long time scales of the order T, with $T \to \infty$, unless the electron essentially performs a "free flight" in the limit $L \to \infty$. The present paper is concerned with the so-called low-density regime (or: Boltzmann–Grad regime) where the ratio $T \sim L^d$ is prescribed. In this scaling indeed, the obstacles occupy a proportion $\sim 1/L^d$ of the total volume, so that the probability for the electron to hit an obstacle *once* per unit time on this time scale is unity.

The issue in considering such a model is the following: it is physically expected (see, e.g., [Pa], [VH1,2,3], [KL1,2], [Ku], [Pr], [Vk], [Zw] or also [Ck], see [Fi] for recent developments) that the present system tends to be described by a linear Boltzmann equation in the low-density asymptotics, and precise convergence results in this direction have been actually proved in various situations where the obstacles are *randomly* distributed (see, e.g., [Sp1], [HLW], [La], [EY]). In particular, the initially time-reversible model is expected to be asymptotically described by a time-irreversible equation. Contrary to the "random" situation, the present paper deals at variance with a model which is both *deterministic* and *periodic*, which is a very strong constraint as well as a non-generic case. While the stochastic approach somehow ensures that the desired convergence towards a linear Boltzmann equation holds for almost every distribution of obstacles, the present paper wishes to investigate the same convergence in *one particular* configuration, namely the periodic one.

Obviously, the periodic situation leads to specific coherence, or resonance effects, which are somehow smoothed out in the random situation. These effects turn out to be extremely strong, and to abnormally dominate the limiting procedure: it is actually proved in [CD1,2] that the direct limit $L \to \infty$, $T \sim L^d$ in the original periodic Von-Neumann equation *does not* lead to the expected linear Boltzmann equation. The two papers [CD1,2] show in fact that the above mentionned coherence effects can be precisely quantified making use of number theoretical considerations, and the limiting dynamics is proved to remain time-reversible in this case. For this reason, the present paper introduces some "noise" in the model, in that we let the system {electron + potential} additionaly interact with another system, typically a bath of photons or phonons. This leads to the adding of an additional damping term in the original Von-Neumann equation, which modelizes at a phenomenologic level ([NM], [SSL]) the above mentionned interaction. It is measured by the relaxation time $1/\alpha > 0$. It makes the modified Von-Neuman equation (2.8) in which we pass to the limit readily time-irreversible. This damping term, which at first sight can be viewed as an artificial trick, is actually present in most physically realistic cases [Boy], [Lo], [NM], see also [Hu] for the necessity of considering such additional interactions.

Our main result is the following: in the low-density limit $L \to \infty$, $T \sim L^d$, *followed* by the limit $\alpha \to 0$ where the interaction with the external system vanishes, the modified dynamics of the electron is asymptotically described by a linear Boltzmann equation (Theorem 3.3). Moreover, the cross-section involved in the limiting Boltzmann equation is given by a full power series expansion in the potential (3.32), (3.34), and the lower order term satisfies Fermi's Golden Rule (3.35). Lengthy calculations which are deferred to another work [Ca2] actually prove that this expansion coincides with the usual Born series expansion of conventional scattering theory (3.38), (3.39) . In view of the negative results proved in [CP1,2], the two limits in L and α do not commute. The results presented here heavily rely on the control of some oscillatory integrals in large dimensions (Lemma 3.1).

We close this introduction with some references. The first *formal* derivations of the Pauli Master Equation are due to [Pa], [KL1,2], [Ku], [VH1,2,3]. Other works in this direction are due to [Zw], [Pr], [Ja], [Mei] and recently, to [Fi]. Later, many authors did indeed *rigorously* justify this derivation [Sp1], [La], [HLW], and more recently , [EY], but all these references deal with random potentials. The present paper is, to our knowledge, the first to present a derivation of the Quantum Boltzmann Equation for deterministic potentials and to follow the formal approach based on time-dependent scattering theory as outlined in the appendix. Similar questions are dealt with in the framework of classical mechanics in [Sp2,3] and [VbLLS]. We also mention [Ni1,2], where the square of the scattering matrix is proved to be the right object allowing to describe some semi-classical limits, but only finitely many fixed scatterers are considered. Finally, we mention [Ca1], in which the size of the box is kept fixed and the limit equation is a reversible retarded time integral equation.

A review about the convergence result presented here and the non-convergence results proved in [CP1,2] can be found in [Ca3].

1.2. Motivation of the Present Work

We give here two remarks motivating the present work.

At first, we wish to underline a strong parallel between the results discussed here at the quantum level, and other, somehow similar, results valid at the classical level, since it is a major motivation for this paper as well as [CP1,2]. The present paper investigates at the quantum level the convergence of the dynamics of an electron in a *periodic* distribution of obstacles in the low-density limit. Adding a damping term which modelizes the interaction of the electron with an external "reservoir" (a standard procedure in many contexts of statistical physics, see [Sp2,3], see also [CEFM]), we prove the expected convergence towards a linear Boltzmann equation in the appropriate limit. Though the addition of a damping term makes our model time-irreversible while the stochastic approach proves the convergence (in expectation) of a true time-reversible dynamics towards an irreversible dynamics, the present result is somehow analogous, in a deterministic framework, to the convergence results established in the stochastic framework. On the other hand, the results proved in [CP1,2] indicates that the true periodic situation in the case of zero damping leads to specific coherence effects, measured in terms of number theoretical arguments, which in turn prevent the convergence towards the desired Boltzmann equation. These convergence, respectively non-convergence results at the quantum level have the following important analogon at the classical level: it has been proved in [BBS] that the classical dynamics of an electron in a *random* distribution of obstacles converges, in the appropriate low-density limit, towards a linear Boltzmann equation. However, the work [BGW] proves that, when the distribution is *periodic*, the convergence towards a Boltzmann equation *cannot* hold, thus showing that the periodic situation is degenerate in the sense that it is in the zero-measure set where the expected convergence fails. On the more, the non-convergence result of [BGW] relies as in [CP1,2] on "coherence" effects specific to the periodic case which can be precisely quantified thanks to number theoretical considerations. Roughly speaking, we may say that too many trajectories never hit any obstacle in the periodic situation, which makes this situation specific both at the classical and at the quantum level.

A second strong motivation for the present work, and more precisely for the limit in L we consider here, is the following. This paper aims at giving a rigorous derivation of the Pauli Master Equation (or Quantum Boltzmann Equation) starting from the Quantum Liouville Equation (or Von-Neumann Equation). This problem has received considerable interest since the early formal derivation of Pauli [Pa]. Our approach actually tries to mimic the elementary derivation of Fermi's Golden Rule based on time-dependent scattering theory which can be found in many textbooks, e.g., [Boh], [CTDRG], [CTDL], [Mes], [SSL], and which has been recently revived in [Co]. (We recall that Fermi's Golden Rule gives the expression of the transition rate involved in the Pauli Master Equation). This is where our limit in L originates. Elementary time-dependent scattering theory [Boh] considers indeed a Hamiltonian of the form $H_0 + V$ in a *finite* box of size L, where H_0 is the free kinetic energy. Initially, particles are supposed concentrated on an eigenstate state ψ_n of H_0 associated with the energy $\varepsilon_n \approx n^2/L^2$. The goal is to compute the time asymptotics of the population $|C_p(t)|^2 = |(\psi(t), \psi_p)|^2$ of the initially void states of energy ε_p, $p \neq n$, where $\psi(t)$ denotes the wave-function of the particle at time t. It is well known that, if the energy levels remain discrete (i.e., if the size of the box is left unchanged), the behaviour of $|C_p(t)|^2$ is either an oscillatory function of time if the energies are different ($\varepsilon_p \neq \varepsilon_n$) or a quadratic function of time if the energies are equal ($\varepsilon_p = \varepsilon_n$), but can by no means be a linear function of time. However, scattering theory aims at producing a rate of change of the populations, i.e., a probability per unit of time. Therefore, one looks for a linear in time behaviour of $|C_p(t)|^2$. To remove this apparent paradox, one must therefore let the size of the box go to infinity. Indeed, when the level spacings are set to zero, i.e., as $L \to \infty$, the oscillatory function of time $|C_{\mathbf{p}}(t)|^2$, where now $\mathbf{p}$ is a continuous variable ranging in the wave-vector space $\mathbb{R}^3$, formally is, in the sense of distributions of the $\mathbf{p}$ variable, asymptotic as time goes to infinity to a linear function of time multiplied by a delta function of the differences of the energies of the initial and final states $\delta(\varepsilon_n - \varepsilon_p)$. In this sense, one recovers the usual Fermi Golden Rule as a succession of two limits $L \to \infty$ then $t \to \infty$. Note that we recall these standard and formal computations below in the appendix. In particular, the process of taking the size of the box to infinity is of primary importance and not just a technicality, because one cannot deal from the onset with an infinite medium, due to the above mentionned reasons: in an infinite box, the eigenstates of the unperturbed Hamiltonian H_0 are not normalized, and therefore unphysical, and it cannot be given any meaning to the quantity $|C_p(t)|^2$. This point of view thus emphasizes the contrast between the case where the spectrum is discrete, and the case where it becomes continuous. On this particular point, we wish to quote the work [Co], where the effect of "discretizing the spectrum" is studied from a physical point of view, [CP1,2] where this effect is quantitatively studied in the periodic case, as well as [Ca1] for a mathematical work showing that the large-time/small potential limit (analogous to the weak-coupling limit) *cannot* give the physically expected linear Boltzmann equation when studied in a periodic box of fixed finite size.

1.3. Presentation of the Results

The present paper follows the subsequent lines:

1- (Section 2)

1a- As a starting point (Section 2.1), we write down the equation describing the dynamics of an electron in a periodic box, and we introduce the phenomenological damping term needed in our analysis. We also introduce the appropriate scalings and initial data under consideration. We are thus led to considering a (damped) Von-Neumann equation posed on the so-called density matrix of the electron. We recall that the diagonal part of the density matrix (in the momentum representation ψ_n), denoted by $\rho_d^{L,\alpha}(t,n)$ (see below for the notations), precisely gives the populations $|C_n(t)|^2$. Note that the damping term acts on the off-diagonal part of the density matrix only.

1b- Then (Section 2.2), we follow the computations in [Ca1]: the discreteness of the energy levels and the fact that the evolution of the diagonal part only depends on the action of the perturbed Hamiltonian on the off-diagonal part (a universal phenomenon due to the commutator structure of the equation) allow us to write a *closed* equation for the populations, which is equivalent to the original quantum Liouville equation (Theorem 2.1). This equation has the form of a *retarded* time integral equation (non-Markovian dynamics),

$$\frac{\partial}{\partial t}\rho_d^{L,\alpha}(t,n)=\sum_{k\in\mathbb{Z}^3}\int_0^t \sigma^{L,\alpha}(s,n,k)\,\rho_d^{L,\alpha}(s,k)\,ds-\int_0^t \tilde{\sigma}^{L,\alpha}(s,n)\,\rho_d^{L,\alpha}(s,n)\,ds, \tag{1.1}$$

for some cross-sections $\sigma^{L,\alpha}$ and $\tilde{\sigma}^{L,\alpha}$ depending on the scaling parameters L and α, whose explicit value is computed as a power series in the potential V. We refer to the sequel for the precise meaning of the notations.

1c- Then (Section 2.3), we present a *formal* approach *in the case of zero damping*. It indicates that the low-density limit $L\to\infty$, $T\sim L^3$ (which, in the language of conventional scattering theory used in Section 1.2, provides at the same time the two limits, i.e., the size of the box to infinity and the time to infinity), turns out to *formally* give the desired convergence towards a pointwise in time (Markovian) Boltzmann equation, with a cross-section satisfying the Fermi–Golden–Rule at the lower order. However, we mention that this formal limit *cannot* be rigorously justified because it involves a limit in an oscillatory series which becomes an oscillatory integral, a situation which is not described by the classical stationary phase theorem. Moreover, the formal result is actually *wrong* in one dimension as well as in large dimensions $d\geqslant 3$, as it is proved in [CP1,2].

2- (Section 3) To *rigorously* obtain the true Quantum Boltzmann equation, one needs therefore to make use of the damping term: from a technical point of view, it provides us with a regularizing parameter

$\alpha > 0$, additional to the scaling parameter L describing the low-density process. In the language of Section 1.2, this parameter allows to somehow decouple the limits $L \to \infty$ and $t \to \infty$. Now we perform the various limiting procedures:

2a- (Theorem 3.1) Firstly, the convergence proof relies on establishing various *a priori* estimates which are independent of L (but not on α).

2b- (Theorem 3.2) The limit $L \to \infty$ is then taken first and takes the original damped retarded time integral equation to a damped *local-in-time* equation of the form (see below for the notations),

$$\frac{\partial}{\partial t} \rho_d^\alpha(t, \mathbf{n}) = \int_{\mathbb{R}^3} \sigma^\alpha(\mathbf{n}, \mathbf{k}) \, \rho_d^\alpha(t, \mathbf{k}) \, d\mathbf{k} - \tilde{\sigma}^\alpha(\mathbf{n}) \, \rho_d^\alpha(t, \mathbf{n}), \tag{1.2}$$

for some cross-sections σ^α and $\tilde{\sigma}^\alpha$ which we explicitely compute as power series in the potential V. In particular, we see that the dynamics of the electron *becomes* Markovian along the asymptotic process, while being by no means Markovian initially, see also [EY] on this point.

2c- (Theorem 3.3) The limit $\alpha \to 0$ now allows to remove the damping and to obtain (see below for the notations),

$$\frac{\partial}{\partial t} \rho_d(t, \mathbf{n}) = \int_{\mathbb{R}^3} \sigma(\mathbf{n}, \mathbf{k}) \, \rho_d(t, \mathbf{k}) \, d\mathbf{k} - \tilde{\sigma}(\mathbf{n}) \, \rho_d(t, \mathbf{n}), \tag{1.3}$$

where the cross sections σ and $\tilde{\sigma}$ are given as power series of the potential V, and they satisfy the Fermi Golden Rule at lower order in V (Theorem 3.3), i.e.,

$$\sigma(\mathbf{n}, \mathbf{k}) = 2\pi\delta(\mathbf{n}^2 - \mathbf{k}^2) \, |\hat{V}(\mathbf{n} - \mathbf{k})|^2 + O(|\hat{V}|^3). \tag{1.4}$$

The full series defining σ can actually be proved to be identical with the celebrated Born series—see [Ca2]—a fact which is far from obvious in view of formulae given in Theorem 3.3.

2d- (Lemma 3.1) The last limit $\alpha \to 0$ relies in an absolutely essential way on the control of the singularity and the growth with the dimension of certain oscillatory integrals with quadratic phases in large dimension. This Lemma lies at the core of the convergence proof presented here. It gives the estimates independent of α needed along the asymptotic process. Also, since the cross-section involved in (1.3) appears as a power-series in the potential, this lemma allows to control the convergence of these power series.

3- (Section 4) The full convergence proofs of the above statements are given.

Our main results are Theorem 2.1 (getting a closed equation for the diagonal part only), Theorem 3.1 (a priori bounds on the solution to the Von-Neumann equation), Theorem 3.2 (the limit $L \to \infty$, where the dynamics becomes Markovian), Theorem 3.3 (the limit $\alpha \to 0$, where we recover the Quantum Boltzmann equation with the correct cross-section), as well as the key Lemma 3.1 (control of oscillatory integrals in higher dimensions).

2. THE MODEL AND ITS FORMAL ASYMPTOTICS

2.1. The Mathematical Model under Consideration

Before writing down the equation in which we actually perform the asymptotic process and introducing the damping term, we write, as a first step, the equation describing the evolution of an electron evolving on a Torus $[0, 2\pi L]^3$ under the mere influence of a potential V. As is well known, it is actually described by the periodic Von-Neumann equation in the box $[0, 2\pi L]^3$, with periodic boundary conditions,

$$i\partial_t \tilde{\rho}(t, x, y) = (-\Delta_x + \Delta_y)\, \tilde{\rho}(t, x, y) + (V(x) - V(y))\, \tilde{\rho}(t, x, y), \qquad (2.1)$$

where $\tilde{\rho}(t, x, y)$ is the particle density matrix, which is the mathematical object describing the state of the electron at time $t \in \mathbb{R}$ (see [CTDL]), depending on two space variables x and y both belonging to $[0, 2\pi L]^3$. We mention that the boundary conditions can easily be modified into Dirichlet or Neumann boundary conditions, see Section 5.

Here and throughout the paper, we make the following important assumption on the given potential $V(x)$,

$$\begin{cases} V(\mathbf{x}) \text{ is real-valued and compactly supported, } \mathrm{Supp}(V(\mathbf{x})) \subset]0, 2\pi L[^3, \\ V(\mathbf{x}) \text{ is a ``smooth'' function of } \mathbf{x} \in \mathbb{R}^3, \end{cases} \qquad (2.2)$$

where the precise "smoothness" assumption on V is written in the next section (see Definition 3.1 and assumption (3.5)). The compactness assumption ensures that the potential (or: obstacle) occupies a volume of the order $O(1)$ in a cell of the order $O(L^3)$, which is the natural low-density situation. Note that this assumption can somewhat be relaxed, and the results that we present are also valid if the potential $V = V^L$ depends on L and converges to a fixed profile V^∞ belonging to the same spaces as in Definition 3.1 and (3.5).

Now, the various asymptotic processes are naturally performed in the Fourier space rather than directly on (2.1). For this reason, we define, for any n and $p \in \mathbb{Z}^3$, the following Fourier transforms,

$$\rho(t,n,p) := \int_{[0,2\pi L]^6} \tilde{\rho}(t,x,y) \frac{1}{(2\pi L)^{\frac{3}{2}}} \exp\left(+i\frac{n\cdot y}{L}\right) \frac{1}{(2\pi L)^{\frac{3}{2}}} \exp\left(-i\frac{p\cdot x}{L}\right) dx\,dy, \tag{2.3}$$

as well as the more standard,

$$\hat{V}(\mathbf{n}) := \int_{[0,2\pi L]^3} V(x)\exp(-i\mathbf{n}\cdot x)\,dx \quad \left(= \int_{\mathbb{R}^3} V(\mathbf{x})\exp(-i\mathbf{n}\cdot\mathbf{x})\,dx\right), \tag{2.4}$$

for any $\mathbf{n} \in \mathbb{R}^3$. The last equality comes from the assumption on the support of V and $\hat{V}(\cdot)$ is by assumption a fixed "smooth" profile. Here, bold letters $\mathbf{n}$, $\mathbf{p}$,... denote continuous variables belonging typically to $\mathbb{R}^3$, whereas plain letters n, p,... denote discrete variables belonging typically to $\mathbb{Z}^3$, a convention used throughout the paper. With these notations, the original Von-Neumann equation (2.1) becomes,

$$\frac{\partial}{\partial t}\rho(t,n,p) = -i\frac{p^2-n^2}{L^2}\rho(t,n,p) + \frac{i}{(2\pi L)^3}\sum_{k\in\mathbb{Z}^3}\left\{\hat{V}\left(\frac{k-n}{L}\right)\rho(t,k,p) - \hat{V}\left(\frac{p-k}{L}\right)\rho(t,n,k)\right\}. \tag{2.5}$$

Note that the definition (2.3) is the natural one since the functions, $\psi_n(x) := (2\pi L)^{-d/2}\exp(-in\cdot x/L)$, $(n \in \mathbb{Z}^3)$ are the eigenfunctions of the operator $-\Delta_x$ on the space of periodic functions in the box $[0, 2\pi L]^3$, with degenerate eigenvalues, $E_n := n^2/L^2$ $(n \in \mathbb{Z}^3)$.

Before proceeding further, we now define the diagonal and off-diagonal parts of ρ respectively as,

$$\rho_d(t,n) := \rho(t,n,n), \qquad \rho_{nd}(t,n,p) := \rho(t,n,p)\,\mathbf{1}(n \neq p), \tag{2.6}$$

where $\mathbf{1}(n\neq p)$ denotes the characteristic function of the set $\{n \neq p\}$. The diagonal part $\rho_d(t,n)$ represents the occupation number of the nth eigenstate of the Laplacian, whereas the non-diagonal part represents the correlations between the occupation numbers of the nth and pth eigenstates.

We now come to writing the model in which we shall actually perform the asymptotic process. This needs the introduction a phenomenological damping term on the off-diagonal elements in the original Eq. (2.5). Also, this leads to rescaling the various quantities, namely time, potential and absorption. More precisely, let T denote the time-scale, λ the typical amplitude of the potential, and α the damping parameter. Our starting point reads, with these notations,

$$\begin{aligned}\frac{1}{T}\frac{\partial}{\partial t}\rho^{L,\alpha}(t,n,p)\\ &= -i\,\frac{p^2-n^2}{L^2}\,\rho^{L,\alpha}(t,n,p)-\alpha\rho^{L,\alpha}(t,n,p)\,\mathbf{1}(n\neq p)\\ &+\frac{i\lambda}{(2\pi L)^3}\sum_{k\in\mathbb{Z}^3}\left\{\hat{V}\left(\frac{k-n}{L}\right)\rho^{L,\alpha}(t,k,p)-\hat{V}\left(\frac{p-k}{L}\right)\rho^{L,\alpha}(t,n,k)\right\},\end{aligned} \tag{2.7}$$

(compare with (2.5)), where we now explicitely index the dependence of the density matrix upon the scaling parameters L and α (and write $\rho_d^{L,\alpha}$ and $\rho_{nd}^{L,\alpha}$ as well for the diagonal and off-diagonal parts of $\rho^{L,\alpha}$ respectively). Equation (2.7) also reads, upon splitting $\rho^{L,\alpha}$ into its diagonal and off-diagonal parts,

$$\left\{\begin{aligned}&T^{-1}\partial_t\rho_{nd}^{L,\alpha}(t,n,p)\\ &\quad= +i\,\frac{n^2-p^2}{L^2}\,\rho_{nd}^{L,\alpha}(t,n,p)-\alpha\rho_{nd}^{L,\alpha}(t,n,p)\\ &\quad\quad+i\,\frac{\lambda}{(2\pi L)^3}\,\hat{V}\left(\frac{p-n}{L}\right)\{\rho_d^{L,\alpha}(t,p)-\rho_d^{L,\alpha}(t,n)\}\\ &\quad\quad+i\,\frac{\lambda}{(2\pi L)^3}\sum_{k\neq p}\hat{V}\left(\frac{k-n}{L}\right)\rho_{nd}^{L,\alpha}(t,k,p)\\ &\quad\quad-\frac{i\lambda}{(2\pi L)^3}\sum_{k\neq n}\hat{V}\left(\frac{p-k}{L}\right)\rho_{nd}^{L,\alpha}(t,n,k),\\ &T^{-1}\partial_t\rho_d^{L,\alpha}(t,n)\\ &\quad= +\frac{i\lambda}{(2\pi L)^3}\sum_{k\neq n}\left\{\hat{V}\left(\frac{k-n}{L}\right)\rho_{nd}^{L,\alpha}(t,k,n)-\hat{V}\left(\frac{n-k}{L}\right)\rho_{nd}^{L,\alpha}(t,n,k)\right\},\end{aligned}\right. \tag{2.8}$$

To be complete, we now precise the exact asymptotic regime and the specific initial data under consideration. Firstly, we are interested in the following low density regime,

$$T = (2\pi L)^3, \qquad |\lambda| \leqslant \lambda_0, \tag{2.9}$$

where λ_0 is some (small) constant independent of α and L. Note that Eq. (2.7) introduces a damping scaled by α *in the new time scale* T, which is an extremely strong damping. Secondly, and as it is standard in this field (see, e.g., [Ku], [KL1,2], [Ck], [Zw]) we are only interested in performing the asymptotics $L \to \infty$, $\alpha \to 0$ in (2.8) for particular initial data which are stationary states of the *free* Von-Neuman equation $iT^{-1}\partial\tilde{\rho}/\partial t = (-\Delta_x + \Delta_y)\,\tilde{\rho}$. In other words, we wish to quantify the large time influence of the potential for initial states which are equilibrium states of the unperturbed hamiltonian $-\Delta_x$. The initial data of interest in the present paper are thus taken of the form,

$$\begin{cases} \rho_{nd}^{L,\alpha}(t, n, p)|_{t=0} = 0, \\ \rho_d^{L,\alpha}(t, n)|_{t=0} = (2\pi L)^{-3}\, \rho_d^0\left(\dfrac{n}{L}\right), \\ \rho_d^0(\mathbf{n}) \geqslant 0 \text{ is a given ``smooth'' function of } \mathbf{n} \in \mathbb{R}^3, \end{cases} \tag{2.10}$$

where again the precise "smoothness" assumption needed on ρ_d^0 is written in the next section (see Definition 3.1 and assumption (3.5)). The assumption (2.10) generalizes both the case of initial thermodynamical equilibrium where $\rho^{L,\alpha}(t, n, p)|_{t=0} \approx L^{-3} \exp(-\beta n^2/L^2)\, \mathbf{1}[n = p]$ and β is the inverse temperature, and the more general case where $\rho^{L,\alpha}(t=0)$ is an arbitrary function of the energy $\rho^{L,\alpha}(t, n, p)|_{t=0} \sim L^{-3} f(n^2/L^2)\, \mathbf{1}[n = p]$ for some "reasonable" function f. Summarizing, we are interested in obtaining a linear Boltzmann equation on the (non-commuting) limit $\rho_d = \lim_{\alpha \to 0} \lim_{L \to \infty} \rho_d^{L,\alpha}$, in (2.8), (2.10), (2.9).

