UNIVERSITÀ DEGLI STUDI DI TRIESTE
Sede amministrativa del Dottorato di Ricerca
DIPARTIMENTO DI FISICA

XXVIII CICLO DEL
DOTTORATO DI RICERCA IN FISICA

Collisional Models for a Quantum Particle in a Gas

Settore scientifico-disciplinare FIS/02

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Introduction

In 1872 Boltzmann proposed his famous equation to explain the properties of dilute gases, *i.e.*

$$\frac{\partial \rho(\mathbf{x},\mathbf{p})}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla \rho(\mathbf{x},\mathbf{p}) + \mathbf{F} \cdot \frac{\partial \rho(\mathbf{x},\mathbf{p})}{\partial \mathbf{p}} = \left(\frac{\partial \rho(\mathbf{x},\mathbf{p})}{\partial t} \right)_{coll} \tag{1}$$

The equation describes the dynamics of the single particle marginal of the gas ($\rho(\mathbf{x},\mathbf{p})$), under the influence of an external force $\hat{F}$, approximating the complicated interaction with other particles by collisions:

$$\left(\frac{\partial \rho(\mathbf{x},\mathbf{p})}{\partial t} \right)_{coll} = n_{gas} \int d\Omega d\mathbf{k} \frac{\mathbf{p}_r}{m^*} \sigma(\mathbf{p}_r, \Omega)[\rho(\mathbf{p},t)\rho(\mathbf{k},t) - \rho(\mathbf{p}',t)\rho(\mathbf{k}',t)] \tag{2}$$

where $\sigma(\mathbf{p}_r, \Omega)$, is the scattering cross section between two particles of mass m that are scattered by an angle Ω and with relative momentum $\mathbf{p}_r$, and the momenta $\mathbf{p}'$ and $\mathbf{k}'$ are implicitly determined by the conservation law $\mathbf{p} + \mathbf{k} = \mathbf{p}' + \mathbf{k}'$ (for a detailed derivation see [1–3]). The Botlzmann equation is so successful in describing the behavior of dilute gases that it is now recognized as a fundamental equation in the kinetic theory of gases and is a paradigm for the description of classical systems far from equilibrium [4,5].

Guided by the simplicity and the elegance of Boltzmann's derivation many physicist were attracted by the idea of extending Boltzmann's model to the quantum mechanical case [6–16]. Several efforts has been also done in mathematical physics to find a rigorous derivation of the quantum version of the Boltzmann equation [17–21]. However, even a rigorous treatment of the classical equation is missing due to the complexity of the problem (see [22–33] and literature there in for partial results and development).
The situation becomes more tractable if one restricts the problem to the case of a single

particle interacting with a rarefied thermal bath, indeed the non linear term of the Boltzmann equation described in Eq. (1) becomes [2]

$$\left(\frac{\partial\rho(\mathbf{x},\mathbf{p})}{\partial t}\right)_{coll} = \int d\Omega d\mathbf{q}\mathbf{p}_r\sigma(\mathbf{p}_r,\Omega)[\rho(\mathbf{p},t)\rho_g(\mathbf{p}') - \rho(\mathbf{p}',t)\rho_g(\mathbf{q}')] \tag{3}$$

where $\rho_q(\mathbf{p})$ describes the stationary state of the rarefied thermal bath, and Eq. (3) becomes the so called linear Boltzmann equation. Since the linear problem are easier, most promising results have been achieved in the study of the quantum behavior of a test particle in a gas, leading to the well established field of collisional decoherence [34–47]. This field of research was born to explain the emergent classicality -loss of quantum coherence- in the macroscopic world but it is now interested in studying the general decoherence effects on a quantum system due to collisional interaction with the surrounding environment.

The beginning of collisional decoehrence theory dates back to 1985 when Joos and Zeh [34] proposed the first quantum collisional model describing the evolution of a system affected by the interaction with a thermal bath. The main achievement of the Joos-Zeh model is to show the presence of an irreversible damping of the system's spatial interference due to the environmental interaction, the so called spatial decoherence. Even if the model is of great importance for the development of the theory, it is just a first step in understanding the behavior of a quantum system affected by environmental interactions. Indeed, this model is limited to the description of a very massive object in a regime where no friction and only small spatial coherences are present. A drawback of the Joos-Zeh model is an infinite growth of the system's energy for long time scales, which is unphysical because one expects a thermalization process that equilibrates the system's energy with the gas thermal energy.

In 1990 a step towards a consistent model describing a quantum particle in a thermal bath was made by Gallis and Flemming [35]. They extended the Joos-Zeh result, deriving an equation that correctly describes the dynamics of spatial coherences at all length scales. However, they were not able to include friction. The first attempt in this direction has been done in 1995, when Diósi published a work containing a collisional model describing the dissipative behavior of massive particle in a thermal bath [36].

Five years later Hornberger and Vacchini extended Diósi's result by removing the constraint of very massive particle [40]. They also claimed to have derived the quantum counterpart of the linear Boltzmann equation, describing the classical dynamics of a test particle affected by a rarefied thermal gas.

However this result was obtained by making use of several heuristic arguments. These were somehow necessary to overcome the difficulties which prevented the previous authors from finding a consistent and general model describing the quantum dynamics of a test particle affected by a rarefied thermal gas. The presence of inconsistencies in the heuristic arguments adopted by Hornberger-Vacchini has been independently pointed out by Kamleitner and Diósi [39, 48]. Furthermore, Diósi proposed a new model based on incomplete collisions process [39], in the attempt to avoid the problems encounter by Hornberger-Vacchini. Anyhow, as later pointed out by Honrberger-Vacchini, also this model by Diósi is not satisfactory [49].

To summarize, important steps forward have been done in the last decades to understand of the quantum behavior of a test particle affected by a thermal bath. However the most refined theoretical collisional models proposed so far seem not to be in agreement with each other. Furthermore, the open debate about which model is the one that correctly describes a particle in a gas is a witness that the validity of these models is still unclear. A better understanding of the quantum behavior of test particles in gases is not only desirable, but would also help in understanding the non-classical process of decoherence, which is believed to be of crucial importance in the quantum-classical transition. It is a wide spread belief that the emergent of the classical properties in macroscopic systems is due to decoherence phenomena produced by the unavoidable interaction with the surrounding environment.

The aim of this thesis is to critically analyze the collisional models for the quantum behavior of a test particle interacting with a rarefied thermal bath, in order to understand their validity. We start with a critical review of the state of the art in quantum collisional models. Then, we study a very simple system, which is exactly solvable: A two-particle system interacting via a Dirac delta potential in one dimension. We analyze the interaction and estimate the collision time for Gaussian wave packets.
Then, we focus on the main problem of this thesis: the dynamics of a test particle in a quantum gas. We first tackle it with an original technique that combines the Hartree variational method with stochastic calculus techniques. In this way we properly describe the non dissipative behavior of the test particle, and we gather interesting insight on the dissipative process. Eventually, we provide a microscopic derivation of the collisional dynamics for a test particle in a rarefied thermal bath. We, shows the limits of this approach, providing necessary conditions for the validity of collisional equation. We then conclude

by summarizing the main results of this thesis.

Chapter 1

State of the Art

We critically review the state of the art of quantum collisional models. We can divide the review into two parts, each of which is presented in a different section The first includes models for infinitely heavy test particles. This assumption leads to recoil-less collisions, where any change of the test particle's position is neglected. The second includes models which relax this hypothesis, and study the full interplay between friction, diffusion and decoherence of a test particle interacting with a thermal bath. A review of all the models except for the "linear Boltzmann equation with finite intercollision" time proposed by Diosi can also be found in [50] , where the authors use the so called "Quantum Linear Boltzmann equation" to make the comparison.

1.1 Recoil-less Collisional Dynamics

The first model of a particle in a gas was given by Joos and Zeh [34]. It was derived in the attempt to understand how the classical behavior of the macroscopic world emerges from the quantum mechanical laws. Their idea was that classicality is a consequence of the unavoidable interaction among macroscopic objects and the surrounding environment. Precisely in the attempt to build a model describing the evolution of a macroscopic object under the influence of photons or dust particles, they assumed the interaction to be collisional. In particular, they assumed that the duration of the scattering process between the macroscopic object and an environmental particle is short compared to the typical evolution time scales of the macro-object itself. Under this assumption, they claim, the dynamics of the macroscopic object can be described by the free evolution, suddenly and randomly perturbed by scattering events; formally they write:

$$i\hbar\frac{\partial\hat{\rho}}{\partial t} = \left[\hat{H}_0\,,\hat{\rho}\right] + \left.\frac{\partial\hat{\rho}}{\partial t}\right|_{scatt.}, \tag{1.1}$$

where $\hat{\rho}$ is the statistical operator describing the state of the system, $\hat{H}_0$ is the hamiltonian generating the free evolution and $\frac{\partial\hat{\rho}}{\partial t}|_{scatt.}$ is the collisional contribution to the dynamics. In order to find the analytic expression for such a collisional term in Eq. (1.1), the authors make the key assumption of a *recoil free* scattering, *i.e.* they assume that the scattering process does not affect the position of the macroscopic system :

$$|\mathbf{x}\rangle\,|\chi\rangle \xrightarrow{scattering} \hat{S}\,|\mathbf{x}\rangle\,|\chi\rangle = |\mathbf{x}\rangle\,\hat{S}_{\mathbf{x}}\,|\chi_{\mathbf{x}}\rangle = |\mathbf{x}\rangle\,|\chi_{\mathbf{x}}\rangle\,, \tag{1.2}$$

where $\hat{S}$ is the scattering operator describing the collision process between the macro object and the environmental particle, $\hat{S}_{\mathbf{x}} = \langle\mathbf{x}|\,\hat{S}\,|\mathbf{x}\rangle$ is the scattering matrix for a macro-object with center of mass in $\mathbf{x}$, $|\chi\rangle$ is the state of the environmental particle before the scattering, and $|\chi_{\mathbf{x}}\rangle$ is the state of the environmental particle after the scattering, that obviously depends on the position of the macro-object. The hypothesis of a recoil free scattering is justified when the mass of the macroscopic object is much larger than the mass of the environmental particle, a condition that the authors assume to be satisfied for a scattering with dust or light. Describing the macroscopic object by a wave function $\varphi(\mathbf{x})$ in the position basis, the authors write the density matrix of the scattering center $\mathbf{x}$ as

$$\hat{\rho}(\mathbf{x},\mathbf{x}') = \varphi(\mathbf{x})\varphi^*(\mathbf{x}')\,\langle\chi|\,\hat{S}^\dagger_{\mathbf{x}'}\hat{S}_{\mathbf{x}}\,|\chi\rangle\,. \tag{1.3}$$

In order to consider a very general recoil free collision process, they make the natural assumption of translational invariant interactions. Accordingly, they find

$$\begin{aligned}\langle\chi|\,\hat{S}^\dagger_{\mathbf{x}'}\hat{S}_{\mathbf{x}}\,|\chi\rangle &= \int d\mathbf{k}\,d\mathbf{k}'d\mathbf{k}''\,S_{\mathbf{x}'}(\mathbf{k},\mathbf{k}')S^*_{\mathbf{x}}(\mathbf{k},\mathbf{k}'')\chi(\mathbf{k}')\chi(\mathbf{k}'')\\ &= \int d\mathbf{k}\,d\mathbf{k}'d\mathbf{k}''\,S(\mathbf{k},\mathbf{k}')S^*(\mathbf{k},\mathbf{k}'')e^{-i\mathbf{k}'(\mathbf{x}-\mathbf{x}')}e^{-i\mathbf{k}''(\mathbf{x}-\mathbf{x}')}\chi(\mathbf{k}')\chi(\mathbf{k}''),\end{aligned} \tag{1.4}$$

with $S(\mathbf{k},\mathbf{k}')$ the usual scattering matrix in momentum, $S^*(\mathbf{k},\mathbf{k}')$ its complex conjugate and $\chi(\mathbf{k}) = \langle\mathbf{k}|\chi\rangle$ the environmental wave function in momentum. They express the scattering matrix in terms of the scattering amplitude $f(\mathbf{k},\mathbf{k}')$, *i.e.*

$$S(\mathbf{k},\mathbf{k}') = \delta^3(\mathbf{k}-\mathbf{k}') + \frac{i}{2\pi k} f(\mathbf{k},\mathbf{k}')\delta(k-k'), \tag{1.5}$$

and they further approximate the environmental particle state with a momentum eigenstate:

$$\chi(\mathbf{k}) \simeq L^{-3/2}\delta^3(\mathbf{k}-\mathbf{k}_0), \tag{1.6}$$

where $\mathbf{k}_0$ is the momentum of the incident particle and L^3 the normalization volume. The approximation in Eq. (1.6) is justified under the very natural assumption that the interacting environment is a rarefied gas in thermal equilibrium. Substituting Eq. (1.5) and Eq. (1.6) in Eq. (1.4) one gets

$$\langle\chi|\,\hat{S}^\dagger_{\mathbf{x}'}\hat{S}_{\mathbf{x}}\,|\chi\rangle = \int \frac{d\mathbf{k}}{L^3}\,[\delta^3(\mathbf{k}-\mathbf{k}_0)]^2 + \frac{1}{\pi^2 k^2}\,|f(\mathbf{k},\mathbf{k}_0)|^2\,[\delta(k-k_0)]^2 e^{-i(\mathbf{k}-\mathbf{k}_0)(\mathbf{x}-\mathbf{x}')}. \tag{1.7}$$

This equation displays an ill-defined squared delta function, that needs to be handled carefully. The square delta function problem is very common in scattering physics [51] and is usually cured by adopting a specific replacement scheme for the divergent terms, *i.e.*

$$\begin{aligned} [\delta\left(\frac{k^2-k_0^2}{2m}\right)]^2 &\rightarrow \frac{T}{2\pi}\left(\frac{k^2-k_0^2}{2m}\right) \\ [\delta^3(\mathbf{k}-\mathbf{k}_0)]^2 &\rightarrow \frac{L^3}{2\pi}\delta^3(\mathbf{P}) \end{aligned} \tag{1.8}$$

where T is the duration time of the scattering process, and m is the mass of the scattered particle. The replacement scheme in Eq. (1.8) can be easily understood in the framework of time dependent perturbation theory, where the energy Dirac delta function is generated by

$$\lim_{T\to\infty}\frac{1}{2\pi}\int_{-T}^{T} d\tau\, e^{i\frac{\mathbf{k}^2-\mathbf{k}_0^2}{2m}\tau} = \delta\left(\frac{k^2-k_0^2}{2m}\right) = \frac{m}{k}\delta(k-k_0), \tag{1.9}$$

and the three dimensional Dirac delta function is generated by

$$\lim_{L\to\infty}\frac{1}{(2\pi)^3}\int_{L^3} d\mathbf{x}\, e^{i\mathbf{k}\cdot\mathbf{x}} = \delta^3(\mathbf{k}-\mathbf{k}_0). \tag{1.10}$$

However, even if the authors do no explicitly state it, from their calculations one finds out that they cure the divergent term by making the following replacement:

$$\begin{aligned} \delta^3(\mathbf{k}-\mathbf{k}_0)]^2 &\simeq L^3\,\delta^3(\mathbf{k}-\mathbf{k}_0) \\ [\delta(k-k_0)]^2 &\simeq L\,\delta(k-k_0). \end{aligned} \tag{1.11}$$

They where probably guided by the fact that the Fourier representation of the momentum Dirac delta function in one dimension is given by Eq. (1.10)

$$\delta(k) = \frac{1}{(2\pi)} \int dx e^{ikx} \tag{1.12}$$

from which it follows directly that

$$[\delta(k)]^2 = \delta(k)\delta(0) = \frac{1}{(2\pi)^2} \int_L dx' e^{\frac{i}{\hbar}kx'} \int_L dx = \frac{L}{(2\pi)}\delta(k), \tag{1.13}$$

that is similar to the replacement in Eq. (1.11). As we will see, the unjustified replacement adopted by Joos and Zeh in their computation will later lead Hornberger and Sipe [37] to carry out a wave packet analysis of the scattering process and provide an un-usual replacement rule (see Eq. (1.44) in this section) for the ill-defined square delta function. Coming back to the work of Joos-Zeh, using the replacement rule in Eq. (1.11) one gets for Eq. (1.7) the well defined expression

$$\langle\chi|\,\hat{S}^\dagger_{\mathbf{x}'}\hat{S}_{\mathbf{x}}\,|\chi\rangle = 1 + \frac{i}{4\pi^2 L^2} \int \frac{d\mathbf{k}}{k}\,|f(\mathbf{k},\mathbf{k}_0)|^2\,\delta(k-k_0) e^{-i(\mathbf{k}-\mathbf{k}_0)(\mathbf{x}-\mathbf{x}')}. \tag{1.14}$$

Expanding the exponential up to the second order, and integrating over the solid angle of $\mathbf{k}$ the authors eventually obtain

$$\rho(\mathbf{x},\mathbf{x}') \xrightarrow{scattering} \hat{\rho}(\mathbf{x},\mathbf{x}') \left(1 - \frac{(k_0\ |\mathbf{x}-\mathbf{x}'|)^2}{8\pi^2 L^2}\sigma_{eff}\right) \simeq \rho(\mathbf{x},\mathbf{x}') \exp\left(-\frac{(k_0\ |\mathbf{x}-\mathbf{x}'|)^2}{8\pi^2 L^2}\sigma_{eff}\right), \tag{1.15}$$

where

$$\sigma_{eff} := \frac{\pi}{2} \int d\cos\theta\,|f(cos\theta)|^2 \left[(2-\cos\theta)^2 - 1\right] \tag{1.16}$$

is the effective scattering cross-section. The result of Eq. (1.15) is then extended to n subsequent independent scattering processes by multiplying the effective cross-section by the factor n. Joos-Zeh furthermore identify the number of scattering process n as the number of particles passing trough the surface L^2 of the normalization volume L^3 in a time interval t, *i.e.*

$$n = L^2 \cdot flux \cdot t = L^2 \cdot \text{particle density} \cdot \text{mean velocity} \cdot t = L^2 \frac{N}{V} v t, \tag{1.17}$$

which leads to

$$\rho(\mathbf{x}, \mathbf{x}') \xrightarrow{n-scattering} \rho(\mathbf{x}, \mathbf{x}') \exp\left(-\Lambda(\mathbf{x} - \mathbf{x}')^2 t\right) \tag{1.18}$$

where Λ is the localization rate and is defined by

$$\Lambda := \frac{k_0^2 \sigma_{eff} N v}{8\pi^2 V}. \tag{1.19}$$

Performing the time derivative of Eq. (1.18) they eventually obtain

$$\left.\frac{\partial \rho(\mathbf{x}, \mathbf{x}')}{\partial t}\right|_{scatt.} = -\Lambda(\mathbf{x} - \mathbf{x}')^2 \rho(\mathbf{x}, \mathbf{x}') \tag{1.20}$$

or in an equivalent operatorial form

$$\left.\frac{\partial \hat{\rho}}{\partial t}\right|_{scatt.} = -\Lambda \left[\hat{\mathbf{x}}\,, \left[\hat{\mathbf{x}}\,, \hat{\rho}\right]\right]. \tag{1.21}$$

This is the well known Joos and Zeh master equation for collisional decoherence.

One observes that Eq. (1.20) describes an irreversible damping of the interference terms of the density matrix $\hat{\rho}(\mathbf{x}, \mathbf{x}')$, due to the interaction of the system with the environment. One furthermore observes that the decay rate $\Lambda(\mathbf{x} - \mathbf{x}')^2$ of spatial interferences, grows to infinity when $|\mathbf{x} - \mathbf{x}'| \to \infty$, proving an unphysical behavior of the equation for long length-scales [35]. This is not surprising because the approximation performed to obtain Eq. (1.15) from Eq. (1.14) (Taylor expansion) is valid only for small values of $(\mathbf{k} - \mathbf{k}_0)(\mathbf{x} - \mathbf{x}')$. This implies that the Joos-Zeh master equation is not able to correctly describe the system behavior in presence of spatial interference phenomena on large length scales.

Gallis and Fleming [35] later extended the Joos-Zeh result to all length scales. They did so by keeping the exact expression of Eq. (1.14), (without expanding the exponential). Calculations very similar to those performed by Joos and Zeh lead to the following result:

$$\left.\frac{\partial \hat{\rho}}{\partial t}\right|_{scatt.} = \int d\mathbf{k} d\mathbf{k}' \frac{n(k) v(k)}{2k^4} \delta(k - k') \left|f(\mathbf{k}, \mathbf{k}')\right|^2 \left(e^{\frac{i}{\hbar}(\mathbf{k}-\mathbf{k}')\cdot\hat{\mathbf{x}}} \hat{\rho} e^{-\frac{i}{\hbar}(\mathbf{k}-\mathbf{k}')\cdot\hat{\mathbf{x}}} - \hat{\rho}\right); \tag{1.22}$$

where $n(k)$ is the number density of scattering particles with momentum k and $v(k) = k/m$ is their speed. Eq. (1.22) is the well known collisional term of the Gallis-Fleming master equation. One can observe that Eq. (1.22) is well behaved for $|\mathbf{x}-\mathbf{x}'| \to \infty$, indeed

$$\lim_{|\mathbf{x}-\mathbf{x}'|\to\infty} \left.\frac{\partial\rho(\mathbf{x},\mathbf{x}')}{\partial t}\right|_{scatt.} = \int d\mathbf{k}\frac{n(k)v(k)}{2k^4}\left|f(\mathbf{k},\mathbf{k})\right|^2\rho(\mathbf{x},\mathbf{x}'), \tag{1.23}$$

which is finite and independent from the spatial separation $|\mathbf{x}-\mathbf{x}'|$, as one expects from physical considerations [35].

As previously mentioned the replacement rule of Eq. (1.11), adopted both by Joos-Zeh and Gallis-Fleming, is not a consistent replacement rule for the square delta function that appears in Eq. (1.7). Motivated by this fact and by a discrepancy among the experiment and the theoretical predictions [42], Hornberger and Sipe re-derived the Gallis-Fleming master equation. They carried out a careful wave packet analysis of the scattering process. After a cumbersome and lengthy calculation, they were able to reproduce the Gallis-Fleming result rescaled by a $1/2\pi$ factor, which is confirmed by experiments [42]. They furthermore provide a new replacement rule for the ill-defined square delta function in Eq. (1.7), *i.e.*

$$|\delta(k-k_0)f(\mathbf{k},\mathbf{k}_0)|^2 \to \frac{L^3}{2\pi\sigma(\mathbf{k})}\delta(k-k_0)\left|f(\mathbf{k},\mathbf{k}_0)\right|^2, \tag{1.24}$$

claiming the necessity of this replacement when treating the problem without passing trough a wave packet analysis. Adler, in a later work [52], showed that it is possible to obtain Hornberger-Sipe results without passing through a wave packet calculation, nor using the unusual replacement rule in Eq. (1.24). Following the strategy earlier adopted by Diósi in [36] (where the correct replacement rule in Eq. (1.8) is adopted), Adler was able to re-derive Eq. (1.22) with the correct 2π factor. He continued his analysis by making a comparison between Hornberger-Sipe result [37] and Diósi work [36]. We will not report here the details.

In the next section we will discuss the more interesting result obtained by Diósi in [36] in the attempt to overcome the limitations of the Gallis-Fleming and Joos-Zeh models. As it is shown in [53, 54], the assumption of recoil-free collisions in these models leads to an infinite growth of the system's kinetic energy on long time scales. This divergent heating effect restricts the validity of the models to only short times. We will discuss the most relevant attempt to overcome this problem, by including recoil and friction effects in collisional dynamics.

