Relaxation dynamics of a quantum Brownian particle in an ideal gas

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Abstract. We show how the quantum analog of the Fokker-Planck equation for describing Brownian motion can be obtained as the diffusive limit of the quantum linear Boltzmann equation. The latter describes the quantum dynamics of a tracer particle in a dilute, ideal gas by means of a translation-covariant master equation. We discuss the type of approximations required to obtain the generalized form of the Caldeira-Leggett master equation, along with their physical justification. Microscopic expressions for the diffusion and relaxation coefficients are obtained by analyzing the limiting form of the equation in both the Schrödinger and the Heisenberg picture.

1 Introduction

1.1 Quantum Brownian motion

One of the classic problems in open quantum dynamics is the question of quantum Brownian motion, asking how a distinguished 'Brownian' quantum particle experiences friction, diffusion, and thermalization due to the interaction with an unobserved surrounding liquid or gas. Starting with the work of Caldeira and Leggett [1] the bulk of studies on this problem treat the environment in a phenomenological way, usually by linearly coupling the Brownian particle position to a continuous thermal bath of harmonic oscillators, whose spectral density is then chosen as to reproduce the desired relaxation and diffusion constants.

Using the Feynman-Vernon path integral approach [2] these linear models can even be solved exactly for some cases [3–6]. However, as is well known, these non-Markovian dynamical solutions also have limitations. Firstly, they usually have to assume that the Brownian particle and the environment are initially in a product state, leading to an unphysical initial transient dynamics due to the re-adjustment of the energies once the coupling is switched on [7]. Secondly, the generic assumption of a linear coupling with the unbounded position operator, leading to spatial correlations over any length scale, can be justified at best for a restricted class of initial states. It will be valid if the Brownian particle state is close to a classical state, but may lead to unphysically large decoherence rates if the Brownian state is characterized by macroscopically large coherence lengths [8].

In a more concise sense, one should therefore characterize those situations as generic quantum Brownian motion (i) where one is interested in timescales such that the Markov assumption is permissible and (ii) where the motional states considered are close to a classical state in the

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sense that the coherence scales are not macroscopic. This is the regime of the *Caldeira-Leggett master equation* for free quantum Brownian motion [1]. It is obtained from the path integral approach in a high-temperature limit and, apart from the temperature T, it contains a friction constant η as a phenomenological parameter, see section 3.1 below. As in the corresponding case of the classical Kramers equation (section 3.2), the diffusion constant D_{pp} is determined by η and T according to $D_{pp} = \eta M k_\mathrm{B} T$, with M the mass of the Brownian particle. This is an instance of the fluctuation-dissipation theorem.

An issue of much debate is the fact that the Caldeira-Leggett master equation is not of Lindblad-form and therefore does not preserve the positivity of some initial states. As is well known [9], this can be healed by adding a "position-diffusion" term provided the corresponding coefficient D_{xx} satisfies $D_{xx} \geqslant \eta^2 \hbar^2 / (16 D_{pp})$, which in turn leads to "momentum localization". Various authors proposed the 'correct' value for D_{xx} based either on formal arguments, on improved evaluations of the high-temperature limit, and, above all, on more specific descriptions of the environmental interaction process [7,9–14] . In view of this, it seems quite plausible that a definite answer concerning the value of D_{xx} can only be given by accounting for the environment in a way which is microscopically more realistic.

1.2 Microscopically realistic environments

Given the large body of work on quantum Brownian motion it is perhaps surprising that attempts to justify the Caldeira-Leggett master equation by a realistic microscopic description of the environment received much less attention. The main reason is the notorious difficulty of obtaining realistic effective dynamic equations for the Brownian quantum particle in terms of the microscopic properties of a given liquid or gas. Provided such a realistic master equation is available in Lindblad form, one has then to take an appropriate limit, which will be called "*diffusive limit*" below, to end up with a master equation of the form of Caldeira-Leggett plus the "position-diffusion" term. Importantly, the coefficients η, D_{pp}, and D_{xx} are then no longer phenomenological constants, but they are determined by the microscopic description of the particular environment considered.