We end the presentation of the model with two comments.

Physically, the damping term accounts for elastic interactions of the particles with an external bath of, typically, ions, atoms, phonons, photons, etc. (see, e.g., [SSL], Chap. 7.3 for applications to light-matter interaction). Under such interactions indeed, the off-diagonal terms of the density matrix (i.e., the correlations between the energy levels) are exponentially damped due to random changes of phases of the particle wave-functions, while, simultaneously, the diagonal part is left unchanged due to the elastic character of the collisions (see also [Lo], [Boy], [NM]). In the most general case, when both elastic and inelastic interactions are present, the latter act on much longer time scales than the former. Consequently, the decay of the off-diagonal terms of the density matrix by elastic collisions is much quicker than that of the diagonal terms by inelastic collisions [NM]. The damping of the off-diagonal terms bears similarities with the so-called "Random Phase Approximation" [VH1,2,3], [Zw], [Kr], [Pr]. Also, the effect of this damping term is similar to that of an average over random variables like in [Sp1], [La], [HLW], [EY].

Finally, for the sake of completeness, me mention the following lemma, the proof of which is given in Section 4 later. It states that the damping term in (2.8) preserves the positivity of the density matrix. It actually satisfies the stronger "Lindblad" property [Li].

Lemma 2.1. Assume (2.2). Then, the solution $\rho^{L,\alpha}(t,n,p)$ to (2.8) with initial data $\rho^{L,\alpha}(t,n,p)|_{t=0}$ satisfying (2.10) is unique in $C^0(\mathbb{R}_t; l^2(\mathbb{Z}^6_{n,p}))$. Besides, for all *non-negative* values of time $t \geqslant 0$, $\rho^{L,\alpha}(t,n,p)$ is a hermitian, positive, and trace-class operator acting on $l^2(\mathbb{Z}^3)$. In particular, we have, for all $t \geqslant 0$,

$$\rho_d^{L,\alpha}(t,n) \geqslant 0 \qquad \text{and} \qquad \rho_{nd}^{L,\alpha}(t,n,p) = (\rho_{nd}^{L,\alpha}(t,p,n))^*. \tag{2.11}$$

2.2. Elimination of the Non-Diagonal Part

We wish to derive the Pauli master equation for the occupation number $\rho_d^{L,\alpha}(t,n)$ in the asymptotic limits $L \to \infty$, $\alpha \to 0$, starting from the coupled system (2.8) on $\rho_d^{L,\alpha}$ and $\rho_{nd}^{L,\alpha}$. As formally observed in [Zw], [Pr], it is actually possible to write a closed equation on $\rho_d^{L,\alpha}$ before any scaling limit. Following [Ca1], the next theorem gives the explicit form of the equation on $\rho_d^{L,\alpha}$. Its proof is deferred to Section 4.

Theorem 2.1. Assume (2.2). Let $\rho_d^{L,\alpha}(t,n)$, $\rho_{nd}^{L,\alpha}(t,n,p)$ be the unique solution to the rescaled system (2.8) with initial data given by (2.10). Then, for positive values of time, $t \geqslant 0$, $\rho_d^{L,\alpha}(t,n)$ satisfies the following *closed* equation of Boltzmann-type,

$$\partial_t \rho_d^{L,\alpha}(t,n) = \sum_{l=1}^{+\infty} \lambda^{l+1} (Q_l^{L,\alpha} \rho_d^{L,\alpha})(t,n), \tag{2.12}$$

where the "damped collision operators" $Q_l^{L,\alpha}$ are given by,

$$
\begin{aligned}
&(Q_l^{L,\alpha}\rho_d^{L,\alpha})(t,n)\\
&\quad=\frac{T}{(2\pi L)^{3(l+1)}}(-2\Re)\sum_{\varepsilon_1,\dots,\varepsilon_l}\sum_{k_1,\dots,k_l}\int_{u_1,\dots,u_l}(-1)^{\tilde\varepsilon_1+\cdots+\tilde\varepsilon_l}\\
&\qquad\times\exp\left(i\,\frac{(n+\varepsilon_1k_1)^2-(n-\tilde\varepsilon_1k_1)^2}{L^2}\,u_1-\alpha u_1\right)\\
&\qquad\times\exp\left(i\,\frac{(n+\varepsilon_1k_1+\varepsilon_2k_2)^2-(n-\tilde\varepsilon_1k_1-\tilde\varepsilon_2k_2)^2}{L^2}\,u_2-\alpha u_2\right)\\
&\qquad\times\cdots\times\\
&\qquad\times\exp\left(i\,\frac{(n+\varepsilon_1k_1+\cdots+\varepsilon_lk_l)^2-(n-\tilde\varepsilon_1k_1-\cdots-\tilde\varepsilon_lk_l)^2}{L^2}\,u_l-\alpha u_l\right)\\
&\qquad\times\left[i\widehat V\left(\frac{k_1}{L}\right)\right]\left[i\widehat V\left(\frac{k_2}{L}\right)\right]\cdots\left[i\widehat V\left(\frac{k_l}{L}\right)\right]\left[i\widehat V^*\left(\frac{k_1+k_2+\cdots k_l}{L}\right)\right]\\
&\qquad\times\rho_d^{L,\alpha}(t-T^{-1}(u_1+u_2+\cdots+u_l),\,n+\varepsilon_1k_1+\varepsilon_2k_2+\cdots+\varepsilon_lk_l).
\end{aligned}
\tag{2.13}
$$

Here and in the sequel, $\Re$ denotes the real part of a complex number. Also, the sums $\sum_{\varepsilon_1,\dots,\varepsilon_l}\sum_{k_1,\dots,k_l}$ carry over the variables $(\varepsilon_1,\dots,\varepsilon_l)\in\{0,1\}^l$ and $(k_1,\dots,k_l)\in(\mathbb{Z}^3)^l$ such that,

$$k_1\neq 0,\ k_1+k_2\neq 0,\dots,\ k_1+k_2+\cdots+k_l\neq 0, \tag{2.14}$$

and we have made the convention,

$$\forall j=1,\dots,l\qquad \tilde\varepsilon_j=(1-\varepsilon_j)=1\ \text{ or }\ 0. \tag{2.15}$$

Finally, the integrals $\int_{u_1,\dots,u_l}$ carry over the set,

$$0\leqslant u_1\leqslant Tt,\ 0\leqslant u_2\leqslant Tt-u_1,\ \dots,\ 0\leqslant u_l\leqslant Tt-u_1-\cdots-u_{l-1}. \tag{2.16}$$

Moreover, the first collision operator $Q_1^{L,\alpha}$ (case $l=1$ above) has the more explicit value,

$$
\begin{aligned}
\lambda^2(Q_1^{L,\alpha}\rho_d^{L,\alpha})(t,n)&=2\,\frac{\lambda^2}{(2\pi L)^6}\int_{u=0}^{Tt}\sum_{k\neq 0}\exp(-\alpha u)\cos\left(\frac{n^2-k^2}{L^2}\,u\right)\\
&\quad\times|\widehat V|^2\left(\frac{n-k}{L}\right)[\rho_d^{L,\alpha}(t-T^{-1}u,k)-\rho_d^{L,\alpha}(t-T^{-1}u,n)]\,du.
\end{aligned}
\tag{2.17}
$$

Remarks. **1.** The system (2.12)–(2.13) is a linear Boltzmann-like equation with memory in time, of the form (1.1). The typical "gain-loss" structure of the right-hand-side of (2.12)–(2.13) is particularly transparent on the first collision operator $\lambda^2 Q_1^{L,\alpha}$, in spite of the fact that the (time dependent) "scattering rate,"

$$2\,\frac{\lambda^2}{(2\pi L)^6}\exp(-\alpha u)\cos\left(\frac{n^2-k^2}{L^2}\,u\right)|\hat{V}|^2\left(\frac{n-k}{L}\right), \tag{2.18}$$

is not positive. More generally, each term $\lambda^{l+1}Q_l^{L,\alpha}\rho_d^{L,\alpha}$ describes how the occupation numbers $\rho_d^{L,\alpha}(t,n)$ are affected by $(l+1)$ consecutive interactions with the potential V, so that the expansion $\sum_l \lambda^{l+1}Q_l^{L,\alpha}$ is also a power series in V. Obviously, its structure could be illustrated by means of a Feynman diagram.

2. We can readily observe that, for fixed t, we have the following bound on the right-hand-side of (2.12),

$$\begin{aligned}
\|\lambda^{l+1}Q_l^{L,\alpha}\rho_d^{L,\alpha}\|_{l_n^2} &\leqslant T\left[\frac{2\lambda}{(2\pi L)^3}\right]^{l+1}\frac{T^l\,|t|^l}{l!}\left[\left\|(2\pi L)^{-3}\,\hat{V}\left(\frac{k}{L}\right)\right\|_{l_k^1}\right]^l\\
&\quad\times\left\|(2\pi L)^{-3}\,\hat{V}\left(\frac{k}{L}\right)\right\|_{l_k^\infty}\|\rho_d^{L,\alpha}(t,n)\|_{l_n^2},\\
&\quad\left(\text{use that }\int_{u_1=0}^{t}\cdots\int_{u_l=0}^{t-u_1-\cdots-u_{l-1}}1\,du_1\cdots du_l=t^l/l!\right)\\
&\leqslant\left[\frac{C\lambda T t}{L^3}\right]^{l+1}\frac{1}{l!}\|\rho^{L,\alpha}(t,n,p)\|_{l_{n,p}^2}\\
&\quad\text{(for some constant } C\text{, thanks to (2.2)),}\\
&\leqslant\left[\frac{C\lambda T t}{L^3}\right]^{l+1}\frac{1}{l!}\,C'(t),
\end{aligned}$$

for some time dependent function $C'(t)$, because $\rho^{L,\alpha}(t)\in C^0(l^2)$ (Lemma 2.1). Obviously, this is enough to give a rigorous meaning to the series involved in Theorem 2.1, at least for *fixed* values of the scaling parameters T and L.

2.3. A Formal Investigation of the Infinite Volume Limit in the Case of Zero Damping

We are interested in the infinite volume limit $(L\to+\infty)$ in (2.12)–(2.13) when the damping is set to zero. On the one hand, we describe the main scaling properties of Eqs. (2.12)–(2.13), which lead to thinking that the direct and formal limit $L \to \infty$ in (2.12)–(2.13) with $\alpha \equiv 0$ *could* give the Quantum Boltzmann equation. Simultaneously, we indicate that this rough and formal limit *cannot* be made rigorous.

To simplify the presentation we restrict ourselves to the leading order term namely, $\partial_t \rho_d^L = \lambda^2 Q_1^L \rho_d^L + O(\lambda^3)$, with vanishing damping, i.e.,

$$\left\{\begin{aligned} \partial_t \rho_d^L(t,n) &= 2T\lambda^2 (2\pi L)^{-6} \int_{u=0}^{t} \sum_{k \neq 0} \cos\left(\frac{n^2-k^2}{L^2}\, u\right) \\ &\quad \times |\hat{V}|^2 \left(\frac{n-k}{L}\right) [\rho_d^L(t-u,k) - \rho_d^L(t-u,n)]\, du + O(\lambda^3), \\ \rho_d^L(t=0,n) &= \frac{1}{(2\pi L)^3}\, \rho_d^0\left(\frac{n}{L}\right). \end{aligned}\right. \tag{2.19}$$

We first observe that formula (2.19) ressembles the following basic formula, valid for all "smooth" functions ψ, $L^{-N} \sum_{k \in \mathbb{Z}^N} \psi(k/L) \xrightarrow[L \to \infty]{} \int_{\mathbf{k} \in \mathbb{R}^N} \psi(\mathbf{k})\, d\mathbf{k}$, but the factor $(2\pi L)^{-6}$ in front of the sum $\sum_k$ is too strong, since the vector k belongs to the 3-dimensional space only. Therefore, the low-density scaling $T = (2\pi L)^3$ is natural in (2.19). With this rescaling in time we obtain indeed,

$$\left\{\begin{aligned} \partial_t \rho_d^L(t,n) &= 2\lambda^2 (2\pi L)^{-3} \int_{u=0}^{(2\pi L)^3 t} \sum_{k \neq 0} \cos\left(\frac{n^2-k^2}{L^2}\, u\right) |\hat{V}|^2 \left(\frac{n-k}{L}\right) \\ &\quad \times \left[\rho_d\left(t - \frac{u}{(2\pi L)^3}, k\right) - \rho_d\left(t - \frac{u}{(2\pi L)^3}, n\right)\right] du + O(\lambda^3), \\ \rho_d^L|_{t=0}(n) &= (2\pi L)^{-3}\, \rho_d^0(n/L). \end{aligned}\right. \tag{2.20}$$

If we now try to perform the infinite volume limit on (2.20), three distinct phenomena take place, at least formally:

1. The model should converge towards a model where $\sum_k (\cdots)(k/L, n/L)$ is replaced by $\int_{\mathbf{k}} (\cdots)(\mathbf{k}, \mathbf{n})\, \frac{d\mathbf{k}}{(2\pi)^3}$ as $L \to \infty$, and with the initial data in (2.20) simply replaced by $\rho_d|_{t=0} = (2\pi)^{-3}\, \rho_d^0(\mathbf{n})$.

2. The time integration $u \in [0, t]$ in the original model (2.12)–(2.13) has become, after rescaling in time, $u \in [0, (2\pi L)^3 t]$. Therefore, for *positive* values of time t (this is where time irreversibility appears), the limit $L \to +\infty$ in (2.20) should give rise to an integral over the positive real line, $\int_{u=0}^{+\infty} \cdots$.

3. The factor $\rho_d^L(t-T^{-1}u, n)$ in the original equation has become $\rho_d^L(t-\frac{u}{(2\pi L)^3}, n)$ and should converge towards $\rho_d(t, \mathbf{n})$ in the limit $L \to +\infty$. In particular, the infinite volume limit seems to transform an equation *with memory in time* into a Boltzmann equation *without memory in time*.

For all these reasons, the infinite volume limit $L \to \infty$ in (2.20) *formally* gives the asymptotic behaviour,

$$\partial_t \rho_d(t, \mathbf{n}) \sim 2\lambda^2 \int_0^{+\infty} \int_{\mathbb{R}^3} \cos([\mathbf{n}^2 - \mathbf{k}^2]\, u) \times |\hat{V}|^2\, (\mathbf{n}-\mathbf{k})\, [\rho_d(t, \mathbf{k}) - \rho_d(t, \mathbf{n})]\, \frac{d\mathbf{k}}{(2\pi)^3}\, du + O(\lambda^3). \quad (2.21)$$

In particular, the time integral $\int_{u=0}^{+\infty} \cdots$ in (2.21) has a meaning as an *oscillatory integral*, and (2.21) gives (see Lemma 3.1 and the subsequent remarks),

$$\partial_t \rho_d(t, \mathbf{n}) \sim 2\pi\lambda^2 \int_{\mathbb{R}^3} \delta(\mathbf{n}^2 - \mathbf{k}^2)\, |\hat{V}|^2\, (\mathbf{n}-\mathbf{k}) [\rho_d(t, \mathbf{k}) - \rho_d(t, \mathbf{n})]\, \frac{d\mathbf{k}}{(2\pi)^3} + O(\lambda^3), \quad (2.22)$$

which is precisely the Quantum Boltzmann equation that we are looking for.

The first two steps cannot be justified because they involve the transformation of a discrete series into an oscillatory integral. Indeed, the notion of oscillatory integral heavily relies on the fact that the **k**, **n** variables are continuous. Moreover, it can be proved [CP1,2] that, at least in dimension one as well as in large dimensions ($d \geqslant 3$), this formal analysis is actually false, and the limiting equation remains reversible. This is the reason of our introduction of the damping variable α. This is also the reason why, in previous works, expectation values over random phases were considered [Sp1], [La], [HLW], [EY].

3. STATEMENT OF THE THEOREMS

3.1. The Rigorous Convergence Results

We are now able to describe the asymptotics $L \to +\infty$, $\alpha \to 0$ in Theorem 2.1. We begin with some notations.

Definition 3.1. (i) For any $D \geqslant 0$, we define the following spaces of test functions,

$$\mathcal{T}_D(\mathbb{R}^N) := \{\Psi(\mathbf{n}) \in C^0(\mathbb{R}^N) \text{ s.t. } \langle \mathbf{n} \rangle^D \Psi(\mathbf{n}) \in L^\infty(\mathbb{R}^N)\}, \tag{3.1}$$

where we use the usual notation, $\langle \mathbf{n} \rangle := (1+\mathbf{n}^2)^{1/2}$. In the sequel, $\mathcal{T}_D(\mathbb{R}^N)$ will often be written in short $\mathcal{T}_D$, without refering to the actual dimension of the underlying space $\mathbb{R}^N$. The space $\mathcal{T}_D$ is a Banach space, and its norm is given by,

$$\|\Psi\|_{\mathcal{T}_D} := \|\langle \mathbf{n} \rangle^D \Psi(\mathbf{n})\|_{L^\infty}. \tag{3.2}$$

(ii) For any $D \geqslant 0$, we define,

$$\mathcal{S}_D(\mathbb{R}^N) := \{\Psi(\mathbf{n}) \in C^0(\mathbb{R}^N) \text{ s.t. } \langle \mathbf{n} \rangle^a \langle \partial_{\mathbf{n}} \rangle^b \Psi(\mathbf{n}) \in C^0(\mathbb{R}^N), \forall 0 \leqslant a, b \leqslant D\}, \tag{3.3}$$

where as usual, $\langle \partial_{\mathbf{n}} \rangle := (1-\Delta_{\mathbf{n}})^{1/2}$. The space $\mathcal{S}_D$ is a Banach space, and its norm is given by,

$$\|\Psi\|_{\mathcal{S}_D} := \sum_{a,b=0}^{D} \|\langle \mathbf{n} \rangle^a \langle \partial_{\mathbf{n}} \rangle^b \Psi(\mathbf{n})\|_{L^\infty}. \tag{3.4}$$

Using these notations, we shall assume throughout the paper that the profiles ρ_d^0 and $\hat{V}$ (the data of the problem) satisfy,

$$\rho_d^0(\mathbf{n}) \in \mathcal{T}_D, \quad \hat{V}(\mathbf{n}) \in \mathcal{S}_{2D}, \quad \text{for some large (but fixed) } D, \text{ say } D \geqslant 4. \tag{3.5}$$

Also, we pick up a coupling parameter λ satisfying, $|\lambda| \leqslant \lambda_0$, where λ_0 is some small constant, whose actual value only depends on the norms $\|\rho_d^0(\mathbf{n})\|_{\mathcal{T}_D}$ and $\|\hat{V}(\mathbf{n})\|_{\mathcal{S}_{2D}}$, but it does not depend on L nor on α.

We are now in position to state the three main theorems of the present paper.

Theorem 3.1 (A priori bounds and existence of weak limits). Let $\rho_d^{L,\alpha}(t, n)$ and $\rho_{nd}^{L,\alpha}(t, n, p)$ be the unique solutions to (2.8) in $C_t^0(l_n^2)$ and $C_t^0(l_{n,p}^2)$ respectively. Assume that the initial datum satisfies (2.10), and the potential satisfies (2.2), with profiles ρ_d^0 and $\hat{V}$ satisfying (3.5). Then the following holds.