1.2 Collisional Dynamics with Recoil

To our knowledge, the first attempt to deal with the problem of the infinite heating effect in collisional models was done by Diósi in [36]. The author considers a single collision in the interaction picture (I):

$$\hat{\rho}^I_{\mathcal{S}\mathcal{E}} \xrightarrow{scattering} \hat{S}\hat{\rho}^I_{\mathcal{S}\mathcal{E}}\hat{S}^\dagger, \tag{1.25}$$

where $\hat{S}$ is the unitary scattering operator and $\hat{\rho}_{\mathcal{S}\mathcal{E}}$ the statistical operator describing the system plus environment. Equation (1.25) is analogous to the one in Eq. (1.2) by Joos-Zeh; however here no assumption of recoil-free scattering is made. After introducing the transition operator $\hat{T}$, through the relation $\hat{S} = \mathbf{1} + i\hat{T}$, Diósi finds that the change of the statistical operator $\hat{\rho}_{\mathcal{S}\mathcal{E}}$ due to one collision is

$$\Delta\hat{\rho}^I_{\mathcal{S}\mathcal{E}} = \hat{S}\hat{\rho}^I_{\mathcal{S}\mathcal{E}}\hat{S}^\dagger - \hat{\rho}^I_{\mathcal{S}\mathcal{E}} = \frac{i}{2}\left[\hat{T} + \hat{T}^\dagger\,,\hat{\rho}^I_{\mathcal{S}\mathcal{E}}\right] + \hat{T}\hat{\rho}^I_{\mathcal{S}\mathcal{E}}\hat{T}^\dagger - \frac{1}{2}\left\{\hat{T}^\dagger\hat{T}\,,\hat{\rho}^I_{\mathcal{S}\mathcal{E}}\right\}. \tag{1.26}$$

In order to obtain a collisional master equation, he assumes that the time derivative of the statistical operator in the interaction picture can be approximated by the change due to a collision over the collision time Δt, *i.e.*

$$\frac{\partial\hat{\rho}^I_{\mathcal{S}}}{\partial t} \simeq \frac{\Delta\hat{\rho}^I_{\mathcal{S}}}{\Delta t} = \frac{1}{\Delta t}\mathrm{Tr}_{\mathcal{E}}\Delta\hat{\rho}^I_{\mathcal{S}\mathcal{E}}. \tag{1.27}$$

With Eq. (1.27) he implicitly assumes that the collision described by Eq. (1.26) lasts for very short time scales. This assumption is equivalent to the assumption of short collision time made by Joos and Zeh in [34]. He further assumes that the collision incoming states are uncorrelated[1], *i.e.* the incoming state is in a factorized product $\hat{\rho}_{\mathcal{S}\mathcal{E}} = \hat{\rho}_{\mathcal{S}} \otimes \hat{\rho}_{\mathcal{E}}$, where $\hat{\rho}_{\mathcal{S}}$ and $\hat{\rho}_{\mathcal{E}}$ describes the state of the system and of the environment respectively. The environmental state $\hat{\rho}_{\mathcal{E}}$ describes n uncorrelated identical particles per unit volume, all of them in the same stationary state $\rho_{\mathcal{E}}(\mathbf{k})$. He then introduces the standard representation

[1] This assumption is the quantum analogous to the molecular chaos assumption made by Boltzmann in his seminal work.

of the transition operator,

$$\hat{T} = \frac{1}{2\pi m^*} \int d\mathbf{P}_i d\mathbf{k}_f d\mathbf{k}_i f(\mathbf{k}_f^*, \mathbf{k}_i^*) \delta(E_{\mathbf{k}_f^*} - E_{\mathbf{k}_i^*}) \left| \mathbf{P}_i - \mathbf{k}_f + \mathbf{k}_i, \mathbf{k}_f \right\rangle \left\langle \mathbf{P}_i, \mathbf{k}_i \right| \tag{1.28}$$

where

$$M^* = M + m, \quad m^* = \frac{mM}{M^*}, \quad \mathbf{k}_i^* = \frac{M}{M^*}\mathbf{k}_i - \frac{m}{M^*}\mathbf{P}_i, \quad \mathbf{k}_f^* = \mathbf{k}_f - \frac{m}{M^*}(\mathbf{k}_i + \mathbf{P}_i), \tag{1.29}$$

M, $\vec{P}$ and m, $\vec{k}$ are respectively the mass and the momentum of the system and of the gas particle. In this way Diósi derives the following identity:

$$\begin{aligned} \mathrm{Tr}_{\mathcal{E}} \left(\hat{T} \hat{\rho}_{\mathcal{S}}^I \otimes \hat{\rho}_{\mathcal{E}} \hat{T}^\dagger \right) &= \frac{2\pi n}{m^{*2}} \int d\mathbf{P}_i d\mathbf{P'}_i d\mathbf{k}_i d\mathbf{k}_f \, \rho_{\mathcal{E}}(\mathbf{k}_i) \left\langle \mathbf{P}_i \right| \hat{\rho}_{\mathcal{S}}^I \left| \mathbf{P'}_i \right\rangle \\ &\cdot f(\mathbf{k}_f^*, \mathbf{k'}_i^*) \delta(E_{\mathbf{k}_f^*} - E_{\mathbf{k}_i^*}) \left| \mathbf{P}_i + \mathbf{k}_i - \mathbf{k}_f \right\rangle \left\langle \mathbf{P'}_i + \mathbf{k}_i - \mathbf{k}_f \right| f^*(\mathbf{k'}_f^*, \mathbf{k'}_i^*) \delta(E_{\mathbf{k'}_f^*} - E_{\mathbf{k'}_i^*}). \end{aligned} \tag{1.30}$$

By observing that $\left| \mathbf{k'}_i^* - \mathbf{k}_i^* \right| = \left| \mathbf{k'}_f^* - \mathbf{k}_f^* \right| = (m/M^*) \left| \mathbf{P'}_i - \mathbf{P}_i \right|$, and under the assumption that the system's density matrix in momentum representation $\hat{\rho}_s(\mathbf{P}_i, \mathbf{P'}_i)$ is almost diagonal, *i.e.* $(m/M^*) \left| \mathbf{P'}_i - \mathbf{P}_i \right| \simeq 0$, the author approximates

$$\mathbf{k'}_f^* \simeq \mathbf{k}_f^*, \qquad \mathbf{k'}_i^* \simeq \mathbf{k}_i^*. \tag{1.31}$$

Exploiting this prescription in Eq. (1.30), he eventually obtains

$$\begin{aligned} \mathrm{Tr}_{\mathcal{E}} \left(\hat{T} \hat{\rho}_{\mathcal{S}}^I \otimes \hat{\rho}_{\mathcal{E}} \hat{T}^\dagger \right) &= \frac{2\pi n}{m^{*2}} \left(\frac{M^*}{M} \right)^3 \int d\mathbf{k}_i^* d\mathbf{k}_f^* \, \left| f(\mathbf{k}_f^*, \mathbf{k'}_i^*) \right|^2 \\ &[\delta(E_{\mathbf{k}_f^*} - E_{\mathbf{k}_i^*})]^2 \sqrt{\rho_{\mathcal{E}}(\mathbf{k}_i)} e^{-i(\mathbf{k}_f^* - \mathbf{k}_i^*)\hat{\mathbf{x}}} \hat{\rho}_{\mathcal{S}}^I e^{i(\mathbf{k}_f^* - \mathbf{k}_i^*)\hat{\mathbf{x}}} \sqrt{\rho_{\mathcal{E}}(\mathbf{k}_i)}. \end{aligned} \tag{1.32}$$

The approximation just performed leads to an ill-defined square delta function in Eq. (1.32), that Diósi cures with the standard replacement of Eq.(1.8), *i.e.*

$$\delta(E)|_{E=0} = \Delta t / 2\pi. \tag{1.33}$$

By rewriting Eq. (1.32) in polar coordinates and integrating over the modulus of the vector $\mathbf{k}_i$ one obtains

$$\begin{aligned} \left. \frac{\partial \hat{\rho}_{\mathcal{S}}^I}{\partial t} \right|_{scatt.} &= \frac{n}{m^{*2}} \left(\frac{M^*}{M} \right)^3 \int dE d\Omega_i^* d\Omega_f^* \, k^{*2} \frac{d\sigma(\theta^*, E^*)}{d\Omega_f^*} \\ &\cdot \left(\hat{V}_{\mathbf{k}^*_f \mathbf{k}^*_i} \hat{\rho}_{\mathcal{S}}^I \hat{V}_{\mathbf{k}^*_f \mathbf{k}^*_i}^\dagger - \frac{1}{2} \left\{ \hat{V}_{\mathbf{k}^*_f \mathbf{k}^*_i}^\dagger \hat{V}_{\mathbf{k}^*_f \mathbf{k}^*_i} , \hat{\rho}_{\mathcal{S}}^I \right\} \right), \end{aligned} \tag{1.34}$$

where $d\sigma/d\Omega = |f|^2$ is the center of mass differential cross-section and

$$\hat{V}_{\mathbf{k}^*{}_f\mathbf{k}^*{}_i} = \sqrt{\hat{\rho}_\mathcal{E}\left(\mathbf{k}^*_i + \frac{m}{M}(\hat{\mathbf{P}} + \mathbf{k}^*_f)\right)}e^{-i(\mathbf{k}^*_f - \mathbf{k}^*_i)\cdot\hat{\mathbf{X}}}. \tag{1.35}$$

Equation (1.34) is the main result of Diósi's paper. One observes that Eq. (1.35) is a function not only of the system position operator $\hat{\mathbf{x}}$ but also of the system momentum operator $\hat{\mathbf{P}}$. The presence of the momentum operator $\hat{\mathbf{p}}$ in Eq. (1.35) is a witnesses that Eq. (1.34) accounts for recoil effects. In fact, as it can be easily shown, the collisional process described by Eq. (1.34) does not preserve the position states of the system, *i.e.*

$$\left.\frac{\partial\,|\mathbf{x}\rangle\langle\mathbf{x}|}{\partial t}\right|_{scatt.} \neq 0. \tag{1.36}$$

The author then proves the existence of a steady state for the dynamics described by Eq. (1.34) and that such a steady state is the Gibbs state $\propto \exp[-\beta\mathbf{P}^2/2M]$, with inverse temperature β. This fact guarantees that the system kinetic energy goes to the finite asymptotic value $E = \frac{3}{2}\beta^{-1}$ on the long time scale, witnessing the presence of friction in the dyamics.

An equation similar to Eq. (1.34) was later developed by Vacchini, exploiting the formalism of multi-particle quantum field theory in [55]. Since a detailed analysis of Vacchini's work goes beyond the purposes of this review, we just stress the fact that the main difference of the results in [55] from Eq. (1.34) is due to a different approximation scheme adopted by Vacchini. The author, differently from Diósi, applied the following approximation scheme along the derivation (compare with. Eq. (1.31))

$$\mathbf{k}^*_i \simeq \frac{\mathbf{k}^*_i + \mathbf{k}'^*_i}{2} \simeq \mathbf{k}'^*_i \qquad\qquad \mathbf{k}^*_f \simeq \frac{\mathbf{k}^*_f + \mathbf{k}'^*_f}{2} \simeq \mathbf{k}'^*_f \tag{1.37}$$

This replacement leads to a different formula from Eq. (1.34). However, it is easy to show that Vacchini and Diósi results are equivalent when in Vacchini's work the gas is chosen to be described by Boltzmann statistics. We stress that the assumption of almost diagonal system state $\hat{\rho}_\mathcal{S}$ in momentum representation is a crucial point in Vacchini and Diósi results. In fact, the replacement in Eq. (1.37) and Eq. (1.31) holds true only in this case.

Hornberger and Vacchini [40] later proposed a new approach to remove the limitations of the previous derivations. They started from Eq. (1.25) but, differently from Diósi, they explicitly introduce a rate operator $\hat{\Gamma}$ to take into account the collision probability in a small time interval Δt. The authors then assume the rate operator $\hat{\Gamma}$ to be the classical collision rate function promoted to an operator function:

$$\hat{\Gamma} = \frac{n}{m^*} \left| \mathrm{rel}(\hat{\mathbf{P}}, \hat{\mathbf{k}}) \right| \sigma_{\mathrm{tot}}(\mathrm{rel}(\hat{\mathbf{P}}, \hat{\mathbf{k}})), \tag{1.38}$$

where $\hat{\mathbf{P}}$ and $\hat{\mathbf{k}}$ are respectively the momentum operators of the system and of the gas particle, $\mathrm{rel}(\mathbf{P}, \mathbf{k})$ the relative momentum between the system and a gas particle and n the gas particles density. Exploiting the monitoring approach [56] and assuming a factorized incoming state $\hat{\rho}_{S\mathcal{E}} = \hat{\rho}_s \otimes \hat{\rho}_{\mathcal{E}}$, the authors obtain the following effective equation of motion

$$\frac{\partial \hat{\rho}_S}{\partial t} = \frac{1}{i\hbar}\left[\hat{H}\,, \hat{\rho}_s\right] + \mathcal{L}\hat{\rho}_S + \mathcal{R}\hat{\rho}_S \tag{1.39}$$

where the superoperators $\mathcal{L}$ and $\mathcal{R}$ depend on the transition ($\hat{T}$) and rate ($\hat{\Gamma}$) operators as follows:

$$\mathcal{L}\hat{\rho}_S = \mathrm{Tr}_{\mathcal{E}}\left(\hat{T}\hat{\Gamma}^{1/2}[\hat{\rho}_s \otimes \hat{\rho}_{\mathcal{E}}]\hat{\Gamma}^{1/2}\hat{T}^\dagger\right) - \frac{1}{2}\mathrm{Tr}_{\mathcal{E}}\left(\left\{\hat{\Gamma}^{1/2}\hat{T}\hat{T}^\dagger\hat{\Gamma}^{1/2}\,, [\hat{\rho}_S \otimes \hat{\rho}_{\mathcal{E}}]\right\}\right), \tag{1.40}$$

$$\mathcal{R}\hat{\rho}_S = i\mathrm{Tr}_{\mathcal{E}}\left(\left[\hat{\Gamma}^{1/2}\frac{\hat{T} + \hat{T}^\dagger}{2}\hat{\Gamma}^{1/2}\,, \hat{\rho}_S \otimes \hat{\rho}_{\mathcal{E}}\right]\right). \tag{1.41}$$

In order to find an explicit expression for Eq. (1.39) they assume the environment to be described by the Botlzmann distribution $\mu(\mathbf{k})$ of box normalized momentum states

$$\hat{\rho}_{\mathcal{E}}(\mathbf{k}, \mathbf{k}) = \frac{(2\pi\hbar)^3}{\Omega}\mu(\mathbf{k}), \tag{1.42}$$

and with the help of Eq. (1.28) they rewrite the first term of Eq. (1.40) as follows:

$$\langle \mathbf{P}_f |\, \mathrm{Tr}_{\mathcal{E}}\left(\hat{T}\,\hat{\Gamma}^{1/2}[\hat{\rho}_S \otimes \hat{\rho}_{\mathcal{E}}]\hat{\Gamma}^{1/2}\hat{T}^\dagger\right)\left|\mathbf{P'}_f\right\rangle = \frac{(2\pi\hbar)^3}{\Omega}\frac{2\pi n}{m^{*2}}\int d\mathbf{k}_i d\mathbf{k}_f\, \mu\left(\mathbf{k}_i\right)$$
$$\cdot f(\mathbf{k}_f^*, \mathbf{k}_i^*)\delta(E_{\mathbf{k}_f^*} - E_{\mathbf{k}_i^*})\sqrt{\Gamma(\mathbf{k}_i^*)}\langle \mathbf{P}_f - \mathbf{k}_{fi}|\hat{\rho}_S\left|\mathbf{P'}_f - \mathbf{k}_{fi}\right\rangle\sqrt{\Gamma(\mathbf{k'}_i^*)}f^*(\mathbf{k'}_f^*, \mathbf{k'}_i^*)\delta(E_{\mathbf{k'}_f^*} - E_{\mathbf{k'}_i^*}). \tag{1.43}$$

If one considers the diagonal matrix elements of Eq. (1.43) one obtains a squared Dirac delta function, that the authors regularize by introducing the replacement rule

$$\frac{(2\pi\hbar)^2}{|\Omega|}\left|f(\mathbf{k}_f^*, \mathbf{k}_i^*)\delta(E_{\mathbf{k}_f^*} - E_{\mathbf{k}_i^*})\right|^2 \to \frac{\delta(E_{\mathbf{k}_f^*} - E_{\mathbf{k}_i^*})\left|f(\mathbf{k}_f^*, \mathbf{k}_i^*)\right|^2}{\Gamma(\mathbf{k}_i^*)} \tag{1.44}$$

previously proposed by Hornberger and Sipe [37] (see Eq. (1.24) sec. 1.1). As previously mentioned the replacement rule in Eq. (1.44) is unusual. However, the authors choose to use this for two reasons: first, the standard replacement in Eq. (1.8) would lead to the presence of an un-wanted Δt factor in the collisional term, and more importantly this unusual replacement scheme allows the authors to remove the rate operators ($\hat{\Gamma}$) dependence in Eq. (1.43), which would produce a quadratic dependency of the collision term on the scattering cross section. They also extend the replacement in Eq. (1.44) to the off-diagonal matrix elements of Eq. (1.43) by formally taking the square root of Eq. (1.44), *i.e.*

$$\frac{2\pi\hbar}{\sqrt{\Omega}} f(\mathbf{k}_f^*, \mathbf{k}_i^*)\delta(E_{\mathbf{k}_f^*} - E_{\mathbf{k}_i^*}) \to \frac{\sqrt{\delta(E_{\mathbf{k}_f^*} - E_{\mathbf{k}_i^*})} f(\mathbf{k}_f^*, \mathbf{k}_i^*)}{\sqrt{\Gamma(\mathbf{k}_i^*)}}. \tag{1.45}$$

This extension is here needed to remove the rate operator $\hat{\Gamma}$ also in the non diagonal terms. Exploiting Eq. (1.45) one ends up with the square root of a product of two energy conserving-delta functions with argument $\frac{\mathbf{k}_f^{*2} - \mathbf{k}_i^{*2}}{2} - (\mathbf{k}_f^* - \mathbf{k}_i^*) \cdot \mathbf{Q}$, where $\mathbf{Q} = \frac{m}{M^*} \frac{\mathbf{P}_i - \mathbf{P'}_i}{2}$. The authors argue that $\mathbf{Q}$ should be replaced by $\mathbf{Q}_\perp$, *i.e.* the component of $\mathbf{Q}$ orthogonal to $\mathbf{k}_f^* - \mathbf{k}_i^*$, and, by resorting to Eqs. (1.39 ,1.40, 1.41), they eventually end up with the following master equation:

$$\frac{\partial \hat{\rho}_s}{\partial t} = \frac{1}{i\hbar}\left[\hat{H}\,,\hat{\rho}_s\right] + \int d\mathbf{Q} \int_{\mathbf{Q}_\perp} \frac{d\mathbf{k}}{|\mathbf{Q}|} \left(\hat{L}_{\mathbf{Q},\mathbf{k}} \hat{\rho}_S \hat{L}^\dagger_{\mathbf{Q},\mathbf{k}} - \frac{1}{2}\hat{\rho}_S \hat{L}^\dagger_{\mathbf{Q},\mathbf{k}} \hat{L}_{\mathbf{Q},\mathbf{k}} - \frac{1}{2}\hat{L}_{\mathbf{Q},\mathbf{k}} \hat{L}_{\mathbf{Q},\mathbf{k}} \hat{\rho}_S \right), \tag{1.46}$$

with $\hat{L}_{\mathbf{Q},\mathbf{k}} = e^{i\hat{\mathbf{x}}\cdot\mathbf{Q}} \hat{L}_{\mathbf{k},\mathbf{Q}}(\hat{\mathbf{P}})$ and

$$\hat{L}_{\mathbf{k},\mathbf{Q}}(\hat{\mathbf{P}}) = \frac{n\,m}{m^{2*}} f\left[\mathrm{rel}(\mathbf{k}_{\perp\mathbf{Q}}, \mathbf{P}_{\perp\mathbf{Q}}) - \frac{\mathbf{Q}}{2} \mathrm{rel}(\mathbf{k}_{\perp\mathbf{Q}}, \mathbf{P}_{\perp\mathbf{Q}} + \frac{\mathbf{Q}}{2}) \right] \sqrt{\hat{\rho}_\varepsilon(\mathbf{P}_{\perp\mathbf{Q}} + \frac{m}{m^*}\frac{\mathbf{Q}}{2} + \frac{m}{M}\mathbf{P}_{\|\mathbf{Q}})} \tag{1.47}$$

where the integration over the gas particle momentum $\mathbf{k}$ is performed over the plane perpendicular to the momentum transfer $\mathbf{Q}$, and the vector with index $\|\mathbf{Q}$ denotes vector components parallel $\mathbf{Q}$.

In the original paper the authors derive, as limiting cases, Joos-Zeh [34], Gallis-Fleming [35] (with the correct 2π factor) and Vacchini [55] results, showing the generality of Eq. (1.46). Later, Diósi [39] and Kamleitner [48], independently, questioned on the validity of Hornberger-Vacchini derivation. In particular, they questioned the fact that the replacement adopted by Hornberger-Vacchini for the off-diagonal terms of Eq. (1.43) is not justified, because the off-diagonal terms do not present any divergence to be cured, unlike the diagonal terms. Diósi and Kamlaitner also notice that a complete collision event described by Eq. (1.43) would destroy all momentum coherences in the state of the system [39, 48], but the replacement ($\mathbf{Q} \to \mathbf{Q}_\perp$) adopted by Hornberger and Vacchini for the off-diagonal terms removes this feature of the collision event.