The simplest realistic environment in that sense is clearly given by an ideal gas in a thermal state. The gas particles then do not interact with each other, but they influence the Brownian particle via two-body forces, which should be taken sufficiently short-ranged to permit a scattering theory description of the interaction processes. The corresponding effective equation of motion for the quantum Brownian particle is called *quantum linear Boltzmann equation*[1]. Such a Lindblad master equation was obtained recently by implementing the Markov assumption before performing the partial trace over the gas particles in a non-perturbative calculation [16,17]. It is supposed to be valid if the gas is sufficiently dilute to justify both the neglect of three-body collisions and the Markov approximation. Moreover, unlike the master equations for quantum Brownian motion, it is supposed to be valid even for very non-classical motional states, such as the superposition states found in an interferometer.

The purpose of the present article is to use this quantum linear Boltzmann equation as a starting point for obtaining the extended Caldeira-Leggett master equation. We will discuss what kind of assumptions and approximations are required to end up in that form and how this *diffusive limit* can be justified by using both the operator and the Wigner-Weyl formulation of quantum mechanics in the Schrödinger and the Heisenberg picture. In all cases we will find that the friction and diffusion coefficients η and D_{pp} are uniquely specified by combining the thermodynamic quantities of the gas with the relevant microscopic properties of its constituent particles, namely their mass and their suitably averaged cross section. Moreover, we will see that the coefficient of the "position-diffusion" term D_{xx}, which is required for complete positivity, is completely determined by η and D_{pp} at its smallest possible value, $D_{xx} = \eta^2 \hbar^2 / (16 D_{pp})$.

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[1] This is the quantum analogue of the classical linear Boltzmann equation for a tracer particle [15]. It is important not to confuse this equation, which is non-perturbative, with the *linearized* quantum equation for the reduced single particle gas state of a self-interacting quantum gas.

The structure of the article is as follows. In section 2 we briefly review the form of the quantum linear Boltzmann equation in operator representation and in the momentum basis. section 3 discusses the diffusive limit of the equation in the Schrödinger picture, both in operator form and in the Wigner-Weyl phase space representation. In section 4 we formulate the same limit in the Heisenberg picture and discuss the equations of motion for the energy and momentum operator. We present our conclusions in section 5.

2 The quantum linear Boltzmann equation

Before we present the full form of the quantum linear Boltzmann equation let us briefly collect some important steps that lead to its derivation. The idea of using a scattering theory formulation for obtaining Markovian master equations goes back to the work by Joos and Zeh on collisional decoherence [18]. However, their master equation, which was later formulated in a non-perturbative fashion [19,20], cannot describe friction, since the Brownian mass M is assumed to be infinitely large compared to the gas mass m, so that energy exchange cannot be accommodated. An early proposal for finite mass ratios m/M is the master equation of Diósi [12], which is quite close to the present formulation of the quantum linear Boltzmann equation, but, as we will see, it differs in some crucial aspects, such as the inferred value of D_{xx}. A perturbative form of the present quantum linear Boltzmann equation was obtained in [16, 21,22], pointing to a connection with the van Hove relation and the dynamic structure factor of the gas. While other important contributions dealt with specific aspects [23], the present non-perturbative form is a quite recent result [17], based on a monitoring approach for deriving Markovian master equations [24].

2.1 Operator form

In the following, we will denote the density operator for the motional state of the Brownian particle by ρ, and its momentum operator by P. The quantum linear Boltzmann equation then reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = \frac{1}{\mathrm{i}\hbar}\left[\frac{\mathsf{P}^2}{2M},\rho\right] + \mathcal{L}\rho, \tag{1}$$

where the mapping $\mathcal{L}$ which describes the incoherent effects of the gas environment is given by [17]

$$\mathcal{L}\rho = \int \mathrm{d}\boldsymbol{Q} \int_{\boldsymbol{Q}^\perp} \mathrm{d}\boldsymbol{p} \left\{ \mathsf{L}_{\boldsymbol{Q},\boldsymbol{p}}\rho\mathsf{L}_{\boldsymbol{Q},\boldsymbol{p}}^\dagger - \frac{1}{2}\rho\mathsf{L}_{\boldsymbol{Q},\boldsymbol{p}}^\dagger\mathsf{L}_{\boldsymbol{Q},\boldsymbol{p}} - \frac{1}{2}\mathsf{L}_{\boldsymbol{Q},\boldsymbol{p}}^\dagger\mathsf{L}_{\boldsymbol{Q},\boldsymbol{p}}\rho \right\}. \tag{2}$$