(i) For any $t \geqslant 0$, the following a-priori estimates hold for the diagonal part,

$$\|\rho_d^{L,\alpha}(t,n)\|_{l_n^1} \leqslant C \qquad \text{(preservation of trace)}, \tag{3.6}$$

$$\|\rho_d^{L,\alpha}(t,n)\|_{l_n^\infty} \leqslant \frac{C}{L^3} \qquad \text{(maximum principle)}, \tag{3.7}$$

$$\|\rho_d^{L,\alpha}(t,n)\|_{l_n^2} \leqslant \frac{C}{L^{3/2}} \qquad \text{(interpolation)}, \tag{3.8}$$

where the constant C is of the form,

$$C := C(\|\rho_d^0(\mathbf{n})\|_{\mathcal{T}_D}, \|\hat{V}(\mathbf{n})\|_{\mathcal{S}_{2D}}), \tag{3.9}$$

but C is independent of t and α, a convention that we shall use throughout the paper. Also, the non-diagonal part satisfies, for any $t \geqslant 0$,

$$\|\rho_{nd}^{L,\alpha}(t,n,p)\|_{l_{n,p}^2} \leqslant \frac{C}{\alpha L^3}. \tag{3.10}$$

(ii) Under the same circumstances, the following estimate on the derivative in time $\partial_t \rho_{nd}^{L,\alpha}$ holds, for any $t \geqslant 0$,

$$\int_{s=0}^{t} \|\partial_t \rho_{nd}^{L,\alpha}(s,n,p)\|_{l_{n,p}^2}^2 \, ds \leqslant \frac{C}{\alpha L^3}. \tag{3.11}$$

(iii) Finally, the sequence $\rho_d^{L,\alpha}(t)$ is uniformly differentiable in time, in the sense that for any $t \geqslant 0$,

$$\|\partial_t \rho_d^{L,\alpha}(t,n)\|_{l_n^2} \leqslant \frac{C}{\alpha L^{3/2}}. \tag{3.12}$$

(iv) Define now the distributions $\rho_d^{L,\alpha}(t)$ and $\rho_{nd}^{L,\alpha}(t)$ (denoted by the same name for convenience) acting respectively on functions $\phi(\mathbf{n}) \in C_c^\infty(\mathbb{R}^3)$ and $\Phi(\mathbf{n},\mathbf{p}) \in C_c^\infty(\mathbb{R}^3 \times \mathbb{R}^3)$ through formulae,

$$\langle \rho_d^{L,\alpha}(t), \phi \rangle := \sum_n \rho_d^{L,\alpha}(t,n)\, \phi\left(\frac{n}{L}\right), \tag{3.13}$$

$$\langle \rho_{nd}^{L,\alpha}(t), \Phi \rangle := \sum_{n,p} \rho_{nd}^{L,\alpha}(t,n,p)\, \Phi\left(\frac{n}{L}, \frac{p}{L}\right). \tag{3.14}$$

Then $\rho_d^{L,\alpha}(t)$ and $\rho_{nd}^{L,\alpha}(t)$ extend continuously to the spaces $\mathcal{T}_D(\mathbb{R}^3)$ and $\mathcal{T}_D(\mathbb{R}^6)$ respectively, and, for any $t \geqslant 0$, the following estimates hold,

$$|\langle \rho_d^{L,\alpha}(t), \phi \rangle| \leqslant C \, \|\phi(\mathbf{n})\|_{\mathcal{T}_D(\mathbb{R}^3)}, \tag{3.15}$$

$$|\langle \partial_t \rho_d^{L,\alpha}(t), \phi \rangle| \leqslant \frac{C}{\alpha} \, \|\phi(\mathbf{n})\|_{\mathcal{T}_D(\mathbb{R}^3)}, \tag{3.16}$$

$$|\langle \rho_{nd}^{L,\alpha}(t), \Phi \rangle| \leqslant \frac{C}{\alpha} \, \|\Phi(\mathbf{n}, \mathbf{p})\|_{\mathcal{T}_D(\mathbb{R}^6)}. \tag{3.17}$$

In particular, up to extracting subsequences, the distributions $\rho_d^{L,\alpha}(t)$ and $\rho_{nd}^{L,\alpha}(t)$ both possess weak limits as $L \to \infty$, denoted by $\rho_d^{\alpha}(t)$ and $\rho_{nd}^{\alpha}(t)$, so that,

$$\rho_d^{L,\alpha}(t) \xrightarrow[L \to \infty]{} \rho_d^{\alpha}(t) \quad \text{in} \quad C^0(\mathbb{R}_t^+; [\mathcal{T}_D(\mathbb{R}^3)]^*\text{-weak}^*), \tag{3.18}$$

$$\partial_t \rho_d^{L,\alpha}(t) \xrightarrow[L \to \infty]{} \partial_t \rho_d^{\alpha}(t) \quad \text{in} \quad [L^1(\mathbb{R}_t^+; \mathcal{T}_D(\mathbb{R}^3))]^*\text{-weak}^*, \tag{3.19}$$

$$\rho_{nd}^{L,\alpha}(t) \xrightarrow[L \to \infty]{} \rho_{nd}^{\alpha}(t) \quad \text{in} \quad [L^1(\mathbb{R}_t^+; \mathcal{T}_D(\mathbb{R}^6))]^*\text{-weak}^*. \tag{3.20}$$

Furthermore, $\rho_d^{\alpha}(t)$ possesses in turn a weak limit as $\alpha \to 0$, say $\rho_d(t)$, so that,

$$\rho_d^{\alpha}(t) \xrightarrow[L \to 0]{} \rho_d(t) \quad \text{in} \quad [L^1(\mathbb{R}_t^+; \mathcal{T}_D(\mathbb{R}^3))]^*\text{-weak}^*. \tag{3.21}$$

Remarks. 1. The estimates (i) should be seen as *scaling* estimates in terms of the parameter L. They tell us, in some sense, that for each $t \geqslant 0$, the sequences $\rho_d^{L,\alpha}(t, n)$ and $\rho_{nd}^{L,\alpha}(t, n, p)$ behave in the same way as sequences of the form,

$$\frac{1}{L^3} u\left(t, \frac{n}{L}\right) \quad \text{and} \quad \frac{1}{L^6} v\left(t, \frac{n}{L}, \frac{p}{L}\right), \tag{3.22}$$

respectively, where $u(t, \mathbf{n})$ and $v(t, \mathbf{n}, \mathbf{p})$ should be, say, smooth profiles defined on the whole space.

This fact is naturally obvious at time 0. On the more, if one explicitely solves the Von-Neumann equation (2.8) using Neumann-series and expressing $\rho_{nd}^{L,\alpha}(t)$ as well as $\rho_d^{L,\alpha}(t)$ in terms of the initial datum, this is also *formally* the case at time t if we do not ask questions of convergence. However the series built up in this way is very difficult to bound in a non-trivial way, for we are not able to take advantadge of the many oscillations present at the discrete level. We may indeed draw the following parallel: when the continuous limit $L \to \infty$ has been taken (see Theorem 3.2), we are led to manipulate series of collision operators (see (3.26) and (3.27)) which involve iterated oscillating integrals. The oscillations then allow to make the series converge in a nice way, thanks to Lemma 3.1 below. Now obviously this kind of argument is completely forbidden *while* performing the continuous limit, where we still have to deal with discrete sums.

The part (i) of the theorem makes sure in this perspective that the natural scaling properties in L of the solution to the Von-Neumann equation is *actually* propagated through time-evolution, without writing down the above-mentionned Neumann series. This leads however to worse estimates (ii) than expected, but fortunately these will be enough to take care of the continuous limit.

Note finally that Theorem 3.1 is a priori *false* for negative values of time.

2. As mentionned above, the estimate (ii) on the derivative in time $\partial_t \rho_{nd}^{L,\alpha}$ is somehow weaker than what one would expect, in two respects: firstly, the estimate (ii) holds for *averages in time*, and we do not know whether it holds true pointwise ; secondly, the scaling parameter L^{-3} on the right-hand-side of (3.11) is much weaker than the L^{-6} one would expect for profiles of the form (3.22). However, it is surprising that estimate (ii) hold *uniformly* in t.

3. This theorem relies in an absolutely essential way on the following features of the Von-Neumann equation under consideration: the Von-Neumann equation (2.8) has the so-called Lindblad property (it preserves the positivity of the density matrix—see Lemma 2.1) ; the initial data is purely diagonal (see (2.10)); the equation on the diagonal part involves the non-diagonal part only on the right-hand-side. We emphasize in this respect that the l^∞ bound (3.7) is very specific (it is actually a direct consequence of the Lindblad property), and it is not at all a general feature of Schrödinger-like equations.

Armed with the a priori bounds of Theorem 3.1, we are now able to characterize the consecutive asymptotics $L \to \infty$ and $\alpha \to 0$, as follows.

Theorem 3.2 (Convergence as $L \to \infty$: The equation becomes Markovian). Let $\rho_d^{L,\alpha}(t)$ and $\rho_{nd}^{L,\alpha}(t)$ be as in Theorem 3.1 and define their weak limits $\rho_d^\alpha(t)$ and $\rho_{nd}^\alpha(t)$ as stated in Theorem 3.1. Then the following holds,

(i) The weak limits satisfy the following system of equations,

$$\partial_t \rho_d^\alpha(t,\mathbf{n}) = i\lambda \int_{\mathbb{R}^3} [\hat{V}(\mathbf{n}-\mathbf{k})\, \rho_{nd}^\alpha(t,\mathbf{k},\mathbf{n}) - \hat{V}(\mathbf{k}-\mathbf{n})\, \rho_{nd}^\alpha(t,\mathbf{n},\mathbf{k})] \frac{d\mathbf{k}}{(2\pi)^3}, \tag{3.23}$$

$$\begin{aligned}\rho_{nd}^\alpha(t,\mathbf{n},\mathbf{p}) = {} & \frac{i\lambda}{(2\pi)^3} \int_{u=0}^{+\infty} e^{[i(\mathbf{n}^2-\mathbf{p}^2)-\alpha]\,u} \hat{V}(\mathbf{p}-\mathbf{n}) [\rho_d^\alpha(t,\mathbf{p}) - \rho_d^\alpha(t,\mathbf{n})]\, du \\ & + i\lambda \int_{u=0}^{+\infty} \int_{\mathbb{R}^3} e^{[i(\mathbf{n}^2-\mathbf{p}^2)-\alpha]\,u} [\hat{V}(\mathbf{k}-\mathbf{n})\, \rho_{nd}^\alpha(t,\mathbf{k},\mathbf{p}) \\ & - \hat{V}(\mathbf{p}-\mathbf{k})\, \rho_{nd}^\alpha(t,\mathbf{n},\mathbf{k})] \frac{d\mathbf{k}}{(2\pi)^3}\, du, \end{aligned} \tag{3.24}$$

with initial datum,

$$\rho_d^\alpha(t,\mathbf{n})|_{t=0} = \rho_d^0(\mathbf{n}). \tag{3.25}$$

The equations (3.23) and (3.24) hold between distributions belonging to $[L^1(\mathbb{R}_t^+; \mathcal{T}_D)]^*$.

(ii) The system (3.23)–(3.24) implies that the following Boltzmann equation is satisfied,

$$\partial_t \rho_d^\alpha(t,\mathbf{n}) = \sum_{l\geqslant 1} \lambda^{l+1} [Q_l^\alpha \rho_d^\alpha](t,\mathbf{n}), \tag{3.26}$$

with initial datum (3.25), where the collision operators Q_l^α are defined as,

$$\begin{aligned} & [Q_l^\alpha \rho_d^\alpha](t,\mathbf{n}) \\ & := (2\pi)^{-3l} (-2\Re) \sum_{\varepsilon_1,\ldots,\varepsilon_l} \int_{\mathbb{R}^{3l}} \int_{u_1=0}^{+\infty} \int_{u_2=0}^{+\infty} \cdots \int_{u_l=0}^{+\infty} (-1)^{\tilde{\varepsilon}_1+\cdots+\tilde{\varepsilon}_l} \\ & \quad \times \exp(i[(\mathbf{n}+\varepsilon_1\mathbf{k}_1)^2 - (\mathbf{n}-\tilde{\varepsilon}_1\mathbf{k}_1)^2]\, u_1 - \alpha u_1) \\ & \quad \times \cdots \times \\ & \quad \times \exp(i[(\mathbf{n}+\varepsilon_1\mathbf{k}_1+\cdots+\varepsilon_l\mathbf{k}_l)^2 - (\mathbf{n}-\tilde{\varepsilon}_1\mathbf{k}_1 - \cdots \tilde{\varepsilon}_l\mathbf{k}_l)^2]\, u_l - \alpha u_l) \\ & \quad \times [i\hat{V}(\mathbf{k}_1)] \cdots [i\hat{V}(\mathbf{k}_l)] \times [i\hat{V}^*(\mathbf{k}_1+\cdots+\mathbf{k}_l)] \\ & \quad \times \rho_d^\alpha(t,\mathbf{n}+\varepsilon_1\mathbf{k}_1+\cdots+\varepsilon_l\mathbf{k}_l)\, d\mathbf{k}_1 \cdots d\mathbf{k}_l. \end{aligned} \tag{3.27}$$

Here, variables $\varepsilon_1,..., \varepsilon_l$ are as in Theorem 2.1. Also, the leading term in the series (3.26) is,

$$\lambda^2[Q_1^\alpha \rho_d^\alpha](t, \mathbf{n}) = 2 \int_{\mathbb{R}^3} \int_{u=0}^{+\infty} \exp(-\alpha u) \cos([\mathbf{n}^2 - \mathbf{k}^2]\, u) \times |\hat{V}(\mathbf{n}-\mathbf{k})|^2\, [\rho_d^\alpha(t, \mathbf{k}) - \rho_d^\alpha(t, \mathbf{n})] \frac{d\mathbf{k}}{(2\pi)^3}. \quad (3.28)$$

(iii) The Eq. (3.26) makes sense weakly, when tested against test functions $\phi(\mathbf{n}) \in \mathscr{S}_{2D}(\mathbb{R}^3)$. More precisely, for any such ϕ, we have,

$$\langle \partial_t \rho_d^\alpha(t), \phi \rangle = \sum_{l \geqslant 0} \lambda^{l+1} \langle \rho_d^\alpha(t), {}^t Q_l^\alpha \phi \rangle, \quad (3.29)$$

where ${}^t Q_l^\alpha \phi$ denotes the formal adjoint of Q_l^α, defined as,

$$\begin{aligned}
&[{}^t Q_l^\alpha \phi](t, \mathbf{n}) \\
&:= (2\pi)^{-3l} (+2\mathfrak{R}) \sum_{\varepsilon_1,..., \varepsilon_l} \int_{\mathbb{R}^{3l}} \int_{u_1=0}^{+\infty} \int_{u_2=0}^{+\infty} \cdots \int_{u_l=0}^{+\infty} (-1)^{\varepsilon_1 + \cdots + \varepsilon_l} \\
&\quad \times \exp(i[(\mathbf{n} + \varepsilon_2 \mathbf{k}_2 + \cdots + \varepsilon_l \mathbf{k}_l)^2 - (\mathbf{n} + \mathbf{k}_1 + \varepsilon_2 \mathbf{k}_2 + \cdots + \varepsilon_l \mathbf{k}_l)^2]\, u_1 - \alpha u_1) \\
&\quad \times \exp(i[(\mathbf{n} + \varepsilon_3 \mathbf{k}_3 + \cdots + \varepsilon_l \mathbf{k}_l)^2 - (\mathbf{n} + \mathbf{k}_1 + \mathbf{k}_2 + \varepsilon_3 \mathbf{k}_3 + \cdots + \varepsilon_l \mathbf{k}_l)^2]\, u_1 - \alpha u_1) \\
&\quad \times \cdots \times \\
&\quad \times \exp(i[\mathbf{n}^2 - (\mathbf{n} + \mathbf{k}_1 + \cdots + \mathbf{k}_l)^2]\, u_l - \alpha u_l) \\
&\quad \times [i\hat{V}(\mathbf{k}_1)] \cdots [i\hat{V}(\mathbf{k}_l)] \times [i\hat{V}^*(\mathbf{k}_1 + \cdots + \mathbf{k}_l)] \\
&\quad \times \phi(t, \mathbf{n} + \varepsilon_1 \mathbf{k}_1 + \cdots + \varepsilon_l \mathbf{k}_l)\, d\mathbf{k}_1 \cdots d\mathbf{k}_l. \quad (3.30)
\end{aligned}$$

Also, the following estimate holds,

$$\lambda^{l+1} |\langle \rho_d^\alpha(t), {}^t Q_l^\alpha \phi \rangle| \leqslant \lambda^{l+1} C C_0^l\, \|\hat{V}(\mathbf{n})\|_{\mathscr{S}_{2D}}^{l+1}\, \|\phi\|_{\mathscr{S}_{2D}}, \quad (3.31)$$

for some universal constant C_0, together with some constant C of the form (3.9). The estimate (3.31) implies the convergence of the series (3.29), at least for λ small enough. Also, the estimate (3.31) together with the equation (3.29) imply that $\rho_d^\alpha(t)$ is actually uniformly (in α) bounded in the space,

$$C^1(\mathbb{R}_t^+; [\mathscr{S}_{2D}]^*\text{-weak*}),$$

so that the weak convergence $\rho_d^\alpha(t) \to \rho_d(t)$ also holds in $C^0(\mathbb{R}_t^+; [\mathscr{S}_{2D}]^*\text{-weak}^*)$.

Theorem 3.3 (Convergence as $\alpha \to 0$: Obtaining the Quantum Boltzmann equation). Let $\rho_d^\alpha(t)$ be as in Theorem 3.2 and define its weak limit $\rho_d(t)$ as stated in Theorem 3.1. Then the following holds,

(i) The following Boltzmann equation is satisfied,

$$\partial_t \rho_d(t, \mathbf{n}) = \sum_{l \geqslant 1} \lambda^{l+1} [Q_l \rho_d](t), \tag{3.32}$$

with initial datum,

$$\rho_d(t, \mathbf{n})|_{t=0} = \rho_d^0(\mathbf{n}), \tag{3.33}$$

where the collision operators Q_l are defined as,

$$\begin{aligned}
[Q_l \rho_d](t, \mathbf{n}) := (2\pi)^{-3l} (-2\Re) \sum_{\varepsilon_1,\dots,\varepsilon_l} \int_{\mathbb{R}^{3l}} \int_{u_1=0}^{+\infty} \int_{u_2=0}^{+\infty} \cdots \int_{u_l=0}^{+\infty} (-1)^{\tilde{\varepsilon}_1+\cdots+\tilde{\varepsilon}_l} \\
&\times \exp(i[(\mathbf{n}+\varepsilon_1 \mathbf{k}_1)^2 - (\mathbf{n}-\tilde{\varepsilon}_1 \mathbf{k}_1)^2]\, u_1) \\
&\times \cdots \times \\
&\times \exp(i[(\mathbf{n}+\varepsilon_1 \mathbf{k}_1 + \cdots + \varepsilon_l \mathbf{k}_l)^2 - (\mathbf{n}-\tilde{\varepsilon}_1 \mathbf{k}_1 - \cdots \tilde{\varepsilon}_l \mathbf{k}_l)^2]\, u_l) \\
&\times [i\hat{V}(\mathbf{k}_1)] \cdots [i\hat{V}(\mathbf{k}_l)] \times [i\hat{V}^*(\mathbf{k}_1 + \cdots + \mathbf{k}_l)] \\
&\times \rho_d(t, \mathbf{n}+\varepsilon_1 \mathbf{k}_1 + \cdots + \varepsilon_l \mathbf{k}_l)\, d\mathbf{k}_1 \cdots d\mathbf{k}_l.
\end{aligned} \tag{3.34}$$

Here, variables $\varepsilon_1,\dots, \varepsilon_l$ are as in Theorem 2.1. The Eqs. (3.32), (3.33) and (3.34) hold between distributions belonging to, say, $L^\infty(\mathbb{R}_t^+; [\mathscr{S}_{2D}]^*\text{-weak}^*)$.

(ii) Also, the leading term in the series (3.32) is,

$$\lambda^2 [Q_1 \rho_d](t, \mathbf{n}) = 2\pi\lambda^2 \int_{\mathbb{R}^3} \delta(\mathbf{k}^2 - \mathbf{n}^2)\, |\hat{V}(\mathbf{n}-\mathbf{k})|^2\, [\rho_d(t, \mathbf{k}) - \rho_d(t, \mathbf{n})]\, \frac{d\mathbf{k}}{(2\pi)^3}, \tag{3.35}$$

as predicted by the Fermi Golden Rule.

(iii) The Eq. (3.26) makes sense weakly, when tested against test functions $\phi(\mathbf{n}) \in \mathscr{S}_{2D}(\mathbb{R}^3)$. More precisely, for any such ϕ, we have,

$$\langle \partial_t \rho_d(t), \phi \rangle = \sum_{l \geqslant 0} \lambda^{l+1} \langle \rho_d(t), {}^t Q_l \phi \rangle, \tag{3.36}$$

where ${}^t Q_l \phi$ denotes the formal adjoint of Q_l (see (3.30)), and where the following estimate holds,

$$\lambda^{l+1}\, |\langle \rho_d(t),\, {}^t Q_l \phi \rangle| \leqslant \lambda^{l+1} C C_0^l\, \|\hat{V}(\mathbf{n})\|_{\mathscr{S}_{2D}}^{l+1}\, \|\phi\|_{\mathscr{S}_{2D}}, \tag{3.37}$$

for some universal constant C_0, together with some constant C of the form (3.9).

Remark. Firstly, Eqs. (3.26) and (3.32) are indeed of the form (1.2) and (1.3) respectively. Secondly, it can be proved that the full series in the potential which defines the cross-section in (3.32) is nothing else than the celebrated Born series. By this, we mean that the Eq. (3.32) can be put under the form,

$$\partial_t \rho_d(t, \mathbf{n}) = 2\pi \int_{\mathbb{R}^3} \delta(\mathbf{k}^2 - \mathbf{n}^2)\, b(\mathbf{k}, \mathbf{n}) [\rho_d(t, \mathbf{k}) - \rho_d(t, \mathbf{n})]\, d\mathbf{k}, \tag{3.38}$$

where the coefficient $b(\mathbf{k}, \mathbf{n})$ is given by the Born series,

$$b(\mathbf{k}, \mathbf{n}) = \lambda^2\, |\hat{V}|^2\, (\mathbf{n} - \mathbf{k}) - 2\lambda^3 \Im \int_{\mathbb{R}^3} \frac{\hat{V}(\mathbf{n} - \mathbf{k})\, \hat{V}(\mathbf{k} - \mathbf{k}')\, \hat{V}(\mathbf{k}' - \mathbf{n})}{\mathbf{k}'^2 - \mathbf{n}^2 + i0}\, d\mathbf{k}' + \cdots \tag{3.39}$$

This point is not obvious from the expression (3.34). The proof will be detailed in a future work [Ca2].

3.2. An Oscillatory Integral Estimate

Before turning to the proofs of the above theorems, we state the key estimate which allows to pass to the limit $L \to \infty$ *and* $\alpha \to 0$ in (2.8). This estimate allows to control the oscillations produced by the free Hamiltonian so as to recover the oscillatory integrals in Theorem 3.3 and in particular the Dirac mass in energy in formula (3.35) as $\alpha \to 0$. Also, since our method relies on the iteration of Duhamel's formula and leads therefore to oscillatory integrals in large dimensions, it allows to control the growth of the oscillatory integrals with the dimension. Both aspects are of key importance (see Remarks 2 and 3 later). This lemma heavily relies on the commutation structure $i\partial_t \tilde{\rho} = (-\Delta_x + \Delta_y)\, \tilde{\rho} + \cdots$ of the original Von-Neumann equation.

Lemma 3.1 (Oscillatory Integrals with quadratic phases in large dimensions). Let $\psi(\mathbf{n})$ satisfy $\psi \in L^\infty(\mathbb{R}^3)$. Then, the collision kernel $Q_l(\psi)(\mathbf{n})$ as defined in Theorem 3.3 is well defined and acts continuously on the Sobolev space $W^{4,\infty}(\mathbb{R}^3)$. More precisely, for any choice of the test function $\phi \in W^{4,\infty}(\mathbb{R}^3)$, and for any choice of $\varepsilon := (\varepsilon_1,..., \varepsilon_l)$ as in Theorem 2.1, we have,

(i) The following oscillatory integral makes sense,

$$\begin{aligned}\langle {}^{\varepsilon}Q_l(\psi), \phi\rangle := \int_{u_1=0}^{+\infty} \cdots \int_{u_l=0}^{+\infty} \int_{\mathbb{R}^{3(l+1)}} & \exp(i[(\mathbf{n}+\varepsilon_1\mathbf{k}_1)^2-(\mathbf{n}-\tilde{\varepsilon}_1\mathbf{k}_1)^2]\, u_1) \\ & \times \exp(i[(\mathbf{n}+\varepsilon_1\mathbf{k}_1+\varepsilon_2\mathbf{k}_2)^2-(\mathbf{n}-\tilde{\varepsilon}_1\mathbf{k}_1-\tilde{\varepsilon}_2\mathbf{k}_2)^2]\, u_2) \\ & \times \cdots \times \\ & \times \exp(i[(\mathbf{n}+\varepsilon_1\mathbf{k}_1+\cdots+\varepsilon_l\mathbf{k}_l)^2-(\mathbf{n}-\tilde{\varepsilon}_1\mathbf{k}_1-\cdots-\tilde{\varepsilon}_l\mathbf{k}_l)^2]\, u_l) \\ & \times \hat{V}(\mathbf{k}_1)\, \hat{V}(\mathbf{k}_2) \cdots \hat{V}(\mathbf{k}_l)\, \hat{V}^*(\mathbf{k}_1+\cdots+\mathbf{k}_l) \\ & \times \psi(\mathbf{n}+\varepsilon_1\mathbf{k}_1+\cdots+\varepsilon_l\mathbf{k}_l)\, \phi(\mathbf{n})\, d\mathbf{n}\, d\mathbf{k}_1 \cdots d\mathbf{k}_l\, du_1 \cdots du_l.\end{aligned}$$

(ii) Moreover, the integral defining $\langle {}^{\varepsilon}Q_l(\psi), \phi\rangle$ converges *absolutely* in the variables $u_1,..., u_l$. In particular,

$$\begin{aligned}&\lim_{\alpha\to 0^+} \langle {}^{\varepsilon}Q_l^{\alpha}(\psi), \phi\rangle \\ &:= \lim_{\alpha\to 0^+} \int_{u_1=0}^{+\infty} \cdots \int_{u_l=0}^{+\infty} \int_{\mathbb{R}^{3(l+1)}} \exp(i[(\mathbf{n}+\varepsilon_1\mathbf{k}_1)^2-(\mathbf{n}-\tilde{\varepsilon}_1\mathbf{k}_1)^2]\, u_1-\alpha u_1) \times \cdots \times \\ &\quad \times \exp(i[(\mathbf{n}+\varepsilon_1\mathbf{k}_1+\cdots+\varepsilon_l\mathbf{k}_l)^2-(\mathbf{n}-\tilde{\varepsilon}_1\mathbf{k}_1-\cdots-\tilde{\varepsilon}_l\mathbf{k}_l)^2]\, u_l-\alpha u_l) \\ &\quad \times \hat{V}(\mathbf{k}_1) \cdots \hat{V}(\mathbf{k}_l)\, \hat{V}^*(\mathbf{k}_1+\cdots+\mathbf{k}_l)\, \psi(\mathbf{n}+\varepsilon_1\mathbf{k}_1+\cdots+\varepsilon_l\mathbf{k}_l)\, \phi(\mathbf{n}) \\ &= \langle {}^{\varepsilon}Q_l(\psi), \phi\rangle.\end{aligned}$$

(iii) Finally, the following exponential bound holds, for some universal constant C_0,

$$|\langle {}^{\varepsilon}Q_l(\psi), \phi\rangle| \leqslant C_0^l\, \|\hat{V}\|_{W^{8,1}(\mathbb{R}^3)}^{l+1}\, \|\psi\|_{L^{\infty}(\mathbb{R}^3)}\, \|\phi\|_{W^{4,\infty}(\mathbb{R}^3)}, \tag{3.40}$$

and the same bound (with a different absolute constant) obviously holds for $\langle Q_l(\psi), \phi\rangle$ as well, since $Q_l = \sum_{\varepsilon} {}^{\varepsilon}Q_l$, where the sum carries over all possible sequences ε.