Motivated by these observations Kamleitner made a detailed study of the interaction process of two particles in one dimension [57], and further derived a master equation for the one dimensional dynamics of a quantum particle undergoing random collisions with gas particles [48]. Diósi, instead, proposed a new collisional equation where a finite inter-collision time is explicitly present [39]. He stresses that the presence of a finite inter-collision time is in contrast with the infinite time necessary for the process leading from an ingoing collision state to an outgoing collision state in standard scattering theory. Diósi suggested then the possibility of a non complete scattering process, introducing a finite time in the collision process. To introduce a finite time in the collision and further solve the problems related to the energy delta functions present in previous works, he replaces the energy dirac delta functions in Eq. (1.30), with a "smoothened" delta function

$$\delta(E) \to \delta_\tau(E) = \frac{\sin(\tau E/2)}{\pi E}. \tag{1.48}$$

probably guided by the fact that the energy Dirac delta function in the scattering matrix is generated by

$$\delta(E) = \frac{1}{2\pi} \lim_{\tau\to\infty} \int_{-\tau/2}^{\tau/2} ds\, e^{-iE\,s} = \lim_{\tau\to\infty} \frac{\sin(\tau E)}{\pi E}. \tag{1.49}$$

He then estimates the inter-collision time to be

$$\tau = \frac{\sqrt{\pi\beta m}}{\sigma n} \tag{1.50}$$

where σ is the total scattering cross section, n the gas density, β the inverse temperature, m the mass of the gas particle. Exploiting Eq. (1.26), Eq. (1.30) and the replacement in Eq. (1.48), he eventually obtains the following dynamical equation

$$\frac{\partial\hat{\rho}_s}{\partial t} = -\frac{i}{\hbar}\left[\hat{H}\,,\hat{\rho}_S\right] + \frac{2\pi n}{\tau m^{*2}}\int d\mathbf{k}d\mathbf{Q}\,\hat{\rho}_{\mathcal{E}}(\mathbf{k})\left(\hat{V}(\mathbf{k},\mathbf{Q})\hat{\rho}_S\hat{V}^\dagger(\mathbf{k},\mathbf{Q}) - \frac{1}{2}\left\{\hat{V}^\dagger(\mathbf{k},\mathbf{Q})\hat{V}(\mathbf{k},\mathbf{Q})\,,\hat{\rho}_S\right\}\right), \tag{1.51}$$

where

$$\hat{V}(\mathbf{k},\mathbf{Q}) = e^{\frac{i}{\hbar}\mathbf{Q}\cdot\hat{\mathbf{X}}} f(\hat{k}_f^*, \hat{k}_i^*)\delta_\tau(\hat{E}_{fi}). \tag{1.52}$$

Furthermore in his work Diósi stresses the fact that the coherence between different momentum eigenstates is heavily suppressed by a complete scattering process and the persistence of any coherent dynamics is only due to incomplete quantum collisions, contrary to the previous understanding of the behavior of a quantum particle in a gas. (for example, Hornberger-Vacchini's model displays a persistent coherence in momentum that is suppressed only after several complete collision events). However, Diósi's work is not free form inconsistencies, as pointed out by Hornberger and Vacchini in [49]. The collisional contribution to the dynamics described by Eq. (1.51) is non linear in the gas density n_{gas}, because of the definition of the inter-collision time τ in Eq. (1.50). However, from the physical point of view one would expect a linear dependence on n_{gas} in Eq. (1.51) [49]. Moreover, the definition of the inter-collision time τ in Eq. (1.50) depends on the gas state only, but the inter-collision time should depend both on the test and the gas particles. However Hornberger and Vacchini show that a more appropriate definition of the inter-collision time, *i.e.*

$$\tau^{-1}[\hat{\rho}_{\mathcal{S}}] = \int d\mathbf{P}\, \langle\mathbf{P}|\, \hat{\rho}_{\mathcal{S}}\, |\mathbf{P}\rangle\, n_{gas} \int \rho_{\mathcal{E}}(\mathbf{P}) v_{rel}(\mathbf{k},\mathbf{P})\sigma[E_{rel} = m_* v_{rel}^2(\mathbf{k},\mathbf{P})/2] \tag{1.53}$$

where $v_{rel}(\mathbf{P},\mathbf{P}) = [\mathbf{k}/m - \mathbf{P}/M]$ the relative velocity, and m_* the relative mass, would yield to a non linear time evolution equation for the state $\hat{\rho}_{\mathcal{S}}$. They furthermore show that the master equation in Eq. (1.51) displays an infinite position diffusion effect in the limit of $n_{gas} \to 0$. However, in this regime the master equation should describe a free evolution, and diffusion effects produced by collisional contributions should disappear.
From this review on collisional models of decoherence, one may deduce that there is not a common understanding of the dynamics of a quantum particle in a gas. While recoil-less collisional models have been experimentally tested [42], it is still not clear the validity of collisional models in presence of dissipative phenomena. The presence of two different heuristic models describing the same physical situation with different predictions, shows a lack of understanding in the fundamental process underlying the behavior of a quantum particle in a gas.

In order to make a step forward in the understanding of the problem we will analyse the case study of two particles interacting via a dirac delta potential in one dimension. This simple model has the virtue of being exactly solvable, allowing us to achieve a better understanding of the collision process, disregarding complicated mathematical details. We will then study the case of a test particle in a thermal gas, exploiting a technique based on the Hartree variational method combined with stochastic calculus techniques. This original treatment of the problem will allow us to correctly describe the non dissipative behavior of the test particle, and further to have insight on the dissipative phenomena. Last, in order to show the limits of a collisional treatment in the quantum mechanical framework, we provide a microscopic derivation of a quantum collisional dynamics for the test particle in a gas. Unlike previous derivations we obtain the collisional dynamics starting from the Hamiltonian dynamics of a test particle interacting with an ideal N particle gas.

Chapter 2

Trials

We discuss the lack of a common understanding in the dynamics of a quantum test particle in a rarefied gas. The origin of problems is probably related to the difficulties that one encounters in setting necessary conditions for a collisional description of the interactions. To find the origin of these difficulties, we start our analysis by following Kamleitner steps [57]. We analyze the dynamics of two particles interacting via an infinite Dirac delta potential in one dimension (Section 2.1). This model is exactly solvable and can be exploited to gain insight on the interaction dynamics of two particles. However, the model is too simple to achieve a full understanding of the three dimensional interaction process. However, it is not possible to solve this model in more than one dimension, thus preventing the possibility of having a detailed analysis of a two particle interaction process in three dimensions.

Because of the impossibility of finding an exactly solvable model for the interaction of two particles in three dimensions, we looked at the problem from a completely new perspective. Starting from the full Hamiltonian describing N+1 particles and exploiting the Hartree variational method, we reduce the problem to the effective dynamics of a single particle affected by an external stochastic potential (Section 2.2). This stochastic approach gives useful insight on the recoil effects in a collisional dynamics, but it is still too simple to correctly describe the full dynamics of a quantum particle in a gas. Accordingly we decided to approach the problem from a fully microscopic point of view, in order to understand the limits of a collisional approach in the quantum mechanical framework. This will be presented in chapter 3.

2.1 Collison in one Dimension

We analyze the case two particles interacting via an infinite Dirac delta potential, in one dimension. This analysis will help us to understand the process that governs a collision without taking into account unnecessary details. A similar analysis has been already performed by Kamleitner in [48] to obtain a quantum 1-Dimensional Brownian model; however different resolutive method is here used and different conclusions are reached. The Schrödinger equation in the position representation is given by

$$i\hbar\frac{\partial}{\partial t}\psi(x_1,x_2;t)=\mathcal{H}(x_1,x_2)\psi(x_1,x_2) \tag{2.1}$$

where the Hamiltonian $\mathcal{H}(x_1,x_2)$ is

$$\mathcal{H}(x_1,x_2)=\frac{\hbar}{2m_1}\frac{\partial^2}{\partial x_1^2}+\frac{\hbar}{2m_2}\frac{\partial^2}{\partial x_2^2}+\lim_{\alpha\to\infty}\alpha\delta(x_1-x_2) \tag{2.2}$$

with m_1 (m_2) the mass and x_1 (x_2) the position of the first (second) particle. It is convenient to introduce the centre of mass (x_s) and relative coordinates(x_r), which are defined by

$$(x_1,x_2)=(x_s+\mu_2x_r;\ x_s-\mu_1x_r), \qquad (x_r,x_s)=(x_1-x_2;\ \mu_1x_1+\mu_2x_2) \tag{2.3}$$

with $\mu_i=m_i/(m_1+m_2)$. Equation (2.3) allows to rewrite Eq. (2.2) in the more convenient form

$$i\hbar\frac{\partial}{\partial t}\tilde{\psi}(x_r,x_s;t)=\tilde{\mathcal{H}}(x_r,x_s)\tilde{\psi}(x_r,x_s), \tag{2.4}$$

with

$$\tilde{\psi}(x_r,x_s)\equiv\psi(x_s+\mu_2x_r;\ x_s-\mu_1x_r), \tag{2.5}$$

$$\tilde{\mathcal{H}}(x_r,x_s)\equiv\mathcal{H}(x_s+\mu_2x_r,\ x_s-\mu_1x_r)=\frac{\hbar}{2m_r}\frac{\partial^2}{\partial x_r^2}+\frac{\hbar}{2m_s}\frac{\partial^2}{\partial x_s^2}+\lim_{\alpha\to\infty}\alpha\delta(x_r) \tag{2.6}$$

where $m_s=m_1+m_2$ and $m_r=m_1m_2/m_s$ are respectively the total and the reduced mass of the two-particle system. The problem of finding the solution of Eq. (2.4), can now be replaced by the equivalent problem of finding a $\tilde{\psi}(x_r, x_s, t)$ such that:

$$\tilde{\psi}(x_r, x_s; t) = 0 \text{ for } x_r = 0; \tag{2.7a}$$

$$\tilde{\psi}(x_r, x_s; t) \text{ is continuous around } x_r = 0; \tag{2.7b}$$

$$\tilde{\psi}(x_r, x_s; t) \text{ is a solution of the } \textit{free} \text{ Schrödinger equation , if } x_r \neq 0. \tag{2.7c}$$

A wave function that satisfies these conditions can be written as follows

$$\tilde{\psi}(x_r, x_r; t) = N[\phi(x_r, x_s, t) - \phi(-x_r, x_s, t)], \tag{2.8}$$

where N is a normalization constant, and $\phi(x_r, x_s, t)$ is a generic solution of the *free* Schrödinger equation. Conditions (2.7a) and (2.7b) are trivially satisfied by Eq. (2.8). What is left to show is that also condition (2.7c) is satisfied. To prove this, one may notice that $\phi(-x_r, x_s, t)$ can be obtained from $\phi(x_r, x_s, t)$ by the action of the parity transformation P_r defined as

$$P_r : (x_r, x_s) \to (-x_r, x_s). \tag{2.9}$$

Since such a transformation leaves the Hamiltonian unchanged, *i.e.*

$$\tilde{\mathcal{H}}(-x_r, x_s) = \tilde{\mathcal{H}}(x_r, x_s), \tag{2.10}$$

if $\phi(x_r, x_s, t)$ is a solution of the free Schrödinger equation, then also $\phi(-x_r, x_s, t)$ is. By linearity one finds that condition (2.7c) is satisfied.

The center of mass reference frame is a very useful tool to find the solution of Eq. (2.2), but we are interested in the expression in the original reference frame, where the dependence on the two particles' coordinates is explicit. Exploiting Eq. (2.3), one may rewrite the solution of the problem in the original coordinates system, *i.e.*

$$\psi(x_1, x_2, t) = N[\phi(x_1, x_2, t) - \phi(\tilde{x}_1, \tilde{x}_2, t)] \tag{2.11}$$

where $\phi(x_1, x_2, t)$ is a solution of the *free* Schrödinger equation and

$$(\tilde{x}_1, \tilde{x}_2) = (2\mu_2 x_2 + \mu_r x_1, 2\mu_1 x_1 - \mu_r x_2) \tag{2.12}$$

with $\mu_r = (\mu_1 - \mu_2)$.
We notice that Eq. (2.11) does not allow for localized particles states, because it describes a superposition state between $\phi(x_1, x_2, t)$ and $\phi(\tilde{x}_1, \tilde{x}_2, t)$. This unphysical behaviour can

be removed by restricting the space of solutions of Eq. (2.1) to the half plane described by $x_1 < x_2$. In fact an infinite potential prevents the two particles to cross each other, implying that the request that at the initial time particle 1 is on the left of particle 2 $\psi(x_1, x_2, 0) = 0$ for $x_1 > x_2$, restricts the configuration space to the half plane with $x_1 < x_2$. This condition can be implemented by multiplying Eq. (2.11) by a step function that sets the wave function to zero if $x_1 > x_2$, *i.e.*

$$\psi(x_1, x_2, t) = N^{'}[\phi(x_1, x_2, t) - \phi(\tilde{x}_1, \tilde{x}_2, t)]\theta(x_2 - x_1). \tag{2.13}$$

The term $\phi(x_1, x_2, t)$ may be now understood as the in-going state and $\phi(\tilde{x}_1, \tilde{x}_2, t)$ as the out-going state of the interaction process.

In order to describe the full interaction process, we require that the two particle are not interacting at the initial time and also that they did not interact before that time. In other words the contribution of the out-going state to the wave function must be negligible at $t = 0$:

$$P_{int}(t = 0) \simeq 0, \tag{2.14}$$

where

$$P_{int}(t) = \int dx_1 dx_2 \left|\phi(\tilde{x}_1, \tilde{x}_2, t)\theta(x_2 - x_1)\right|^2 . \tag{2.15}$$

gives the probability that the two particles have already interacted. Under condition (2.14), one may define the collision time as the time in which the probability that the two particles have already interacted passes from a negligible contribution, ε (approximately small), to a significant contribution, $1 - \varepsilon$:

$$\tau_c = t_2 - t_1 \text{ , with } [t_1, t_1] = \{t > 0 \quad | \quad \varepsilon \leq P_{int}(t) \leq 1 - \varepsilon\}. \tag{2.16}$$

The parameter ε is necessarily arbitrary, though small. The only restriction is that one cannot choose $\epsilon = 0$, because it would imply an infinite collision time.

Since an explicit formula for the collision time cannot be derived from (2.16) for an arbitrary initial state, we now restrict the analysis of the collision time to the case of Gaussian initial states (a similar analysis was already provided by Kamleitner in [57]), *i.e.*

$$\psi_0(x_1, x_2) = N^2[\phi_1(x_1)\phi_2(x_2) - \phi_1(\tilde{x}_1)\phi_2(\tilde{x}_2)]\theta(x_2 - x_1) \tag{2.17}$$

where

$$\phi_i(x) \equiv \frac{1}{\sqrt[4]{\pi\sigma_i^2}} \exp\left(-\frac{(x-x_{i0})^2}{2\sigma_i^2} + \frac{i}{\hbar}k_{i0}x\right) \tag{2.18}$$

with x_{i0}, k_{i0} and σ_i the average initial position, the average initial momentum and the initial variance of the i-th particle. Exploiting Eq. (2.15) and Eq. (2.18), and after a lengthy calculation one finds

$$P_{int}(t=0) = \frac{1}{\sqrt{\pi}} \int_{\frac{x_{10}-x_{20}}{\sqrt{\sigma_1+\sigma_2}}}^{\infty} dx\, e^{-x^2}. \tag{2.19}$$

The condition (2.14) leads to the following constraint on the initial state

$$|x_{10} - x_{20}| \gg \sqrt{\sigma_1^2 + \sigma_2^2}. \tag{2.20}$$

This inequality is telling that the two particles are freely evolving only if their wave functions have negligible overlap. Extending the results of Eq. (2.19) the state at a generic time t, one obtains

$$P_{int}(t) = \frac{1}{\sqrt{\pi}} \int_{a_t}^{\infty} dx e^{-x^2}, \tag{2.21}$$

with

$$a_t = \frac{x_{1t} - x_{2t}}{\sqrt{\sigma_{1t}^2 + \sigma_{2t}^2}}, \tag{2.22}$$

where

$$\sigma_{it}^2 = \sigma_i^2 + (m_i\hbar\sigma_i)^{-2}t^2, \qquad x_{it} = x_i + \frac{k_i}{m_i}t. \tag{2.23}$$

If t_1 and t_2 in Eq. (2.16) are chosen such that $a_{t_1} \simeq -1$ and $a_{t_2} \simeq 1$, which implies that during the collision process $P_{int}(t)$ goes from a value of cca. 0.1 to a value of cca. 0.9 one obtains the following inequality

$$-1 < \frac{x_{1t} - x_{2t}}{\sqrt{\sigma_{1t}^2 + \sigma_{2t}^2}} < 1. \tag{2.24}$$

From this inequality and exploiting the definitions (2.23) it is now easy to obtain the following collision time

$$\tau_c = \frac{2t_r m_r (\sigma_1^2 + \sigma_1^2)^{1/2}}{k_r^2 t_r^2 - (\sigma_1^2 + \sigma_1^2) m_r^2} \tag{2.25}$$

where $t_r = \hbar^{-1}\sqrt{((m_1\sigma_1)^{-2} + (m_2\sigma_2)^{-2})(\sigma_1^2 + \sigma_1^2)}$ is the characteristic time scale in which the spread of the gaussian wave packet doubles, and $k_r = k_1\mu_2 - k_2\mu_1$ is the mean relative momentum between the two particles. It is interesting to note that under the assumption $t_r \gg t$ the inequality (2.24) can be approximated to

$$-1 < \frac{x_{1t} - x_{2t}}{\sqrt{\sigma_1^2 + \sigma_2^2}} < 1 \tag{2.26}$$

and then the collision time is

$$\tau_c \simeq 2\sqrt{\sigma_1^2 + \sigma_2^2}\frac{m_r}{k_r} = 2\sqrt{\sigma_1^2 + \sigma_2^2}v_r^{-1} \tag{2.27}$$

which is the time needed to travel twice the total initial spread of the two gaussians $\sqrt{\sigma_1^2 + \sigma_2^2}$ with the mean relative velocity $v_r = k_r/m_r$ between the particles.

It is important to notice that the collision time τ_c differs from zero even with a Dirac delta potential, contrary to what happens in the classical case, where we have instantaneous interactions in the case of a contact potential. A non zero collision time, even with a zero range potential, depends on the fact that the wave functions are spatially extended. In fact from Eq. (2.27) one may deduce that the collision time is proportional to the time needed for the two Gaussians to cross each-other. This result suggests that in order to set the collision time to zero one should also set the spatial extension of the wave function to zero, leading to a classical description of the dynamics, contrary to the original goal of providing a quantum description of the collision.

If we restrict the analysis to the case $m_1 \gg m_2$, and the two particles have momenta of the same magnitude, and Eq. (2.27) can be further simplified as

$$\tau_c \simeq 2\sqrt{\sigma_1^2 + \sigma_2^2}\, v_2^{-1}. \tag{2.28}$$

The above equation suggests that, in the regime $m_1 \gg m_2$, the collision dynamics is fully determined by the light particle. Equation (2.28) also suggests that, if the light particle is fast enough, the collision process can be considered as instantaneous, even if the wave packets of the two particles are spatially extended. Since the condition $m_1 \gg m_2$ is directly connected to the recoil-free assumption made by Joos-Zeh and Gallis-Flemming, this analysis confirms the validity of the recoil-free collisional models in the quantum mechanical framework, but, on the other side, this also suggests that when the condition $m_1 \gg m_2$ does not hold, a collisional description can be achieved only in the classical regime.

However, the model here considered is too simple to give a conclusive answer on the validity of a collisional approach in quantum theory, and further analysis is required. The first step would be to extend the analysis made for Gaussian states to generic wave packets. This is not an achievable task, because it requires the inversion of the condition (2.16), that can be done only in simple cases. One could also think to extend the analysis to the 3-dimensional case, however the procedure used here to solve Eq. (2.1) cannot be exploited for systems in more than 1 dimension. Indeed, in n dimensions with n>1 there is no transformation like Eq. (2.9), that preserve the free Hamiltonian and, at the same time, can be used to write a solution for the interacting problem in the form (2.11). The fact that finding exact solutions for the Schrödinger equation (2.1) in tree dimensions (whose potential is the simplest possible one) is a very difficult task, combined with the fact that the analysis here performed can be carried out explicitly only for specific wave functions suggest that an alternative approach is needed to gain further insight in the quantum collisional dynamics.

2.2 Variational Method for Collisional Dynamics

In this section we study the evolution of a target particle interacting with a rarefied thermal bath, by exploiting the Hartree variational method combined with stochastic calculus techniques. This method allows to unravel interesting details related to dissipation in collisional dynamics, bypassing the problem encountered in the previous section of finding exact solutions to the dynamics. To our knowledge, this is the first time that these two method are combined together in the field of open quantum systems. The full Hamiltonian of a test particle interacting with other N particles is given by

$$\hat{H} = \frac{\hat{\mathbf{P}}^2}{2M} + \sum_{i=1}^{N} \frac{\hat{\mathbf{p}}_i^2}{2m} + \sum_{i<j}^{N} \hat{V}_{ij} + \sum_{i}^{N} \hat{V}(\hat{\mathbf{X}} - \hat{\mathbf{x}}_j) \tag{2.29}$$

where capital letters labels the target particle and i,j the gas particles. Since solving explicitly the dynamics is not an achievable task, we simplify the problem by making use of the Hartree variational method. We assume that the gas particles, in thermal equilibrium, are described by un-correlated wave functions, and that the correlation produced by the interaction between the test particle and one bath particle are quickly removed by the bath particles' mutual interaction. Accordingly, we restrict the Hilbert space to the subspace of the factorized state vectors:

$$|\Psi\rangle = |\psi_{\mathcal{S}}\rangle |\phi_1\rangle |\phi_2\rangle \ldots . |\phi_n\rangle \tag{2.30}$$

We then consider the mean value of the Hamiltonian $\langle\Psi| \hat{H} |\Psi\rangle$ as a functional, and we look for the stationary solution of this functional, with the constraint $\langle\Psi|\Psi\rangle = 1$, *i.e.*

$$\delta\{\langle\Psi| \hat{H} |\Psi\rangle - \lambda[\langle\Psi|\Psi\rangle - 1]\} = 0 \tag{2.31}$$

where the Lagrange multiplier λ is associated to the state vector normalization constraint $\langle\Psi|\Psi\rangle = 1$. The general variation of the state (2.30) is given by

$$|\delta\Psi\rangle = |\delta\psi_{\mathcal{S}}\rangle |\phi_1\rangle |\phi_2\rangle \ldots |\phi_n\rangle + \sum_{i=1}^{n} |\psi_{\mathcal{S}}\rangle |\phi_1\rangle \ldots |\delta\phi_i\rangle \ldots |\phi_n\rangle \,. \tag{2.32}$$

Actually it is not necessary to consider the above general variation, to find an effective equation for the test particle alone. It is sufficient to restrict the analysis to variations along the test particle's direction

$$|\delta_{\mathcal{S}}\Psi\rangle = |\delta\psi_{\mathcal{S}}\rangle |\phi_1\rangle |\phi_2\rangle \ldots |\phi_n\rangle \,. \tag{2.33}$$

Indeed, variations along the bath particles direction would give an unsolvable equation describing the effective dynamics of the bath particles, which we are not interested in. Exploiting Eq. (2.31) and Eq. (2.33) one obtains

$$\lambda |\psi_{\mathcal{S}}\rangle = \left\{ \frac{\hat{\mathbf{P}}^2}{2M} + \sum_{i=1}^{n} \langle\phi_i| \hat{V}(\hat{\mathbf{X}} - \hat{\mathbf{x}}_i) |\phi_i\rangle \right\} |\psi_{\mathcal{S}}\rangle \,. \tag{2.34}$$

form which one reads the test particle effective Hamiltonian to be

$$\hat{H}_{eff} = \frac{\hat{\mathbf{P}}^2}{2M} + \sum_{i=1}^{n} \langle\phi_i| \hat{V}(\hat{\mathbf{X}} - \hat{\mathbf{x}}_i) |\phi_i\rangle \,. \tag{2.35}$$

It is worth to stress that Eq. (2.35) is valid only under the hypothesis that Eq. (2.30) is a good approximation for the state at any time.