Here the integration is over all momentum transfers $\boldsymbol{Q}$, and for fixed $\boldsymbol{Q}$ also over the perpendicular plane $\boldsymbol{Q}^\perp = \{\boldsymbol{p} \in \mathbb{R}^3 : \boldsymbol{p} \cdot \boldsymbol{Q} = 0\}$. The Lindblad operators have the form

$$\mathsf{L}_{\boldsymbol{Q},\boldsymbol{p}} = \mathrm{e}^{i\boldsymbol{Q}\cdot\mathsf{X}/\hbar}L(\boldsymbol{p},\mathsf{P};\boldsymbol{Q}) \tag{3}$$

where X is the position operator of the Brownian particle. The first term in (3) thus effects a momentum transfer determined by $\boldsymbol{Q}$. It is important to stress that the form (2) of $\mathcal{L}\rho$ fits the general structure of a translation-covariant and completely positive master equation as characterized by Holevo [25] (see [26,27] for a discussion).

The function L, which is operator-valued in (3), contains all the details of the collisional interaction with the gas. It involves the momentum distribution function $\mu(\boldsymbol{p})$ of the gas, its number density n_{gas} and the elastic scattering amplitude $f(\boldsymbol{p}_f, \boldsymbol{p}_i)$, which determines the differential cross section

$$\sigma(\boldsymbol{p}_f, \boldsymbol{p}_i) = |f(\boldsymbol{p}_f, \boldsymbol{p}_i)|^2,$$

as well as the total cross section

$$\sigma_{\text{tot}}\left(\boldsymbol{p}_i\right) = \int \mathrm{d}\boldsymbol{n} \left|f\left(p_i\boldsymbol{n},\boldsymbol{p}_i\right)\right|^2,$$

where $\boldsymbol{n}$ is a unit vector with $\mathrm{d}\boldsymbol{n}$ the associated solid angle element.

In order to specify L let us denote, for any given momentum exchange $\boldsymbol{Q} \neq 0$, the parallel and the perpendicular contribution of a vector $\boldsymbol{P}$ by $\boldsymbol{P}_{\|\boldsymbol{Q}} = \left(\boldsymbol{P}\cdot\boldsymbol{Q}\right)\boldsymbol{Q}/Q^2$ and by $\boldsymbol{P}_{\perp\boldsymbol{Q}} = \boldsymbol{P}-\boldsymbol{P}_{\|\boldsymbol{Q}}$, respectively. With these definitions the function L is defined by

$$L\left(\boldsymbol{p},\boldsymbol{P};\boldsymbol{Q}\right) = \sqrt{\frac{n_{\text{gas}}m}{Qm_*^2}}\mu^{\frac{1}{2}}\left(\boldsymbol{p}_{\perp\boldsymbol{Q}} + \left(1+\frac{m}{M}\right)\frac{\boldsymbol{Q}}{2} + \frac{m}{M}\boldsymbol{P}_{\|\boldsymbol{Q}}\right)$$
$$\times f\left(\text{rel}\left(\boldsymbol{p}_{\perp\boldsymbol{Q}},\boldsymbol{P}_{\perp\boldsymbol{Q}}\right) - \frac{\boldsymbol{Q}}{2},\text{rel}\left(\boldsymbol{p}_{\perp\boldsymbol{Q}},\boldsymbol{P}_{\perp\boldsymbol{Q}}\right) + \frac{\boldsymbol{Q}}{2}\right). \tag{4}$$

The most natural choice for μ is of course the Maxwell-Boltzmann distribution

$$\mu_\beta\left(\boldsymbol{p}\right) = \frac{1}{\pi^{3/2}p_\beta^3}\exp\left(-\frac{\boldsymbol{p}^2}{p_\beta^2}\right) \tag{5}$$

with $p_\beta^2 = 2m/\beta$ the most probable momentum at temperature $T = 1/\left(k_{\text{B}}\beta\right)$. Moreover, in (4) we have denoted the reduced mass by $m_* = mM/\left(M+m\right)$ and relative momenta by

$$\text{rel}\left(\boldsymbol{p},\boldsymbol{P}\right) := \frac{m_*}{m}\boldsymbol{p} - \frac{m_*}{M}\boldsymbol{P}.$$