Remarks. 1. The method of proof given below allows to establish various estimates of the same kind than (3.40). For instance, we may mention without proof the estimate,

$$|\langle {}^{\varepsilon}Q_l(\psi), \phi\rangle| \leqslant C_0^l \, \|\hat{V}\|^{l+1}_{W^{8,1}(\mathbb{R}^3) \cap W^{8,\infty}(\mathbb{R}^3)} \, \|\psi\|_{\mathscr{M}_b(\mathbb{R}^3)} \, \|\phi\|_{W^{4,\infty}(\mathbb{R}^3)}, \tag{3.41}$$

where $\mathscr{M}_b$ stands for the space of bounded measures.

2. The idea of the proof is the following: all the above quantities are of the form,

$$\int_{\mathbb{R}^{3(l+1)}} \int_{u_1,\dots,u_l=0}^{+\infty} \exp[iq_{u_1,\dots,u_l}(\mathbf{x})] \, \Phi(\mathbf{x}) \, d\mathbf{x} \, du_1 \cdots du_l, \tag{3.42}$$

where $q_{u_1,\dots,u_l}(\mathbf{x})$ is a quadratic form in $\mathbf{x}$, whose coefficients depend on $u_1,\dots, u_l$, and the difficulty stems from the need to integrate (3.42) up to $u_1 = \cdots = u_l = \infty$. By the stationnary phase formula, we know that the quantity $\int \exp[iq_{u_1,\dots,u_l}(\mathbf{x})] \, \Phi(\mathbf{x}) \, d\mathbf{x}$ decays like $|\det(q_{u_1,\dots,u_l})|^{-1/2}$ at infinity as a function of the u-variables, at least if the function Φ is sufficiently smooth. Hence the control of quantities like (3.42) reduces to controlling that $\det(q_{u_1,\dots,u_l})$ grows fast enough at infinity, as well as to controlling the number of derivatives needed by the use of the stationnary phase formula.

3. The bound (3.40) is important in two respects. Firstly, the left-hand-side is uniformly bounded using a *fixed* (independent of l) number of derivatives in $\hat{V}$, ϕ, although the singularity created by the oscillatory exponentials apparently grows with l. In other words, the oscillatory integrals above do not act as *iterated* derivatives on ϕ, but rather as distributions of *fixed* order. Secondly, the constant involved in (3.40) grows geometrically with l. Both points are crucial since the case of iterated derivatives could lead to a growth of $\langle {}^{\varepsilon}Q_l(\psi), \phi\rangle$ like $l!$ (hence to diverging series).

4. Up to some change of variables, one can see this lemma as a definition of distributions like,

$$(\mathbf{n}^2 - \mathbf{k}_1^2 + i0)^{-1} \times (\mathbf{n}^2 - \mathbf{k}_2^2 + i0)^{-1} \times \cdots \times (\mathbf{n}^2 - \mathbf{k}_l^2 + i0)^{-1} \tag{3.43}$$

in $\mathscr{D}'(\mathbb{R}^{3(l+1)})$. Indeed, Lemma 3.1 should be compared with the well-known formula, valid in $\mathscr{D}'(\mathbb{R})$,

$$\int_{s=0}^{+\infty} \exp(is\mathbf{x}) \, ds = +\pi\delta(\mathbf{x}) + iv.p.(1/\mathbf{x}) = -i(\mathbf{x}+i0)^{-1}.$$

However, the definition of distributions like (3.43) *is not* in general a consequence of the usual theorems about the prolongation and composition of homogeneous distributions (see [Hö]), nor it is a consequence of the usual theorems about the composition and products of distribution with "well-behaved" wave-fronts. This is due to the fact that the singularity near the origin $\mathbf{n}^2 = \mathbf{k}_1^2 = \cdots = \mathbf{k}_l^2 = 0$ and near all the axes is too severe. In particular, the definition of such distributions a priori involves *products* of Dirac masses, a forbidden operation. The above lemma shows that this is fortunately not the case, and this relies on the fact that the $+i0$ and $-i0$ occur at the right places due to the specific commutator structure of the original equation (see (4.20) and the last step of the proof of this lemma). This is *formally* in analogy with the well-known fact that the distribution $(\mathbf{x}+i0)^{-2}$ is well-defined, whereas the product $(\mathbf{x}+i0)^{-1}(\mathbf{x}-i0)^{-1}$ does not make sense.

5. In the particular case $l = 1$, we can identify the oscillatory integrals as,

$$\Re \int_{u=0}^{+\infty} \int_{\mathbb{R}^6} \exp(i[\mathbf{n}^2-\mathbf{k}^2]\, u)\, \psi(\mathbf{n}, \mathbf{k})\, d\mathbf{n}\, d\mathbf{k}\, du = \pi \int_{\mathbb{R}^6} \delta(\mathbf{n}^2-\mathbf{k}^2)\, \psi(\mathbf{n}, \mathbf{k})\, d\mathbf{n}\, d\mathbf{k}, \tag{3.44}$$

where the distribution $\delta(\mathbf{n}^2-\mathbf{k}^2)$ has the usual meaning (see [Hö]).

5. The proof below goes through when the variables $\mathbf{n}$, $\mathbf{k}_1$, etc. in Lemma 3.1 belong to the d-dimensional space $\mathbb{R}^d$, *for any dimension* $d \geqslant 3$ (see (4.25)), up to replacing $\|\widehat{V}\|_{W^{8,1}(\mathbb{R}^3)}$ by $\|\widehat{V}\|_{W^{2(d+1),1}(\mathbb{R}^d)}$, and $\|\phi\|_{W^{4,\infty}(\mathbb{R}^3)}$ by $\|\phi\|_{W^{d+1,\infty}(\mathbb{R}^d)}$. We mention in passing the obvious imbedding $\mathcal{S}_8(\mathbb{R}^3) \subset W^{8,1}(\mathbb{R}^3)$.

4. PROOFS

4.1. Proof of Lemma 2.1: Positivity of the Density Matrix

Equation (2.5) is linear. For fixed time, we can obviously bound the $l^2(\mathbb{Z}^6_{n,p})$-norm of the right-hand-side of (2.5) by,

$$\|\cdots\|_{l^2} \leqslant 2\, \|(2\pi L)^{-3}\, \widehat{V}(k/L)\|_{l^1(\mathbb{Z}^3_k)}\, \|\rho(t, n, p)\|_{l^2(\mathbb{Z}^6_{n,p})},$$

The quantity $\|(2\pi L)^{-3}\, \widehat{V}(k/L)\|_{l^1(\mathbb{Z}^3_k)}$ is obviously bounded for fixed L if V satisfies (2.2). Also the l^2-norm of $\rho(t, n, p)|_{t=0}$ is bounded initially. Indeed,

$$\|\rho(t, n, p)|_{t=0}\|_{l^2_{n,p}} \leqslant \|(2\pi L)^{-3}\, \rho^0_d(n/L)\|_{l^2_n},$$

and this last quantity is bounded for fixed L since ρ_d^0 decays nicely (assumption (2.10)). All this clearly proves the first part of the lemma (existence and uniqueness in $C^0(l^2)$).

The second part of the lemma is proved by observing that the system (2.8) is of Linblad-form. More precisely, let $\tilde{\rho}(t, x, y)$ be the inverse Fourier transform of $\rho(t, n, p)$. Then $\tilde{\rho}$ satisfies,

$$T^{-1}\partial_t\tilde{\rho}(t, x, y) = -i(-\Delta_x + \Delta_y)\,\tilde{\rho}(t, x, y) \\ -i\lambda(V(x) - V(y))\,\tilde{\rho}(t, x, y) + \alpha F(\tilde{\rho})(t, x, y), \qquad (4.1)$$

where the linear operator F reads,

$$F(\tilde{\rho}) = \tfrac{1}{2}\sum_{n \in \mathbb{Z}} 2L_n\tilde{\rho}L_n^* - L_n^*L_n\tilde{\rho} - \tilde{\rho}L_n^*L_n, \qquad (4.2)$$

up to defining the linear operators L_n, and their hermite-conjugates L_n^*, acting on $L^2([0, 2\pi L]^3)$, as,

$$L_n(x, y) = \frac{\exp(inx/L)}{(2\pi L)^{3/2}} \times \frac{\exp(-iny/L)}{(2\pi L)^{3/2}},$$

i.e., to each function $\phi(x) \in L^2([0; 2\pi L]^3)$, L_n associates,

$$(L_n\phi)(x) := \int_{y \in [0;\, 2\pi L]^3} L_n(x, y)\,\phi(y)\,dy.$$

We clearly have $L_n = L_n^*$. Note that we do not give any details about the problems of convergence in the series defining F. We leave the simple limiting argument to the reader, which involves a truncated sum and then goes to the infinite series defining F. The proof of (4.2) is obtained by observing that (here, $\mathscr{F}$ denotes Fourier transform on the Torus $(\mathbb{R}/2\pi L)^3$),

$$\begin{aligned} F(\tilde{\rho})(t, x, y) &= -\mathscr{F}^{-1}[\rho(t, n, p)\,\mathbf{1}(n \neq p)] \\ &= \mathscr{F}^{-1}[\rho(t, n, p)\,\mathbf{1}(n = p) - \rho(t, n, p)] \\ &= \sum_n L_n(x, y) \int_{(a, b) \in \mathbb{R}^6} L_n(b, a)\,\tilde{\rho}(t, a, b)\,da\,db - \tilde{\rho}(t, x, y), \end{aligned}$$

and formula (4.2) follows.

This proves that equation (4.1) (or: (2.8)) is of Lindblad form, and in particular, the density matrix $\tilde{\rho}$ remains positive (as an operator) for all non-negative values of time [Li]. This implies the non-negativity of ρ_d for $t \geqslant 0$. The hermitianity is easily seen by uniqueness. ▌

4.2. Proof of Theorem 2.1: A Closed Equation on the Diagonal Part of the Density Matrix

We follow the computations in [Ca1].

First Step. *Getting an Abstract Equation for* $\rho_d^{L,\alpha}$

We first rewrite the original system (2.8) on $\rho_{nd}^{L,\alpha}$, $\rho_d^{L,\alpha}$ in the following form,

$$\partial_t \rho_{nd}^{L,\alpha}(t,n,p) = +i\,\frac{n^2-p^2}{L^2}\,\rho_{nd}^{L,\alpha} + -\alpha\rho_{nd}^{L,\alpha}$$

$$+(A\rho_d^{L,\alpha})(t,n,p)+(B\rho_{nd}^{L,\alpha})(t,n,p), \tag{4.3}$$

$$\partial_t \rho_d^{L,\alpha}(t,n,p) = (B\rho_{nd}^{L,\alpha})(t,n,n), \tag{4.4}$$

where we have introduced the following notations,

$$\begin{cases} (A\rho_d^{L,\alpha})(t,n,p) = +\dfrac{i\lambda T}{(2\pi L)^3}\,\hat{V}\left(\dfrac{p-n}{L}\right)[\rho_d^{L,\alpha}(t,p)-\rho_d^{L,\alpha}(t,n)], \\ (B\rho_{nd}^{L,\alpha})(t,n,p) \\ \quad = +\dfrac{i\lambda T}{(2\pi L)^3}\displaystyle\sum_{k\neq p}\left[\hat{V}\left(\dfrac{k-n}{L}\right)\rho_{nd}^{L,\alpha}(t,k,p)-\hat{V}\left(\dfrac{p-k}{L}\right)\rho_{nd}^{L,\alpha}(t,n,k)\right]. \end{cases} \tag{4.5}$$

Now, we first use (4.3) in order to compute $\rho_{nd}^{L,\alpha}$ as an explicit function of $\rho_d^{L,\alpha}$, and then insert the corresponding formula for $\rho_{nd}^{L,\alpha}$ into the right-hand-side of (4.4). For that purpose, we introduce the following operator,

$$(S\rho_{nd}^{L,\alpha})(t,n,p) = \int_0^{Tt}\exp\left(+i\,\frac{n^2-p^2}{L^2}\,s-\alpha s\right)\rho_{nd}^{L,\alpha}(t-T^{-1}s,n,p)\,ds, \tag{4.6}$$

and the same formula when $\rho_{nd}^{L,\alpha}$ is replaced by any function $v(t,n,p)$. Obviously here S stands for "Schrödinger," since for any function $v(t,n,p)$, the associated function $(Sv)(t,n,p) := w(t,n,p)$ is the unique solution to the equation,

$$\begin{cases} T^{-1}\partial_t w(t,n,p) = +i\,\dfrac{n^2-p^2}{L^2}\,w(t,n,p)-\alpha w(t,n,p)+v(t,n,p), \\ w(t=0,n,p)=0. \end{cases}$$

With these notations, we easily integrate (4.3), using the fact that $\rho_{nd}^{L,\alpha}$ vanishes initially, and obtain,

$$\rho_{nd}^{L,\alpha}(t, n, p) = (SA\rho_d^{L,\alpha})(t, n, p) + (SB\rho_{nd}^{L,\alpha})(t, n, p). \tag{4.7}$$

Therefore, iterating this formula gives the following Neumann series for $\rho_{nd}^{L,\alpha}$,

$$\rho_{nd}^{L,\alpha}(t, n, p) = \sum_{l=0}^{+\infty} ([SB]^l (SA\rho_d^{L,\alpha}))(t, n, p). \tag{4.8}$$

We now insert this expression into the equation (4.4), and obtain,

$$\partial_t \rho_d^{L,\alpha}(t, n) = \sum_{l=0}^{+\infty} (B[SB]^l (SA\rho_d^{L,\alpha}))(t, n, n) = \sum_{l=1}^{+\infty} ([BS]^l (A\rho_d^{L,\alpha}))(t, n, n). \tag{4.9}$$

This is the abstract form of Theorem 2.1. Obviously, we have used here the fact that $\partial_t \rho_d^{L,\alpha}$ depends on $\rho_{nd}^{L,\alpha}$ only in (4.4) (see above).

Second Step. *Getting an Explicit Equation on* $\rho_d^{L,\alpha}$

It remains now to translate (4.9) into a more explicit formula. For that purpose, we rewrite the definition of the operator B (see (4.5)) into the following form,

$$\begin{aligned}(B\rho_{nd}^{L,\alpha})(t, n, p) &= +\frac{i\lambda T}{(2\pi L)^3} \sum_{k_1} \hat{V}\left(\frac{k_1}{L}\right) [\rho_{nd}^{L,\alpha}(t, n+k_1, p)\, \mathbf{1}(n+k_1 \neq p) \\ &\quad - \rho_{nd}^{L,\alpha}(t, n, p-k_1)\, \mathbf{1}(n \neq p-k_1)] \\ &= \frac{\lambda T}{(2\pi L)^3} \sum_{\varepsilon_1, k_1} (-1)^{\tilde{\varepsilon}_1} \left[i\hat{V}\left(\frac{k_1}{L}\right)\right] \rho_{nd}^{L,\alpha}(t, n+\varepsilon_1 k_1, p-\tilde{\varepsilon}_1 k_1) \\ &\quad \times \mathbf{1}(n+\varepsilon_1 k_1 \neq p-\tilde{\varepsilon}_1 k_1).\end{aligned} \tag{4.10}$$

Here, the same convention as in Theorem 2.1 has been used, namely,

$$\varepsilon_1 = 0 \quad \text{or} \quad 1, \qquad \tilde{\varepsilon}_1 = 1 - \varepsilon_1.$$

We iterate formula (4.10), and use (4.6), in order to compute the explicit value of each term $[BS]^l (A\rho_d^{L,\alpha})(t, n, n)$ in (4.9). This easily gives,

$$\partial_t \rho_d^{L,\alpha}(t, n) = \sum_{l=1}^{+\infty} (Q'_l \rho_d^{L,\alpha})(t, n), \tag{4.11}$$

with,

$$
\begin{aligned}
&(Q'_l \rho_d^{L,\alpha})(t,n)\\
&\quad = T\left[\frac{\lambda}{(2\pi L)^3}\right]^{(l+1)} \sum_{\varepsilon_1,\dots,\varepsilon_l} \sum_{k_1,\dots,k_l} \int_{u_1,\dots,u_l} (-1)^{\tilde{\varepsilon}_1+\cdots+\tilde{\varepsilon}_l}\\
&\qquad \times \exp\left(i\,\frac{(n+\varepsilon_1 k_1)^2-(n-\tilde{\varepsilon}_1 k_1)^2}{L^2}\,u_1-\alpha u_1\right)\\
&\qquad \times \exp\left(i\,\frac{(n+\varepsilon_1 k_1+\varepsilon_2 k_2)^2-(n-\tilde{\varepsilon}_1 k_1-\tilde{\varepsilon}_2 k_2)^2}{L^2}\,u_2-\alpha u_2\right)\\
&\qquad \times \cdots \times \exp\left(i\,\frac{(n+\varepsilon_1 k_1+\cdots+\varepsilon_l k_l)^2-(n-\tilde{\varepsilon}_1 k_1-\cdots-\tilde{\varepsilon}_l k_l)^2}{L^2}\,u_l-\alpha u_l\right)\\
&\qquad \times \left[i\hat{V}\left(\frac{k_1}{L}\right)\right]\left[i\hat{V}\left(\frac{k_2}{L}\right)\right]\cdots\left[i\hat{V}\left(\frac{k_l}{L}\right)\right]\times\left[i\hat{V}\left(-\frac{k_1+k_2+\cdots k_l}{L}\right)\right]\\
&\qquad \times [\rho_d^{L,\alpha}(t-T^{-1}(u_1+u_2+\cdots+u_l), n-\tilde{\varepsilon}_1 k_1-\tilde{\varepsilon}_2 k_2-\cdots-\tilde{\varepsilon}_l k_l)\\
&\qquad - \rho_d^{L,\alpha}(t-T^{-1}(u_1+u_2+\cdots+u_l), n+\varepsilon_1 k_1+\varepsilon_2 k_2+\cdots+\varepsilon_l k_l)].
\end{aligned}
\tag{4.12}
$$

On the more, iterating also (4.6), and the characteristic function $\mathbf{1}(n+\varepsilon_1 k_1 \neq p-\tilde{\varepsilon}_1 k_1)$ appearing in (4.10), we easily observe that the sums $\sum_{\varepsilon_1,\dots,\varepsilon_l}\sum_{k_1,\dots,k_l}$ and integrals $\int_{u_1,\dots,u_l}$ in (4.12), carry over the sets (2.14), (2.15), (2.16) given in Theorem 2.1.