Expanding the bath particles states $|\phi_i\rangle$ in position eigenbasis, Eq. (2.35) can be rewritten as

$$\hat{H}_{eff} = \frac{\hat{\mathbf{p}}_{\mathcal{S}}^2}{2M} + \int dy \; \eta(\mathbf{y}, t) V(\hat{\mathbf{X}} - \mathbf{y}) \tag{2.36}$$

where $\eta(\mathbf{y},t) = \sum_i |\langle\phi_{i,t}|\mathbf{y},\mathbf{t}\rangle|^2$ can be understood as the local gas density. This association allow us to rewrite $\eta(\mathbf{y},t)$ as

$$\eta(\mathbf{y},t) = \bar{\eta} + \zeta(\mathbf{y},t) \tag{2.37}$$

where $\bar{\eta} = N/V$ is the average number of particles per unit area, and $\zeta(\mathbf{y},t)$ describes the fluctuations around the average $\bar{\eta}$. In order to model these fluctuations, we assume $\zeta(\mathbf{y},t)$ to be a real gaussian stochastic field with mean and variance defined as

$$\begin{aligned}\mathbb{E}\left[\zeta(\mathbf{x},t)\right] &= \bar{\zeta}(\mathbf{x},t),\\ \mathbb{E}\left[\zeta(\mathbf{x},t)\zeta(\mathbf{y},\tau)\right] &= f(\mathbf{x},t;\mathbf{y},\tau),\end{aligned} \tag{2.38}$$

where $f(\mathbf{x},t;\mathbf{y},\tau)$ is a symmetric function under exchange $(\mathbf{x},t)\to(\mathbf{y},\tau)$, and $\mathbb{E}[\dots]$ denotes the average over the probability distribution of $\zeta(\mathbf{x},t)$. Since the gas is in thermal equilibrium it is reasonable to assume stationary and translationally invariant fluctuations with zero mean, *i.e.*

$$\begin{aligned}\bar{\zeta}(\mathbf{x},t) &= 0\\ f(\mathbf{x},t;\mathbf{y},\tau) &= f(\mathbf{x}-\mathbf{y},t-\tau).\end{aligned} \tag{2.39}$$

We furthermore expect the thermal bath dynamics to be much faster than the test particle's dynamics, so we also assume the fluctuations to be delta correlated in time, *i.e.*

$$f(\mathbf{x},t;\mathbf{y},\tau) = g(\mathbf{x}-\mathbf{y})\delta(t-\tau). \tag{2.40}$$

Under these assumptions, one finds that the system state $\hat{\rho}(t)$ evolves accordingly to the following average master equation (see app. A for detailed calculations)

$$\begin{aligned}\frac{\partial}{\partial t}\hat{\rho}(t) = &-\frac{i}{\hbar}\left[\frac{\hat{\mathbf{P}}^2}{2M},\hat{\rho}(t)\right]\\ &-\frac{1}{2\hbar^2}\int_0^\infty d\tau\int d\mathbf{y}d\mathbf{z}\,\mathbb{E}[\zeta(\mathbf{x},t)\zeta(\mathbf{y},\tau)]\left[V(\mathbf{y}-\hat{\mathbf{X}}),\left[V(\mathbf{z}-\hat{\mathbf{X}}),\hat{\rho}(t)\right]\right]\\ = &-\frac{i}{\hbar}\left[\frac{\hat{\mathbf{P}}^2}{2M},\hat{\rho}(t)\right]-\frac{1}{2\hbar^2}\int d\mathbf{y}d\mathbf{z}\,g(\mathbf{x}-\mathbf{y})\left[V(\mathbf{y}-\hat{\mathbf{X}}),\left[V(\mathbf{z}-\hat{\mathbf{X}}),\hat{\rho}(t)\right]\right]\end{aligned} \tag{2.41}$$

Rewriting the interaction term $V(\hat{\mathbf{x}}_\mathcal{S}-\mathbf{y})$ in Fourier components, *i.e.*

$$V(\hat{\mathbf{X}}-\mathbf{y}) = \frac{1}{(2\pi\hbar)^3}\int d\mathbf{Q}\,\tilde{V}(\mathbf{Q})\,e^{\frac{i}{\hbar}\mathbf{Q}\cdot(\mathbf{y}-\hat{\mathbf{X}})} \tag{2.42}$$

and performing the spatial integrals in Eq. (2.41), one eventually obtains

$$\frac{\partial}{\partial t}\hat{\rho}(t) = -\frac{i}{\hbar}\left[\frac{\hat{\mathbf{P}}^2}{2m}, \hat{\rho}(t)\right] + \frac{1}{2\hbar^2(2\pi\hbar)^3}\int d\mathbf{Q}\,\tilde{g}(\mathbf{Q})|V(\mathbf{Q})|^2(e^{\frac{i}{\hbar}\mathbf{Q}\cdot\hat{\mathbf{X}}}\hat{\rho}(t)e^{-\frac{i}{\hbar}\mathbf{Q}\cdot\hat{\mathbf{X}}} - \hat{\rho}(t)). \tag{2.43}$$

with

$$\tilde{g}(\mathbf{Q}) = \int d\mathbf{y} e^{\frac{i}{\hbar}\mathbf{Q}\cdot(\mathbf{x}-\mathbf{y})} g(\mathbf{x}-\mathbf{y}) = \int_0^\infty d\tau\,\mathbb{E}\left[\zeta(\mathbf{x},t)\zeta(\mathbf{y},t-\tau)\right] e^{\frac{i}{\hbar}\mathbf{Q}\cdot(\mathbf{x}-\mathbf{y})}. \tag{2.44}$$

Equation (2.44) can be theoretically computed with the help of thermal quantum field theory [58]. Let $\hat{\rho}_\mathcal{E} = \mathcal{Z}^{-1}e^{-\beta\hat{H}_\mathcal{E}}$ be the state of the thermal bath, $\phi^\dagger(\mathbf{x})$ and $\phi(\mathbf{x})$ the creation and annihilation fields of the bath and $\hat{\eta}(\mathbf{x}) = \hat{\phi}^\dagger(\mathbf{x})\hat{\phi}^\dagger(\mathbf{x})$ its density operator. One may write the average spatial density as

$$\begin{aligned}\bar{\eta} \equiv \mathbb{E}\left[\eta(\mathbf{x})\right] &= \mathrm{Tr}_\mathcal{E}\left(\hat{\phi}^\dagger(\mathbf{x})\hat{\phi}(\mathbf{x})\,\hat{\rho}_\mathcal{E}\right)\\ &= \int d\mathbf{k}d\mathbf{Q}\,e^{\frac{i}{\hbar}\mathbf{Q}\cdot\mathbf{x}}\,\mathrm{Tr}_\mathcal{E}\left(\hat{a}^\dagger(\mathbf{k})\hat{a}(\mathbf{k}+\mathbf{Q})\,\hat{\rho}_\mathcal{E}\right) = \int d\mathbf{k}d\mathbf{Q}\,\delta(\mathbf{q})\mathrm{Tr}_\mathcal{E}\left(\hat{a}^\dagger(\mathbf{k}+\mathbf{Q})\hat{a}(\mathbf{k})\,\hat{\rho}_\mathcal{E}\right)\end{aligned} \tag{2.45}$$

where $\hat{a}^\dagger(\mathbf{k})$ and $\hat{a}(\mathbf{k})$ are respectively the creation and annihilation field in momentum representation, and write the gas fluctuations as the real part of the quantum transition amplitude, *i.e.*

$$\begin{aligned}&\mathbb{E}\left[\zeta(\mathbf{x},t)\zeta(\mathbf{y},\tau)\right] = \mathbb{E}\left[\eta(\mathbf{x},t)\eta(\mathbf{y},\tau)\right] - \mathbb{E}\left[\eta(\mathbf{x})\right]\mathbb{E}\left[\eta(\mathbf{y})\right]\\ &= \mathrm{Re}\left[\mathrm{Tr}_\mathcal{E}\left(\hat{\phi}\dagger(\mathbf{x};t)\hat{\phi}(\mathbf{x};t)\hat{\phi}^\dagger(\mathbf{y};\tau)\hat{\phi}(\mathbf{y};\tau)\,\hat{\rho}_\mathcal{E}\right) - \mathrm{Tr}_\mathcal{E}\left(\hat{\eta}(\mathbf{x})\,\hat{\rho}_\mathcal{E}\right)\mathrm{Tr}_\mathcal{E}\left(\hat{\eta}(\mathbf{y})\,\hat{\rho}_\mathcal{E}\right)\right]\\ &= \int d\mathbf{k}d\mathbf{k}'d\mathbf{Q}d\mathbf{Q}'e^{\frac{i}{\hbar}\mathbf{Q}\cdot\mathbf{x}}\mathrm{Re}\left[e^{\frac{i}{\hbar}\mathbf{Q}'\cdot\mathbf{y}}e^{\frac{i}{\hbar}\frac{\mathbf{k}^2-(\mathbf{k}-\mathbf{Q})^2}{2m}t}e^{\frac{i}{\hbar}\frac{\mathbf{k}'^2-(\mathbf{k}'-\mathbf{Q}')^2}{2m}\tau}\right]\\ &\qquad\qquad \mathrm{Tr}_\mathcal{E}\left(\hat{a}^\dagger(\mathbf{k})\hat{a}(\mathbf{k}-\mathbf{Q})\hat{a}^\dagger(\mathbf{k}')\hat{a}(\mathbf{k}'-\mathbf{Q}')\,\hat{\rho}_\mathcal{E}\right) - \bar{\eta}^2\end{aligned} \tag{2.46}$$

with $\hat{\phi}(\mathbf{x},t) \equiv e^{i\hat{H}_\mathcal{E}t}\hat{\phi}(x)e^{-i\hat{H}_\mathcal{E}t}$. Exploiting Wick's theorem at finite temperature one may rewrite the trace in Eq. (2.46) as

$$\begin{aligned}&\mathrm{Tr}_\mathcal{E}\left(\hat{a}^\dagger(\mathbf{k})\hat{a}(\mathbf{k}-\mathbf{Q})\hat{a}^\dagger(\mathbf{k}')\hat{a}(\mathbf{k}'-\mathbf{Q}')\,\hat{\rho}_\mathcal{E}\right) =\\ &\delta(\mathbf{Q}+\mathbf{Q}')\delta(\mathbf{k}'-\mathbf{k}-\mathbf{Q})\mathrm{Tr}_\mathcal{E}\left(\hat{a}^\dagger(\mathbf{k})\hat{a}(\mathbf{k})\,\hat{\rho}_\mathcal{E}\right)\left(1 \pm \mathrm{Tr}_\mathcal{E}\left(\hat{a}^\dagger(\mathbf{k}')\hat{a}(\mathbf{k}')\,\hat{\rho}_\mathcal{E}\right)\right)\\ &+\delta(\mathbf{Q})\delta(\mathbf{Q}')\mathrm{Tr}_\mathcal{E}\left(\hat{a}^\dagger(\mathbf{k})\hat{a}^\dagger(\mathbf{k})\,\hat{\rho}_\mathcal{E}\right)\mathrm{Tr}_\mathcal{E}\left(\hat{a}^\dagger(\mathbf{k}')\hat{a}^\dagger(\mathbf{k}')\,\hat{\rho}_\mathcal{E}\right)\end{aligned} \tag{2.47}$$

to eventually obtain

$$
\begin{aligned}
\mathbb{E}\left[\zeta(\mathbf{x},t)\zeta(\mathbf{y},\tau)\right] = & \int d\mathbf{k}d\mathbf{q}\, Re\left[e^{\frac{i}{\hbar}(\mathbf{x}-\mathbf{y})\mathbf{Q}}\, e^{\frac{i}{\hbar}\frac{\mathbf{k}^2-(\mathbf{k}-\mathbf{Q})^2}{2m}(t-\tau)}\right] \\
& \cdot \mathrm{Tr}_{\mathcal{E}}\left(\hat{a}^\dagger(\mathbf{k})\hat{a}(\mathbf{k})\,\hat{\rho}_{\mathcal{E}}\right)\left(1 \pm \mathrm{Tr}_{\mathcal{E}}\left(\hat{a}^\dagger(\mathbf{k}-\mathbf{Q})\hat{a}(\mathbf{k}-\mathbf{Q})\,\hat{\rho}_{\mathcal{E}}\right)\right) \\
= & \int d\mathbf{k}d\mathbf{q}\, Re\left[e^{\frac{i}{\hbar}(\mathbf{x}-\mathbf{y})\mathbf{Q}}\, e^{\frac{i}{\hbar}\frac{\mathbf{k}^2-(\mathbf{k}-\mathbf{Q})^2}{2m}(t-\tau)}\right] n(\mathbf{k})(1 \pm n(\mathbf{k}-\mathbf{Q})) \quad (2.48)
\end{aligned}
$$

where $\eta(\mathbf{k}) = \mathrm{Tr}_{\mathcal{E}}\left(\hat{a}^\dagger(\mathbf{k})\hat{a}(\mathbf{k})\,\hat{\rho}_{\mathcal{E}}\right)$ is the gas particles. Neglecting this quantum mechanical correction[1] in Eq. (2.48) , exploiting Eq. (2.44) and the identity,

$$
\frac{1}{\pi}\int_0^\infty d\tau e^{\pm ix\tau} = \delta(x) \pm i\mathcal{P}\left(\frac{1}{x}\right) \quad (2.49)
$$

where $\mathcal{P}(\cdot)$ denotes the principal value, one may rewrite Eq. (2.44) as follows:

$$
\tilde{g}(\mathbf{Q}) = \delta\left(\frac{\mathbf{k}^2}{2m} - \frac{(\mathbf{k}-\mathbf{Q})^2}{2m}\right) n(\mathbf{k}). \quad (2.50)
$$

Replacing the above expression in Eq. (2.43) one eventually obtains

$$
\begin{aligned}
\frac{\partial}{\partial t}\hat{\rho}(t) = & -\frac{i}{\hbar}\left[\frac{\hat{\mathbf{P}}^2}{2m}, \hat{\rho}(t)\right] \\
& + \frac{2\pi}{m^2}\int d\mathbf{Q}\,\delta\left(\frac{\mathbf{k}^2}{2m} - \frac{(\mathbf{k}-\mathbf{Q})^2}{2m}\right) n(\mathbf{k})|f_b(\mathbf{Q})|^2 (e^{\frac{i}{\hbar}\mathbf{Q}\cdot\hat{\mathbf{X}}}\hat{\rho}(t)e^{-\frac{i}{\hbar}\mathbf{Q}\cdot\hat{\mathbf{X}}} - \hat{\rho}(t)) \quad (2.51)
\end{aligned}
$$

where

$$
f_b(\mathbf{Q}) = -(2\pi)^2\hbar m\,|V(\mathbf{Q})|\,. \quad (2.52)
$$

and $f_b(\mathbf{Q})$ is the scattering amplitude in Born approximation [51]. One can easily check that Eq. (2.51) is equivalent to the Born approximation of the Gallis-Flemming master equation accordingly, it does not take into account recoil effects on the test particle. However, the derivation of the master equation Eq. (2.51) here presented suggests that dissipation cannot appear under the assumption assumption in Eq. (2.40) of delta correlated bath time fluctuations, or in other words, zero collision time. Indeed one can see from $\tilde{g}(\mathbf{Q})$ in Eq. (2.48) and the derivation that lead to the expression in Eq. (2.50), that the bath energy dirac delta, and with that, the dependence on the bath particle momentum in the

[1] note that $n(\mathbf{k}) \ll 1$ because we restrict to the case of a rarefied thermal gas

collisional term of Eq. (2.43), is strictly related to the possibility that the gas particle has to evolve during the interaction process. On the other side, there is no dependence on the test particle momentum in the collision term, and the free evolution contribution of the test particle during the interaction process is zero because the bath fluctuations are Dirac delta correlated in time. In order to verify this hypothesis, we relax the assumption in Eq. (2.40) of delta correlated fluctuations in time, and we assume a finite correlation time τ_c, *i.e.*

$$\mathbb{E}\left[\zeta(\mathbf{x},t)\zeta(\mathbf{y},\tau)\right] = f(\mathbf{x}-\mathbf{y},t-\tau) = 0 \qquad \forall\, t \geq \tau_c. \tag{2.53}$$

Similarly to what done for Eq. (2.41), in the app. A we also provide detailed calculation for the average master equation generated in the case of a finite correlation in time. Exploiting this results in the case of study, we obtain the following master equation

$$\begin{aligned}\frac{\partial}{\partial t}\hat{\rho}(t) = &-\frac{i}{\hbar}\left[\frac{\hat{\mathbf{P}}^2}{2M}\,,\hat{\rho}(t)\right]\\ &+\frac{1}{2\hbar^2}\int_0^\infty d\tau\int d\mathbf{y}d\mathbf{z}\,f(\mathbf{y}-\mathbf{z};\tau)\left[V(\hat{\mathbf{X}}-\mathbf{y})\,,\left[V_I(\hat{\mathbf{X}}-\mathbf{z};-\tau)\,,\hat{\rho}(t)\right]\right]+\mathcal{O}((\tau_c/t)^2)\quad \forall t>\tau_c,\end{aligned} \tag{2.54}$$

with $V_I(\hat{\mathbf{x}}_\mathcal{S}-\mathbf{y},\tau)$ the interaction potential in interaction picture defined as

$$V_I(\hat{\mathbf{x}}_\mathcal{S}-\mathbf{y};\tau) = e^{\frac{i}{\hbar}\frac{\hat{\mathbf{P}}^2}{2M}\tau}V(\hat{\mathbf{X}}-\mathbf{y})e^{-\frac{i}{\hbar}\frac{\hat{\mathbf{P}}^2}{2M}\tau}. \tag{2.55}$$

Expanding the correlation function in Fourier components, *i.e.*

$$f(\mathbf{x},t) = \frac{1}{(2\pi\hbar)^4}\int d\mathbf{Q}d\omega\, e^{\frac{i}{\hbar}(\mathbf{Q}\cdot\mathbf{x}+\omega t)}\tilde{f}(\mathbf{Q},\omega) \tag{2.56}$$

and integrating Eq. (2.54) over the spatial variables $d\mathbf{y}$, $d\mathbf{z}$, one obtains

$$\begin{aligned}\frac{\partial}{\partial t}\hat{\rho}(t) = &-\frac{i}{\hbar}\left[\frac{\hat{\mathbf{P}}^2}{2M}\,,\hat{\rho}(t)\right]+\frac{1}{8\pi\hbar^3}\int d\mathbf{Q}d\omega\,\tilde{f}(\mathbf{Q},\omega)e^{-\frac{i}{\hbar}\omega\tau}\left|V(\mathbf{Q})\right|^2\\ &\cdot\int_0^\infty d\tau\left[e^{-\frac{i}{\hbar}\mathbf{Q}\cdot\hat{\mathbf{X}}}\,,\left[e^{-\frac{i}{\hbar}\frac{\hat{\mathbf{P}}^2}{2M}\tau}\,e^{\frac{i}{\hbar}\mathbf{Q}\cdot\hat{\mathbf{X}}}\,e^{\frac{i}{\hbar}\frac{\hat{\mathbf{P}}^2}{2M}\tau}\,,\hat{\rho}(t)\right]\right]+\mathcal{O}((\tau_c/t)^2).\end{aligned} \tag{2.57}$$

Exploiting the canonical commutation relation $[\hat{x}\,,\hat{p}]\;=\;i\hbar$, and recalling the symmetry property of the correlation function, ($f(\mathbf{Q},\omega)=f(-\mathbf{Q},-\omega)$), one obtains

$$\begin{aligned}\frac{\partial}{\partial t}\hat{\rho}(t) = &-\frac{i}{\hbar}\left[\frac{\hat{\mathbf{P}}^2}{2M}\,,\hat{\rho}(t)\right]+\frac{1}{8\pi\hbar^3}\int d\mathbf{Q}d\omega\,\tilde{f}(\mathbf{Q},\omega)\,|V(\mathbf{Q})|^2\\ &\left[\int_0^\infty d\tau e^{\frac{i}{\hbar}\left(\frac{\hat{\mathbf{P}}^2}{2M}-\frac{(\hat{\mathbf{P}}-\mathbf{Q})^2}{2M}-\omega\right)\tau}\left(e^{\frac{i}{\hbar}\hat{\mathbf{x}}\mathbf{Q}}\hat{\rho}(t)e^{\frac{i}{\hbar}\hat{\mathbf{x}}\mathbf{Q}}-\hat{\rho}(t)\right)\right.\\ &\left.+\int_0^\infty d\tau\left(e^{\frac{i}{\hbar}\hat{\mathbf{X}}\cdot\mathbf{Q}}\hat{\rho}(t)e^{\frac{i}{\hbar}\hat{\mathbf{X}}\cdot\mathbf{Q}}-\hat{\rho}(t)\right)e^{-\frac{i}{\hbar}\left(\frac{\hat{\mathbf{P}}^2}{2M}-\frac{(\hat{\mathbf{P}}-\mathbf{Q})^2}{2M}-\omega\right)\tau}\right]+\mathcal{O}((\tau_c/t)^2). \quad (2.58)\end{aligned}$$

This equation can be rewritten in a more explicit manner by exploiting Eq. (2.49) to eventually obtain[2]

$$\begin{aligned}\frac{\partial\hat{\rho}(t)}{\partial t} = &-\frac{i}{\hbar}\left[\frac{\hat{\mathbf{P}}^2}{2M}\,,\hat{\rho}(t)\right]+\frac{1}{8\hbar^2}\int d\mathbf{Q}d\omega\,\tilde{f}(\mathbf{Q},\omega)\,|V(\mathbf{Q})|^2\\ &\cdot\left[\left\{\delta\left(\frac{\hat{\mathbf{P}}^2}{2M}-\frac{(\hat{\mathbf{P}}-\mathbf{Q})^2}{2M}-\omega\right),\left(e^{\frac{i}{\hbar}\hat{\mathbf{X}}\cdot\mathbf{Q}}\hat{\rho}(t)e^{-\frac{i}{\hbar}\hat{\mathbf{X}}\cdot\mathbf{Q}}-\hat{\rho}(t)\right)\right\}\right.\\ &\left.+\mathcal{P}\left(\left[\left(\frac{\hat{\mathbf{P}}^2}{2M}-\frac{(\hat{\mathbf{P}}-\mathbf{Q})^2}{2M}-\omega\right)^{-1},\left(e^{\frac{i}{\hbar}\hat{\mathbf{X}}\cdot\mathbf{Q}}\hat{\rho}(t)e^{-\frac{i}{\hbar}\hat{\mathbf{X}}\cdot\mathbf{Q}}-\hat{\rho}(t)\right)\right]\right)\right]+\mathcal{O}((\tau_c/t)^2).\end{aligned} \quad (2.59)$$

One can easily check that the equation above displays recoil effects. It is sufficient to see that the collision term of the above master equation does not leave the position state unchanged, because of its dependence on the momentum operator $\hat{\mathbf{p}}$. This confirms the necessity of bath fluctuations with correlation time different from zero to have dissipative phenomena. It is also worth noticing that, under the assumption of almost diagonal system's state in momentum representation, *i.e.*

$$\left[\frac{\hat{\mathbf{P}}}{M}\,,\hat{\rho}(t)\right]\simeq 0, \quad (2.60)$$

[2] A careful reader may notice that this equation is not in Lindblad form and is then a not completely positive equation. However, Eq. (2.59) has been derived under the assumption $\tau_c \ll \tau$, meaning that cannot be used to describe the early stage of the evolution but only such states that are evolved at time t by the action of Eq. (A.8). It is exactly the action of Eq. (A.8) that select the class of possible states that are accessible when $\tau_c \ll t$ and consequently the class of state compatible with the approximated dynamics.

Eq. (2.59) takes the following simpler expression

$$\frac{\partial}{\partial t}\hat{\rho}(t) \simeq -\frac{i}{\hbar}\left[\frac{\hat{\mathbf{P}}^2}{2M}, \hat{\rho}(t)\right] + \frac{1}{4\hbar^2}\int d\mathbf{Q}d\omega\,\tilde{f}(\mathbf{Q},\omega)\,|V(\mathbf{Q})|^2\,\delta\left(\frac{\hat{\mathbf{P}}^2}{2M} - \frac{(\hat{\mathbf{P}}-\mathbf{Q})^2}{2M} - \omega\right)\left(e^{\frac{i}{\hbar}\hat{\mathbf{X}}\cdot\mathbf{Q}}\hat{\rho}(t)e^{-\frac{i}{\hbar}\hat{\mathbf{X}}\cdot\mathbf{Q}} - \hat{\rho}(t)\right). \tag{2.61}$$

This equation is very similar to Eq. (2.43), with the only difference of the collisional term that here displays an explicit dependence on the test particle momentum. Moreover, the presence of an energy Dirac delta function guarantees an energy preserving collision process where $\mathbf{Q}$ is the transferred momentum.