One limiting form of the quantum linear Boltzmann equation is obtained by replacing the scattering amplitudes in (4) by their Born approximation. This simplifies the equation considerably, since the Born amplitude depends only on the difference of the momenta, $f_B\left(\boldsymbol{p}_f,\boldsymbol{p}_i\right) = f_B\left(\boldsymbol{p}_f - \boldsymbol{p}_i,0\right)$, which removes the operator-valuedness of the scattering amplitudes. In this approximation one has

$$L_B\left(\boldsymbol{p},\boldsymbol{P};\boldsymbol{Q}\right) = \sqrt{\frac{n_{\text{gas}}m}{Qm_*^2}}\mu^{\frac{1}{2}}\left(\boldsymbol{p}_{\perp\boldsymbol{Q}} + \left(1+\frac{m}{M}\right)\frac{\boldsymbol{Q}}{2} + \frac{m}{M}\boldsymbol{P}_{\|\boldsymbol{Q}}\right)f_B\left(-\boldsymbol{Q},0\right)$$

so that the $\mathrm{d}\boldsymbol{p}_{\perp\boldsymbol{Q}}$-integration in (2) can be carried out. The resulting equation thus reduces to the one proposed in [16, 21].

Another limiting form of the master equation is the case of an infinitely massive Brownian particle, $m/M \to 0$, where it describes no dissipation, but pure spatial decoherence. As one expects, the quantum linear Boltzmann equation reduces in this limit to the proper master equation for collisional decoherence [20, 27, 28], which was recently tested experimentally [29–31].

2.2 Momentum representation

Although the operator form (2)–(5) of $\mathcal{L}$ will be quite useful for the discussion of the diffusive limit below, the physics described by the master equation is more easily understood in momentum representation. Let us denote matrix elements of ρ in the basis of improper momentum eigenkets as $\langle\boldsymbol{P}|\rho|\boldsymbol{P}'\rangle = \rho\left(\boldsymbol{P},\boldsymbol{P}'\right)$. The incoherent part (2) of the quantum linear Boltzmann equation then takes the form

$$\langle\boldsymbol{P}|\mathcal{L}\rho|\boldsymbol{P}'\rangle = \int \mathrm{d}\boldsymbol{Q}\,\rho\left(\boldsymbol{P}-\boldsymbol{Q},\boldsymbol{P}'-\boldsymbol{Q}\right)M_{\text{in}}\left(\boldsymbol{P},\boldsymbol{P}';\boldsymbol{Q}\right)$$
$$-\rho\left(\boldsymbol{P},\boldsymbol{P}'\right)\frac{1}{2}\int \mathrm{d}\boldsymbol{Q}\left[M_{\text{in}}\left(\boldsymbol{P}+\boldsymbol{Q},\boldsymbol{P}+\boldsymbol{Q};\boldsymbol{Q}\right) + M_{\text{in}}\left(\boldsymbol{P}'+\boldsymbol{Q},\boldsymbol{P}'+\boldsymbol{Q};\boldsymbol{Q}\right)\right]$$

with the complex function $M_{\mathrm{in}}\left(\boldsymbol{P}, \boldsymbol{P}'; \boldsymbol{Q}\right)$ defined by

$$M_{\mathrm{in}}\left(\boldsymbol{P}, \boldsymbol{P}'; \boldsymbol{Q}\right) = \int_{\boldsymbol{Q}^{\perp}} \mathrm{d}\boldsymbol{p} L\left(\boldsymbol{p}, \boldsymbol{P} - \boldsymbol{Q}; \boldsymbol{Q}\right) L^*\left(\boldsymbol{p}, \boldsymbol{P}' - \boldsymbol{Q}; \boldsymbol{Q}\right). \tag{6}$$