Last Step. *Getting the Theorem*

As a last step, we finally transform (4.12) into the form (2.12), (2.13) given in Theorem 2.1. We first observe that, due to the factor $[\rho_d^{L,\alpha}(t-T^{-1}(u_1+\cdots), n-\tilde{\varepsilon}_1 k_1-\cdots)-\rho_d^{L,\alpha}(t-T^{-1}(u_1+\cdots), n+\varepsilon_1 k_1+\cdots)]$ in (4.12), the term $Q'_l\rho_d^{L,\alpha}$ naturally splits into two terms,

$$Q'_l\rho_d^{L,\alpha} = Q_l^{(1)}\rho_d^{L,\alpha} - Q_l^{(2)}\rho_d^{L,\alpha}, \tag{4.13}$$

using the obvious notation. On the other hand, due to (2.2), V is real-valued, so that,

$$\forall k, \qquad \hat{V}(-k) = \hat{V}^*(k),$$

and we are able to replace in (4.12),

$$\hat{V}\left(-\frac{k_1+k_2+\cdots k_l}{L}\right) = \hat{V}^*\left(\frac{k_1+k_2+\cdots k_l}{L}\right).$$

This, together with the fact that $\rho_d^{L,\alpha}$ is real-valued (see Lemma 2.1), yields,

$$
\begin{aligned}
&(Q_l^{(1)}\rho_d^{L,\alpha})(t,n)\\
&:= T\left[\frac{\lambda}{(2\pi L)^3}\right]^{(l+1)} \sum_{\varepsilon_1,\dots,\varepsilon_l}\sum_{k_1,\dots,k_l}\int_{u_1,\dots,u_l}(-1)^{\tilde\varepsilon_1+\tilde\varepsilon_2+\cdots+\tilde\varepsilon_l}\\
&\quad\times\exp\left(i\,\frac{(n+\varepsilon_1k_1)^2-(n-\tilde\varepsilon_1k_1)^2}{L^2}\,u_1-\alpha u_1\right)\\
&\quad\times\exp\left(i\,\frac{(n+\varepsilon_1k_1+\varepsilon_2k_2)^2-(n-\tilde\varepsilon_1k_1-\tilde\varepsilon_2k_2)^2}{L^2}\,u_2-\alpha u_2\right)\\
&\quad\times\cdots\times\\
&\quad\times\exp\left(i\,\frac{(n+\varepsilon_1k_+\cdots+\varepsilon_lk_l)^2-(n-\tilde\varepsilon_1k_1-\cdots-\tilde\varepsilon_lk_l)^2}{L^2}\,u_l-\alpha u_l\right)\\
&\quad\times\left[i\hat V\left(\frac{k_1}{L}\right)\right]\left[i\hat V\left(\frac{k_2}{L}\right)\right]\cdots\left[i\hat V\left(\frac{k_l}{L}\right)\right]\times\left[i\hat V^*\left(\frac{k_1+k_2+\cdots k_l}{L}\right)\right]\\
&\quad\times\rho_d^{L,\alpha}(t-T^{-1}(u_1+u_2+\cdots+u_l),\,n-\tilde\varepsilon_1k_1-\tilde\varepsilon_2k_2-\cdots-\tilde\varepsilon_lk_l)
\end{aligned}
$$

$= $ (perform the change of variables $\tilde\varepsilon_j\to\varepsilon_j$, and $k_j\to -k_j$, for all $1\leqslant j\leqslant l$, and use $\hat V(-k)=\hat V^*(k)$),

$$
\begin{aligned}
&= -\Bigg(T\left[\frac{\lambda}{(2\pi L)^3}\right]^{(l+1)} \sum_{\varepsilon_1,\dots,\varepsilon_l}\sum_{k_1,\dots,k_l}\int_{u_1,\dots,u_l}(-1)^{\tilde\varepsilon_1+\tilde\varepsilon_2+\cdots+\tilde\varepsilon_l}\\
&\quad\times\exp\left(i\,\frac{(n+\varepsilon_1k_1)^2-(n-\tilde\varepsilon_1k_1)^2}{L^2}\,u_1-\alpha u_1\right)\\
&\quad\times\exp\left(i\,\frac{(n+\varepsilon_1k_1+\varepsilon_2k_2)^2-(n-\tilde\varepsilon_1k_1-\tilde\varepsilon_2k_2)^2}{L^2}\,u_2-\alpha u_2\right)\\
&\quad\times\cdots\times\\
&\quad\times\exp\left(i\,\frac{(n+\varepsilon_1k_1+\cdots+\varepsilon_lk_l)^2-(n-\tilde\varepsilon_1k_1-\cdots-\tilde\varepsilon_lk_l)^2}{L^2}\,u_l-\alpha u_l\right)\\
&\quad\times\left[i\hat V\left(\frac{k_1}{L}\right)\right]\left[i\hat V\left(\frac{k_2}{L}\right)\right]\cdots\left[i\hat V\left(\frac{k_l}{L}\right)\right]\times\left[i\hat V^*\left(\frac{k_1+k_2+\cdots k_l}{L}\right)\right]\\
&\quad\times\rho_d^{L,\alpha}(t-T^{-1}(u_1+u_2+\cdots+u_l),\,n+\varepsilon_1k_1+\varepsilon_2k_2+\cdots+\varepsilon_lk_l)\Bigg)^*\\
&= -(Q_l^{(2)}\rho_d^{L,\alpha}(t,n))^*.
\end{aligned}
$$

Therefore, equation (4.12) has the form,

$$\partial_t \rho_d^{L,\alpha} = \sum_{l=1}^{+\infty} Q'_l \rho_d^{L,\alpha} = \sum_{l=1}^{+\infty} Q_l^{(1)} \rho_d^{L,\alpha} - Q_l^{(2)} \rho_d^{L,\alpha} = \sum_{l=1}^{+\infty} -(Q_l^{(2)} \rho_d^{L,\alpha})^* - Q_l^{(2)} \rho_d^{L,\alpha}$$

$$= -2\Re \sum_{l=1}^{+\infty} Q_l^{(2)} \rho_d^{L,\alpha}.$$

This is exactly the formula given in Theorem 2.1. This ends the proof. ∎

4.3. Proof of Lemma 3.1: Controlling Oscillatory Integrals

The proof is given in three steps.

First Step. *Changing Variables*

Let us look at the first exponential in Lemma 3.1. If $\varepsilon_1 = 0$, its argument involves the quantity $\mathbf{n}^2 - (\mathbf{n} - \mathbf{k}_1)^2$, in which case one should change variables $\mathbf{N} = \mathbf{n}$, $\mathbf{K}_1 = \mathbf{n} - \mathbf{k}_1$, and the exponential becomes,

$$\exp(i[\mathbf{N}^2 - \mathbf{K}_1^2]\, u_1). \tag{4.14}$$

On the other hand, if $\varepsilon_1 = 1$, the argument in the first exponential is $(\mathbf{n} + \mathbf{k}_1)^2 - \mathbf{n}^2$, and one should change variables $\mathbf{N} = \mathbf{n}$, $\mathbf{K}_1 = \mathbf{n} + \mathbf{k}_1$ and get,

$$\exp(i[\mathbf{K}_1^2 - \mathbf{N}^2]\, u_1). \tag{4.15}$$

In order to fix the ideas, let us consider we are in the case $\varepsilon_1 = 0$.

We now come to the second exponential. If $\varepsilon_2 = 0$, we change variables, $\mathbf{K}_2 = \mathbf{n} - \mathbf{k}_1 - \mathbf{k}_2$, and the first two exponentials give,

$$\exp(i[\mathbf{N}^2 - \mathbf{K}_1^2]\, u_1) \exp(i[\mathbf{N}^2 - \mathbf{K}_2^2]\, u_2), \tag{4.16}$$

while in the case $\varepsilon_2 = 1$, we come up against the change of variables $\mathbf{K}_2 = \mathbf{n} + \mathbf{k}_2$ and obtain,

$$\exp(i[\mathbf{N}^2 - \mathbf{K}_1^2]\, u_1) \exp(i[\mathbf{K}_2^2 - \mathbf{K}_1^2]\, u_2). \tag{4.17}$$

Proceeding further gives therefore the following typical product of exponentials, say,

$$\begin{aligned}
&\exp(i[\mathbf{N}^2-\mathbf{K}_1^2]\,u_1)\exp(i[\mathbf{K}_2^2-\mathbf{K}_1^2]\,u_2)\\
&\qquad\times\exp(i[\mathbf{K}_3^2-\mathbf{K}_1^2]\,u_3)\exp(i[\mathbf{K}_3^2-\mathbf{K}_4^2]\,u_4)\cdots\\
&\quad=\exp(+i\mathbf{N}^2u_1)\exp(-i\mathbf{K}_1^2[u_1+u_2+u_3])\exp(+i\mathbf{K}_2^2u_2)\\
&\qquad\times\exp(+i\mathbf{K}_3^2[u_3+u_4])\exp(-i\mathbf{K}_4^2u_4)\;\cdots.
\end{aligned}\tag{4.18}$$

Now let us decribe this procedure in the general case.

The linear change of coordinates needed in this approach obviously depends on the values of $\varepsilon_1,\ldots,\ \varepsilon_l$ in $\langle {}^{\varepsilon}Q_l(\psi),\phi\rangle$, but its Jacobian has always the value ± 1 (its matrix is a triangle with ± 1 on the diagonal). Actually, the exact value of this linear change of variables is in any case,

$$\begin{aligned}
&\mathbf{N}=\mathbf{n},\\
&\mathbf{K}_1=\mathbf{n}+\varepsilon_1\mathbf{k}_1\quad\text{if } \varepsilon_1=1,\ \mathbf{n}-\tilde{\varepsilon}_1\mathbf{k}_1\ \text{ else},\\
&\mathbf{K}_2=\mathbf{n}+\varepsilon_1\mathbf{k}_1+\varepsilon_2\mathbf{k}_2\quad\text{if } \varepsilon_2=1,\ \mathbf{n}-\tilde{\varepsilon}_1\mathbf{k}_1-\tilde{\varepsilon}_2\mathbf{k}_2\ \text{ else},\\
&\quad\vdots\\
&\mathbf{K}_l=\mathbf{n}+\varepsilon_1\mathbf{k}_1+\varepsilon_2\mathbf{k}_2+\cdots++\varepsilon_l\mathbf{k}_l\quad\text{if } \varepsilon_l=1,\ \mathbf{n}-\tilde{\varepsilon}_1\mathbf{k}_1-\tilde{\varepsilon}_2\mathbf{k}_2-\tilde{\varepsilon}_l\mathbf{k}_l\ \text{ else}.
\end{aligned}\tag{4.19}$$

Also, and in any case, the change of variables (4.19) transforms the oscillatory exponentials $\exp\{iu_1[(\mathbf{n}+\varepsilon_1\mathbf{k}_1)^2-(\mathbf{n}+\tilde{\varepsilon}_1\mathbf{k}_1)^2]\}\cdots$ in the old variables into the following typical oscillating exponential in the new variables,

$$\begin{aligned}
&\exp\{i[\pm\mathbf{N}^2(u_1+u_2+u_3)\pm\mathbf{K}_1^2u_1\pm\mathbf{K}_2^2u_2\pm\mathbf{K}_3(u_3+u_4+u_5)\\
&\qquad\pm\mathbf{K}_4^2u_4\pm\mathbf{K}_5^2(u_5+u_6)\cdots]\},
\end{aligned}\tag{4.20}$$

or, in a more abstract form,

$$\begin{aligned}
&\exp\left\{i\left[\ \pm\mathbf{N}^2(u_1+\cdots+u_{i_0})+\sum_{i=1}^{i_0-1}\ \pm\mathbf{K}_i^2u_i\right.\right.\\
&\qquad\left.\left.\pm\mathbf{K}_{i_0}^2(u_{i_0}+\cdots+u_{i_1})+\sum_{i=i_0+1}^{i_1-1}\ \pm\mathbf{K}_i^2u_i\pm\mathbf{K}_{i_1}^2(u_{i_1}+\cdots+u_{i_2})+\cdots\right]\right\},
\end{aligned}\tag{4.21}$$

for some indices $1\leqslant i_0\leqslant i_1\leqslant\cdots$ depending on the exact value of the ε's, and where the signs $\pm$ in (4.20)–(4.21) have some unimportant value, depending on the ε's as well.

We have now described the effect of the change of variables (4.19) on the oscillating exponentials appearing in the definition of $\langle {}^{\varepsilon}Q_l(\psi),\phi\rangle$.

Before ending this first step, we now mention the effect of this change of variables on the function $\hat{V}(\mathbf{k}_1)\cdots\hat{V}(\mathbf{k}_l)\,\hat{V}^*(\mathbf{k}_1+\cdots+\mathbf{k}_l)\,\psi(\mathbf{n}+\varepsilon_1\mathbf{k}_1+\cdots+\varepsilon_l\mathbf{k}_l)\,\phi(\mathbf{n})$ appearing in $\langle{}^{\varepsilon}Q_l(\psi),\phi\rangle$. It is straightforward to see that this function becomes, in the new variables,

$$\hat{V}(\mathbf{N}-\mathbf{K}_1)\,\hat{V}(\mathbf{K}_1-\mathbf{K}_2)\cdots\hat{V}(\mathbf{K}_{l-1}-\mathbf{K}_l)\,\hat{V}(\mathbf{K}_l-\mathbf{N})\,\psi(\mathbf{N})\,\phi(\mathbf{N}), \tag{4.22}$$

if $\varepsilon=(\varepsilon_1,\ldots,\varepsilon_l)=(0,\ldots,0)$ (this is the so-called "gain-term" in the full collision kernel $Q_l=\sum_{\varepsilon}{}^{\varepsilon}Q_l$). If $\varepsilon\neq(0,\ldots,0)$ (the "loss"-terms), we recover the typical value (say),

$$\hat{V}(\mathbf{N}-\mathbf{K}_1)\,\hat{V}(\mathbf{N}-\mathbf{K}_2)\,\cdots\hat{V}(\mathbf{K}_{l-1}-\mathbf{K}_l)\,\hat{V}^*(\mathbf{K}_a-\mathbf{K}_l)\,\psi(\mathbf{K}_a)\,\phi(\mathbf{N}), \tag{4.23}$$

for some value of the index a, where, as in the gain term, each of the variables $\mathbf{N}$, $\mathbf{K}_1,\ldots,\mathbf{K}_l$ appear *twice* as the argument of the function $\hat{V}$, and amongst these variables, one (and only one) of them appears also as the argument of the test function ψ.

Again, the exact values of the indices in formula (4.23) depend on the exact value of the sequence ε, but the above described structure is present for any ε.

Second Step. *Proving the Lemma when $\varepsilon_1=\varepsilon_2=\cdots=\varepsilon_l=0$—The Gain Term*

We are now led to studying the convergence of the integrals $\langle{}^{\varepsilon}Q_l(\psi),\phi\rangle$ where the exponentials have the form (4.20) (or: (4.21)) above.

We begin by studying the easier case where $\varepsilon_1=\varepsilon_2=\cdots=\varepsilon_l=0$.

In this case, as we explained in the first step above, the change of variables (4.19) leads to studying,

$$\begin{aligned}\langle{}^{\varepsilon}Q_l(\psi),\phi\rangle := \int_{u_1=0}^{+\infty}\cdots\int_{u_l=0}^{+\infty}\int_{\mathbb{R}^{3(l+1)}} &\exp(+i\mathbf{N}^2[u_1+\cdots+u_l])\\ &\times\exp(-i\mathbf{K}_1^2u_1)\exp(-i\mathbf{K}_2^2u_2)\cdots\exp(-i\mathbf{K}_l^2u_l)\\ &\times\hat{V}(\mathbf{N}-\mathbf{K}_1)\,\hat{V}(\mathbf{K}_1-\mathbf{K}_2)\,\cdots\hat{V}(\mathbf{K}_{l-1}-\mathbf{K}_l)\,\hat{V}^*(\mathbf{N}-\mathbf{K}_l)\\ &\times\psi(\mathbf{N})\,\phi(\mathbf{N})\,d\mathbf{N}\,d\mathbf{K}_1\cdots d\mathbf{K}_l\,du_1\cdots du_l.\end{aligned} \tag{4.24}$$

Now we split the time integral $\int du_1\cdots\int du_l$ according to the 2^l different cases: $u_1\geqslant$ or $\leqslant 1$, $u_2\geqslant$ or $\leqslant 1,\ldots,u_l\geqslant$ or $\leqslant 1$.

∗ On the set where $u_1,u_2,\ldots,u_l$ are *all* $\leqslant 1$, we observe that the corresponding contribution to $\langle{}^{\varepsilon}Q_l(\psi),\phi\rangle$ is,

$$\leqslant C_1 \, \|\psi\|_{L^\infty(\mathbb{R}^3)} \int_{\mathbb{R}^{3(l+1)}} |\hat{V}(\mathbf{N}-\mathbf{K}_1)\, \hat{V}(\mathbf{K}_1-\mathbf{K}_2) \cdots \hat{V}(\mathbf{K}_{l-1}-\mathbf{K}_l)$$
$$\times \hat{V}^*(\mathbf{N}-\mathbf{K}_l)\, \phi(\mathbf{N})| \, d\mathbf{N}\, d\mathbf{K}_1 \cdots d\mathbf{K}_l,$$

for some universal constant C_1, and therefore it is bounded by,

$$\leqslant C_1 \, \|\hat{V}\|^{l+1}_{L^1(\mathbb{R}^3)} \, \|\psi\|_{L^\infty(\mathbb{R}^3)} \, \|\phi\|_{L^\infty(\mathbb{R}^3)}.$$

* If, say, u_1 is $\geqslant 1$, and all the other variables are $\leqslant 1$, we use Parseval formula in the $\mathbf{K}_1$ variable, and rely on the well-known formula,

$$\int_{x \in \mathbb{R}^3} \exp\left(i \frac{\lambda x^2}{2}\right) f(x)\, dx = C_2 \int_{\xi \in \mathbb{R}^3} \lambda^{-3/2} \exp\left(-i \frac{\xi^2}{2\lambda}\right) \hat{f}(\xi)\, d\xi, \quad (4.25)$$

for some universal constant C_2. This gives that the corresponding contribution to $\langle {}^\varepsilon Q_l(\psi), \phi \rangle$ is, for some other universal constant C_3 related to C_2,

$$= C_3 \int_{u_1=1}^{+\infty} \int_{u_2=0}^{1} \cdots \int_{u_l=0}^{1} \int_{\mathbb{R}^{3(l+1)}} \exp(+i\mathbf{N}^2[u_1 + \cdots + u_l])$$
$$\times \frac{\exp\left(+i \frac{\xi_1^2}{u_1}\right)}{u_1^{3/2}} \times \exp(-i\mathbf{K}_2^2 u_2) \cdots \exp(-i\mathbf{K}_l^2 u_l)$$
$$\times (\mathscr{F}_{\mathbf{K}_1 \to \xi_1} \hat{V}(\mathbf{N}-\mathbf{K}_1) \cdots \hat{V}(\mathbf{K}_{l-1}-\mathbf{K}_l)\, \hat{V}^*(\mathbf{N}-\mathbf{K}_l)\, \psi(\mathbf{N})\, \phi(\mathbf{N}))$$
$$\times d\mathbf{N}\, d\xi_1\, d\mathbf{K}_2 \cdots d\mathbf{K}_l\, du_1 \cdots du_l. \quad (4.26)$$

Obviously, we can bound (4.26) by,

$$\leqslant C_3 \times \int_{u_1=1}^{+\infty} \frac{du_1}{u_1^{3/2}} \|\psi\|_{L^\infty(\mathbb{R}^3)} \int_{\mathbb{R}^{3(l+1)}} |\mathscr{F}_{\mathbf{K}_1 \to \xi_1} \hat{V}(\mathbf{N}-\mathbf{K}_1) \cdots \hat{V}(\mathbf{K}_{l-1}-\mathbf{K}_l)$$
$$\times \hat{V}^*(\mathbf{N}-\mathbf{K}_l)\, \phi(\mathbf{N})| \, d\mathbf{N}\, d\xi_1\, d\mathbf{K}_2 \cdots d\mathbf{K}_l$$
$$\leqslant C_4 \, \|\psi\|_{L^\infty(\mathbb{R}^3)} \times \left[\int_{\mathbb{R}^3} (1+|\mathbf{x}|^4)^{-1}\, d\mathbf{x} \right] \times \int_{\mathbb{R}^{3(l+1)}} |(1-\Delta^2_{\mathbf{K}_1})[\hat{V}(\mathbf{N}-\mathbf{K}_1)$$
$$\times \hat{V}(\mathbf{K}_1-\mathbf{K}_2) \cdots \hat{V}^*(\mathbf{N}-\mathbf{K}_l)\, \phi(\mathbf{N})]| \, d\mathbf{N}\, d\mathbf{K}_1\, d\mathbf{K}_2 \cdots d\mathbf{K}_l$$
$$\leqslant C_5 \, \|\hat{V}\|^2_{W^{4,1}(\mathbb{R}^3)} \, \|\hat{V}\|^{l-1}_{L^1(\mathbb{R}^3)} \, \|\psi\|_{L^\infty(\mathbb{R}^3)} \, \|\phi\|_{L^\infty(\mathbb{R}^3)}$$
$$\leqslant C_6 \, \|\hat{V}\|^{l+1}_{W^{4,1}(\mathbb{R}^3)} \, \|\psi\|_{L^\infty(\mathbb{R}^3)} \, \|\phi\|_{L^\infty(\mathbb{R}^3)}. \quad (4.27)$$

Here C_3,..., C_5 are universal constants.

$*$ If, say, u_1 and u_2 are $\geqslant 1$, the other variables being $\leqslant 1$, the same method (Fourier transform in $\mathbf{K}_1$ and $\mathbf{K}_2$) obviously leads to bounding the corresponding contribution to $\langle {}^{\varepsilon}Q_l(\psi), \phi\rangle$ by,

$$\leqslant C_7 \, \|\psi\|_{L^\infty(\mathbb{R}^3)} \int_{\mathbb{R}^{3(l+1)}} |(1-\Delta^2_{\mathbf{K}_1})(1-\Delta^2_{\mathbf{K}_2})[\hat{V}(\mathbf{N}-\mathbf{K}_1)\, \hat{V}(\mathbf{K}_1-\mathbf{K}_2) \cdots$$

$$\cdots \hat{V}^*(\mathbf{N}-\mathbf{K}_l)\, \phi(\mathbf{N})]| \, d\mathbf{N} \, d\mathbf{K}_1 \cdots d\mathbf{K}_l$$

$$\leqslant C_8 \, \|\psi\|_{L^\infty(\mathbb{R}^3)} \, \|\hat{V}\|^3_{W^{8,1}(\mathbb{R}^3)} \, \|\hat{V}\|^{l-2}_{L^1(\mathbb{R}^3)} \, \|\phi\|_{L^\infty(\mathbb{R}^3)},$$

hence this is bounded by,

$$\leqslant C_8 \, \|\psi\|_{L^\infty(\mathbb{R}^3)} \, \|\hat{V}\|^{l+1}_{W^{8,1}(\mathbb{R}^3)} \, \|\phi\|_{L^\infty(\mathbb{R}^3)}.$$

$*$ Continuing this procedure allows to bound all the contributions to $\langle {}^{\varepsilon}Q_l(\psi), \phi\rangle$, including the worst case where *all* the u_j's are $\geqslant 1$. Indeed, in this case we Fourier transform in $\mathbf{K}_1, \ldots, \mathbf{K}_l$, and obtain a bound like,

$$\leqslant C_9^l \times \int_{u_1=1}^{+\infty} \cdots \int_{u_l=1}^{+\infty} [u_1 u_2 \cdots u_l]^{-3/2} du_1 \cdots du_l \, \|\psi\|_{L^\infty(\mathbb{R}^3)}$$

$$\times \int_{\mathbb{R}^{3(l+1)}} |(1-\Delta^2_{\mathbf{K}_1}) \cdots (1-\Delta^2_{\mathbf{K}_l})$$

$$\times [\hat{V}(\mathbf{N}-\mathbf{K}_1) \cdots \hat{V}^*(\mathbf{N}-\mathbf{K}_l)\, \phi(\mathbf{N})]| \, d\mathbf{N} \, d\mathbf{K}_1 \cdots d\mathbf{K}_l$$

$$\leqslant C_{10}^l \, \|\psi\|_{L^\infty(\mathbb{R}^3)} \, \|\hat{V}\|^{l+1}_{W^{8,1}(\mathbb{R}^3)} \, \|\phi\|_{L^\infty(\mathbb{R}^3)}.$$

Note that we never differentiate nor use the Parseval formula in the $\mathbf{N}$ variable, hence we do not need differentiability properties of the function ψ.

Now, all the constants appearing while bounding $\langle {}^{\varepsilon}Q_l(\psi), \phi\rangle$ depend geometrically on l, including the number of terms in which one is led to split $I_l(\psi, \phi)$ (this number is 2^l). This gives the following bound on the gain term (i.e., in the particular case $\varepsilon_1 = \cdots = \varepsilon_l = 0$),

$$|\langle {}^{\varepsilon}Q_l(\psi), \phi\rangle| \leqslant C_{11}^l \, \|\psi\|_{L^\infty(\mathbb{R}^3)} \, \|\hat{V}\|_{W^{8,1}(\mathbb{R}^3)} \, \|\phi\|_{L^\infty(\mathbb{R}^3)}, \tag{4.28}$$

where C_{11} is some universal constant.

We emphasize the fact that this bound implies the corresponding bound in Lemma 3.1, but it is actually much better an estimate. Indeed, the bound (4.28) says that the operator ${}^{\varepsilon}Q_l$ (in the case $\varepsilon_1 = \cdots = \varepsilon_l = 0$) sends $L^\infty(\mathbb{R}^3)$ into its dual continuously, whereas Lemma 3.1 implies a loss of four derivatives.

We finally mention that the absolute convergence in the u-variables of the integrals defining ${}^{\varepsilon}Q_l$ is an obvious consequence of the above computations (i.e., of the absolute convergence of $\int_1^\infty u^{-3/2}\,du$).

Last Step. *The General Case—The Loss Terms*

The method indicated above in the special case $\varepsilon_1 = \cdots = \varepsilon_l = 0$ works without any modification for *any* value of the numbers ε_j. However, the bound on $\langle {}^{\varepsilon}Q_l(\psi), \phi\rangle$ given by this method in the case of the "loss"-terms differs from the one obtained in the case of the "gain"-term (see (4.28)) in that we shall now obtain a bound *with* loss of derivatives.