Even if Eq. (2.61) seems a good dissipative equation, its dynamics does not allow the thermal state

$$\rho_{eq}(\hat{\mathbf{P}}) = \mathcal{Z}_\beta e^{-\frac{\mathbf{P}_\mathcal{S}^2}{2M}} \tag{2.62}$$

as stationary state (as one would expect from physical considerations), forcing us to reject the equation as a good dissipative equation. To prove that $\rho_{eq}(\hat{\mathbf{P}})$ is not a stationary solution of Eq. (2.61), we replace Eq. (2.62) in Eq. (2.59) and exploit the symmetry of Eq.(2.62)

$$\rho_{eq}(\hat{\mathbf{P}}) = e^{\beta\left(\frac{\mathbf{Q}^2+2\mathbf{Q}\cdot\hat{\mathbf{P}}}{2M}\right)}\rho_{eq}(\hat{\mathbf{P}}+\mathbf{Q}). \tag{2.63}$$

The result is

$$\frac{\partial\rho_{eq}(\hat{\mathbf{P}})}{\partial t} = \frac{1}{4\hbar^2}\int d\mathbf{Q}d\omega\left\{\tilde{f}(\mathbf{Q},\omega)\left|\tilde{V}(\mathbf{Q})\right|^2\delta\left(\frac{(\hat{\mathbf{p}}_\mathcal{S}+\mathbf{Q})^2}{2m} - \frac{\hat{\mathbf{P}}^2}{2m} - \omega\right)\rho_{eq}(\hat{\mathbf{p}}-\mathbf{Q}) - \tilde{f}(\mathbf{Q},\omega)\left|\tilde{V}(\mathbf{Q})\right|^2\delta\left(\frac{\hat{\mathbf{P}}^2}{2M} - \frac{(\hat{\mathbf{P}}-\mathbf{Q})^2}{2M} - \omega\right)e^{\beta\frac{\mathbf{Q}^2+2\mathbf{Q}\cdot\hat{\mathbf{P}}}{2M}}\rho_{eq}(\hat{\mathbf{P}}+\mathbf{Q})\right\}. \tag{2.64}$$

From Eq. (2.64) it is easy to show that $\frac{\partial\rho_{eq}}{\partial t} = 0$ only if

$$\left[\tilde{f}(\mathbf{Q},\omega)\delta\left(\frac{(\hat{\mathbf{P}}+\mathbf{Q})^2}{2M} - \frac{\hat{\mathbf{P}}^2}{2M} - \omega\right) = \tilde{f}(-\mathbf{Q},\omega)\delta\left(\frac{\hat{\mathbf{P}}^2}{2M} - \frac{(\hat{\mathbf{P}}+\mathbf{Q})^2}{2M} - \omega\right)e^{\beta\frac{\mathbf{Q}^2-2\mathbf{Q}\cdot\hat{\mathbf{P}}}{2M}}\right]. \tag{2.65}$$

Equation (2.65) holds true only for $\tilde{f}(\mathbf{Q},\omega) = 0$, (because of the symmetry $\tilde{f}(\mathbf{Q},\omega) = \tilde{f}(-\mathbf{Q},-\omega)$ imposed by the assumption of real Gaussian bath fluctuations), proving that ρ_{eq} is not a stationary state of the dynamics described by Eq. (2.59). This argument leads us to conclude that a stochastic approach based on real Gaussian noise is not enough to describe the behaviour of a particle in a gas when also dissipative phenomena are present. One could then think to use a complex Gaussian noise to model the bath fluctuations, *i.e.*

$$\mathbb{E}\left[\zeta(\mathbf{x},t)\zeta(\mathbf{y},\tau)\right] = g(\mathbf{x}-\mathbf{y},t-\tau), \qquad \mathbb{E}\left[\zeta(\mathbf{x},t)\zeta^*(\mathbf{y},\tau)\right] = f(\mathbf{x}-\mathbf{y},t-\tau). \tag{2.66}$$

However this choice would lead to a non Hermitian coupling in Eq. (2.36) and consequently lead to a dynamics that would violate the very basic request of trace preservance and positivity. In order to restore trace preservance and positivity of one might modify Eq. (2.36) as follows:

$$\begin{aligned}\hat{H}_{eff}(t) = \frac{\hat{\mathbf{P}}^2}{2M} &+ \int dy\, \eta(\mathbf{y},t)V(\hat{\mathbf{X}}-\mathbf{y}) \\ &+ \int_0^t d\tau \int d\mathbf{y}d\mathbf{z}V(\hat{\mathbf{X}}-\mathbf{y})[f(\mathbf{y}-\mathbf{z},t-\tau) - g(\mathbf{y}-\mathbf{z},t-\tau)]\frac{\delta}{\delta\zeta(\mathbf{z},\tau)}\end{aligned} \tag{2.67}$$

where $\delta\zeta(\mathbf{z},\tau)$ is a functional derivative on the noise field, as it is usually done in other fields of research [59]. This equation differs from Eq. (2.36) for the term in the second line. However, the addition of this term has no evident physical explanation, preventing any motivated interpretation for the modified Hamiltonian in Eq. (2.67) and its dynamics. This fact prevents us from exploiting the method here developed in order to derive a consistent dissipative model for the dynamics. Due to the impossibility of further exploiting this method to gather more information on the mechanism underling dissipative dynamics, we decided to tackle the problem of a the collisional dynamics from a purely microscopic perspective.

Chapter 3

Microscopic treatment of Collisional Dynamics

Starting from a full Hamiltonian treatment we derive the short time scale evolution of a test particle in a rarefied thermal bath. Exploiting this result and physically motivated arguments, we build a piece-wise model for the long time behaviour of the test particle. The piece-wise model provide a natural scheme to obtain a coarse-grained theory where instantaneous collisions appears. The collision term obtained from the coarse-graining is not expressed in terms of the standard scattering operator, as one expect. However we, show that -in the limit of a collisional description- it can be replaced by a new operator fully characterized by scattering operator provided by the standard scattering theory. Eventually we estimate the free evolution time scale and the collision time scale proving the limits of a collisional dynamics in the quantum mechanical framework.

3.1 Test particle in a dilute gas

The aim of this section is to derive a model describing the behaviour of a test particle in a thermal bath from a microscopic treatment of the dynamics.
We consider an ideal gas ($\mathcal{E}$) of N-indistinguishable,[1] non interacting particles, with mass

[1] here the indistinguishability should be understood in a wide sense: either lack of information or a property of the quantum particle.

m, confined in a box of large volume Ω with periodic boundary conditions, described by the Hamiltonian

$$\hat{H}_{\mathcal{E}} = \sum_{i=1}^{N} \hat{H}_i = \sum_{i=1}^{N} \frac{\hat{\mathbf{p}}_i^2}{2m}, \tag{3.1}$$

where $\hat{\mathbf{x}}_i$ and $\hat{\mathbf{p}}_i$ are position and momentum operators of the i-th gas particle. A test particle ($\mathcal{S}$) described by the Hamiltonian

$$\hat{H}_{\mathcal{S}} = \frac{\hat{\mathbf{P}}^2}{2M} \tag{3.2}$$

interacts with the gas through the following interaction potential

$$\hat{H}_{int} = \sum_{i=1}^{N} V(\hat{\mathbf{X}} - \hat{\mathbf{x}}_i) \tag{3.3}$$

where $\hat{\mathbf{X}}$ and $\hat{\mathbf{P}}$ are the position and the momentum operator, and and M is the mass of the test particle.
We also assume the system and environment state $\hat{\varrho}_{\mathcal{S}\mathcal{E}}$ to be initially uncorrelated, *i.e.*

$$\hat{\varrho}_{\mathcal{S}\mathcal{E}}(0) = \hat{\varrho}_{\mathcal{S}} \otimes \hat{\varrho}_{\mathcal{E}}. \tag{3.4}$$

The dynamics of the whole system is described by the following Liouville von Neuman equation

$$\frac{\partial \hat{\varrho}_{\mathcal{S}\mathcal{E}}(t)}{\partial t} = -\frac{i}{\hbar}\left[\hat{H}_{\mathcal{S}} + \hat{H}_{\mathcal{E}} + \hat{H}_{int}\, , \hat{\varrho}_{\mathcal{S}\mathcal{E}}(t)\right]. \tag{3.5}$$

Tracing Eq. (3.5) over the N particles degrees of freedom, one obtains the test particle reduced dynamics, described by

$$\begin{aligned}\frac{\partial \hat{\varrho}_{\mathcal{S}}(t)}{\partial t} &= -\frac{i}{\hbar}\mathrm{Tr}_{[1\ldots N]}\left[\hat{H}_{\mathcal{S}} + \hat{H}_{\mathcal{E}} + \hat{H}_{int}\, , \hat{\varrho}_{\mathcal{S}\mathcal{E}}(t)\right] \\ &= -\frac{i}{\hbar}\left[\hat{H}_{\mathcal{S}}\, , \hat{\varrho}_{\mathcal{S}}(t)\right] - \frac{i}{\hbar}\sum_{i=1}^{N}\mathrm{Tr}_i\left[V(\hat{\mathbf{X}} - \hat{\mathbf{x}}_i)\, , \hat{\varrho}_{\mathcal{S},i}(t)\right]\end{aligned} \tag{3.6}$$

where $\mathrm{Tr}_i[\cdot]$ is the trace over the degrees of freedom of the i-th particle of the gas, $\mathrm{Tr}_{[1\ldots N]}[\cdot] = \prod_{I=1}^{N}\mathrm{Tr}_i[\ldots[\cdot]]$, $\hat{\varrho}_{\mathcal{S}} = \mathrm{Tr}_{[1\ldots N]}[\hat{\varrho}_{\mathcal{S}\mathcal{E}}]$ is the reduced statistical operator of the test particle ($\mathcal{S}$) and $\hat{\varrho}_{\mathcal{S},i} = \mathrm{Tr}_{[1\ldots i-1,i+1\ldots N]}[\hat{\varrho}_{\mathcal{S}\mathcal{E}}]$ the reduced statistical operator of the system composed by the test particle ($\mathcal{S}$) and the i-th particle of the gas.

Under the assumption of indistinguishable gas particles $\hat{\varrho}_{\mathcal{S},i} = \hat{\varrho}_{\mathcal{S},j} \; \forall i,j \in 1,\ldots,N$, Eq. (3.6) can be rewritten as

$$\frac{\partial \hat{\varrho}_{\mathcal{S}}(t)}{\partial t} = -\frac{i}{\hbar}\left[\hat{H}_{\mathcal{S}}\,,\hat{\varrho}_{\mathcal{S}}(t)\right] - \frac{i}{\hbar}N\,\mathrm{Tr}_1\left[V(\hat{\mathbf{X}}-\hat{\mathbf{x}}_1)\,,\hat{\varrho}_{\mathcal{S},1}(t)\right] \tag{3.7}$$

where the interaction with an N particles gas is reduced to the interaction with a single particle of the gas.

In order to fully determine the reduced dynamics of $\hat{\varrho}_{\mathcal{S}}(t)$ one needs to determine the evolution of $\hat{\varrho}_{\mathcal{S},1}(t)$. A dynamical equation for $\hat{\varrho}_{\mathcal{S},1}(t)$ can be easily obtained by tracing Eq. (3.5) over the degrees of freedom of the gas particles $2,\ldots N$:

$$\frac{\partial \hat{\varrho}_{\mathcal{S},1}(t)}{\partial t} = -\frac{i}{\hbar}\left[\hat{H}_{\mathcal{S}} + \hat{H}_1 + V(\hat{\mathbf{X}}-\hat{\mathbf{x}}_1)\,,\hat{\varrho}_{\mathcal{S},1}(t)\right]. \tag{3.8}$$

Since there is no interaction between the particles of the gas, Eq. (3.8) is a closed equation and, if combined with Eq. (3.7), it allows to describe the reduced dynamics of the system. It is convenient to rewrite the system of Eq. (3.7) and Eq. (3.8) in their respective interaction pictures, labelled by the superscript I :

$$\hat{\varrho}^{\mathrm{I}}_{\mathcal{S},1}(t) = \hat{U}^{\dagger}_0(t)\hat{\varrho}_{\mathcal{S},1}(t)\hat{U}_0(t) \qquad , \qquad \hat{\varrho}^{\mathrm{I}}_{\mathcal{S}}(t) = \hat{U}^{\dagger}_{\mathcal{S}}(t)\hat{\varrho}^{\mathrm{I}}_{\mathcal{S}}(t)\hat{U}_{\mathcal{S}}(t) \tag{3.9}$$

with:

$$\hat{U}_0(t) = e^{-\frac{i}{\hbar}(\hat{H}_s+\hat{H}_1)t} \qquad , \qquad \hat{U}_{\mathcal{S}}(t) = e^{-\frac{i}{\hbar}\hat{H}_s t}. \tag{3.10}$$

Equations (3.7) and (3.8) now become

$$\begin{cases} \dfrac{\partial \hat{\varrho}^{\mathrm{I}}_{\mathcal{S}}(t)}{\partial t} = N\,\mathrm{Tr}_1\left[\dfrac{\partial \hat{\varrho}^{\mathrm{I}}_{\mathcal{S},1}(t)}{\partial t}\right] & \text{(3.11a)} \\ \dfrac{\partial \hat{\varrho}^{\mathrm{I}}_{\mathcal{S},1}(t)}{\partial t} = -\dfrac{i}{\hbar}\left[V_I(\hat{\mathbf{X}}-\hat{\mathbf{x}}_1;t)\,,\hat{\varrho}^{\mathrm{I}}_{\mathcal{S},1}(t)\right] & \text{(3.11b)} \end{cases}$$

with:

$$\hat{V}_I(\hat{\mathbf{X}}-\hat{\mathbf{x}}_1;t) = \hat{U}_0(t)\hat{V}(\hat{\mathbf{X}}-\hat{\mathbf{x}}_1)\hat{U}^{\dagger}_0(t). \tag{3.12}$$

The formal solution of the system of Eqs. (3.11a, 3.11b) with initial condition $\hat{\varrho}_{s,1}(t_0) = \hat{\varrho}_s \otimes \hat{\varrho}_1$ can now be written in the from

$$\hat{\varrho}^{\mathrm{I}}_{\mathcal{S}}(t) = \mathcal{M}^{\mathrm{I}}_t(\hat{\varrho}_s) = N\mathrm{Tr}_1\left(\hat{U}_{\mathrm{I}}(t)\hat{\varrho}_{\mathcal{S}} \otimes \hat{\varrho}_1\hat{U}^{\dagger}_{\mathrm{I}}(t) - \hat{\varrho}_{\mathcal{S}} \otimes \hat{\varrho}_1\right) + \hat{\varrho}_s \tag{3.13}$$

where

$$\hat{U}_I(t) = \mathcal{T}\left\{e^{-\frac{i}{\hbar}\int_0^t d\tau \hat{V}_I(\tau)}\right\} \tag{3.14}$$

and $\mathcal{T}\{\dots\}$ is the time ordering operator (in writing the interaction operator $V_{\rm I}(\tau)$, we have suppressed the explicit dependency on $\mathbf{X}$ and $\mathbf{x}_1$ to keep the notation compact). Equation (3.13) can be now conveniently rewritten in the Schrödinger picture:

$$\hat{\varrho}_{\mathcal{S}}(t) = \mathcal{M}_t(\hat{\varrho}_{\mathcal{S}}) = \mathcal{U}_t^{\mathcal{S}}(\mathcal{M}_t^{\rm I}(\hat{\varrho}_{s})) \tag{3.15}$$

with $\mathcal{U}_\tau^{\mathcal{S}}(\cdot)$ the free-evolution dynamical map defined by

$$\mathcal{U}_t^{\mathcal{S}}(\hat{\varrho}_{\mathcal{S}}) = \hat{U}_{\mathcal{S}}(t)\hat{\varrho}_{\mathcal{S}}(t)\hat{U}_{\mathcal{S}}^{\dagger}(t). \tag{3.16}$$

It is important to keep in mind that Eq. (3.13) describes the interaction dynamics of a single particle in a gas under the assumption of non-interacting gas particles. This approximation holds in the case of a rarefied gas in thermal equilibrium, where the average contribution to the dynamics due to the mutual interaction of the gas particles is negligible.

The lack of interaction between the particles of the gas does not allow the gas to equilibrate back after having interacted with the test particle, asymptotically bringing the gas far from the equilibrium. This means that the model in Eq. (3.13) describes the correct short time behaviour of the test particle interacting with a rarefied thermal bath, but fails in describing the long time behaviour of the test particle. However, under the assumption that the bath re-equilibration time (τ_r) is negligible compared to the typical times of the test particle dynamics[2], one can approximate the bath re-equilibration process as an instantaneous event that restores the gas to equilibrium after the interaction process between the bath and the test particle. This assumption allows to describe the long time behaviour of a test particle in a thermal bath through a piecewise dynamics: the test particle evolves according to the Eq. (3.13), for short time intervals τ, and at the end of each time interval, the gas particle is traced out and replaced by a new one in a thermal equilibrium state

$$\hat{\varrho}_{\mathcal{S}}(t = n\tau) = \underbrace{\mathcal{M}_\tau \circ \cdots \circ \mathcal{M}_\tau}_{n-times}(\hat{\varrho}_{\mathcal{S}}) \tag{3.17}$$

[2]It is important to notice that the test particle dynamics is governed not only by the free evolution but also by the interaction with the bath, accordingly the typical re-equilibration time of the bath should be much faster than both the typical variation time of the freely evolving particle and of the typical variation time of the interaction dynamics.

where $\mathcal{M}_\tau$ is the dynamical map describing the short time dynamics of the test particle according to Eq. (3.15), *i.e.*

$$\begin{aligned}\mathcal{M}_\tau(\hat{\varrho}_S) &= \mathcal{U}^S_\tau(\mathcal{M}^{\rm I}_\tau(\hat{\varrho}_S)) \\ &= \hat{U}_S(\tau) N \mathrm{Tr}_1 \left(\hat{U}_{\rm I}(\tau)\hat{\varrho}_S \otimes \hat{\varrho}_1 \hat{U}^\dagger_{\rm I}(\tau) - \hat{\varrho}_s \otimes \hat{\varrho}_1 \right) \hat{U}^\dagger_S(\tau) + \hat{U}_S(\tau)\hat{\varrho}_S \hat{U}^\dagger_S(\tau),\end{aligned} \tag{3.18}$$

$\hat{\varrho}_1$ descirbes the typical particle of a rarefied bath in thermal equilibrium and is therefore given by the Boltzmann distribution $\mu(\hat{\mathbf{p}}_1)$ in a box normalized momentum states, *i.e.*

$$\hat{\varrho}_1 = \frac{(2\pi\hbar)^3}{\Omega}\mu(\hat{\mathbf{p}}_1) = \frac{(2\pi\hbar)^3}{\Omega}\left(\frac{\beta}{2\pi m}\right)^{3/2} e^{-\beta\frac{\hat{\mathbf{p}}_1^2}{2m}}. \tag{3.19}$$

Clearly the piecewise dynamics here derived is in general highly dependent on the choice of the time interval τ. This fact prevents Eq. (3.17) from being a good dynamical description of the system in exam. However, if the time interval τ is much bigger than the typical variation time (τ_{int}) of the interaction process (in such a way to let the interaction exhausts his contribution on the dynamics), but much smaller then the typical variation time of the freely evolving particle (τ_{free}) (because the model in Eqs. (3.11a) and (3.11b) fails in describing the long time behaviour of the test particle, as mentioned in the previous page), one can obtain a piecewise dynamics independent from the time interval τ.

Summarising, a piecewise dynamics described by Eq. (3.17) should satisfy the following conditions

$$\tau_r \ll \tau_{int} \ll \tau \ll \tau_{free}. \tag{3.20}$$

Now that we have outlined a scheme to treat the dynamics of a particle in a gas, we want to understand if within this scheme the interaction process between the test particle and the gas can be described as a collision, like in the classical case. In the next section we explore this possibility.

3.2 Collisional Effective Dynamics

Aim of this section is to describe the interaction between the test particle and a gas particle occurring in the time interval τ of the piecewise dynamics described by Eq. (3.17) as a collision event. We follow the idea that the collision is an emergent dynamical property of the dynamics in which bounded states of the interaction are not allowed: the interaction is effective only in specific regions of the configuration space of the system and it does not allow the system to remain confined in these regions. We furthermore assume that the typical variation time of the interacting system (τ_{int}) is much shorter than the typical variation time (τ_{free}) of the freely evolving system:

$$\tau_{int} \ll \tau_{free}. \tag{3.21}$$

This condition allows to define a time scale τ, in which the free evolution gives negligible contributions to the dynamics, whereas the interaction process has enough time to evolve the system to a steady state of the interaction. The outcome of the interaction process after a time interval τ is understood as a *collision* if time scales smaller than τ are unaccessible to the theory. In this framework, a system satisfying (3.21) and described by an effective theory having temporal resolution τ such that $\tau_{int} \ll \tau \ll \tau_{free}$, is expected to display an effective dynamics dominated by free evolution suddenly interrupted by instantaneous collision events.

A simple example of emergent collision is the interaction process of two classical charged particles. The fundamental laws of physics explain the interaction process as the influence of electromagnetic field generated by one particle to the motion of the other, and vice versa. Since the electromagnetic field is spatially extended, the interaction process lasts for a finite time t, related to the initial velocity of the particles and the strength of the interaction. However, a coarse-grained theory in which both the spatial extension of the e.m. field and the time length of the interaction process are unaccessible, describes the interaction process between the two particles as a local and instantaneous collision.

The model developed in sec. 3.1 satisfies (3.21), meaning that a satisfactory piecewise dynamics can always be reduced to a collisional dynamics.

An interesting feature of the piecewise dynamics defined by Eq. (3.17) is that it provides a natural scheme to develop the coarse-grained theory with a time resolution bigger than τ. Indeed, Eq. (3.17) can be rewritten as

$$\hat{\varrho}_S(t = n\tau) = \sum_{i=0}^{n} \Delta\hat{\varrho}_S(t_i) \tag{3.22}$$

where $t_0 = 0$ and

$$\Delta\hat{\varrho}_S(t_i) \equiv \mathcal{M}_\tau(\hat{\varrho}_S(t_i)) - \hat{\varrho}_S(t_i) \tag{3.23}$$

with $\mathcal{M}_\tau(\hat{\varrho}_s)$ the dynamical map describing the short time behaviour of the test particle, as defined by Eq. (3.18). The request of a time resolution bigger than τ is mathematically equivalent to performing the limit $\tau \to 0$ in Eq. (3.22), under the constraints of Eq. (3.20). Multiplying and dividing Eq. (3.22) by τ and performing the limit one eventually obtains:

$$\hat{\varrho}_S(t) = \lim_{\tau \to 0} \sum_{i=0}^{n} \frac{\Delta \hat{\varrho}_S(t_i)}{\tau} \tau = \int_0^t \frac{\partial \hat{\varrho}_S(\tau)}{\partial \tau} d\tau. \tag{3.24}$$

If this limit exists, Eq. (3.24) describes the effective collisional theory unable to resolve time scales smaller than τ. In the next section we perform a detailed analysis of Eq. (3.24) in order to find necessary conditions on the existence of a collisional dynamics describing the behaviour of a test particle in a gas under the very natural assumption that collisions should be described by the action of the standard scattering operator $\hat{S}$ defined by

$$\hat{S} = \lim_{\tau \to +\infty} \mathcal{T} \left\{ e^{-\frac{i}{\hbar} \int_{-\tau}^{\tau} \hat{V}_I(s) ds} \right\}. \tag{3.25}$$

3.2.1 General conditions for collisional dynamics

We now analyse the term $\frac{\Delta \hat{\varrho}_s}{\tau}$ of Eq. (3.24) in order to find general conditions for the existence of the limit $\tau \to 0$ in Eq. (3.24).
Substituting Eq. (3.18) in Eq. (3.23) one obtains

$$\frac{\Delta \hat{\varrho}_S(t)}{\tau} = \frac{\mathcal{U}_\tau^S(\hat{\varrho}_S(t)) - \hat{\varrho}_S(t)}{\tau} + \frac{\mathcal{U}_\tau^S[\mathcal{M}_\tau^{\mathrm{I}}(\hat{\varrho}_S(t)) - \hat{\varrho}_S(t)]}{\tau}. \tag{3.26}$$

The first term on r.h.s. represents the change of the system due to the free evolution: it describes the dynamics of the system when there is no interaction at all. The second term is an additional contribution to the dynamics produced by the interaction with the thermal bath. One observes that this second term is composed by $\mathcal{M}_\tau^{\mathrm{I}}(\hat{\varrho}_S(t)) - \hat{\varrho}_S(t)$, that represents the change of the system due to the interaction with the thermal bath, and the action of the free-evolution map $\mathcal{U}_\tau^S$, representing residual changes of the system due to the free evolution, after the interaction process. This considerations allow to understand $\mathcal{M}_\tau^{\mathrm{I}}(\hat{\varrho}_S(t)) - \hat{\varrho}_S(t) \equiv \Delta \hat{\varrho}_S|_{coll}$ as the generator of the collision events in the coarse grained theory, if conditions (3.20) are satisfied.
Under the assumption

$$\tau \ll \tau_{free} \tag{3.27}$$

one expects the free-dynamics to give a negligible contribution. This allows to expand the free evolution super-operator defined by Eq. (3.16) in Taylor series and truncate the expansion to the first perturbative order, *i.e.*

$$\mathcal{U}^{\mathcal{S}}_{\tau}(\,\cdot\,) = \mathbb{1} - \frac{i}{\hbar}\mathcal{H}_{\mathcal{S}}(\,\cdot\,)\tau + \mathcal{O}(\tau^2/\tau^2_{free}) \tag{3.28}$$

where $\mathcal{H}_{\mathcal{S}}$ is the infinitesimal change given by the free-dynamics:

$$\mathcal{H}_{\mathcal{S}}(\hat{\varrho}_{\mathcal{S}}) = \left[\hat{H}_{\mathcal{S}}\,, \hat{\varrho}_{\mathcal{S}}\right]. \tag{3.29}$$

Under the further assumption

$$\tau_{int} \ll \tau \tag{3.30}$$

one is allowed to Taylor expand the collision term around $\tau = \infty$ to obtain

$$\mathcal{M}^{\mathrm{I}}_{\tau}(\hat{\varrho}_{\mathcal{S}}) - \hat{\varrho}_{\mathcal{S}} = [\mathcal{M}^{\mathrm{I}}_{\tau}(\hat{\varrho}_{\mathcal{S}}) - \hat{\varrho}_{\mathcal{S}}]|_{\tau=\infty} + \mathcal{O}(\tau_{int}/\tau) \tag{3.31}$$

where $(\mathcal{M}_{\tau}(\cdot) - \hat{\varrho}_{\mathcal{S}})|_{\tau=\infty} = \Delta\hat{\varrho}_{\mathcal{S}}|_{coll}$ is the change of the system given by a full collision. Exploiting Eq. (3.28) and Eq. (3.31) one may now rewrite Eq. (3.26) as follows

$$\frac{\Delta\hat{\varrho}_{\mathcal{S}}(t)}{\tau} = -\frac{i}{\hbar}\left[\hat{H}_{\mathcal{S}}\,, \hat{\varrho}_{\mathcal{S}}\right] + \frac{\Delta\hat{\varrho}_{\mathcal{S}}(t)|_{coll}}{\tau} - \frac{i}{\hbar}\left[\hat{H}_{\mathcal{S}}\,, \Delta\hat{\varrho}_{\mathcal{S}}|_{coll}\right] \tag{3.32}$$

where the first term describes the infinitesimal change of the system given by the free evolution, the second term the change of the system given by collisions and the third term the interplay between free-evolution and collisions occurring in the time interval τ.