One can show that for $\boldsymbol{P} = \boldsymbol{P}'$ this function is equal to the rate density, found in the classical linear Boltzmann equation, of the particle ending up with momentum $\boldsymbol{P}$ after a momentum gain of $\boldsymbol{Q}$ due to a gas collision. In other words, we have $M_{\mathrm{in}}\left(\boldsymbol{P}, \boldsymbol{P}; \boldsymbol{Q}\right) = M_{\mathrm{in}}^{\mathrm{cl}}\left(\boldsymbol{P}; \boldsymbol{Q}\right)$ with

$$M_{\mathrm{in}}^{\mathrm{cl}}\left(\boldsymbol{P}; \boldsymbol{Q}\right) = \frac{n_{\mathrm{gas}}}{m_*} \int \mathrm{d}\boldsymbol{p}_0 \mu\left(\boldsymbol{p}_0\right) \sigma\left(\mathrm{rel}\left(\boldsymbol{p}_0 - \boldsymbol{Q}, \boldsymbol{P}\right), \mathrm{rel}\left(\boldsymbol{p}_0, \boldsymbol{P} - \boldsymbol{Q}\right)\right)$$

$$\times \delta\left(\frac{|\mathrm{rel}\left(\boldsymbol{p}_0 - \boldsymbol{Q}, \boldsymbol{P}\right)|^2 - |\mathrm{rel}\left(\boldsymbol{p}_0, \boldsymbol{P} - \boldsymbol{Q}\right)|^2}{2}\right). \tag{7}$$

We can equally consider the corresponding classical rate density for the particle with momentum $\boldsymbol{P}$ to end up at a different momentum,

$$M_{\mathrm{out}}^{\mathrm{cl}}\left(\boldsymbol{P}\right) := \int \mathrm{d}\boldsymbol{Q}\, M_{\mathrm{in}}^{\mathrm{cl}}\left(\boldsymbol{P} + \boldsymbol{Q}; \boldsymbol{Q}\right)$$

$$= \frac{n_{\mathrm{gas}}}{m_*} \int \mathrm{d}\boldsymbol{p}_0 \mathrm{d}\boldsymbol{Q} \mu\left(\boldsymbol{p}_0\right) \sigma\left(\mathrm{rel}\left(\boldsymbol{p}_0, \boldsymbol{P}\right) + \boldsymbol{Q}, \mathrm{rel}\left(\boldsymbol{p}_0, \boldsymbol{P}\right)\right)$$

$$\times \delta\left(\frac{|\mathrm{rel}\left(\boldsymbol{p}_0, \boldsymbol{P}\right)|^2 - |\mathrm{rel}\left(\boldsymbol{p}_0, \boldsymbol{P}\right) + \boldsymbol{Q}|^2}{2}\right). \tag{8}$$

This can be used to put the master equation into the shorter form

$$\langle\boldsymbol{P}|\mathcal{L}\rho|\boldsymbol{P}'\rangle = \int \mathrm{d}\boldsymbol{Q}\, M_{\mathrm{in}}\left(\boldsymbol{P}, \boldsymbol{P}'; \boldsymbol{Q}\right) \rho\left(\boldsymbol{P} - \boldsymbol{Q}, \boldsymbol{P}' - \boldsymbol{Q}\right) - \frac{1}{2}\left[M_{\mathrm{out}}^{\mathrm{cl}}\left(\boldsymbol{P}\right) + M_{\mathrm{out}}^{\mathrm{cl}}\left(\boldsymbol{P}'\right)\right] \rho\left(\boldsymbol{P}, \boldsymbol{P}'\right). \tag{9}$$

For $\boldsymbol{P} \neq \boldsymbol{P}'$ the function M_{in} is in general complex and cannot be related to a classical rate, but still the analogy to the classical case seems quite intuitive.

3 Diffusive limit in the Schrödinger picture

We now want to consider the Brownian motion limit of the quantum linear Boltzmann equation, using arguments similar to the treatment that turns the classical linear Boltzmann equation into the Fokker-Planck equation [32]. The situation is actually more complicated in the quantum case, since one is dealing with operators whose values can be estimated in a meaningful way only when suitable matrix elements are considered.