Indeed, for any value of the ε's we know from the first step above that it is possible to change variables as in (4.19) so as to recover an oscillatory integral involving on the one hand exponentials of the form (4.20) (or: (4.21)), and on the other hand the particular structure (4.23) persists for the non-oscillatory part of the integral.

In order to fix the ideas, let us now bound the typical quantity,

$$\begin{aligned}&\int_{\mathbb{R}^{3(l+1)}}\int_{u_1,\dots,u_l=0}^{+\infty} \exp\{i[\mathbf{N}^2u_1 - \mathbf{K}_1^2(u_1+u_2)\\ &\quad+\mathbf{K}_2^2(u_2+u_3+\cdots+u_l) - \mathbf{K}_3^2u_3 - \cdots - \mathbf{K}_l^2u_l]\}\\ &\quad\times \hat{V}(\mathbf{N}-\mathbf{K}_1)\,\hat{V}(\mathbf{K}_2-\mathbf{N})\,\hat{V}(\mathbf{K}_1-\mathbf{K}_3)\,\hat{V}(\mathbf{K}_3-\mathbf{K}_4)\cdots\hat{V}(\mathbf{K}_{l-1}-\mathbf{K}_l)\,\hat{V}(\mathbf{K}_l-\mathbf{K}_2)\\ &\quad\times \psi(\mathbf{K}_2)\,\phi(\mathbf{N})\,d\mathbf{N}\,d\mathbf{K}_1\cdots d\mathbf{K}_l\,du_1\cdots du_l.\end{aligned} \tag{4.29}$$

(This quantity corresponds to $\varepsilon_1 = 0$, $\varepsilon_2 = 1$, $\varepsilon_3 = \cdots = \varepsilon_l = 0$). Following the procedure used in the second step above, we may use the Parseval formula in the $\mathbf{K}_1$, $\mathbf{K}_3$,..., $\mathbf{K}_l$ variables (and not in $\mathbf{K}_2$, which is the variable appearing as the argument of ψ).

This provides the decay of the $d\mathbf{N}\,d\mathbf{K}_1\,d\mathbf{K}_2\,d\mathbf{K}_3\,d\mathbf{K}_4\cdots d\mathbf{K}_l$ integral involved in (4.29) like,

$$(1+u_1)^{-3/2}\,(1+u_1+u_2)^{-3/2}\,(1+u_3)^{-3/2}\,(1+u_4)^{-3/2}\cdots(1+u_l)^{-3/2}, \tag{4.30}$$

up to the use of eight derivatives of $\hat{V}$, and four derivatives in ϕ, but no derivatives of ψ is needed to get this decay. We do not precise the exact manipulations, which are exactly the same as in the second step. Now, the function appearing in (4.30) is integrable over $[0,+\infty[^l$. Collecting these informations gives the bound,

$$\leqslant C_{12}^l\,\|\hat{V}\|_{W^{8,1}(\mathbb{R}^3)}^{l+1}\,\|\psi\|_{L^\infty(\mathbb{R}^3)}\,\|\phi\|_{W^{4,\infty}(\mathbb{R}^3)}.$$

Now, collecting bounds over the 2^l possible values of the ε's gives therefore the theorem. ∎

4.4. Proof of Theorem 3.1: Getting a priori Bounds

First Step. *Proof of (iv)*

Clearly, points (i), (ii), and (iii), imply (iv). For instance, we may write indeed,

$$
\begin{aligned}
|\langle \rho_d^{L,\alpha}(t), \phi \rangle| &\leqslant \|\rho_d^{L,\alpha}(t,n)\|_{l_n^2} \left\| \phi\left(\frac{n}{L}\right)\right\|_{l_n^2} \\
&\leqslant C \left\| \frac{1}{L^{3/2}} \phi\left(\frac{n}{L}\right)\right\|_{l_n^2} \qquad \text{(here we used (3.8))} \\
&\leqslant C \left[\frac{1}{L^3} \sum_n \left\langle \frac{n}{L} \right\rangle^{-2D} \right]^{1/2} \|\phi(\mathbf{n})\|_{\mathscr{T}_D} \leqslant C \|\phi(\mathbf{n})\|_{\mathscr{T}_D},
\end{aligned}
$$

for some constant C as in (3.9), so that (3.8) implies (3.15). Using this argument several times shows that (iv) is a simple consequence of (i), (ii), and (iii), so that we now concentrate on the proof of these points.

Second Step. *Proof of (i)—The Diagonal Part*

Since the original Von-Neumann equation (2.8) has the so-called Linblad property, it preserves the positivity of the density-matrix as an operator for any *non-negative* values of time $t \geqslant 0$. In particular, as we already saw, the diagonal coefficients of the density-matrix, $\rho_d^{L,\alpha}(t,n)$ are non-negative (as numbers) for any $t \geqslant 0$.

Now define the following density-matrix $\tilde{u}(x, y)$ through its Fourier coefficients,

$$
u(n, p) := \mathbf{1}[n = p] \left[\frac{1}{L^3} \|\rho_d^0(\mathbf{n})\|_{L^\infty(\mathbb{R}^3)} - \frac{1}{L^3} \rho_d^0\left(\frac{n}{L}\right)\right], \tag{4.31}
$$

for any n and p in $\mathbb{Z}^3$, and let $u(t, n, p)$ be the value at time t of the corresponding solution to the Von-Neumann equation (2.8) with initial data $u(n, p)$. It is clear that initially, $u(n, p)$ defines a positive density matrix $\tilde{u}(x, y)$ (as an operator), so that the corresponding density matrix $\tilde{u}(t, x, y)$ (with Fourier coefficients $u(t, n, p)$) remains positive (as an operator) for any time $t \geqslant 0$. In particular, the diagonal coefficients $u(t, n, n)$ are non-negative (as numbers) for any $t \geqslant 0$.

On the other hand, it is readily seen that the actual value of $u(t, n, p)$ at time t is given through,

$$
u(t, n, n) = \frac{1}{L^3} \|\rho_d^0(\mathbf{n})\|_{L^\infty(\mathbb{R}^3)} - \rho_d^{L,\alpha}(t, n), \tag{4.32}
$$

for the diagonal part of u, and, if $n \neq p$,

$$u(t, n, p) = -\rho_{nd}^{L,\alpha}(t, n, p). \tag{4.33}$$

As an obvious consequence, we now deduce from the preceding considerations that, for any $t \geqslant 0$, we have,

$$0 \leqslant \rho_{nd}^{L,\alpha}(t, n) \leqslant \frac{1}{L^3} \|\rho_d^0(\mathbf{n})\|_{L^\infty(\mathbb{R}^3)}. \tag{4.34}$$

This already proves (3.7).

On the other hand, the Von-Neumann equation (2.8) clearly preserves the trace of the operator $\tilde{\rho}$. Indeed, in view of the positivity of the diagonal coefficients $\rho_d^{L,\alpha}(t, n)$, we have,

$$\operatorname{Tr}\tilde{\rho}(t, x, y) = \sum_n \rho_d^{L,\alpha}(t, n, n), \tag{4.35}$$

and it is clear from the Von-Neumann equation (2.8) that,

$$\partial_t \left[\sum_n \rho_d^{L,\alpha}(t, n, n) \right] = 0. \tag{4.36}$$

From (4.36) it follows that,

$$\sum_n \rho_d^{L,\alpha}(t, n, n) = \sum_n \frac{1}{L^3} \rho_d^0\left(\frac{n}{L}\right) = C, \tag{4.37}$$

and (3.6) is proved. The estimate (3.8) follows by interpolation between (3.6) and (3.7).

Third Step. *Proof of (i)—The Non-Diagonal Part*

The first way to (try to) get an l^2 bound on $\rho_{nd}^{L,\alpha}$ is the following. The Von-Neumann equation (2.8) preserves the $l_{n,p}^2$ norm of the *full* density matrix $\rho^{L,\alpha}(t) := \rho_d^{L,\alpha}(t) + \rho_{nd}^{L,\alpha}(t)$, and more precisely we have,

$$\partial_t [\|\rho_d^{L,\alpha}(t)\|_{l_n^2}^2 + \|\rho_{nd}^{L,\alpha}(t)\|_{l_{n,p}^2}^2] = -2\alpha L^3 \|\rho_{nd}^{L,\alpha}(t)\|_{l_{n,p}^2}^2 \leqslant 0. \tag{4.38}$$

Hence we readily obtain,

$$\|\rho_{nd}^{L,\alpha}(t)\|_{l_{n,p}^2} \leqslant \|\rho^{L,\alpha}(t=0)\|_{l_{n,p}^2} = \left\| \frac{1}{L^3} \rho_d^0\left(\frac{n}{L}\right) \right\|_{l_n^2} = \frac{C}{L^{3/2}}.$$

Unfortunately, this first attempt gives too small a decay in L on the right-hand-side, since we shall need in the sequel a decay like L^{-3} (see (3.10)).

This is the reason why we work out the estimate of $\rho_{nd}^{L,\alpha}(t)$ in more detail. Using the equation satisfied by $\rho_{nd}^{L,\alpha}(t)$, we readily write,

$$\begin{aligned}
&\partial_t \|\rho_{nd}^{L,\alpha}(t)\|_{l^2_{n,p}}^2 \\
&\quad = -2\alpha L^3 \|\rho_{nd}^{L,\alpha}(t)\|_{l^2_{n,p}}^2 \\
&\qquad + 2L^3 \Re \left\langle \rho_{nd}^{L,\alpha}(t,n,p), \frac{\lambda}{L^3} \hat{V}\left(\frac{p-n}{L}\right)[\rho_d^{L,\alpha}(t,p) - \rho_d^{L,\alpha}(t,n)] \right\rangle_{l^2_{n,p}} \\
&\quad \leqslant -2\alpha L^3 \|\rho_{nd}^{L,\alpha}(t)\|_{l^2_{n,p}}^2 + 4L^3 \|\rho_{nd}^{L,\alpha}(t)\|_{l^2_{n,p}} \left\| \frac{\lambda}{L^3} \hat{V}\left(\frac{p-n}{L}\right) \right\|_{l^\infty_n(l^2_p)} \|\rho_d^{L,\alpha}(t,n)\|_{l^2_n} \\
&\quad \leqslant -2\alpha L^3 \|\rho_{nd}^{L,\alpha}(t)\|_{l^2_{n,p}}^2 + 4L^3 \|\rho_{nd}^{L,\alpha}(t)\|_{l^2_{n,p}} \times \frac{C}{L^{3/2}} \times \frac{C}{L^{3/2}},
\end{aligned}$$

where we used the bound (3.8) together with the fact that,

$$\left\| \frac{1}{L^{3/2}} \hat{V}\left(\frac{n}{L}\right) \right\|_{l^2_n} \leqslant \|\hat{V}(\mathbf{n})\|_{\mathcal{T}_D}. \tag{4.39}$$

Hence, we obtain,

$$\partial_t \|\rho_{nd}^{L,\alpha}(t)\|_{l^2_{n,p}}^2 \leqslant -2\alpha L^3 \|\rho_{nd}^{L,\alpha}(t)\|_{l^2_{n,p}}^2 + C \|\rho_{nd}^{L,\alpha}(t)\|_{l^2_{n,p}}. \tag{4.40}$$

From (4.40) together with the (crucial) fact that $\rho_{nd}^{L,\alpha}(t)$ vanishes initially we deduce,

$$\begin{aligned}
\|\rho_{nd}^{L,\alpha}(t)\|_{l^2_{n,p}}^2 &\leqslant C \int_{s=0}^t \exp(-2\alpha L^3(t-s)) \|\rho_{nd}^{L,\alpha}(s)\|_{l^2_{n,p}} \\
&\leqslant C \int_{s=0}^t \exp(-2\alpha L^3 s)\, ds \sup_{0\leqslant s\leqslant t} \|\rho_{nd}^{L,\alpha}(s)\|_{l^2_{n,p}} \\
&\leqslant \frac{C}{\alpha L^3} \sup_{0\leqslant s\leqslant t} \|\rho_{nd}^{L,\alpha}(s)\|_{l^2_{n,p}}.
\end{aligned}$$

Hence,

$$\forall t \geqslant 0, \quad \|\rho_{nd}^{L,\alpha}(t)\|_{l^2_{n,p}} \leqslant \frac{C}{\alpha L^3},$$

and (3.10) is proved.

Fourth Step. *Proof of (ii)*

Using again the equations satisfied by $\rho_d^{L,\alpha}(t)$ and $\rho_{nd}^{L,\alpha}(t)$, we readily observe that all the time derivatives $\partial_t^\beta \rho_d^{L,\alpha}(t)$ and $\partial_t^\beta \rho_{nd}^{L,\alpha}(t)$ ($\beta \in \mathbb{N}$) satisfy the *same* Von-Neumann equation (2.8). In particular, the following "conservation law" holds,

$$\partial_t [\|\partial_t^\beta \rho_{nd}^{L,\alpha}(t)\|_{l^2_{n,p}}^2 + \|\partial_t^\beta \rho_d^{L,\alpha}(t)\|_{l^2_n}^2] = -2\alpha L^3 \, \|\partial_t^\beta \rho_{nd}^{L,\alpha}(t)\|_{l^2_{n,p}}^2. \qquad (4.41)$$

Now (4.41) implies,

$$\|\partial_t^\beta \rho_{nd}^{L,\alpha}(t)\|_{l^2_{n,p}}^2 + \|\partial_t^\beta \rho_d^{L,\alpha}(t)\|_{l^2_n}^2$$

$$= \|\partial_t^\beta \rho_{nd}^{L,\alpha}(t=0)\|_{l^2_{n,p}}^2 + \|\partial_t^\beta \rho_d^{L,\alpha}(t=0)\|_{l^2_n}^2 - 2\alpha L^3 \int_{s=0}^t \|\partial_t^\beta \rho_{nd}^{L,\alpha}(s)\|_{l^2_{n,p}}^2 \, ds \geqslant 0,$$

from which the following a-priori bound is derived,

$$\int_{s=0}^t \|\partial_t^\beta \rho_{nd}^{L,\alpha}(s)\|_{l^2_{n,p}}^2 \leqslant \frac{1}{\alpha L^3} \times [\|\partial_t^\beta \rho_{nd}^{L,\alpha}(t=0)\|_{l^2_{n,p}}^2 + \|\partial_t^\beta \rho_d^{L,\alpha}(t=0)\|_{l^2_n}^2]. \qquad (4.42)$$

On the other hand, the actual value of the factor,

$$\|\partial_t^\beta \rho_{nd}^{L,\alpha}(t=0)\|_{l^2_{n,p}}^2 + \|\partial_t^\beta \rho_d^{L,\alpha}(t=0)\|_{l^2_n}^2,$$

in (4.42) is easily computed from the explicit formulae for the particular values $\beta = 0, 1$, namely,

$$\rho_d^{L,\alpha}(t=0) = \frac{1}{L^3} \rho_d^0 \left(\frac{n}{L}\right), \qquad \rho_{nd}^{L,\alpha}(t=0) = 0,$$

$$\partial_t \rho_d^{L,\alpha}(t=0) = 0, \qquad \partial_t \rho_{nd}^{L,\alpha}(t=0) = \frac{i\lambda}{(2\pi)^3 L^3} \hat{V}\left(\frac{p-n}{L}\right)\left[\rho_d^0\left(\frac{p}{L}\right) - \rho_d^0\left(\frac{n}{L}\right)\right],$$

so that the following initial estimates hold,

$$\|\rho_{nd}^{L,\alpha}(t=0)\|_{l^2_{n,p}}^2 + \|\rho_d^{L,\alpha}(t=0)\|_{l^2_n}^2 \leqslant \frac{C}{L^3},$$
$$\|\partial_t \rho_{nd}^{L,\alpha}(t=0)\|_{l^2_{n,p}}^2 + \|\partial_t \rho_d^{L,\alpha}(t=0)\|_{l^2_n}^2 \leqslant C. \qquad (4.43)$$

Now (4.43) together with (4.42) readily give the desired estimates,

$$\int_{s=0}^t \|\rho_{nd}^{L,\alpha}(s)\|_{l^2_{n,p}}^2 \leqslant \frac{C}{\alpha L^6}, \qquad (4.44)$$

$$\int_{s=0}^t \|\partial_t \rho_{nd}^{L,\alpha}(s)\|_{l^2_{n,p}}^2 \leqslant \frac{C}{\alpha L^3}. \qquad (4.45)$$

Note that the bound (4.44) obtained in this way on the non-diagonal part itself (without time-differentiating) is slightly worse than (3.10). This is due to the fact that, when no time derivative is involved, we were able to use much more structure in the third step, and in particular, to use the very special form of the initial density-matrix.

Fifth Step. *Proof of (iii)*

The proof of (iii) is very easy. Using the equation satisfied by $\rho_d^{L,\alpha}(t)$, we readily estimate,

$$\|\partial_t \rho_d^{L,\alpha}(t)\|_{l_n^2} \leqslant \left\| \hat{V}\left(\frac{n}{L}\right)\right\|_{l_n^2} \|\rho_{nd}^{L,\alpha}(t)\|_{l_{n,p}^2} \leqslant CL^{3/2}\frac{1}{\alpha L^3} = \frac{C}{\alpha L^{3/2}},$$

where we made use of (3.10). The point (iii) follows. ▮

4.5. Proof of Theorem 3.2: Convergence as $L \to \infty$

First Step. *Transforming the Original Equation into a System of Integral Equations*

Let $\Phi(\mathbf{n}, \mathbf{p})$ and $\phi(\mathbf{n})$ be smooth test functions. We first transform the Von-Neumann equation (2.8) into (equivalent) integral formulae, as follows. Firstly, the non-diagonal part satisfies (recall that $\rho_{nd}^{L,\alpha}$ vanishes initially),

$$\begin{aligned}
\langle \rho_{nd}^{L,\alpha}(t), \Phi\rangle = {} & i\int_{s=0}^{L^3 t} \sum_{n,p,k} \exp\left(\left[i\frac{n^2-p^2}{L^2}-\alpha\right]s\right)\\
& \times\left[\frac{\lambda}{L^3}\hat{V}\left(\frac{k-n}{L}\right)\rho_{nd}^{L,\alpha}\left(t-\frac{s}{L^3}, k, p\right)\right.\\
& \left. -\frac{\lambda}{L^3}\hat{V}\left(\frac{p-k}{L}\right)\rho_{nd}^{L,\alpha}\left(t-\frac{s}{L^3}, n, k\right)\right]\Phi\left(\frac{n}{L},\frac{p}{L}\right)\\
& +i\int_{s=0}^{L^3 t} \sum_{n,p} \exp\left(\left[i\frac{n^2-p^2}{L^2}-\alpha\right]s\right)\\
& \times\frac{\lambda}{L^3}\hat{V}\left(\frac{p-n}{L}\right)\left[\rho_d^{L,\alpha}\left(t-\frac{s}{L^3}, p\right)-\rho_d^{L,\alpha}\left(t-\frac{s}{L^3}, n\right)\right]\Phi\left(\frac{n}{L},\frac{p}{L}\right),
\end{aligned}$$

and it is an easy computation to transform this relation into,

$$
\begin{aligned}
&\langle \rho_{nd}^{L,\alpha}(t), \Phi \rangle \\
&\quad = \frac{i\lambda}{L^3} \int_{s=0}^{L^3 t} \exp(-\alpha s) \left\langle \rho_{nd}^{L,\alpha}\left(t - \frac{s}{L^3}\right), \sum_k \left[\exp\left(i \frac{k^2 - p^2}{L^2} s\right) \hat{V}\left(\frac{n-k}{L}\right) \right.\right. \\
&\qquad \left.\left. \times \Phi\left(\frac{k}{L}, \frac{p}{L}\right) - \exp\left(i \frac{n^2 - k^2}{L^2} s\right) \hat{V}\left(\frac{k-p}{L}\right) \Phi\left(\frac{n}{L}, \frac{k}{L}\right) \right] \right\rangle \\
&\qquad + \frac{i\lambda}{L^3} \int_{s=0}^{L^3 t} \exp(-\alpha s) \left\langle \rho_{d}^{L,\alpha}\left(t - \frac{s}{L^3}\right), \sum_p \left[\exp\left(i \frac{p^2 - n^2}{L^2} s\right) \hat{V}\left(\frac{n-p}{L}\right) \right.\right. \\
&\qquad \left.\left. \times \Phi\left(\frac{p}{L}, \frac{n}{L}\right) - \exp\left(i \frac{n^2 - p^2}{L^2} s\right) \hat{V}\left(\frac{p-n}{L}\right) \Phi\left(\frac{n}{L}, \frac{p}{L}\right) \right] \right\rangle . \qquad (4.46)
\end{aligned}
$$

In other terms, if we introduce,

$$
\begin{aligned}
(\mathscr{A}^L(s)\, \Phi)(\mathbf{n}, \mathbf{p}) := \frac{\lambda}{L^3} \sum_k \Bigg[& \exp\left(i \left[\frac{k^2}{L^2} - \mathbf{p}^2\right] s\right) \hat{V}\left(\mathbf{n} - \frac{k}{L}\right) \Phi\left(\frac{k}{L}, \mathbf{p}\right) \\
& - \exp\left(i \left[\mathbf{n}^2 - \frac{k^2}{L^2}\right] s\right) \hat{V}\left(\frac{k}{L} - \mathbf{p}\right) \Phi\left(\mathbf{n}, \frac{k}{L}\right) \Bigg] \qquad (4.47)
\end{aligned}
$$

$$
\begin{aligned}
(\mathscr{B}^L(s)\, \Phi)(\mathbf{n}) := \frac{\lambda}{L^3} \sum_p \Bigg[& \exp\left(i \left[\frac{p^2}{L^2} - \mathbf{n}^2\right] s\right) \hat{V}\left(\mathbf{n} - \frac{p}{L}\right) \Phi\left(\frac{p}{L}, \mathbf{n}\right) \\
& - \exp\left(i \left[\mathbf{n}^2 - \frac{p^2}{L^2}\right] s\right) \hat{V}\left(\frac{p}{L} - \mathbf{n}\right) \Phi\left(\mathbf{n}, \frac{p}{L}\right) \Bigg], \qquad (4.48)
\end{aligned}
$$

then (4.46) reads,

$$
\begin{aligned}
\langle \rho_{nd}^{L,\alpha}(t), \Phi \rangle = {} & i \int_{s=0}^{L^3 t} \exp(-\alpha s) \left\langle \rho_{nd}^{L,\alpha}\left(t - \frac{s}{L^3}\right), \mathscr{A}^L(s)\, \Phi \right\rangle \\
& + i \int_{s=0}^{L^3 t} \exp(-\alpha s) \left\langle \rho_{d}^{L,\alpha}\left(t - \frac{s}{L^3}\right), \mathscr{B}^L(s)\, \Phi \right\rangle . \qquad (4.49)
\end{aligned}
$$

We can proceed to the analogous transformation for the diagonal part as well, thus obtaining,

$$\begin{aligned}
&\langle \rho_d^{L,\alpha}(t), \phi\rangle \\
&= \left\langle \frac{1}{L^3} \rho_d^0\left(\frac{n}{L}\right), \phi\right\rangle \\
&\quad + i\lambda \int_{s=0}^t \sum_{n,k} \left[\hat{V}\left(\frac{k-n}{L}\right) \rho_{nd}^{L,\alpha}(s,k,n)\, \phi\left(\frac{n}{L}\right) - \hat{V}\left(\frac{n-k}{L}\right) \rho_{nd}^{L,\alpha}(s,n,k)\, \phi\left(\frac{n}{L}\right)\right] \\
&= \left\langle \frac{1}{L^3} \rho_d^0\left(\frac{n}{L}\right), \phi\right\rangle + i\lambda \int_{s=0}^t \sum_{n,k} \rho_{nd}^{L,\alpha}(s,n,k)\, \hat{V}\left(\frac{n-k}{L}\right)\left[\phi\left(\frac{k}{L}\right) - \phi\left(\frac{n}{L}\right)\right],
\end{aligned}$$

where we used the natural convention,

$$\left\langle \frac{1}{L^3} \rho_d^0\left(\frac{n}{L}\right), \phi\right\rangle := \sum_n \frac{1}{L^3} \rho_d^0\left(\frac{n}{L}\right) \phi\left(\frac{n}{L}\right).$$

In other words, we have obtained,

$$\langle \rho_d^{L,\alpha}(t), \phi\rangle = \left\langle \frac{1}{L^3} \rho_d^0\left(\frac{n}{L}\right), \phi\right\rangle + i \int_{s=0}^t \langle \rho_{nd}^{L,\alpha}(s), \mathscr{C}\phi\rangle, \tag{4.50}$$

up to defining,

$$(\mathscr{C}\phi)(\mathbf{n}, \mathbf{p}) := \lambda \hat{V}(\mathbf{n}-\mathbf{p})[\phi(\mathbf{p}) - \phi(\mathbf{n})]. \tag{4.51}$$

Since now (4.50) only depends on the non-diagonal part through its average in time, we may integrate the equation (4.49) in time. Summarizing, we have thus transformed the original Von-Neumann equation (2.8) into the following system of equations,

$$\langle \rho_d^{L,\alpha}(t), \phi\rangle = \left\langle \frac{1}{L^3} \rho_d^0\left(\frac{n}{L}\right), \phi\right\rangle + i \int_{s=0}^t \langle \rho_{nd}^{L,\alpha}(s), \mathscr{C}\phi\rangle, \tag{4.52}$$

and,

$$\begin{aligned}
\int_{s=0}^t \langle \rho_{nd}^{L,\alpha}(s), \Phi\rangle &= i \int_{s=0}^t \int_{u=0}^{L^3 s} \exp(-\alpha u) \left\langle \rho_{nd}^{L,\alpha}\left(s - \frac{u}{L^3}\right), \mathscr{A}^L(u)\, \Phi\right\rangle \\
&\quad + i \int_{s=0}^t \int_{u=0}^{L^3 s} \exp(-\alpha u) \left\langle \rho_d^{L,\alpha}\left(s - \frac{u}{L^3}\right), \mathscr{B}^L(u)\, \Phi\right\rangle.
\end{aligned} \tag{4.53}$$

Note that the system (4.52)–(4.53) may be solved iteratively if necessary.