One observes that Eq. (3.32) is well defined in the limit for $\tau \to 0$ only if $\Delta\hat{\varrho}_{\mathcal{S}}|_{coll}$ is proportional to τ^n with $n \geq 1$. Moreover $\Delta\hat{\varrho}_{\mathcal{S}}|_{coll}$ gives a finite and non negligible contribution to the coarse-grained dynamics in Eq. (3.24) only if $n = 1$. Accordingly one can conclude that in a good collisional dynamics the rate of collisions should have linear dependency on the time resolution τ, *i.e.*

$$\Delta\hat{\varrho}_{\mathcal{S}}(t)|_{coll} \propto \tau. \tag{3.33}$$

If the relation above holds true, the second term of r.h.s. in Eq. (3.32), describing the interplay between free-evolution and collisions, would be proportional to τ, and it would give negligible contribution in the limit of $\tau \to 0$. Accordingly the coarse-grained dynamics in Eq. (3.24) becomes:

$$\hat{\varrho}_{\mathcal{S}}(t) = \int_0^t \frac{\partial\hat{\varrho}_{\mathcal{S}}(s)}{\partial s} ds \tag{3.34}$$

with

$$\frac{\partial \hat{\varrho}_{\mathcal{S}}(s)}{\partial s} \equiv -\frac{i}{\hbar}\left[\hat{H}_{\mathcal{S}}\,,\hat{\varrho}_{\mathcal{S}}(s)\right] + \left.\frac{\Delta\hat{\varrho}_{\mathcal{S}}(s)}{\tau}\right|_{coll} \tag{3.35}$$

where the first term on r.h.s. of Eq. (3.35) describes the free evolution dynamics and the second term on r.h.s. the collisional contribution to the dynamics defined by

$$\Delta\hat{\varrho}_{\mathcal{S}}|_{coll} = [\mathcal{M}^I_\tau(\hat{\varrho}_{\mathcal{S}}) - \hat{\varrho}_{\mathcal{S}}]|_{\tau=\infty} = N\mathrm{Tr}_1\left(\hat{U}_I(\tau)\hat{\varrho}_{\mathcal{S}}(t)\otimes\hat{\varrho}_1\hat{U}_I(\tau) - \hat{\varrho}_{\mathcal{S}}\otimes\hat{\varrho}_1\right)\Big|_{\tau=\infty} \tag{3.36}$$

where Eq. (3.13) has been used for the last equality. One immediately sees from Eq. (3.36) that the collisional term $\Delta\hat{\varrho}_s|_{coll}$ has an uncommon expression: it is not described by the action of the scattering operator $\hat{S}$ contrary to the equations commonly present in literature [34–36, 39, 40, 55]. However, we will show that it is possible to replace the collision map in Eq. (3.36) with an equivalent map depending only on the scattering operator $\hat{S}$. The replacement will be useful not only for the comparison with the existing literature, but will be also useful to give an estimation of the collision time.

3.2.2 Collisional contribution and scattering operator

In this subsection we focus on the collisional term defined in Eq. (3.36) before taking the limit $\tau \to \infty$, *i.e.*

$$\Delta\hat{\varrho}_s|_{coll} = \mathcal{M}^I_\tau(\hat{\varrho}_s) - \hat{\varrho}_s = N\mathrm{Tr}_1\left(\hat{U}_I(\tau)\hat{\varrho}_{\mathcal{S}}(t)\otimes\hat{\varrho}_1\hat{U}_I(\tau) - \hat{\varrho}_{\mathcal{S}}\otimes\hat{\varrho}_1\right). \tag{3.37}$$

The operator $\hat{U}_I(\tau)$ defined by Eq. (3.14) has a similar structure to the scattering operator in Eq. (3.25), but it is not symmetric in time. However, exploiting the unitarity of the free evolution, $\hat{U}_0^\dagger(\tau)\hat{U}_0(\tau) = \mathbb{1}$, the operator $\hat{U}_I(\tau)$ can be rewritten as

$$\hat{U}_I(\tau) = \hat{U}_0^\dagger(\tau/2)\hat{S}_\tau\hat{U}_0(\tau/2) \tag{3.38}$$

where $\hat{S}_\tau$ is the incomplete scattering operator defined by

$$\hat{S}_\tau = \mathcal{T}\left\{e^{-\frac{i}{\hbar}\int_{-\tau/2}^{\tau/2} ds\,\hat{V}_I(s)}\right\}. \tag{3.39}$$

Exploiting Eq. (3.38), Eq. (3.10), the ciclicity of the trace and the fact that $\left[\hat{H}_1\,,\hat{\varrho}_1\right] = 0$, one may rewrite the collision term of Eq. (3.37) as follows

$$\Delta\hat{\varrho}_{\mathcal{S}}|_{coll} = \hat{U}_{\mathcal{S}}(\tau/2)N\mathrm{Tr}_1\left(\hat{S}_\tau\hat{U}^\dagger_{\mathcal{S}}(\tau/2)\hat{\varrho}_{\mathcal{S}}(t)\otimes\hat{\varrho}_1\hat{U}_{\mathcal{S}}(\tau/2)\hat{S}^\dagger_\tau - \hat{U}^\dagger_{\mathcal{S}}(\tau/2)\hat{\varrho}_s(t)\otimes\hat{\varrho}_1\hat{U}_{\mathcal{S}}(\tau/2)\right)\hat{U}^\dagger_{\mathcal{S}}(\tau/2). \tag{3.40}$$

Similarly one can rewrite the map $\mathcal{M}^{\mathrm{I}}_{\tau}(\hat{\varrho}_{\mathcal{S}})$ as

$$\mathcal{M}^{\mathrm{I}}_{\tau}(\hat{\varrho}_{\mathcal{S}}) - \hat{\varrho}_{\mathcal{S}} = \mathcal{U}^{\mathcal{S}}_{-\tau/2} \circ (\mathcal{C}_{\tau} - \mathbb{1}) \circ \mathcal{U}^{\mathcal{S}}_{\tau/2}(\hat{\varrho}_{\mathcal{S}}) \tag{3.41}$$

where

$$\mathcal{C}_{\tau}(\hat{\varrho}_{\mathcal{S}}) = N\mathrm{Tr}_1\left(\hat{S}_{\tau}\hat{\varrho}_{\mathcal{S}} \otimes \hat{\varrho}_1\hat{S}^{\dagger}_{\tau} - \hat{\varrho}_{\mathcal{S}} \otimes \hat{\varrho}_1\right) + \hat{\varrho}_{\mathcal{S}}, \tag{3.42}$$

that has a structure similar to the collision term heuristically derived in [34–36, 39, 40, 55], exploiting scattering theory. Inverting Eq. (3.41) one obtains

$$C_{\tau}(\hat{\varrho}_{\mathcal{S}}) - \hat{\varrho}_{\mathcal{S}} = \mathcal{U}^{\mathcal{S}}_{\tau/2} \circ (\mathcal{M}^{\mathrm{I}}_{\tau} - 1) \circ \mathcal{U}^{\mathcal{S}}_{-\tau/2}(\hat{\varrho}_{\mathcal{S}}). \tag{3.43}$$

From Eq. (3.28) one can deduce that

$$\mathcal{U}^{\mathcal{S}}_{-\tau}(\hat{\varrho}_{\mathcal{S}}) = \hat{\varrho}_{\mathcal{S}} + \mathcal{O}(\tau), \tag{3.44}$$

and from previous considerations (see Eq. (3.33) and Eq. (3.31)) find that

$$(\mathcal{M}^{I}_{\tau} - \mathbb{1})(\hat{\varrho}_{s}) \propto \tau. \tag{3.45}$$

Exploiting Eq. (3.43) and Eq. (3.45) one eventually ends up with

$$\mathcal{M}^{\mathrm{I}}_{\tau}(\hat{\varrho}_{\mathcal{S}}) = \mathcal{C}_{\tau}(\hat{\varrho}_{\mathcal{S}}) + \mathcal{O}(\tau^3). \tag{3.46}$$

The above equation allows to replace $\mathcal{M}^{I}_{\tau}(\hat{\varrho}_{\mathcal{S}})$ with $\mathcal{C}_{\tau}(\hat{\varrho}_{\mathcal{S}})$ in the coarse-grained dynamics described by Eq. (3.35), to obtain

$$\begin{aligned}\frac{\partial \hat{\varrho}_{\mathcal{S}}(t)}{\partial t} &= -\frac{i}{\hbar}\mathcal{H}_{\mathcal{S}}(\hat{\varrho}_{s}(t)) + \left.\frac{\mathcal{C}_{\tau}(\hat{\varrho}_{s}(t)) - \hat{\varrho}_{s}(t)}{\tau}\right|_{\tau=\infty} \\ &= -\frac{i}{\hbar}\left[\hat{H}_{\mathcal{S}}\,, \hat{\varrho}_{s}(t)\right] + \frac{N}{\tau}\mathrm{Tr}_1\left.\left(\hat{S}_{\tau}\hat{\varrho}_{\mathcal{S}}(t) \otimes \hat{\varrho}_1\hat{S}^{\dagger}_{\tau} - \hat{\varrho}_{\mathcal{S}}(t) \otimes \hat{\varrho}_1\right)\right|_{\tau=\infty}.\end{aligned} \tag{3.47}$$

This equation describes the collisional dynamics of a test particle interacting with a rarefied particles thermal bath. As expected Eq. (3.47) confirms the possibility to describe collisions through the action of the scattering operator $\hat{S}$, under the assumptions in (3.20) and the further assumption

$$(\mathcal{C}_{\tau}(\hat{\varrho}_{\mathcal{S}}(\tau)) - \hat{\varrho}_{\mathcal{S}}) \propto \tau. \tag{3.48}$$

In order to make a comparison with previous literature, we now introduce the incomplete transition operator $\hat{T}_\tau$, by $\hat{S}_\tau = \mathbb{1} + i\hat{T}_\tau$. Exploiting the unitarity of $\hat{S}_\tau$ one obtains $\hat{T}_\tau^\dagger \hat{T}_\tau = i(\hat{T}_\tau - \hat{T}_\tau^\dagger)$. Then, Eq. (3.47) can be rewritten in the more familiar form

$$\left.\frac{\partial \hat{\varrho}_S(t)}{\partial t}\right|_{coll} = \frac{N}{\tau}\mathrm{Tr}_1 \left.\left(\frac{i}{2}[\hat{T}_\tau - \hat{T}_\tau^\dagger, \hat{\varrho}_S(t)\otimes\hat{\varrho}_1] - \frac{1}{2}\{\hat{T}_\tau^\dagger \hat{T}_\tau, \hat{\varrho}_S(t)\otimes\hat{\varrho}_1\} + \hat{T}_\tau(\hat{\varrho}_S(t)\otimes\hat{\varrho}_1)\hat{T}_\tau^\dagger \right)\right|_{\tau=\infty} \tag{3.49}$$

from which one may recognize a Lindblad type structure. The assumption (3.48) can be rewritten as

$$\mathrm{Tr}_1\left([\hat{T}_\tau - \hat{T}_\tau^\dagger, \hat{\varrho}_S(t)\otimes\hat{\varrho}_1]\right) \propto \tau, \qquad \mathrm{Tr}_1\left(\{\hat{T}_\tau^\dagger\hat{T}_\tau, \hat{\varrho}_S(t)\otimes\hat{\varrho}_1\}\right) \propto \tau,$$
$$\mathrm{Tr}_1\left(\hat{T}_\tau(\hat{\varrho}_S(t)\otimes\hat{\varrho}_1)\hat{T}_\tau^\dagger\right) \propto \tau. \tag{3.50}$$

In order to evaluate the action of the incomplete transition operator in Eq. (3.49) and to verify the assumption above, we now focus on the behaviour of the incomplete scattering operator $\hat{S}_\tau$ in the large τ limit.

3.2.3 Incomplete Scattering operator in the large τ limit

According to the definition in Eq. (3.39) the incomplete scattering operator is defined as

$$\hat{S}_\tau |\varphi\rangle \equiv \mathcal{T}\left\{ e^{-\frac{i}{\hbar}\int_{-\tau/2}^{\tau/2} d\tau \hat{V}_I(\tau)} \right\} |\varphi\rangle\,. \tag{3.51}$$

For our purpose it is convenient to use the following equality:

$$\int d\tau \hat{V}_I(\tau) = \int d\tau \lim_{\varepsilon\to 0} e^{\varepsilon\tau}\hat{V}_I(\tau) \tag{3.52}$$

and the Vitali theorem to rewrite Eq. (3.51) as follows

$$\hat{S}_\tau |\varphi\rangle = \lim_{\varepsilon\to 0}\mathcal{T}\left\{ e^{-\frac{i}{\hbar}\int_{-\tau/2}^{\tau/2} d\tau\, e^{\varepsilon\tau}\hat{V}_I(\tau)} \right\} \tag{3.53}$$

This regularized expression for the incomplete scattering operator allow us expand $\hat{S}_\tau$ in the energy eigenbasis avoiding divergence problems that can arise from this expansion, as it will be clear later. Expanding the exponential and resolving the time ordering $\mathcal{T}\{\dots\}$ one obtains the following expression:

$$\hat{S}_\tau = \lim_{\varepsilon\to 0}\sum_{n=0}\frac{(-i)^n}{\hbar^n}\int_{-\tau/2}^{\tau/2} d\tau_1\cdots\int_{-\tau/2}^{\tau_{n-1}} d\tau_n\, e^{\varepsilon\tau_i}\,\hat{V}_I(\tau_1)\dots e^{\varepsilon\tau_n}\,\hat{V}_I(\tau_n). \tag{3.54}$$

Denoting with $|\lambda\rangle$ the basis of eigenstates of the free Hamiltonian, *i.e.* $\hat{H}_0 = \hat{H}_\mathcal{S} + \hat{H}_1$, $\hat{H}_0\,|\lambda\rangle = E_\lambda\,|\lambda\rangle$, and exploiting the definition of $\hat{V}_I(t)$ given in Eq. (3.12) , we rewrite Eq. (3.54) as follows:

$$\hat{S}_\tau = \lim_{\varepsilon\to 0}\sum_{n=0}\frac{(-i)^n}{\hbar^n}\int_{-\tau/2}^{\tau/2} d\tau_1\cdots\int_{-\tau/2}^{\tau_{n-1}} d\tau_n\prod_{i=0}^{n}\left(\int d\lambda_i\right)|\lambda_0\rangle \\ \prod_{i=1}^{n} e^{-i\hbar(E_{\lambda_{i-1}}-E_{\lambda_i}-i\varepsilon)\tau_i}\,\langle\lambda_{i-1}|\,\hat{V}\,|\lambda_i\rangle\,\langle\lambda_n| \tag{3.55}$$

We now focus on the first term of this series, *i.e.*

$$\begin{aligned}\hat{T}_1 &= -\frac{i}{\hbar}\lim_{\varepsilon\to 0}\int d\lambda_0\, d\lambda_1\int_{-\tau/2}^{\tau/2} d\tau\, e^{-\frac{i}{\hbar}(E_{\lambda_1}-E_{\lambda_0}-i\varepsilon\hbar)\tau_1}\,|\lambda_0\rangle\langle\lambda_0|\,\hat{V}\,|\lambda_1\rangle\langle\lambda_1| \\ &= \int d\lambda_0 d\lambda_1 \delta_\tau(E_{\lambda_0}-E_{\lambda_1}) f_1(\lambda_0,\lambda_1)\,|\lambda_0\rangle\langle\lambda_1|\,.\end{aligned} \tag{3.56}$$

with $f_1(\lambda_0,\lambda_1) = -i2\pi\,\langle\lambda_0|\,\hat{V}\,|\lambda_1\rangle$ and

$$\delta_\tau(x) = \frac{1}{2\pi\hbar}\int_{-\tau/2}^{\tau/2} d\tau\, e^{-\frac{i}{\hbar}x\tau} = \frac{\sin(x\tau/2\hbar)}{2\pi x}, \qquad \lim_{\tau\to\infty}\delta_\tau(x) = \delta(x). \tag{3.57}$$

As one may notice the $\delta_\tau(x)$ defined above is exactly the "smoothened" delta function (see (1.48)) used by Diósi to derive Eq. (1.51), describing a collisional dynamics with finite collision time.
The second term of the series in Eq. (3.55), reads

$$\begin{aligned}\hat{T}_2\,|\varphi\rangle = &-\frac{1}{\hbar^2}\lim_{\varepsilon\to 0}\int d\lambda_0\, d\lambda_1\, d\lambda_2\int_{-\tau/2}^{\tau/2} d\tau_1\, e^{-\frac{i}{\hbar}(E_{\lambda_1}-E_{\lambda_0}-i\varepsilon\hbar)\tau_1} \\ &\int_{-\tau/2}^{\tau_1} d\tau_2\, e^{-\frac{i}{\hbar}(E_{\lambda_2}-E_{\lambda_1}-i\varepsilon\hbar)\tau_2}\,|\lambda_0\rangle\langle\lambda_0|\,\hat{V}\,|\lambda_1\rangle\langle\lambda_1|\,\hat{V}\,|\lambda_2\rangle\langle\lambda_2|\varphi\rangle \\ = &-2\pi\lim_{\varepsilon\to 0}\int d\lambda_0\, d\lambda_1\, d\lambda_2\left[\frac{\delta_\tau(E_{\lambda_0}-E_{\lambda_2}-i\hbar\varepsilon)}{(E_{\lambda_1}-E_{\lambda_2}+i\hbar\varepsilon)}\right. \\ &\left.-\frac{\delta_\tau(E_{\lambda_0}-E_{\lambda_1}-i\hbar\varepsilon)e^{-\frac{i}{2\hbar}(E_{\lambda_1}-E_{\lambda_2}-i\varepsilon\hbar)\tau}}{(E_{\lambda_1}-E_{\lambda_2}+i\hbar\varepsilon)}\right]|\lambda_0\rangle\langle\lambda_0|\,\hat{V}\,|\lambda_1\rangle\langle\lambda_1|\,\hat{V}\,|\lambda_2\rangle\langle\lambda_2|\varphi\rangle\,.\end{aligned} \tag{3.58}$$

One observes that the first term in the square brackets in Eq. (3.58) has the same behaviour as $\hat{T}_1$. The second term instead displays an oscillating term and it is consequently suppressed in the limit of large τ. Accordingly, in the limit of $\tau \to \infty$, Eq. (3.58) can be approximated by

$$\hat{T}_2 \simeq \int d\lambda_0 \, d\lambda_2 \, \delta_\tau(E_{\lambda_0} - E_{\lambda_2}) f_2(\lambda_0, \lambda_2) \, |\lambda_0\rangle\langle\lambda_2| \tag{3.59}$$

with:

$$f_2(\lambda_0, \lambda_2) = \lim_{\varepsilon \to 0} 2\pi \int d\lambda_1 \frac{\langle\lambda_0| \, \hat{V} \, |\lambda_1\rangle\langle\lambda_1| \, \hat{V} \, |\lambda_2\rangle}{(E_{\lambda_1} - E_{\lambda_1} + i\hbar\varepsilon)} \tag{3.60}$$

Analyzing the other terms of the expansion in Eq. (3.55) one finds more involved contributions, containing a relevant term proportional to $\delta_\tau(E_{\lambda_f} - E_{\lambda_i})$ and oscillatory terms (that are negligible in the large τ limit). In this regime one is then allowed to write the n-th term of the series as

$$\hat{T}_n = \int d\lambda_f d\lambda_i \delta_\tau(E_{\lambda_f} - E_{\lambda_i}) f(\lambda_f, \lambda_i) \, |\lambda_f\rangle\langle\lambda_i| \tag{3.61}$$

where $f_i(\lambda_f, \lambda_i)$ is the n-th order contribution of the scattering amplitude and contains all the dependence on the interaction potential. Summing up all the terms of the series in Eq. (3.54) we obtain the scattering operator

$$\hat{S}_\tau = \mathbb{1} + i\hat{T}_\tau \tag{3.62}$$

where the incomplete transition operator $\hat{T}_\tau$ is defined by

$$\hat{T}_\tau = \int d\lambda_f \, d\lambda_i \, \delta_\tau(E_{\lambda_f} - E_{\lambda_i}) f(\lambda_f, \lambda_i) \, |\lambda_f\rangle\langle\lambda_i| \tag{3.63}$$

where $f(\lambda_f, \lambda_i) = \sum_{n=1}^{\infty} f_n(\lambda_f, \lambda_i)$ is the scattering amplitude and contains all the dependence on the interaction potential of the scattering process. Associating now the eigenvector $|\lambda\rangle$ with the tensor product of the test and gas particle momentum eigenstates, *i.e* $|\lambda\rangle \equiv |\mathbf{P}, \mathbf{k}\rangle$ and recalling that $\hat{V}$ is invariant under global translationsone obtains the textbook expression [51] of the transition operator, where the energy preserving Dirac delta function has been replaced with the "smoothened" delta function in (3.57), *i.e.*

$$
\begin{aligned}
&\langle \mathbf{P}, \mathbf{k}|\hat{T}_\tau|\mathbf{P}', \mathbf{k}'\rangle = \\
&= \frac{1}{2\pi\hbar m^*}\delta^3\left(\mathbf{P}+\mathbf{k}-\mathbf{P}'-\mathbf{k}'\right)\delta_\tau\left(\frac{\mathbf{P}^2-\mathbf{P}'^2}{2M}+\frac{\mathbf{k}^2-\mathbf{k}'^2}{2m}\right) f\left(\mathrm{rel}(\mathbf{k},\mathbf{P}),\mathrm{rel}(\mathbf{k}',\mathbf{P}')\right) \\
&= \frac{1}{2\pi\hbar m^*}\delta^3\left(\mathbf{P}+\mathbf{k}-\mathbf{P}'-\mathbf{k}'\right)\delta_\tau\left(\frac{\mathrm{rel}(\mathbf{k},\mathbf{P})^2}{2m^*}-\frac{\mathrm{rel}(\mathbf{k}',\mathbf{P}')^2}{2m^*}\right) f\left(\mathrm{rel}(\mathbf{k},\mathbf{P}),\mathrm{rel}(\mathbf{k}',\mathbf{P}')\right)
\end{aligned}
\tag{3.64}
$$

where

$$
\mathrm{rel}(\mathbf{k},\mathbf{P}) = \frac{m^*}{m}\mathbf{k} - \frac{m^*}{M}\mathbf{P} \tag{3.65}
$$

and $m^* = mM/(m+M)$ is the reduced mass.