We will argue that the quantum counterpart of the classical Fokker-Planck equation can be obtained by formally expanding the operators in the collision kernel of the quantum linear Boltzmann equation up to second order contributions in the canonically conjugate operators X and P. As we shall see, the result is *not* equivalent to a naive application of the correspondence principle on the classical result. Such a procedure would simply lead to the original Caldeira-Leggett master equation [1], which does not guarantee to preserve the positivity of the statistical operator. The operator expansion holds under conditions analogous to the classical ones [32], which imply in particular that the statistical operator describes a very massive test particle not far from thermal equilibrium, that is to say, close to diagonal in momentum representation. More specifically, the off-diagonal elements $\langle\boldsymbol{P}|\rho|\boldsymbol{P}'\rangle$ may differ significantly from zero only for $\Delta P := \left|\boldsymbol{P} - \boldsymbol{P}'\right| \lesssim \sqrt{M/\beta}$. In the position representation the validity of the expansion requires that the statistical operator is only coherent over a length of the order of the thermal wavelength of the test particle, so that $\langle\boldsymbol{X}|\rho|\boldsymbol{X}'\rangle$ is appreciably different from zero only within a range

given by the thermal de Broglie wave length $\lambda_{\text{th}} = \sqrt{2\pi\hbar^2\beta/M}$, i.e., for $\Delta X := |\boldsymbol{X} - \boldsymbol{X}'| \lesssim \sqrt{2\pi\hbar^2\beta/M}$. Note that since we require $m/M \ll 1$ it follows that the Brownian thermal wave length is much smaller that the thermal wave length of the gas, $\lambda_{\text{th}} \ll \lambda_{\text{th}}^{\text{gas}} = \sqrt{2\pi\hbar^2\beta/m}$.

3.1 Operator formulation

In order to formulate the Brownian motion limit of the quantum linear Boltzmann equation we come back to its explicit expression (2)–(4) and we confine ourselves to the case of a *constant* scattering cross-section $\left|f\left(\boldsymbol{p}_f, \boldsymbol{p}_i\right)\right|^2 = \sigma_{\text{tot}}/4\pi$. In this case, the operator form of the quantum linear Boltzmann equation is given explicitly by

$$
\begin{aligned}
\mathcal{L}\rho &= n_{\text{gas}} \frac{m}{m_*^2} \frac{\sigma_{\text{tot}}}{4\pi} \int \frac{\mathrm{d}\boldsymbol{Q}}{Q} \int_{\boldsymbol{Q}^\perp} \mathrm{d}\boldsymbol{p} \\
&\times \left[e^{i\boldsymbol{Q}\cdot\mathsf{X}/\hbar} \mu^{\frac{1}{2}} \left(\boldsymbol{p}_{\perp\boldsymbol{Q}} + \frac{m}{m_*}\frac{\boldsymbol{Q}}{2} + \frac{m}{M}\mathsf{P}_{\|\boldsymbol{Q}} \right) \rho \mu^{\frac{1}{2}} \left(\boldsymbol{p}_{\perp\boldsymbol{Q}} + \frac{m}{m_*}\frac{\boldsymbol{Q}}{2} + \frac{m}{M}\mathsf{P}_{\|\boldsymbol{Q}} \right) e^{-i\boldsymbol{Q}\cdot\mathsf{X}/\hbar} \right. \\
&\left. - \frac{1}{2} \left\{ \mu \left(\boldsymbol{p}_{\perp\boldsymbol{Q}} + \frac{m}{m_*}\frac{\boldsymbol{Q}}{2} + \frac{m}{M}\mathsf{P}_{\|\boldsymbol{Q}} \right), \rho \right\} \right]
\end{aligned} \tag{10}
$$

where $\{\cdot,\cdot\}$ denotes the anti-commutator. Specializing to the case of a Maxwell-Boltzmann distribution in the gas (5) we can write

$$
\begin{aligned}
\mathcal{L}\rho &= n_{\text{gas}} \frac{m}{m_*^2} \frac{\sigma_{\text{tot}}}{4\pi} \int \frac{\mathrm{d}\boldsymbol{Q}}{Q} \int_{\boldsymbol{Q}^\perp} \mathrm{d}\boldsymbol{p}\, \mu_\beta \left(\boldsymbol{p}_{\perp\boldsymbol{Q}} + \frac{m}{m_*}\frac{\boldsymbol{Q}}{2} \right) \\
&\times \left[e^{i\boldsymbol{Q}\cdot\mathsf{X}/\hbar} \exp\left(-\beta\frac{m\mathsf{P}_{\|\boldsymbol{Q}}^2}{4M^2} - \beta\frac{m\boldsymbol{Q}\cdot\mathsf{P}}{4Mm_*} \right) \rho \exp\left(-\beta\frac{m\mathsf{P}_{\|\boldsymbol{Q}}^2}{4M^2} - \beta\frac{m\boldsymbol{Q}\cdot\mathsf{P}}{4Mm_*} \right) e^{-i\boldsymbol{Q}\cdot\mathsf{X}/\hbar} \right. \\
&\left. - \frac{1}{2} \left\{ \exp\left(-\beta\frac{m\mathsf{P}_{\|\boldsymbol{Q}}^2}{4M^2} - \beta\frac{m\boldsymbol{Q}\cdot\mathsf{P}}{4Mm_*} \right), \rho \right\} \right].
\end{aligned}
$$