We now derive the necessary a-priori bounds in order to pass to the limit $L \to \infty$ in the integral formulae (4.53) and (4.52).

Second Step. *A Priori Bounds*

First of all, we have the uniform bound,

$$\begin{aligned}
&\left| \int_{s=0}^{L^3 t} \exp(-\alpha s) \left\langle \rho_{nd}^{L,\alpha}\left(t - \frac{s}{L^3}\right), \mathscr{A}^L(s)\,\Phi \right\rangle \right| \\
&\quad \leqslant \frac{1}{\alpha} \sup_{0 \leqslant s \leqslant t} \|\rho_{nd}^{L,\alpha}(s)\|_{l^2_{n,p}} \sup_{s \geqslant 0} \left\| [\mathscr{A}^L(s)\,\Phi]\left(\frac{n}{L}, \frac{p}{L}\right) \right\|_{l^2_{n,p}} \\
&\quad \leqslant \frac{C}{\alpha^2} \sup_{s \geqslant 0} \left\| \frac{1}{L^3} [\mathscr{A}^L(s)\,\Phi]\left(\frac{n}{L}, \frac{p}{L}\right) \right\|_{l^2_{n,p}},
\end{aligned} \tag{4.54}$$

where we used the bound (3.10). On the more, we readily upper-bound the factor $\|\frac{1}{L^3}\mathscr{A}^L(s)\,\Phi\|_{l^2_{n,p}}$ as follows,

$$\begin{aligned}
&\left\| \frac{1}{L^3} [\mathscr{A}^L(s)\,\Phi]\left(\frac{n}{L}, \frac{p}{L}\right) \right\|_{l^2_{n,p}} \\
&\leqslant \frac{|\lambda|}{L^6} \left\| \sum_k \left[|\hat{V}|\left(\frac{n-k}{L}\right) |\Phi|\left(\frac{k}{L}, \frac{p}{L}\right) + |\hat{V}|\left(\frac{k-p}{L}\right) |\Phi|\left(\frac{n}{L}, \frac{k}{L}\right) \right] \right\|_{l^2_{n,p}} \\
&\leqslant \frac{C}{L^6} \left\| \sum_k \left[\left\langle \frac{n-k}{L} \right\rangle^{-D} \left\langle \frac{k}{L} \right\rangle^{-D} \left\langle \frac{p}{L} \right\rangle^{-D} + \left\langle \frac{p-k}{L} \right\rangle^{-D} \left\langle \frac{k}{L} \right\rangle^{-D} \left\langle \frac{n}{L} \right\rangle^{-D} \right] \right\|_{l^2_{n,p}} \\
&\quad \times \|\Phi(\mathbf{n}, \mathbf{p})\|_{\mathscr{T}_D} \\
&\leqslant \frac{C}{L^6} \left\| \left\langle \frac{p}{L} \right\rangle^{-D} \right\|_{l^2_p} \left\| \left\langle \frac{n}{L} \right\rangle^{-D} \right\|_{l^1_n} \left\| \left\langle \frac{k}{L} \right\rangle^{-D} \right\|_{l^2_k} \times \|\Phi(\mathbf{n}, \mathbf{p})\|_{\mathscr{T}_D} \\
&\leqslant C \left\| \frac{1}{L^{3/2}} \left\langle \frac{p}{L} \right\rangle^{-D} \right\|_{l^2_p} \left\| \frac{1}{L^3} \left\langle \frac{k}{L} \right\rangle^{-D} \right\|_{l^1_k} \left\| \frac{1}{L^{3/2}} \left\langle \frac{k}{L} \right\rangle^{-D} \|_{l^2_k} \, \|\Phi(\mathbf{n}, \mathbf{p})\|_{\mathscr{T}_D} \right. \\
&\leqslant C\, \|\Phi(\mathbf{n}, \mathbf{p})\|_{\mathscr{T}_D},
\end{aligned} \tag{4.55}$$

where we used that $D > 3$, together with the Hölder and the Young inequalities. Putting (4.54) and (4.55) together gives the uniform bound,

$$\left| \int_{s=0}^{L^3 t} \exp(-\alpha s) \left\langle \rho_{nd}^{L,\alpha}\left(t - \frac{s}{L^3}\right), \mathscr{A}^L(s)\,\Phi \right\rangle \right| \leqslant \frac{C}{\alpha^2} \|\Phi(\mathbf{n}, \mathbf{p})\|_{\mathscr{T}_D}, \tag{4.56}$$

meaning that the operator on the left-hand-side of (4.56) is uniformly bounded (in L) on the space of test functions $\Phi(\mathbf{n}, \mathbf{p}) \in \mathcal{T}_D(\mathbb{R}^6)$.

The same method gives similar uniform bounds on the two terms,

$$\int_{s=0}^{L^3 t} \exp(-\alpha s) \left\langle \rho_d^{L,\alpha}\left(t-\frac{s}{L^3}\right), \mathcal{B}^L(s)\,\Phi \right\rangle,$$

$$\text{and} \quad \int_{s=0}^{L^3 t} \exp(-\alpha s) \left\langle \rho_{nd}^{L,\alpha}\left(t-\frac{s}{L^3}\right), \mathcal{C}\Phi \right\rangle,$$

as we show now. Indeed, proceeding as in (4.54), we first upper-bound,

$$\left|\int_{s=0}^{L^3 t} \exp(-\alpha s) \left\langle \rho_d^{L,\alpha}\left(t-\frac{s}{L^3}\right), \mathcal{B}^L(s)\,\Phi \right\rangle\right| \leqslant \frac{C}{\alpha} \sup_{0 \leqslant s \leqslant t} \left\| \frac{1}{L^{3/2}} [\mathcal{B}^L(s)\,\Phi]\left(\frac{n}{L}\right)\right\|_{l_n^2},$$

where we made use of the a-priori bound (3.8). Again, we may write as in (4.55),

$$\begin{aligned}\left\| \frac{1}{L^{3/2}} [\mathcal{B}^L(s)\,\Phi]\left(\frac{n}{L}\right)\right\|_{l_n^2} &\leqslant \frac{2}{L^{3/2}} \left\| \sum_p \frac{|\lambda|}{L^3} |\hat{V}| \left(\frac{n-p}{L}\right) |\Phi| \left(\frac{p}{L}, \frac{n}{L}\right)\right\|_{l_n^2} \\ &\leqslant C \left\| \frac{1}{L^{3/2}} \hat{V}\left(\frac{n}{L}\right)\right\|_{l_n^2} \left\| \frac{1}{L^3} \Phi\left(\frac{p}{L}, \frac{n}{L}\right)\right\|_{l_{n,p}^2} \\ &\leqslant C\, \|\Phi(\mathbf{n}, \mathbf{p})\|_{\mathcal{T}_D},\end{aligned}$$

where C is as usual. Hence, we get,

$$\left|\int_{s=0}^{L^3 t} \exp(-\alpha s) \left\langle \rho_d^{L,\alpha}\left(t-\frac{s}{L^3}\right), \mathcal{B}^L(s)\,\Phi \right\rangle\right| \leqslant \frac{C}{\alpha} \|\Phi(\mathbf{n}, \mathbf{p})\|_{\mathcal{T}_D}. \tag{4.57}$$

Finally, we end this step by proving the following upper-bound,

$$\begin{aligned}&\left|\int_{s=0}^{L^3 t} \exp(-\alpha s) \left\langle \rho_{nd}^{L,\alpha}\left(t-\frac{s}{L^3}\right), \mathcal{C}\phi \right\rangle\right| \\ &\leqslant \frac{C}{\alpha^2} \left\| \frac{1}{L^3} [\mathcal{C}\phi]\left(\frac{n}{L}, \frac{p}{L}\right)\right\|_{l_{n,p}^2} \qquad \text{(here we used (3.10))} \\ &\leqslant \frac{C}{\alpha^2} \left\| \frac{1}{L^3} |\hat{V}| \left(\frac{n-p}{L}\right) |\phi| \left(\frac{n}{L}\right)\right\|_{l_{n,p}^2} \\ &\leqslant \frac{C}{\alpha^2} \left\| \frac{1}{L^{3/2}} \hat{V}\left(\frac{n}{L}\right)\right\|_{l_n^2} \left\| \frac{1}{L^{3/2}} \phi\left(\frac{n}{L}\right)\right\|_{l_n^2},\end{aligned}$$

and this finally gives,

$$\left| \int_{s=0}^{L^3 t} \exp(-\alpha s) \left\langle \rho_{nd}^{L,\alpha}\left(t-\frac{s}{L^3}\right), \mathscr{C}\phi \right\rangle \right| \leqslant \frac{C}{\alpha^2} \|\phi(\mathbf{n})\|_{\mathscr{T}_D}.$$

We now have derived all the necessary uniform bounds. We proceed to the convergence proofs.

Third Step. *Passing to the Limit in (4.52)*

We wish to pass to the limit $L \to \infty$ in the integral formulae (4.53) and (4.52).

We begin in this step with the treatment of the easier equation (4.52).

In view of the uniform boundedness of *all* the operators involved in (4.52) as operators on $\mathscr{T}_D(\mathbb{R}^3)$, as we proved in the second step above, it is enough to pass to the limit in (4.52) in the special case where the test function ϕ actually belongs to $C_c^\infty(\mathbb{R}^3)$.

We turn to identifying the limit of each term in (4.52) when $\phi \in C_c^\infty(\mathbb{R}^6)$. We readily have the convergence,

$$\langle \rho_d^{L,\alpha}(t), \phi \rangle \xrightarrow[L \to \infty]{} \langle \rho_d^{\alpha}(t), \phi \rangle \qquad \text{in } C^0(\mathbb{R}_t^+)$$

$$\left\langle \frac{1}{L^3} \rho_d^0\left(\frac{n}{L}\right), \phi \right\rangle \xrightarrow[L \to \infty]{} \langle \rho_d^0, \phi \rangle := \int_{\mathbb{R}^3} \rho_d^0(\mathbf{n})\, \phi(\mathbf{n})\, d\mathbf{n}.$$

The last line is indeed an obvious consequence of both the theorem on the convergence of Riemann sums towards the correponding integrals and the fact that the test function ϕ has been chosen with compact support. The first line is merely a consequence of Theorem 3.1-(iv).

There remains to prove the convergence,

$$\int_{s=0}^{t} \langle \rho_{nd}^{L,\alpha}(s), \mathscr{C}\phi \rangle \xrightarrow[L \to \infty]{} \int_{s=0}^{t} \langle \rho_{nd}^{\alpha}(s), \mathscr{C}\phi \rangle. \tag{4.58}$$

But we know from Theorem 3.1 that the sequence $\rho_{nd}^{L,\alpha}(s)$ converges in $[L^1(\mathbb{R}_t^+; \mathscr{T}_D(\mathbb{R}^6))]^*$-weak*. Hence it suffices to prove that the function $(\mathscr{C}\phi)(\mathbf{n}, \mathbf{p})$ belongs to $\mathscr{T}_D(\mathbb{R}^6)$, knowing that ϕ is C^∞ with compact support and $\hat{V}$ belongs to $\mathscr{T}_D$. This last point is obvious from the very definition (4.51) of $\mathscr{C}$, and (4.58) is thus proved.

Summarizing, we have proved that, as $L \to \infty$, the equation (4.52) transforms into,

$$\langle \rho_d^\alpha(t), \phi \rangle = \langle \rho_d^0, \phi \rangle + \int_{s=0}^{t} \langle \rho_{nd}^\alpha(s), \mathscr{C}\phi \rangle, \tag{4.59}$$

for all $\phi(\mathbf{n}) \in C_c^\infty(\mathbb{R}^3)$, hence for all $\phi \in \mathscr{T}_D(\mathbb{R}^3)$. This ends this third step.

Fourth Step. *Passing to the Limit in (4.53)*

We now come to the more difficult treatment of (4.53).

Again, in view of the uniform boundedness of *all* the operators involved in (4.53) as operators on $\mathscr{T}_D(\mathbb{R}^6)$, it is enough to pass to the limit in (4.53) in the special case where the test function Φ actually belongs to $C_c^\infty(\mathbb{R}^6)$.

We turn to identifying the limit of each term in (4.53) when $\Phi \in C_c^\infty(\mathbb{R}^6)$. In view of the weak convergence of $\rho_{nd}^{L,\alpha}(t)$, as stated in Theorem 3.1-(iv), we readily have,

$$\int_{s=0}^{t} \langle \rho_{nd}^{L,\alpha}(s), \Phi \rangle \xrightarrow[L\to\infty]{} \int_{s=0}^{t} \langle \rho_{nd}^\alpha(s), \Phi \rangle.$$

We now claim that the following convergence results hold as $L \to \infty$,

$$\int_{s=0}^{t} \int_{u=0}^{L^3 s} \exp(-\alpha u) \left\langle \rho_{nd}^{L,\alpha}\left(s - \frac{u}{L^3}\right), \mathscr{A}^L(u)\, \Phi \right\rangle$$

$$\to \int_{s=0}^{t} \int_{u=0}^{+\infty} \exp(-\alpha u) \langle \rho_{nd}^\alpha(s), \mathscr{A}(u)\, \Phi \rangle, \tag{4.60}$$

$$\int_{s=0}^{t} \int_{u=0}^{L^3 s} \exp(-\alpha u) \left\langle \rho_{d}^{L,\alpha}\left(s - \frac{u}{L^3}\right), \mathscr{B}^L(u)\, \Phi \right\rangle$$

$$\to \int_{s=0}^{t} \int_{u=0}^{+\infty} \exp(-\alpha u) \langle \rho_{d}^\alpha(s), \mathscr{B}(u)\, \Phi \rangle, \tag{4.61}$$

where we define,

$$(\mathscr{A}(u)\, \Phi)(\mathbf{n}, \mathbf{p}) := \lambda \int_{\mathbb{R}^3} [\exp(i[\mathbf{k}^2 - \mathbf{p}^2]\, u)\, \hat{V}(\mathbf{n} - \mathbf{k})\, \Phi(\mathbf{k}, \mathbf{p})$$

$$- \exp(i[\mathbf{n}^2 - \mathbf{k}^2]\, u)\, \hat{V}(\mathbf{k} - \mathbf{p})\, \Phi(\mathbf{n}, \mathbf{k})]\, d\mathbf{k} \tag{4.62}$$

$$(\mathscr{B}(u)\, \Phi)(\mathbf{n}) := \lambda \int_{\mathbb{R}^3} [\exp(i[\mathbf{p}^2 - \mathbf{n}^2]\, u)\, \hat{V}(\mathbf{n} - \mathbf{p})\, \Phi(\mathbf{p}, \mathbf{n})$$

$$- \exp(i[\mathbf{n}^2 - \mathbf{p}^2]\, u)\, \hat{V}(\mathbf{p} - \mathbf{n})\, \Phi(\mathbf{n}, \mathbf{p})]. \tag{4.63}$$

We prove this in two distinct steps. We readily mention that the key difficulty lies in proving that the non-local terms of the form $\rho_d^{L,\alpha}(s-\frac{u}{L^3})$ do converge towards $\rho_d^{L,\alpha}(s)$ (the equation becomes Markovian).

Fourth Step–Part a. *Proving (4.61)*

The point (4.61) is easily proved. Indeed, we naturally decompose the left-hand-side of (4.61) into,

$$\begin{aligned}
&\int_{s=0}^{t}\int_{u=0}^{L^3 s} \exp(-\alpha u)\left\langle \rho_d^{L,\alpha}\left(s-\frac{u}{L^3}\right), \mathscr{B}^L(u)\,\Phi\right\rangle\\
&\quad=\int_{s=0}^{t}\int_{u=0}^{L^3 s} \exp(-\alpha u)\left\langle \rho_d^{L,\alpha}\left(s-\frac{u}{L^3}\right)-\rho_d^{L,\alpha}(s), \mathscr{B}^L(u)\,\Phi\right\rangle\\
&\qquad+\int_{s=0}^{t}\int_{u=0}^{L^3 s} \exp(-\alpha u)\langle \rho_d^{L,\alpha}(s), \mathscr{B}^L(u)\,\Phi-\mathscr{B}(u)\,\Phi\rangle\\
&\qquad+\int_{s=0}^{t}\int_{u=0}^{L^3 s} \exp(-\alpha u)\langle \rho_d^{L,\alpha}(s), \mathscr{B}(u)\,\Phi\rangle\\
&\quad:=I+II+III.
\end{aligned}\tag{4.64}$$

∗ It is easily seen that II goes to zero. Indeed, on the one hand,

$$\begin{aligned}
&|\langle \rho_d^{L,\alpha}(s), \mathscr{B}^L(u)\,\Phi-\mathscr{B}(u)\,\Phi\rangle|\\
&\quad\leqslant \frac{C}{L^{3/2}}\left\|[\mathscr{B}^L(u)\,\Phi-\mathscr{B}(u)\,\Phi]\left(\frac{n}{L}\right)\right\|_{l_n^2} \qquad \text{(thanks to estimate (3.8))}\\
&\quad\leqslant C\left[\frac{1}{L^3}\sum_n\left|\sum_p\left(\exp\left(i\left[\frac{p^2-n^2}{L^2}\right]u\right)\frac{\lambda}{L^3}\hat{V}\left(\frac{n-p}{L}\right)\Phi\left(\frac{p}{L},\frac{n}{L}\right)\right.\right.\right.\\
&\quad\quad-\exp\left(i\left[\frac{n^2-p^2}{L^2}\right]u\right)\frac{\lambda}{L^3}\hat{V}\left(\frac{p-n}{L}\right)\Phi\left(\frac{n}{L},\frac{p}{L}\right)\Bigg)\\
&\quad\quad-\lambda\left(\int_{\mathbb{R}^3}\exp\left(i\left[\mathbf{p}^2-\frac{n^2}{L^2}\right]u\right)\hat{V}\left(\frac{n}{L}-\mathbf{p}\right)\Phi\left(\mathbf{p},\frac{n}{L}\right)\right.\\
&\quad\quad\left.\left.\left.-\exp\left(i\left[\frac{n^2}{L^2}-\mathbf{p}^2\right]u\right)\hat{V}\left(\mathbf{p}-\frac{n}{L}\right)\Phi\left(\frac{n}{L},\mathbf{p}\right)\right)\right|^2\right]^{1/2}\to 0,
\end{aligned}$$

thanks to the convergence of Riemann sums towards their integral counterpart, and in view of the decay assumptions we made on $\hat{V}$ and on the test function Φ (which actually has compact support). On the other hand, we readily have the uniform (in u) bound, using (4.57),

$$
\begin{aligned}
&|\langle \rho_d^{L,\alpha}(s), \mathscr{B}^L(u)\,\Phi - \mathscr{B}(u)\,\Phi\rangle| \\
&\quad \leqslant \|\rho_d^{L,\alpha}(s)\|_{l_n^2} \left[\left\| [\mathscr{B}^L(u)\,\Phi]\left(\frac{n}{L}\right)\right\|_{l_n^2} + \left\| [\mathscr{B}(u)\,\Phi]\left(\frac{n}{L}\right)\right\|_{l_n^2} \right] \\
&\quad \leqslant \frac{C}{L^{3/2}} \left[\left\| [\mathscr{B}^L(u)\,\Phi]\left(\frac{n}{L}\right)\right\|_{l_n^2} + \left\| [\mathscr{B}(u)\,\Phi]\left(\frac{n}{L}\right)\right\|_{l_n^2} \right] \\
&\quad \leqslant C\, \|\Phi\|_{\mathscr{T}_D}.
\end{aligned}
$$

Using now the fact that $\exp(-\alpha u)$ is integrable over the positive real axis, the Lebesgue Theorem is enough to obtain the convergence of II towards 0.

∗ The convergence of III is straightforward,

$$
\begin{aligned}
III &= \int_{s=0}^{t} \left\langle \rho_d^{L,\alpha}(s), \int_{u=0}^{L^3 s} \exp(-\alpha u)\, \mathscr{B}(u)\,\Phi \right\rangle \\
&\to \int_{s=0}^{t} \left\langle \rho_d^{\alpha}(t), \int_{u=0}^{+\infty} \exp(-\alpha u)\, \mathscr{B}(u)\,\Phi \right\rangle,
\end{aligned}
$$

in view of the Lebesgue Theorem together with the uniform boundedness of $\mathscr{B}(u)\,\Phi$ in $\mathscr{T}_D$, and using the weak convergence of $\rho_d^{L,\alpha}$ as stated in Theorem 3.1-(iv).