3.2.4 Evaluation of the Collision term

Next, we evaluate the collision contribution of Eq. (3.49) exploiting the result of Eq. (3.64). The term

$$
\hat{\varrho}'_{\mathcal{S}} = \mathrm{Tr}_1\left(\hat{T}_\tau\hat{\varrho}_{\mathcal{S}}\otimes\hat{\varrho}_1\hat{T}_\tau\right), \tag{3.66}
$$

is equivalent to

$$
\langle \mathbf{P}|\hat{\varrho}'_{\mathcal{S}}|\mathbf{P}'\rangle = \int d\mathbf{P}''d\mathbf{P}'''d\mathbf{k}d\mathbf{k}'d\mathbf{k}''\varrho_{\mathcal{S}}(\mathbf{P}'',\mathbf{P}''')\varrho_1(\mathbf{k}',\mathbf{k}'')\langle \mathbf{P},\mathbf{k}|\hat{T}|\mathbf{P}'',\mathbf{k}'\rangle\langle \mathbf{P}''',\mathbf{k}''|\hat{T}|\mathbf{P}',\mathbf{k}\rangle, \tag{3.67}
$$

where

$$
\begin{aligned}
\varrho_{\mathcal{S}}(\mathbf{P}'',\mathbf{P}''') &\equiv \langle \mathbf{P}''|\hat{\varrho}_{\mathcal{S}}|\mathbf{P}'''\rangle \\
\varrho_1(\mathbf{k}',\mathbf{k}'') &\equiv \langle \mathbf{k}'|\hat{\varrho}_1|\mathbf{k}''\rangle.
\end{aligned}
\tag{3.68}
$$

If we introduce the new variable $\mathbf{Q} = \mathbf{P} - \mathbf{P}''$, and replace Eqs. (3.19) and (3.64) in Eq. (3.67), the two δ^3-functions due to momentum conservation imply $\mathbf{k} = \mathbf{k}' - \mathbf{Q}$ and $\mathbf{P}''' = \mathbf{P}' - \mathbf{Q}$. Thus, we end up with

$$
\begin{aligned}
&\langle \mathbf{P}|\hat{\varrho}'_{\mathcal{S}}|\mathbf{P}'\rangle \\
&= \frac{2\pi\hbar}{m^{*2}\Omega}\int d\mathbf{Q}d\mathbf{k}\rho(\mathbf{P}-\mathbf{Q},\mathbf{P}'-\mathbf{Q})\mu(\mathbf{k})\delta_\tau\left(E_f-E_i\right)\delta_\tau\left(E'_f-E'_i\right) f\left(\mathbf{P}_f,\mathbf{P}_i\right) f^*\left(\mathbf{P}'_f,\mathbf{P}'_i\right),
\end{aligned}
\tag{3.69}
$$

where

$$\begin{aligned}\mathbf{P}_i &= \text{rel}\,(\mathbf{k}, \mathbf{P}-\mathbf{Q}) \\ \mathbf{P}_f &= \text{rel}\,(\mathbf{k}-\mathbf{Q}, \mathbf{P}) \\ \mathbf{P'}_i &= \text{rel}\,\big(\mathbf{k}, \mathbf{P'}-\mathbf{Q}\big) \\ \mathbf{P'}_f &= \text{rel}\,\big(\mathbf{k}-\mathbf{Q}, \mathbf{P'}\big)\,, \end{aligned} \tag{3.70}$$

and $E_{i,f} = P_{i,f}^2/(2m^*), E'_{i,f} = P'^2_{i,f}/(2m^*)$ are the corresponding energies; $\mathbf{P}_{i,f}, \mathbf{P'}_{i,f}$ have to be understood as functions of the momenta $\mathbf{k}, \mathbf{Q}, \mathbf{P}$ and $\mathbf{P'}$. From a physical point of view, the interpretation of Eq. (3.69) is straightforward: it displays the product of the two center-of-mass probability amplitudes, as well as a "smothened" δ-functions for the partial energy conservation associated with the incomplete collisions

$$\begin{aligned}\mathbf{P}-\mathbf{Q} &\rightarrow \mathbf{P} \\ \mathbf{k} &\rightarrow \mathbf{k}-\mathbf{Q}\end{aligned} \tag{3.71}$$

and

$$\begin{aligned}\mathbf{P'}-\mathbf{Q} &\rightarrow \mathbf{P'} \\ \mathbf{k} &\rightarrow \mathbf{k}-\mathbf{Q}.\end{aligned} \tag{3.72}$$

Equation (3.69) can be then put in an operatorial form:

$$\hat{\varrho}'_S = \frac{2\pi\hbar}{m^{*2}\,\Omega}\int d\mathbf{Q}d\mathbf{k}\,\mu(\mathbf{k})e^{\frac{i}{\hbar}\mathbf{Q}\cdot\hat{x}}\hat{L}_{\tau,\mathbf{Q},\mathbf{k}}\,\hat{\varrho}_S\,\hat{L}^\dagger_{\tau,\mathbf{Q},\mathbf{k}}e^{-\frac{i}{\hbar}\mathbf{Q}\cdot\hat{x}} \tag{3.73}$$

where:

$$\hat{L}_{\tau,\mathbf{Q},\mathbf{k}}(\hat{\mathbf{P}}) = f(\hat{\mathcal{P}}_f, \hat{\mathcal{P}}_i)\delta_\tau(\hat{\mathcal{E}}_f - \hat{\mathcal{E}}_i), \tag{3.74}$$

with $f(\hat{\mathcal{P}}_f, \hat{\mathcal{P}}_i)$ the scattering amplitude defined in Eq. (3.64), promoted to operator function and

$$\begin{aligned}\hat{\mathcal{P}}_i &= \text{rel}\left(\mathbf{k}, \hat{\mathbf{P}}\right) \\ \hat{\mathcal{P}}_f &= \text{rel}\left(\mathbf{k}-\mathbf{Q}, \hat{\mathbf{P}}+\mathbf{Q}\right) = \hat{\mathcal{P}}_i - \mathbf{Q}, \\ \hat{\mathcal{E}}_{i,f} &= \frac{\hat{\mathcal{P}}^2_{i,f}}{2m^*}.\end{aligned} \tag{3.75}$$

With a straightforward calculation one can rewrite the other terms of Eq. (3.49) in terms of $\hat{L}_{\tau,\mathbf{Q},\mathbf{k}}(\hat{\mathbf{P}})$ as

$$\begin{aligned}\mathrm{Tr}_1\left([\hat{T}_\tau - \hat{T}_\tau^\dagger, \hat{\varrho}_S \otimes \hat{\varrho}_1]\right) &= -\frac{i\,(\pi\hbar)^2}{m^*\Omega}\int d\mathbf{k}\,\mu(\mathbf{k})\left[(\hat{L}_{\tau,0,\mathbf{k}} + \hat{L}^\dagger_{\tau,0,\mathbf{k}})\,,\hat{\varrho}_S(t)\right]\\ \mathrm{Tr}_1\left(\{\hat{T}_\tau^\dagger\hat{T}_\tau, \hat{\varrho}_S \otimes \hat{\varrho}_1\}\right) &= -\frac{(2\pi\hbar)}{m^{*2}\Omega}\int d\mathbf{Q}d\mathbf{k}\,\mu(\mathbf{k})\left\{L^\dagger_{\tau,\mathbf{Q},\mathbf{k}}L_{\tau,\mathbf{Q},\mathbf{k}}\,,\hat{\varrho}_S(t)\right\}.\end{aligned} \tag{3.76}$$

Replacing now Eq. (3.73) and Eq. (3.76) in Eq. (3.49) one obtains

$$\begin{aligned}\left.\frac{\partial\hat{\varrho}_S(t)}{\partial t}\right|_{coll} &= -\frac{i\,n(2\pi\hbar)^2}{2m^*\tau}\int d\mathbf{k}\,\mu(\mathbf{k})\left[(\hat{L}_{\tau,0,\mathbf{k}} + \hat{L}^\dagger_{\tau,0,\mathbf{k}})\,,\hat{\varrho}_S(t)\right]\\ &-\frac{n(2\pi\hbar)}{m^{*2}\tau}\int d\mathbf{Q}d\mathbf{k}\,\mu(\mathbf{k})\left(\frac{1}{2}\left\{L^\dagger_{\tau,\mathbf{Q},\mathbf{k}}L_{\tau,\mathbf{Q},\mathbf{k}}\,,\hat{\varrho}_S(t)\right\} + e^{\frac{i}{\hbar}\mathbf{Q}\cdot\hat{x}}\hat{L}_{\tau,\mathbf{Q},\mathbf{k}}\hat{\varrho}_S(t)\hat{L}^\dagger_{\tau,\mathbf{Q},\mathbf{k}}e^{-\frac{i}{\hbar}\mathbf{Q}\cdot\hat{x}}\right)\Bigg|_{\tau=\infty}\end{aligned} \tag{3.77}$$

where $n = N/\Omega$ is the density of the gas. One observes that the second line of the equation above exactly recovers Diósi master equation (1.51) if the evaluation at $\tau = \infty$ is replaced by Eq. (1.50). The term in the first line instead is a shift of system's energy due to the background gas, which Diósi sets to zero. Recalling now Eq. (3.57) one notices that

$$\begin{aligned}\delta_\tau(0) &= \frac{1}{2\pi\hbar}\int_{-\tau/2}^{\tau/2} = \frac{\tau}{2\pi\hbar},\\ \delta^2_\tau(E) &= \frac{1}{(2\pi\hbar)^2}\int_{-\tau/2}^{\tau/2}ds_1\int_{-\tau/2}^{\tau/2}ds_2 e^{-\frac{i}{\hbar}E(s_1+s_2)} = \frac{\tau}{2\pi\hbar}\delta_\tau(E).\end{aligned} \tag{3.78}$$

Exploiting the above equations and Eq. (3.74) one obtains

$$\begin{aligned}\hat{L}_{\tau,0,\mathbf{k}} &= \frac{\tau}{2\pi\hbar}f(\hat{\mathcal{P}}_i,\hat{\mathcal{P}}_i),\\ \hat{L}^\dagger_{\tau,\mathbf{Q},\mathbf{k}}(\hat{\mathbf{P}})\hat{L}_{\tau,\mathbf{Q},\mathbf{k}}(\hat{\mathbf{P}}) &= \frac{\tau}{2\pi\hbar}\left|f(\hat{\mathcal{P}}_f,\hat{\mathcal{P}}_i)\right|^2\delta_\tau(\hat{\mathcal{E}}_f - \hat{\mathcal{E}}_i).\end{aligned} \tag{3.79}$$

Which can be exploited together with Eq. (3.74) to rewrite Eq. (3.77) in the more explicit form

$$\begin{aligned}\left.\frac{\partial\hat{\varrho}_S(t)}{\partial t}\right|_{coll} &= -\frac{i2\pi\hbar\,n}{m^*}\int d\mathbf{k}\,\mu(\mathbf{k})\left[\mathbf{Re}(f(\hat{\mathcal{P}}_i,\hat{\mathcal{P}}_i)\,,\hat{\varrho}_S(t)\right]\\ &-\frac{n}{m^{*2}}\int d\mathbf{Q}d\mathbf{k}\,\mu(\mathbf{k})\frac{1}{2}\left\{\left|f(\hat{\mathcal{P}}_f,\hat{\mathcal{P}}_i)\right|^2\delta_\tau(\hat{\mathcal{E}}_f - \hat{\mathcal{E}}_i)\,,\hat{\varrho}_S(t)\right\}\\ &+\frac{n(2\pi\hbar)}{\tau m^{*2}}\int d\mathbf{Q}d\mathbf{k}\mu(\mathbf{k})e^{\frac{i}{\hbar}\mathbf{Q}\cdot\hat{x}}f(\hat{\mathcal{P}}_f,\hat{\mathcal{P}}_i)\delta_\tau(\hat{\mathcal{E}}_f - \hat{\mathcal{E}}_i)\hat{\varrho}_S(t)\delta_\tau(\hat{\mathcal{E}}_f - \hat{\mathcal{E}}_i)f^*(\hat{\mathcal{P}}_f,\hat{\mathcal{P}}_i)e^{-\frac{i}{\hbar}\mathbf{Q}\cdot\hat{x}}\Bigg|_{\tau=\infty}.\end{aligned} \tag{3.80}$$

The last term of this equation depends on τ^{-1}, meaning that the condition (3.50) is in general not verified. However, the fact that the dependence on τ is contained also and only in the two energy Dirac delta function indicates that condition (3.50) can be satisfied only in the case where:

$$\delta_\tau(\hat{\mathcal{E}}_f - \hat{\mathcal{E}}_i)\hat{\varrho}_S(t)\delta_\tau(\hat{\mathcal{E}}_f - \hat{\mathcal{E}}_i) \propto \tau \tag{3.81}$$

under the integral $\int d\mathbf{q}d\mathbf{k}$. Equation (3.78) suggests that condition above can be verified in the case where the energy Dirac delta function commutes with the statistical operator $\hat{\varrho}_S(t)$, *i.e.*

$$\left[(\hat{\mathcal{E}}_i - \hat{\mathcal{E}}_f)\,,\hat{\varrho}_s(t)\right] = 0 \tag{3.82}$$

under the integrals $\int d\mathbf{Q}d\mathbf{k}$. Indeed under this assumption, and exploiting Eq. (3.78) it is easy to verify the following

$$\delta_\tau(\hat{\mathcal{E}}_f - \hat{\mathcal{E}}_i)\hat{\varrho}_S(t)\delta_\tau(\hat{\mathcal{E}}_f - \hat{\mathcal{E}}_i) = \frac{\tau}{2\pi\hbar}\delta_\tau(\hat{\mathcal{E}}_f - \hat{\mathcal{E}}_i)\hat{\varrho}_S(t). \tag{3.83}$$

It is now interesting to notice that, exploiting Eq. (3.75), assumption (3.82) can be equivalently rewritten as $\left[\hat{\mathcal{P}}_i \cdot \mathbf{Q}\,,\hat{\varrho}_S(t)\right] = 0$, that can be further reduced to

$$\left[\frac{m}{m+M}\hat{\mathbf{P}}\,,\hat{\varrho}_S(t)\right] = 0 \tag{3.84}$$

exploiting Eq. (3.75), Eq. (3.65) and the arbitrariness of $\mathbf{Q}$. Equation (3.84) shows that assuming (3.82) ensure not only the commutativity of the Energy Dirac delta function with the statistical operator $\hat{\varrho}_S(t)$, but also commutativity of the scattering amplitude $f(\hat{\mathcal{P}}_i, \hat{\mathcal{P}}_f)$ with $\hat{\varrho}_S(t)$ and furthermore constraints the state of the system $\hat{\varrho}_S(t)$ to be diagonal in momentum eigenbasis. Substituting now Eq. (3.83) exploiting the commutativity between $\hat{\varrho}_S(t)$ and $f(\hat{\mathcal{P}}_i, \hat{\mathcal{P}}_f)$ and taking the limit $\tau \to \infty$, one eventually obtains a well defined collisional term:

$$\begin{aligned}\left.\frac{\partial\hat{\varrho}_S(t)}{\partial t}\right|_{coll} &= -\frac{i2\pi\hbar\, n}{m^*}\int d\mathbf{k}\,\mu(\mathbf{k})\left[\mathbf{Re}(f(\hat{\mathcal{P}}_i,\hat{\mathcal{P}}_i))\,,\hat{\varrho}_S(t)\right] \\ &- \frac{n}{2m^{*2}}\int d\mathbf{Q}d\mathbf{k}\,\mu(\mathbf{k})\left\{\left|f(\hat{\mathcal{P}}_f,\hat{\mathcal{P}}_i)\right|^2\delta(\hat{\mathcal{E}}_f - \hat{\mathcal{E}}_i)\,,\hat{\varrho}_S(t)\right\} \\ &+ \frac{n}{m^{*2}}\int d\mathbf{Q}d\mathbf{k}\mu(\mathbf{k})e^{\frac{i}{\hbar}\mathbf{Q}\cdot\hat{x}}\left|f(\hat{\mathcal{P}}_f,\hat{\mathcal{P}}_i)\right|^2\delta(\hat{\mathcal{E}}_f - \hat{\mathcal{E}}_i)\hat{\varrho}_S(t)e^{-\frac{i}{\hbar}\mathbf{Q}\cdot\hat{x}},\end{aligned} \tag{3.85}$$

which displays no explicit dependence on τ, confirming that condition (3.50) is satisfied under assumption (3.82). Notice that even if Eq. (3.85) it is not written in Lindblad form, it is still correct on the subspace of the states that satisfies condition (3.84). Indeed Eq. (3.85) does preserves the diagonal form of $\hat{\varrho}_S(t)$.

Before going further it is convenient to summarize what has been done to obtain Eq. (3.85). We started by deriving the dynamics governing the short time scale evolution of a test particle in a rarefied thermal bath. Exploiting this result, we build a piece-wise model describing not only the short time behavior but also the long time behavior of the test particle, that showed to be valid only under assumption (3.20). This model provided a natural scheme to obtain a coarse-grained theory where (instantaneous) collisions appear, described by Eq. (3.26). From Eq. (3.26) we were able to identify the collisional contribution to the dynamics as in Eq. (3.31). Once identified the collision term we learned the necessity of the condition (3.33) in order to derive a well defined collisional dynamics. We then showed that, under the assumption (3.33), the collisional term in Eq. (3.26) can be equivalently described by Eq. (3.42) where the collisions are described by the action the standard scattering operator $\hat{S}$. We then analyzed the collision term, finding that condition (3.33) is verified under assumption (3.84) and under this assumption we eventually derived Eq. (3.85). Going further one may now notice that the classical regime, where the system's state is described by an ensemble of momentum eigenstates, *i.e.* $\hat{\varrho}_s = \hat{\varrho}_S(\hat{\mathbf{P}})$, and the diffusive regime, where $m/M \to 0$, are probably the only two cases satisfying Eq. (3.84). It is also interesting to notice that the first is the regime in which the classical Linear Boltzmann equation was derived, and the second one is the regime in which Joos-Zeh and Gallis-Flemming models were derived.

Next we explicitly compute the collisional term in Eq. (3.85) for these two particular cases.

Classical case

Under the assumption that the state of the system is described by an ensemble of momentum eigenstates, *i.e.* $\hat{\varrho}_S = \varrho_S(\hat{\mathbf{P}})$, Eq. (3.85) can be rewritten as

$$\left.\frac{\partial \varrho_S(\hat{\mathbf{P}},t)}{\partial t}\right|_{coll} = -\frac{i2\pi\hbar\, n}{m^*}\int d\mathbf{k}\,\mu(\mathbf{k})\left[\mathbf{Re}(f(\hat{\mathcal{P}}_i,\hat{\mathcal{P}}_i)\,,\varrho_S(\hat{\mathbf{P}},t)\right]$$
$$-\frac{n}{m^{*2}}\int d\mathbf{Q}d\mathbf{k}\,\mu(\mathbf{k})\left|f(\hat{\mathcal{P}}_f,\hat{\mathcal{P}}_i)\right|^2\delta(\hat{\mathcal{E}}_f-\hat{\mathcal{E}}_i)\varrho_S(\hat{\mathbf{P}},t)$$
$$+\frac{n}{m^{*2}}\int d\mathbf{Q}d\mathbf{k}\,\mu(\mathbf{k})e^{+\frac{i}{\hbar}\mathbf{Q}\cdot\hat{x}}\left|f(\hat{\mathcal{P}}_f,\hat{\mathcal{P}}_i)\right|^2\delta(\hat{\mathcal{E}}_f-\hat{\mathcal{E}}_i)e^{-\frac{i}{\hbar}\mathbf{Q}\cdot\hat{x}}\varrho_S(\hat{\mathbf{P}}-\mathbf{Q},t) \quad (3.86)$$

Commuting now the first exponential operator, $e^{\frac{i}{\hbar}\mathbf{Q}\cdot\hat{x}}$ in the last line with $\left|f(\hat{\mathcal{P}}_f,\hat{\mathcal{P}}_i)\right|^2\delta_\tau(\hat{\mathcal{E}}_f-\hat{\mathcal{E}}_i)$, performing the change of variable $\mathbf{k}\to\mathbf{k}+\mathbf{Q}$ and then $\mathbf{Q}\to-\mathbf{Q}$, one ends up with

$$\left.\frac{\partial \hat{\varrho}_S(\hat{\mathbf{P}},t)}{\partial t}\right|_{coll}$$
$$= -\frac{n}{m^{*2}}\int d\mathbf{Q}d\mathbf{k}\,\left|f(\hat{\mathcal{P}}_i,\hat{\mathcal{P}}_f)\right|^2\delta(\hat{\mathcal{E}}_f-\hat{\mathcal{E}}_i)\left(\mu(\mathbf{k})\hat{\varrho}_S(\hat{\mathbf{P}},t)-\mu(\mathbf{k}-\mathbf{Q})\hat{\varrho}_S(\hat{\mathbf{P}}+\mathbf{Q},t)\right). \quad (3.87)$$

Since the integrated function is diagonal in the momentum eigenbasis, we are now allowed to perform the following change of variables $\mathbf{Q}\to\mathbf{Q}+\hat{\mathcal{P}}_i$, rewrite $d\mathbf{Q}$ in polar coordinates, and integrating over the modulus of the vector $\mathbf{Q}$ one eventually obtains

$$\left.\frac{\partial \hat{\varrho}_S(t)}{\partial t}\right|_{coll} = -n\int d\mathbf{k}d\mathbf{n}\,\frac{|\hat{\mathcal{P}}_i|}{m^*}\left|f(\hat{\mathcal{P}}_i+\hat{\mathcal{Q}},\hat{\mathcal{P}}_i)\right|^2\left(\mu(\mathbf{k})\varrho_S(\hat{\mathbf{P}})-\mu(\mathbf{k}+\hat{\mathcal{Q}})\varrho_S(\hat{\mathbf{P}}-\hat{\mathcal{Q}})\right) \quad (3.88)$$

with $\mathbf{n}$ the unit vector associated to the solid angle and $\hat{\mathcal{Q}} = \left|\hat{\mathcal{P}}_i\right|\mathbf{n}-\hat{\mathcal{P}}_i$ the collision momentum transfer operator. This Equation describes the classical result obtained by Boltzmann.