Since we are ultimately interested in an expansion up to second order in P, the contributions coming from the terms involving squares of the momentum operator in the exponent will simply cancel out. We can replace them by unity, leading to the much simpler expression

$$
\begin{aligned}
\mathcal{L}\rho &= n_{\text{gas}} \frac{m}{m_*^2} \frac{\sigma_{\text{tot}}}{4\pi} \int \frac{\mathrm{d}\boldsymbol{Q}}{Q} \int_{\boldsymbol{Q}^\perp} \mathrm{d}\boldsymbol{p}\, \mu_\beta \left(\boldsymbol{p}_{\perp\boldsymbol{Q}} + \frac{m}{m_*}\frac{\boldsymbol{Q}}{2} \right) \\
&\times \left[e^{i\boldsymbol{Q}\cdot\mathsf{X}/\hbar} \exp\left(-\beta\frac{m\boldsymbol{Q}\cdot\mathsf{P}}{4Mm_*} \right) \rho \exp\left(-\beta\frac{m\boldsymbol{Q}\cdot\mathsf{P}}{4Mm_*} \right) e^{-i\boldsymbol{Q}\cdot\mathsf{X}/\hbar} - \frac{1}{2} \left\{ \exp\left(-\beta\frac{m\boldsymbol{Q}\cdot\mathsf{P}}{2Mm_*} \right), \rho \right\} \right].
\end{aligned}
$$

For a small mass ratio $m/M \ll 1$ this yields finally

$$
\begin{aligned}
\mathcal{L}\rho &= \frac{n_{\text{gas}}}{m} \frac{\sigma_{\text{tot}}}{4\pi} \int \frac{\mathrm{d}\boldsymbol{Q}}{Q} \int_{\boldsymbol{Q}^\perp} \mathrm{d}\boldsymbol{p}\, \mu_\beta \left(\boldsymbol{p}_{\perp\boldsymbol{Q}} + \frac{\boldsymbol{Q}}{2} \right) \\
&\times \left[e^{i\boldsymbol{Q}\cdot\mathsf{X}/\hbar} \exp\left(-\beta\frac{\boldsymbol{Q}\cdot\mathsf{P}}{4M} \right) \rho \exp\left(-\beta\frac{\boldsymbol{Q}\cdot\mathsf{P}}{4M} \right) e^{-i\boldsymbol{Q}\cdot\mathsf{X}/\hbar} - \frac{1}{2} \left\{ \exp\left(-\beta\frac{\boldsymbol{Q}\cdot\mathsf{P}}{2M} \right), \rho \right\} \right],
\end{aligned} \tag{11}
$$

which we will use as the starting point for expanding in X and P. The main requirement for the expansion is the assumption that the change in momentum of the Brownian particle is small compared to the scales involved in its motional state. More specifically, one has to assume that for typical values of the momentum transfer Q the relevant matrix elements of the statistical operator vanish unless

$$
\frac{Q}{\hbar}\Delta X \ll 1 \qquad \text{and} \qquad \frac{\beta Q}{M}\Delta P \ll 1.
$$

These conditions are both satisfied if the Brownian state is close to thermal and $M \gg m$ since the momentum transfer Q is then typically of the order of the momentum of the colliding gas

particles $p_\beta = \sqrt{2m/\beta}$. This implies in particular that

$$\frac{Q}{\hbar} \approx \sqrt{\frac{m}{2\pi\hbar^2\beta}} = \frac{1}{\lambda_{\text{th}}^{\text{gas}}} \ll \frac{1}{\lambda_{\text{th}}} \lesssim \frac{1}{\Delta X}$$

and

$$\frac{\beta Q}{M} \approx \sqrt{\frac{m}{M}}\sqrt{\frac{\beta}{M}} \ll \sqrt{\frac{\beta}{M}} \lesssim \frac{1}{\Delta P}.$$