∗ There remains to prove that $I \to 0$. In order to do so, it turns out that the uniform Lipschitz estimate (3.12) of Theorem 3.1 is enough. Indeed,

$$
\begin{aligned}
|I| &\leqslant C(\Phi)\, L^{3/2} \int_{s=0}^{t} \int_{u=0}^{L^3 s} \exp(-\alpha u) \left\| \rho_d^{L,\alpha}\left(s - \frac{u}{L^3}\right) - \rho_d^{L,\alpha}(s) \right\|_{l_n^2} \\
&\quad \left(\text{here we used that } \left\| [\mathscr{B}^L(u)\,\Phi]\left(\frac{n}{L}\right)\right\|_{l_n^2} \leqslant C(\Phi)\, L^{3/2}, \right. \\
&\quad \left. \text{for some constant depending on } \Phi, \text{ using (4.57)} \right) \\
&\leqslant C(\Phi)\, L^{3/2} \int_{s=0}^{t} \int_{u=0}^{+\infty} \exp(-\alpha u)\, \frac{u}{L^3}\, \frac{C}{\alpha L^{3/2}} \\
&\quad \text{(thanks to (3.12))} \\
&\leqslant \frac{C \times C(\Phi)}{\alpha^3 L^3},
\end{aligned}
$$

hence,

$$I \to 0 \qquad \text{as} \qquad L \to \infty.$$

Fourth Step–Part b. *Proving (4.60)*

Let us now prove the more delicate point (4.60). We first decompose the left-hand-side of (4.60) in the same way as in part a above, and write,

$$\int_{s=0}^{t} \int_{u=0}^{L^3 s} \exp(-\alpha u) \left\langle \rho_{nd}^{L,\alpha}\left(s - \frac{u}{L^3}\right), \mathscr{A}^L(u)\, \Phi \right\rangle$$

$$= \int_{s=0}^{t} \int_{u=0}^{L^3 s} \exp(-\alpha u) \left\langle \rho_{nd}^{L,\alpha}\left(s - \frac{u}{L^3}\right) - \rho_{nd}^{L,\alpha}(s), \mathscr{A}^L(u)\, \Phi \right\rangle$$

$$+ \int_{s=0}^{t} \int_{u=0}^{L^3 s} \exp(-\alpha u) \langle \rho_{nd}^{L,\alpha}(s), \mathscr{A}^L(u)\, \Phi - \mathscr{A}(u)\, \Phi \rangle$$

$$+ \int_{s=0}^{t} \int_{u=0}^{L^3 s} \exp(-\alpha u) \langle \rho_{nd}^{L,\alpha}(s), \mathscr{A}(u)\, \Phi \rangle$$

$$:= I + II + III. \tag{4.65}$$

(We use the same notations an in part a above).

$*$ The most obvious term in (4.65) is III, which obviously converges towards,

$$III \to \int_{s=0}^{t} \int_{u=0}^{+\infty} \exp(-\alpha u) \langle \rho_{nd}^{\alpha}(s), \mathscr{A}(u)\, \Phi \rangle$$

$$= \int_{s=0}^{t} \left\langle \rho_{nd}^{\alpha}(s), \int_{u=0}^{+\infty} \exp(-\alpha u)\, \mathscr{A}(u)\, \Phi \right\rangle, \tag{4.66}$$

in view of the Lebesgue Theorem together with the uniform (in u) boundedness of $[\mathscr{A}(u)\, \Phi](\mathbf{n}, \mathbf{p})$ in $\mathscr{T}_D(\mathbb{R}^6)$, and using the weak convergence of $\rho_{nd}^{L,\alpha}$ as stated in Theorem 3.1-(iv).

$*$ We now turn to estimating II. The analysis is exactly the same as in part a above. Again, we begin by writing (use (3.10)),

$$\left| \int_{s=0}^{t} \int_{u=0}^{L^3 t} \exp(-\alpha u) \langle \rho_{nd}^{L,\alpha}(s), \mathscr{A}^L(u)\, \Phi - \mathscr{A}(u)\, \Phi \rangle \right|$$

$$\leqslant \frac{C}{\alpha} \int_{s=0}^{t} \int_{u=0}^{+\infty} \exp(-\alpha u) \left\| \frac{1}{L^3} [\mathscr{A}^L(u)\, \Phi - \mathscr{A}(u)\, \Phi]\left(\frac{n}{L}, \frac{p}{L}\right) \right\|_{l^2_{n,p}}. \tag{4.67}$$

Now we are led to estimating $\frac{1}{L^3}\|[\mathscr{A}^L(u)\,\Phi-\mathscr{A}(u)\,\Phi](\frac{n}{L},\frac{p}{L})\|_{l^2_{n,p}}$, a term which can be obviously decomposed as a sum of two symmetric terms, and we simply estimate one of them, as follows,

$$\begin{aligned}&\left\|\frac{1}{L^3}[\mathscr{A}^L(u)\,\Phi-\mathscr{A}(u)\,\Phi]\left(\frac{n}{L},\frac{p}{L}\right)\right\|_{l^2_{n,p}}\\&\approx\left[\sum_{n,p}\frac{1}{L^6}\left|\sum_k\frac{\lambda}{L^3}\exp\left(i\left[\frac{k^2-p^2}{L^2}\right]u\right)\hat{V}\left(\frac{n-k}{L}\right)\Phi\left(\frac{k}{L},\frac{p}{L}\right)\right.\right.\\&\qquad\left.\left.-\int_{\mathbb{R}^3}\exp\left(i\left[\mathbf{k}^2-\frac{p^2}{L^2}\right]u\right)\hat{V}\left(\frac{n}{L}-\mathbf{k}\right)\Phi\left(\mathbf{k},\frac{p}{L}\right)d\mathbf{k}\right|^2\right]^{1/2}\\&\to 0,\end{aligned}$$

in view of the theorem on convergence of Riemann sums, together with the decay assumptions we made on $\hat{V}$ and Φ.

∗ We now turn to the analysis of the most difficult term, namely I. We first write the obvious bound (use (4.55)),

$$\begin{aligned}|I|&\leqslant L^3\int_{s=0}^{t}\int_{u=0}^{L^3s}\exp(-\alpha u)\left\|\rho_{nd}^{L,\alpha}\left(s-\frac{u}{L^3}\right)-\rho_{nd}^{L,\alpha}(s)\right\|_{l^2_{n,p}}\\&\quad\times\left\|\frac{1}{L^3}[\mathscr{A}^L(u)\,\Phi]\left(\frac{n}{L},\frac{p}{L}\right)\right\|_{l^2_{n,p}}\\&\leqslant C(\Phi)\times L^3\int_{s=0}^{t}\int_{u=0}^{L^3s}\exp(-\alpha u)\left\|\rho_{nd}^{L,\alpha}\left(s-\frac{u}{L^3}\right)-\rho_{nd}^{L,\alpha}(s)\right\|_{l^2_{n,p}},\end{aligned}$$

where $C(\Phi)$ denotes some constant depending on Φ.

We now Taylor expand to first order the difference $\rho_{nd}^{L,\alpha}(s-\frac{u}{L^3})-\rho_{nd}^{L,\alpha}(s)$, and use the estimate (ii) of Theorem 3.1. This gives the bound,

$$\begin{aligned}&\leqslant L^3\int_{s=0}^{t}\int_{u=0}^{L^3s}\exp(-\alpha u)\left\|\rho_{nd}^{L,\alpha}\left(s-\frac{u}{L^3}\right)-\rho_{nd}^{L,\alpha}(s)\right\|_{l^2_{n,p}}\\&\leqslant L^3\int_{s=0}^{t}\int_{u=0}^{L^3s}\exp(-\alpha u)\int_{v=s-\frac{u}{L^3}}^{s}\|\partial_t\rho_{nd}^{L,\alpha}(v)\|_{l^2_{n,p}}\\&=L^3\int_{u=0}^{L^3t}\int_{s=\frac{u}{L^3}}^{t}\int_{v=s-\frac{u}{L^3}}^{s}\exp(-\alpha u)\,\|\partial_t\rho_{nd}^{L,\alpha}(v)\|_{l^2_{n,p}}\\&\leqslant L^3\int_{u=0}^{L^3t}\int_{v=0}^{t}\int_{s=v}^{v+\frac{u}{L^3}}\exp(-\alpha u)\,\|\partial_t\rho_{nd}^{L,\alpha}(v)\|_{l^2_{n,p}}\end{aligned}$$

$$\leqslant |t|^{1/2} \int_{u=0}^{L^3 t} u \exp(-\alpha u) \left(\int_{v=0}^{t} \|\partial_t \rho_{nd}^{L,\alpha}(v)\|_{l_{n,p}^2}^2 \right)^{1/2}$$

(by the Cauchy–Schwartz inequality in v)

$$\leqslant C \frac{|t|^{1/2}}{\alpha^{1/2} L^{3/2}} \int_{u=0}^{\infty} u \exp(-\alpha u)$$

(where we used the estimate (3.11))

$$\leqslant C \frac{|t|^{1/2}}{\alpha^{5/2} L^{3/2}}.$$

Note that we did not use the Cauchy–Schwartz inequality in v directly on the integral $s-(u/L^3) \leqslant v \leqslant s$, but rather on the larger domain $0 \leqslant v \leqslant t$ (after interchanging the v and s integrations). Indeed, the first approach leads to an upper-bound of the order one, for we would have lost the L^{-3} factor stemming from the smallness of the interval of integration in s.

This ends part b of the Fourth Step, hence the Fourth step.

Fifth Step. *Conclusion*

As a conclusion of the above four steps, we have proved that, as $L \to \infty$, the weak limits $\rho_d^\alpha(t)$ and $\rho_{nd}^\alpha(t)$ of $\rho_d^{L,\alpha}(t)$ and $\rho_{nd}^{L,\alpha}(t)$ satisfy, for any $\phi(\mathbf{n}) \in \mathscr{T}_D(\mathbb{R}^3)$ and $\Phi(\mathbf{n}, \mathbf{p}) \in \mathscr{T}_D(\mathbb{R}^6)$,

$$\langle \rho_d^\alpha(t), \phi \rangle = \langle \rho_d^0, \phi \rangle + i \int_{s=0}^{t} \langle \rho_{nd}^\alpha(s), \mathscr{C}\phi \rangle, \tag{4.68}$$

and,

$$\int_{s=0}^{t} \langle \rho_{nd}^\alpha(s), \Phi \rangle = i \int_{s=0}^{t} \left\langle \rho_{nd}^{L,\alpha}(s), \int_{u=0}^{+\infty} \exp(-\alpha u)\, \mathscr{A}(u)\, \Phi \right\rangle$$
$$+ i \int_{s=0}^{t} \left\langle \rho_d^{L,\alpha}(s), \int_{u=0}^{+\infty} \exp(-\alpha u)\, \mathscr{B}(u)\, \Phi \right\rangle. \tag{4.69}$$

The operators $\mathscr{A}(u)$, $\mathscr{B}(u)$ and $\mathscr{C}$ have been defined in (4.51), (4.62) and (4.63).

Coming back to the actual value of $\mathscr{A}(u)$, $\mathscr{B}(u)$ and $\mathscr{C}$ and transposing these operators, this means that the following relations hold true in a weak sense,

$$\partial_t \rho_d^\alpha(t) = \frac{i\lambda}{(2\pi)^3} \int_{\mathbb{R}^3} [\hat{V}(\mathbf{k}-\mathbf{n})\, \rho_{nd}^\alpha(t, \mathbf{k}, \mathbf{n}) - \hat{V}(\mathbf{n}-\mathbf{k})\, \rho_{nd}^\alpha(t, \mathbf{n}, \mathbf{k})]\, d\mathbf{k}, \tag{4.70}$$

and,

$$\rho_{nd}^{\alpha}(t,\mathbf{n},\mathbf{p}) = \frac{i\lambda}{(2\pi)^3}\int_0^{+\infty} e^{[i(\mathbf{n}^2-\mathbf{p}^2)-\alpha]\,u}\,\widehat{V}(\mathbf{p}-\mathbf{n})[\rho_d^{\alpha}(t,\mathbf{p})-\rho_d^{\alpha}(t,\mathbf{n})]\,du$$
$$+\frac{i\lambda}{(2\pi)^3}\int_0^{+\infty}\int_{\mathbb{R}^3} e^{[i(\mathbf{p}^2-\mathbf{n}^2)-\alpha]\,u}$$
$$\times[\widehat{V}(\mathbf{k}-\mathbf{n})\,\rho_{nd}^{\alpha}(t,\mathbf{k},\mathbf{p})-\widehat{V}(\mathbf{p}-\mathbf{k})\,\rho_{nd}^{\alpha}(t,\mathbf{n},\mathbf{k})]\,d\mathbf{k}\,du, \quad (4.71)$$

together with the initial datum,

$$\rho_d^{\alpha}(t=0,\mathbf{n}) = \rho_d^{0}(\mathbf{n}). \quad (4.72)$$

Actually we should say that (4.70) and (4.71) hold between distributions in $L^{\infty}(\mathbb{R}_t^+;[\mathcal{T}_D(\mathbb{R}^3)]^*)$ and $L^{\infty}(\mathbb{R}_t^+;[\mathcal{T}_D(\mathbb{R}^6)]^*)$ respectively, where $[\mathcal{T}_D]^*$ stands for the dual of $\mathcal{T}_D$. Also, (4.72) holds in $[\mathcal{T}_D]^*$ since $\rho_d^{\alpha}(t)$ is continuous, with values in $[\mathcal{T}_D]^*$.

Now, we may transform iteratively the system (4.70)–(4.71) into a closed equation on $\rho_d^{\alpha}(t)$. The formal manipulations are exactly the same as in the discrete case (see proof of Theorem 2.1), and lead to formulae (3.26), (3.27) in the statement of Theorem 3.2, which we rewrite briefly in the form,

$$\partial_t\rho_d^{\alpha}(t) = \sum_{l\geqslant 0}\lambda^{l+1}[Q_l^{\alpha}\rho_d^{\alpha}](t). \quad (4.73)$$

More precisely, when solving the system (4.70)–(4.71) iteratively, one comes up with a formula of the form,

$$\partial_t\rho_d^{\alpha}(t) = \sum_{l=0}^{l_0}\lambda^{l+1}[Q_l^{\alpha}\rho_d^{\alpha}](t)+\lambda^{l_0+1}[R_{l_0}^{\alpha}\rho_{nd}^{\alpha}](t), \quad (4.74)$$

where l_0 is some truncation index, and we wish to let $l_0\to\infty$ in order to get (4.73). The term $\lambda^{l_0+1}[R_{l_0}^{\alpha}\rho_{nd}^{\alpha}](t)$ denotes here the remainder term, whose explicit value is easily obtained by means of the computations in Section 4.2, but we skip it here for sake of simplicity. We simply mention in passing that the formula defining $[R_{l_0}^{\alpha}\rho_{nd}](t)$ is very similar in structure to the formula defining $[Q_{l_0}^{\alpha}\rho_d^{0}](t)$, and in particular it involves the same "oscillatory integrals" as treated in Lemma 3.1.

Now, in order to fully justify (4.73), we have to make sure that the remainder in (4.74) actually goes to zero as $l_0\to\infty$. For the sake of simplicity, we shall prove here a slightly weaker result, namely the mere *convergence* of the series involved in (4.73). In view of the actual value of $[R^{\alpha}_{l_0}\rho^{\alpha}_{nd}]$, the convergence towards zero of the remainder term is easily deduced along the same lines.

More precisely, we prove here that the series in (4.73) converges weakly, i.e., for any smooth enough test function $\phi(\mathbf{n})$, we prove that the series,

$$\sum_{l\geqslant 0} \lambda^{l+1}\langle Q^{\alpha}_l\rho^{\alpha}_d(t), \phi\rangle = \sum_{l\geqslant 0} \lambda^{l+1}\langle \rho^{\alpha}_d(t), {}^tQ^{\alpha}_l\phi\rangle, \tag{4.75}$$

converges, where ${}^tQ^{\alpha}_l$ denotes the transpose of Q^{α}_l. Since we simply know that the distribution $\rho^{\alpha}_d(t)$ is well defined in $[\mathcal{T}_D]^*$, the only way to ensure this convergence is to make sure that the series $\sum_{l\geqslant 0} \lambda^{l+1\,t}Q^{\alpha}_l\phi$ converges in $\mathcal{T}_D$, at least for a smooth test function $\phi(\mathbf{n})$.

If we do not take advantage of the oscillations present in the collision operators Q^{α}_l (or ${}^tQ^{\alpha}_l$, which are essentially the same operators), we are instantaneously led to a series of the size $\sum_l (C\lambda/\alpha)^l$ (the denominator α stemming from the integration of the real negative exponentials), and this leads to the constraint $\lambda \leqslant \lambda_0\alpha$, for some small λ_0. In order to avoid such a huge restriction, we rather make use of the crucial Lemma 3.1. More precisely, an easy adaptation of the proof given for this result (see also (3.41)) establishes the estimate,

$$\|\lambda^{l+1}\,{}^tQ^{\alpha}_l\phi\|_{\mathcal{T}_D} \leqslant \lambda^{l+1}C^l_0\,\|\hat{V}(\mathbf{n})\|^{l+1}_{\mathcal{S}_{2D}}\,\|\phi\|_{\mathcal{S}_{2D}}. \tag{4.76}$$

Hence we recover $|\lambda^{l+1}\langle Q^{\alpha}_l\rho^{\alpha}_d(t), \phi\rangle| \leqslant C^l\lambda^{l+1}$ for some constant C depending on the various norms of the profiles, hence the convergence of the series involved in (4.73), at least for small values of λ. This explains the restriction $|\lambda| \leqslant \lambda_0$ we impose in (2.9), as well as in the statement of Theorems 3.2 and 3.3.

This ends the proof of Theorem 3.2. ∎

4.6. Proof of Theorem 3.3: Convergence as $\alpha \to 0$

The proof is obvious in view of the arguments involved in the fifth step of the proof of Theorem 3.2. Indeed, the bound (4.76) established in the previous paragraph indicates that the series (4.73) actually converges *uniformly* with respect to α. On the more (due to the absolute convergence in time of the oscillatory integrals defining Q_l—see Lemma 3.1), the strong convergence,

$$[{}^tQ^{\alpha}_l\phi](\mathbf{n}) \to [{}^tQ_l\phi](\mathbf{n}) \qquad \text{in } \mathcal{T}_D,$$

obviously holds for any $\phi(\mathbf{n}) \in \mathcal{S}_{2D}$.

This ends the proof of Theorem 3.3. ∎

5. CONCLUSION: POSSIBLE EXTENSIONS OF THE PRESENT RESULTS

We have proved that the "damped" Von-Neumann equation posed on a dilated cube with the periodic boundary conditions (2.8) converges towards the Quantum Boltzmann equation when the dilation parameter goes to infinity and the damping parameter to zero (in this order). Since our method heavily relies on *explicit* formulae, the question of its validity for other geometries or boundary conditions is a natural question. For instance, it would be interesting to investigate the case of a dilated domain $L \cdot \Omega$ with Dirichlet boundary conditions, where Ω is some reference domain, and L is the large dilation parameter. One should expect that the same result holds whatever the (smooth enough) shape of the initial domain Ω. This naturally leads to the question of replacing the periodic boundary conditions on the cube by Dirichlet boundary conditions. Our method can easily be adapted to this situation, up to a slight modification of the combinatorics in the formulae that we leave to the reader. However, the case of a more general domain Ω is still open at present.

APPENDIX: THE PHYSISICTS' VIEW OF FERMI'S GOLDEN RULE

In this section, we briefly recall the traditional derivation of Fermi's Golden Rule as given in physics textbooks. Our exposition closely follows that of [Boh], Chapter 21, but many other references can be used as well for instance [CTDRG], [CTDL], [Mes], [SSL].

We denote by, $\psi_n = (2\pi L)^{-3/2} \exp(in \cdot x/L)$, the normalized eigenstates of the free Hamiltonian $H_0 = -\Delta$ on the periodic box $[0, 2\pi L]^3$. Let $C_p(t) = (\psi, \psi_p)$ the p-th component of the wave-function ψ in this eigenfunction basis. Then $C_p(t)$ evolves in time according to,

$$i\,\frac{dC_p}{dt} = (2\pi L)^{-3} \sum_{p'} \hat{V}\left(\frac{p-p'}{L}\right) C_{p'} \exp\left(i\,\frac{|p|^2-|p'|^2}{L^2}\,t\right).$$

We now assume that at time $t=0$, the particle lies entirely in the state n, which means that $C_p(0) = \delta_{p,n}$ where $\delta_{p,n}$ is the Kronecker index. At first order in the potential, we can therefore write for $p \neq n$,

$$i\dot{C}_p \approx (2\pi L)^{-3}\, \hat{V}\left(\frac{p-n}{L}\right) \exp\left(i\,\frac{|p|^2-|n|^2}{L^2}\,t\right),$$

which, after time integration, yields a population $|C_p(t)|^2$ given by,

$$|C_p(t)|^2 = \frac{1}{(2\pi L)^6} \left| \hat{V}\left(\frac{p-n}{L}\right) \right|^2 \frac{\sin^2\left(\frac{(|p|^2-|n|^2)t}{2L^2}\right)}{\left(\frac{|p|^2-|n|^2}{2L^2}\right)^2}.$$

Now we perform the limit $L \to \infty$ and we consider a sequence of states such that p/L, n/L converges to $\mathbf{p}, \mathbf{n} \in \mathbb{R}^3$. Then,

$$(2\pi L)^3\, |C_p(t)|^2 \sim |C_{\mathbf{p}}(t)|^2 = \frac{1}{(2\pi L)^3}\ |\hat{V}(\mathbf{p}-\mathbf{n})|^2\ \frac{\sin^2\left(\frac{(|\mathbf{p}|^2-|\mathbf{n}|^2)t}{2}\right)}{\left(\frac{|\mathbf{p}|^2-|\mathbf{n}|^2}{2}\right)^2}.$$

When t tends to infinity, we have, in the sense of distributions,

$$\frac{\sin^2\left(\frac{(|\mathbf{p}|^2-|\mathbf{n}|^2)t}{2}\right)}{\left(\frac{|\mathbf{p}|^2-|\mathbf{n}|^2}{2}\right)^2} \sim 2\pi t\delta(|\mathbf{p}|^2-|\mathbf{n}|^2)\,, \tag{A.1}$$

and this yields,

$$|C_p(t)|^2/t \sim \frac{2\pi}{(2\pi L)^3}\ |\hat{V}(\mathbf{p}-\mathbf{n})|^2\, \delta(|\mathbf{p}|^2-|\mathbf{n}|^2)\,, \quad \text{as} \quad L \to \infty, \quad t \to \infty, \tag{A.2}$$

which is precisely Fermi's Golden Rule. We note that the dependence of the right-hand side of (A.2) upon L makes it an asymptotic formula rather than a limit. In conventional scattering theory, a collection of N randomly distributed identical potentials is considered. Then, taking the expectation of (A.2) with respect to this random variable, the central limit theorem gives that $\langle |C_p(t)|^2/t \rangle$ is proportional to $N/(2\pi L)^3 = \nu$ where ν is the density of scatterers, an intrinsic property of the scattering medium. Here, we shall not consider a random distribution, but rather absorb L in the scaling.

Finally, to convert formula (A.2) into an expression for the transition rate from state $\mathbf{n}$ to state $\mathbf{p}$, one needs to take the limit $t \to 0$ of (A.2), and transform $|C_p(t)|^2/t$ into a time derivative. Of course, this step is highly questionable since the limit $t \to \infty$ has just been taken before. Obviously, there are two time scales involved, the short one over which elementary scattering events occur (and for which the limit $t \to \infty$ is taken), and the long one over which the populations change macroscopically as the result of the cummulative effects of the elementary scattering events.

Now, this formal computation shows how essential it is to pass from a discrete set of states p to a continuous one $\mathbf{p}$. Indeed, formula (A.1) would have no meaning if the variable $\mathbf{p}$ ranged over the discrete set $\mathbb{Z}^3$. On the other hand, it would not have been possible to start the computation from unnormalized states $\exp(in \cdot x)$ on the whole space $\mathbb{R}^3$, since the populations $|C_p(t)|^2$ would then be meaningless. A basic motivation for this work is to give a mathematically rigorous justification of the formal computation presented above.

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