Diffusive regime

In the diffusive regime, where the mass ratio m/M between the gas particle and the test particle approaches zero and the momenta $\mathbf{k}$ and $\mathbf{P}$ of the gas and the test particle respectively are comparable, condition (3.84) is always verified, giving no constraint on the state of the system $\rho_S(t)$ and the reduced mass and the relative momentum defined Eq. (3.75) can be approximated has follows:

$$\begin{aligned} m^* &= \frac{mM}{m+M} \simeq m \\ \mathrm{rel}(\mathbf{k},\mathbf{P}) &= \frac{m^*}{m}\mathbf{k} - \frac{m^*}{M}\mathbf{P} \simeq \mathbf{k} \end{aligned} \tag{3.89}$$

and $\hat{\mathcal{P}}_i\ \hat{\mathcal{P}}_f$ in Eq. (3.75) become:

$$\begin{aligned} \hat{\mathcal{P}}_i &= \mathbf{k}+\mathbf{Q} \\ \hat{\mathcal{P}}_f &= \mathbf{k} \end{aligned} \tag{3.90}$$

Substituting above relations in Eq. (3.86) one ends up with

$$\begin{aligned} \left.\frac{\partial \hat{\varrho}_S}{\partial t}\right|_{coll} = \frac{n}{m^2}\int d\mathbf{Q}d\mathbf{k}\,\delta\left(\frac{\mathbf{k}^2}{2m} - \frac{(\mathbf{k}+\mathbf{Q})^2}{2m}\right) \\ \mu(\mathbf{k})\,|f(\mathbf{k},\mathbf{k}+\mathbf{Q})|^2\left[e^{\frac{i}{\hbar}\mathbf{Q}\cdot\hat{x}}\hat{\varrho}_S(t)e^{-\frac{i}{\hbar}\mathbf{Q}\cdot\hat{x}} - \hat{\varrho}_S(t)\right]. \end{aligned} \tag{3.91}$$

This equation exactly recover the results for the recoil-free dynamics analysed in sec. 1.1. From a simple comparison with Eq. (1.22) one immediately recognize the Gallis-Flemming collisional term, rescaled of a 2π factor. However, as already discussed in sec. 1.1 only with this rescaling the Gallis-Flemming master equation is able to reproduce experimantal data [42].

3.2.5 Time scales estimation

What is now left to verify is under which regime condition (3.21) holds. In order to do so, in the next section we give an estimation of both the interaction time scale τ_{int} and the free time scale τ_{free}.

Free-time scale

The action of the free evolution in a time interval τ on a generic state ϱ_S is given by

$$\hat{\varrho}_S(t+\tau) = \mathcal{U}^S_\tau(\hat{\varrho}_S(t)) \tag{3.92}$$

where $\mathcal{U}_\tau^{\mathcal{S}}(\cdot)$ is the free-evolution dynamical map defined by Eq. (3.16).
Let us write this equation in Taylor series to obtain

$$\hat{\varrho}_s(t+\tau) = \hat{\varrho}_{\mathcal{S}}(t) + \sum_{n=1}^{\infty}\left(\frac{-i\,\tau}{\hbar}\right)^n \underbrace{\mathcal{H}_s \circ \cdots \circ \mathcal{H}_{\mathcal{S}}}_{n-times}(\hat{\varrho}_s(t)) \tag{3.93}$$

with $\mathcal{H}_{\mathcal{S}}(\cdot)$ the infinitesimal change given by the free dynamics defined in Eq. (3.29). The request that $\tau_{free} \gg \tau$ is equivalent to require that, in the time interval τ, only the first term of the above series contributes, that is

$$\hat{\varrho}_{\mathcal{S}}(t+\tau) = \hat{\varrho}_s(t) + \mathcal{H}_{\mathcal{S}}(\hat{\varrho}_s(t))\tau + \mathcal{O}(\tau^2/\tau_{free}^2). \tag{3.94}$$

In order to estimate τ_{free} we expand Eq. (3.93) in eigenbasis $|\lambda\rangle$ of the free hamiltonian $\hat{H}_s$, $\hat{H}_{\mathcal{S}}\,|\lambda\rangle = E_\lambda\,|\lambda\rangle$ to obtain

$$\hat{\varrho}_{\mathcal{S}}(t+\tau) = \int d\lambda_L d\lambda_R \sum_{n=0} \frac{1}{n!}\left[-\frac{i}{\hbar}(E_{\lambda_L} - E_{\lambda_R})\tau\right]^n |\lambda_L\rangle\langle\lambda_L|\,\hat{\varrho}_{\mathcal{S}}(t)\,|\lambda_R\rangle\langle\lambda_R|\,. \tag{3.95}$$

From the equation above, one immediately sees that the first perturbative term dominates the series only if

$$|(E_{\lambda_L} - E_{\lambda_R})\,\langle\lambda_L|\,\hat{\varrho}_s(t)\,|\lambda_R\rangle\,|\,\frac{\tau}{\hbar} \ll |\,\langle\lambda_L|\,\hat{\varrho}_{\mathcal{S}}(t)\,|\lambda_R\rangle\,| \qquad \forall \quad |\lambda_L\rangle\,, |\lambda_R\rangle\,. \tag{3.96}$$

this is equivalent to requiring

$$\tau \ll \frac{\hbar}{\sup_{\hat{\varrho}_s}|E_{\lambda_R} - E_{\lambda_L}|} \tag{3.97}$$

where $\sup_{\varrho_{\mathcal{S}}}|E_{\lambda_R} - E_{\lambda_L}|$ is the maximum distance of $E_{\lambda_R} - E_{\lambda_L}$ for $\langle\lambda_L|\,\varrho_{\mathcal{S}}\,|\lambda_R\rangle \neq 0$. Since the condition we want to satisfy is $\tau \ll \tau_{free}$, one can now assume that

$$\tau_{free} \equiv \frac{\hbar}{\sup_{\hat{\varrho}_s}|E_{\lambda_R} - E_{\lambda_L}|}. \tag{3.98}$$

The equation above allows us to estimate the time necessary for the free evolution to produce a relevant change in the system's state $\varrho_{\mathcal{S}}$. The definition of τ_{free} given by Eq. (3.98) is formal, however $\sup_{\varrho_{\mathcal{S}}}|E_{\lambda_R} - E_{\lambda_L}|$ can be understood as a measure of quantum coherence in the energy eigen-basis of the system state $\hat{\varrho}_{\mathcal{S}}(t)$, opening the possibility for an experimental estimate of the free evolution time scales, trough a measurement of the coherence in the energy of the system.

Interaction time-scale

Next we give an estimation of the length of time interval τ necessary to contain a complete collision process. A way to estimate the collision time scale is to check in which amount of time after the interaction begin, conservation of the total free kinetic energy is restored. Meaning that the two colliding particles are far enough to not interact anymore. Since the requirement of a perfect conservation law implies an infinite collision time, we require the less stringent condition: the variation of the energy (ΔE_c) of the whole system must be negligible compared to the free energy $\bar{E} \equiv \text{Tr}[(\hat{H}_s + \hat{H}_1)\hat{\varrho}_s \otimes \varrho_1]$ of the interacting system, *i.e.*

$$\Delta E_c \ll \bar{E}. \tag{3.99}$$

Indeed, under this assumption the energy violation produced by the interaction process can be considered irrelevant for the free dynamics and, one can replace $\hat{S}_\tau$ with the full scattering operator $\hat{S}$. We know from Eq. (3.62) and Eq. (3.63) that the incomplete scattering operator takes the following expression

$$\hat{S}_\tau = \mathbb{1} + i \int d\lambda_f d\lambda_i \delta_\tau(E_{\lambda_f} - E_{\lambda_i}) f(\lambda_f, \lambda_i) \left|\lambda_f\right\rangle\!\left\langle\lambda_i\right| \tag{3.100}$$

in the limit of large τ. The $\delta_\tau(E_{\lambda_f} - E_{\lambda_i})$ in the above equation shows that the relevant contributions of the scattering process are given by matrix elements $\langle\lambda_f| \hat{S}_\tau |\lambda_i\rangle$, that satisfy the condition

$$\left|E_{\lambda_f} - E_{\lambda_i}\right| \leq \frac{2\pi\hbar}{\tau}. \tag{3.101}$$

This inequality suggests that the violation of the kinetic energy $\Delta E_c = E_{\lambda_f} - E_{\lambda_i}$ due to the process described by $\hat{S}_\tau$ is proportional to the inverse of the time interval τ during which the collision occurs, *i.e.*

$$\Delta E_{fi} \simeq \frac{2\pi\hbar}{\tau} \tag{3.102}$$

Combining this result with condition (3.99), one eventually obtains that the following inequality

$$\tau \gg \frac{\hbar}{\text{Tr}[(\hat{H}_S + \hat{H}_1)\hat{\varrho}_S \otimes \hat{\varrho}_1]} \tag{3.103}$$

must be satisfied to have complete scattering process. Since the condition that we want to satisfy is $\tau \gg \tau_{int}$, one can now assume that

$$\tau_{int} \simeq \frac{\hbar}{\text{Tr}[(\hat{H}_{\mathcal{S}} + \hat{H}_1)\varrho_{\mathcal{S}} \otimes \varrho_1]} \tag{3.104}$$

and exploiting Eq. (3.19) obtains

$$\tau_{int} \propto \frac{\hbar}{\text{Tr}(\hat{H}_{\mathcal{S}}\hat{\varrho}_s(t)) + \frac{3}{2}\beta^{-1}}. \tag{3.105}$$

Not surprisingly this equation suggests that the time needed for the wave packets to pass trough the interaction region is proportional to the total energy of the test particle plus the bath particle. Even if the interaction time defined in Eq. (3.104) does not contain any information of the interaction potential, it gives the magnitude of the time needed for the wave packet to pass through the interaction region. This can be easily checked under the choice of a Dirac delta potential $\gamma\delta(\mathbf{X} - \mathbf{x}_1)$ where the matrix elements $\langle\lambda|\,\hat{V}\,|\lambda'\rangle$ become constant and no dependence of the shape of the interaction appears in the determination of the relevant components of $\langle\lambda_f|\,\hat{S}\,|\lambda_i\rangle$. Since we expect that the collision time increases with the spatial extension of the interaction potential we deduce that Eq. (3.105) only gives a lower bound for the interaction time.

3.2.6 Regime of Validity for Collisional Equation

Now that we provided an estimation for both τ_{free} and τ_{int} we can discuss the validity of condition (3.20). Substituting Eq. (3.98) and Eq. (3.105) and in (3.20) one obtains the following necessary conditions

$$\sup_{\varrho_{\mathcal{S}}}|E_{\lambda_R} - E_{\lambda_L}| \ll \frac{\hbar}{\tau} \ll \text{Tr}_{\mathcal{S}}\left(\hat{H}_{\mathcal{S}}\hat{\varrho}_{\mathcal{S}}(t)\right) + \frac{3}{2}\beta^{-1}. \tag{3.106}$$

The above inequality suggests that a collisional description can be achieved only if the coherence in energy of the test particle $\varrho_{\mathcal{S}}$ is negligible compared to the energy of the test and the bath particle that interact. One may also notice that the condition (3.84) that seems to be necessary in order to guarantee (3.50) is in complete agreement with (3.106).

Conclusions

Animated by the desire to arrive at a better understanding of the collisional process affecting the quantum dynamics of a test particle in a gas, of the associated process of decoherence, we investigated the limits of a collisional model of this physical situation.

We first analyzed the literature of collisional models. As we have shown in the first chapter, the research in this field, has produced two heuristic models that claim to describe in total generality the behaviour of a quantum particle in a rarefied thermal gas. However these models reach discordant predictions. In order to better understand the dynamics of a collision process in a simple situation, we analyzed a system of two particles interacting via an infinite Dirac delta potential in one dimensional case. As shown in the second chapter this model is exactly solvable and can be exploited to study in full detail the interaction. This model allowed to estimate the duration time of the collision between two Gaussian wave packets. This time is proportional to the spatial extension of the wave packets, suggesting that only the classical behaviour of a point-like particle in a gas can be described in total generality as truly instantaneous collisions.

After this preliminary study we moved to the more interesting case of a test particle in a quantum gas. In order to find a solution for the problem, we combined the Hartree variational method with stochastic calculus techniques. This original treatment of the problem allows to correctly describe the non dissipative behaviour of the test particle, however the method has proved unsuitable to correctly describe dissipative phenomena. Even if this approach is not suitable for taking into account all phenomena underlying the dynamics, it shows that by describing the thermal bath as a system with no correlations in time prevents the possibility to describe dissipative phenomena. This fact suggests that dissipative phenomena can only appears if the collision process is sufficiently slow to let the system evolves during the interaction. Indeed the bath correlation is strictly related

to the duration time of the collision process, and a zero correlation time means that the collision append in a negligible time compared to the free evolution dynamics.
Because of the impossibility to learn more about dissipative phenomena in collisional models starting from heuristic models, we decided to tackle the problem from a different perspective.
In Chapter 3 we provided a microscopic derivation of the collisional dynamics. More importantly, we were able to find necessary conditions for the validity of a collisional approach in the description of a quantum particle in a gas. The very stringent conditions we found, not surprisingly, confirm the validity of a collisional dynamics for quantum systems in classical regime or the diffusive regime (see sec. 3.2.4), where dissipative phenomena are negligible. Moreover, this analysis also suggests that these two cases are the only ones in which a collisional description is possible. These results lead us to conclude that collisional models are not suited for describing systems in which both quantum and dissipative behaviour are present. To our opinion more sophisticated models and and probably are needed in order to tackle the problem of describing dissipative phenomena in the quantum mechanical scenario.

Appendix A

Stochastic master Equation

In this section we the derive approximated master equation associated to the dynamics of a quantum system under the action of an Hermitian operator $\hat{H}$ plus a real stochastic potential $\hat{V}_t$, *i.e.* evolving according to the Schrödinger equation

$$i\hbar\partial_t |\psi_t\rangle = (\hat{H} + \hat{V}(t)) |\psi_t\rangle . \tag{A.1}$$

We restrict to the case of a stochastic potential with Gaussian distribution and zero mean value, *i.e.*

$$\mathbb{E}\left[\hat{V}(t)\right] = 0 \qquad\qquad \mathbb{E}\left[\hat{V}(t)\hat{V}(\tau)\right] \tag{A.2}$$

where $\mathbb{E}[\ldots]$ defines the stochastic average. It is convenient to study the dynamics in interaction picture, where the state of the system $|\psi\rangle$ evolves accordingly to the Schrödinger equation

$$i\hbar\partial_t |\psi_t\rangle = \hat{V}_I(t) |\psi_t\rangle , \tag{A.3}$$

where $\hat{V}_I(t)$ is the time dependent operator $\hat{V}(t)$ in interaction picture and is defined by

$$\hat{V}_I(t) = e^{-\frac{i}{\hbar}\hat{H}t}\hat{V}(t)e^{\frac{i}{\hbar}\hat{H}t}. \tag{A.4}$$

The solution of Eq. (A.3) with initial condition $|\psi\rangle$ may now be formally written in the form

$$|\psi_t\rangle = \mathcal{T}(e^{-\frac{i}{\hbar}\int_0^t d\tau\, \hat{V}_I(\tau)}) |\psi\rangle . \tag{A.5}$$

Exploiting Eq. (A.5), the statistical operator $\hat{\rho}_t \equiv \mathbb{E}\left[|\psi_t\rangle\langle\psi_t|\right]$ is equal to:

$$\hat{\rho}_t \equiv \mathbb{E}\left[\mathcal{T}(e^{-\frac{i}{\hbar}\int_{t_i}^{t} d\tau\,\hat{V}_I(\tau)})\hat{\rho}\mathcal{T}(e^{\frac{i}{\hbar}\int_{t_i}^{t} d\tau\,\hat{V}_I(\tau)})\right] \tag{A.6}$$

where $\hat{\rho} = |\psi\rangle\langle\psi|$ is the initial state[1].
It is now convenient to introduce the super-operator $\mathcal{V}_I(\tau)$ acting on the system state $\hat{\rho}$ such that $\mathcal{V}_I(t)\hat{\rho} \equiv -\hbar^{-1}[\hat{V}_I(t), \hat{\rho}]$ and rewrite Eq. (A.6) as

$$\hat{\rho}_t = \mathbb{E}\left[\mathcal{T}(e^{-i\int_0^t d\tau \mathcal{V}(\tau)})\right]\hat{\rho} \tag{A.7}$$

Exploiting the Gaussianity of the the stochastic operator and the Isserliss theorem one may now rewrite Eq. (A.7) in the more convenient form

$$\hat{\rho}_t = \mathcal{T}(e^{-\frac{1}{2}\int_0^t d\tau' \int_0^t d\tau'' \mathbb{E}[\mathcal{V}_I(\tau')\mathcal{V}_I(\tau'')]})\hat{\rho}, \tag{A.8}$$

The time derivative of Eq. (A.8) yields to the equation

$$\partial_t\hat{\rho}_t = \mathcal{T}\left(\int_0^t d\tau\,\mathbb{E}\left[\mathcal{V}_I(t)\mathcal{V}_I(\tau)\right]\, e^{-\frac{1}{2}\int_0^t d\tau' \int_0^t d\tau'' \mathbb{E}[\mathcal{V}_I(\tau')\mathcal{V}_I(\tau'')]}\right)\hat{\rho} \tag{A.9}$$

but under the hypothesis that exist a time interval τ_c such that

$$\mathbb{E}\left[\mathcal{V}_I(t)\mathcal{V}_I(\tau)\right] \simeq 0 \qquad\qquad |t-\tau| > \tau_c, \tag{A.10}$$

usually called correlation time, one can write Eq. (A.9) as

$$\partial_t\hat{\rho}_t = \mathcal{T}\left(\int_0^\infty d\tau\,\mathbb{E}\left[\mathcal{V}_I(t)\mathcal{V}_I(\tau)\right]\right)\hat{\rho}_t + \mathcal{O}((\tau_c/t)^2) \qquad\qquad \forall\ t > \tau_c \tag{A.11}$$

To show the validity of Eq. (A.11) one may rewrite Eq. (A.9) as

$$\begin{aligned}\partial_t\hat{\rho}_t = &\mathcal{T}(\int_0^t d\tau\,\mathbb{E}\left[\mathcal{V}_I(t)\mathcal{V}_I(\tau)\right] e^{-\frac{1}{2}\int_\tau^t d\tau' \int_\tau^t d\tau'' \mathbb{E}[\mathcal{V}_I(\tau')\mathcal{V}_I(\tau'')]} \\ &e^{-\int_\tau^t d\tau' \int_0^\tau d\tau'' \mathbb{E}[\mathcal{V}_I(\tau')\mathcal{V}_I(\tau'')]} \otimes e^{-\frac{1}{2}\int_0^\tau d\tau' \int_0^\tau d\tau'' \mathbb{E}[\mathcal{V}_I(\tau')\mathcal{V}_I(\tau'')]})\hat{\rho}.\end{aligned} \tag{A.12}$$

Under the assumption that $t > \tau_c$ the term in first line of Eq. (A.12) restricts the variable τ to be

$$\tau \geq (t - \tau_c) \tag{A.13}$$

[1] It is worth to notice the that Eq. (A.6) can be understood a Kraus decomposition of the dynamics ensuring the dynamics to be completely positive

and can be then approximated with

$$\int_0^t d\tau \mathbb{E}\left[\mathcal{V}_I(t)\mathcal{V}_I(\tau) \simeq \int_{t-\tau_c}^t\right] \mathbb{E}\left[\mathcal{V}_I(t)\mathcal{V}_I(\tau)\right] \propto \tau_c. \tag{A.14}$$

With the help of Eq. (A.13), one may also notice that

$$\begin{aligned}
&\int_\tau^t d\tau' \int_\tau^t d\tau'' \mathbb{E}\left[\mathcal{V}_I(\tau')\mathcal{V}_I(\tau'')\right] \simeq \int_{t-\tau_c}^t \int_{t-\tau_c}^t \mathbb{E}\left[\mathcal{V}_I(\tau')\mathcal{V}_I(\tau'')\right] \propto \tau_c^2, \\
&\int_\tau^t d\tau' \int_0^\tau d\tau'' \mathbb{E}\left[\mathcal{V}_I(\tau')\mathcal{V}_I(\tau'')\right] \simeq \int_0^{\tau_c} d\tau' \int_{-\tau_c}^0 d\tau'' \overbrace{\mathcal{V}_I(\tau'-\tau)\mathcal{V}}_I(\tau''+\tau) \propto \tau_c^2, \\
&\int_0^\tau d\tau' \int_0^\tau d\tau'' \mathbb{E}\left[\mathcal{V}_I(\tau')\mathcal{V}_I(\tau'')\right] \simeq \int_0^{t-\tau_c} \int_0^{t-\tau_c} \mathbb{E}\left[\mathcal{V}_I(\tau')\mathcal{V}_I(\tau'')\right] \propto \tau_c t
\end{aligned} \tag{A.15}$$

Exploiting these results one is allowed to approximate Eq. (A.12) as

$$\partial_t \hat{\rho}_\tau = \mathcal{T}(\int_{t-\tau_c}^t d\tau\, \mathbb{E}\left[\mathcal{V}_I(t)\mathcal{V}_I(\tau)\right])\hat{\rho}_\tau + \mathcal{O}((\tau_c/t)^2) \qquad \forall\ t > \tau_c \tag{A.16}$$

which can be equivalently rewritten as

$$\partial_t \hat{\rho}_t = \mathcal{T}(\int_{t-\tau_c}^t d\tau\, \mathbb{E}\left[\mathcal{V}_I(t)\mathcal{V}_I(\tau)\right])\hat{\rho}_t + \mathcal{O}((\tau_c/t)^2) \tag{A.17}$$

because, for $\tau \geq (t-\tau_c)$ and $t > \tau_c$,

$$\hat{\rho}_t = \hat{\rho}_\tau + \mathcal{O}((\tau_c/t)^2). \tag{A.18}$$

Performing now the change of variables $\tau \to (t-\tau)$, Eq. (A.17) may be rewritten as

$$\partial_t \hat{\rho}_t = \mathcal{T}(\int_0^{\tau_c} d\tau\, \mathbb{E}\left[\mathcal{V}_I(t)\mathcal{V}_I(t-\tau)\right])\hat{\rho}_t + \mathcal{O}((\tau_c/t)^2) \tag{A.19}$$

Exploiting the assumption in Eq. (A.10) one may now replace the upper limit of the integral with $+\infty$ to finally obtain

$$\partial_t \hat{\rho}_t = \mathcal{T}(\int_0^{\infty} d\tau\, \mathbb{E}\left[\mathcal{V}_I(t)\mathcal{V}_I(t-\tau)\right])\hat{\rho}_t + \mathcal{O}((\tau_c/t)^2) \tag{A.20}$$

which is the Eq. (A.11). Eq. (A.20) may be furthemrore conveniently rewritten in Schrödinger picture as

$$\partial_t \hat{\rho}_t = -i\mathcal{H}\hat{\rho}_t + \mathcal{T}(\int_0^{\infty} d\tau\, \mathbb{E}\left[\mathcal{V}(t)e^{i\mathcal{H}\tau}\mathcal{V}(t-\tau)\right] e^{-i\mathcal{H}\tau})\hat{\rho}_t + \mathcal{O}((\tau_c/t)^2) \tag{A.21}$$

where $\mathcal{H}\hat{\rho}_t = \hbar^{-1}[\hat{H}, \hat{\rho}_t]$.
It is also worth to notice that in the limit of $\tau_c/t \to 0$, the stochastic process can be assumed to be delta correlated in time, *i.e.*

$$\mathbb{E}\left[\mathcal{V}(t)\mathcal{V}(t-\tau)\right] \propto \delta(\tau) \tag{A.22}$$

and Eq. (A.20) becomes the exact master equation

$$\partial_t \hat{\rho}_t = i\mathcal{H}\hat{\rho}_t + \mathcal{T}(\int_0^\infty d\tau\, \mathbb{E}\left[\mathcal{V}(t)\mathcal{V}(t-\tau)\right])\hat{\rho}_t. \tag{A.23}$$

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