Expanding the terms in the square brackets of (11) one thus arrives at

$$-\frac{1}{2}\sum_{i,j=1}^3 Q_i Q_j \left[\frac{1}{\hbar^2}[\mathsf{X}_i,[\mathsf{X}_j,\rho]] + \left(\frac{\beta}{4M}\right)^2 [\mathsf{P}_i,[\mathsf{P}_j,\rho]] + \frac{i}{\hbar}\frac{\beta}{2M}[\mathsf{X}_i,\{\mathsf{P}_j,\rho\}]\right],$$

where a term linear in the momentum transfer has been omitted since it vanishes upon the integration in (11). It follows that one has to evaluate the integrals

$$\eta_{ij} = \frac{\beta}{2M}\frac{n_{\text{gas}}}{m}\frac{\sigma_{\text{tot}}}{4\pi}\int\frac{\mathrm{d}\boldsymbol{Q}}{Q}\int_{\boldsymbol{Q}^\perp}\mathrm{d}\boldsymbol{p}\,\mu_\beta\left(\boldsymbol{p}_{\perp\boldsymbol{Q}}+\frac{\boldsymbol{Q}}{2}\right)Q_iQ_j,$$

$$= \delta_{ij}\frac{\beta}{6M}\frac{n_{\text{gas}}}{m}\frac{\sigma_{\text{tot}}}{4\pi}\int\mathrm{d}Q\,Q\int_{\boldsymbol{Q}^\perp}\mathrm{d}\boldsymbol{p}\,\mu_\beta\left(\boldsymbol{p}_{\perp\boldsymbol{Q}}+\frac{\boldsymbol{Q}}{2}\right) = \delta_{ij}\eta.$$

The coefficient η is given by

$$\eta = \frac{\beta}{6M}\frac{n_{\text{gas}}}{m}\frac{\sigma_{\text{tot}}}{4\pi}\int\mathrm{d}Q\,Q\mathrm{e}^{-\beta Q^2/(8m)}\int_{\boldsymbol{Q}^\perp}\mathrm{d}\boldsymbol{p}\,\mu_\beta\left(\boldsymbol{p}_{\perp\boldsymbol{Q}}\right) = \frac{16}{3}n_{\text{gas}}\sigma_{\text{tot}}\sqrt{\frac{mk_{\text{B}}T}{2\pi M^2}}. \tag{12}$$

The final result thus takes the form

$$\mathcal{L}\rho = -\frac{i}{\hbar}\frac{\eta}{2}\sum_{i=1}^3[\mathsf{X}_i,\{\mathsf{P}_i,\rho\}] - \frac{D_{pp}}{\hbar^2}\sum_{i=1}^3[\mathsf{X}_i,[\mathsf{X}_i,\rho]] - \frac{D_{xx}}{\hbar^2}\sum_{i=1}^3[\mathsf{P}_i,[\mathsf{P}_i,\rho]], \tag{13}$$

which is an extended version of the Caldeira-Leggett equation. In the original master equation the third term is absent, $D_{xx} = 0$, and η is a phenomenological parameter. In contrast, the diffusive limit of the quantum linear Boltzmann equation yielded a microscopically defined friction constant (12), and also the diffusion coefficients D_{pp} and D_{xx} are directly related to η,

$$D_{pp} = \eta M k_{\text{B}}T \tag{14}$$

and

$$D_{xx} = \eta\frac{\hbar^2}{16Mk_BT} = \left(\frac{\hbar}{4Mk_{\text{B}}T}\right)^2 D_{pp}. \tag{15}$$

Equation (14) is the expected expression of the fluctuation-dissipation relation, while the coefficient (15) of the "position-diffusion term" $\sum_i[\mathsf{P}_i,[\mathsf{P}_i,\rho]]$ has just the minimal value required to ensure the preservation of the positivity of the statistical operator with elapsing time [9]. Since this new contribution appears only in the quantum case, it cannot be read out from the classical Fokker-Planck equation and had to be fixed on the basis of a microscopic derivation at the quantum level, as pointed out in [16]. Note in particular, that Diósi's form of the linear quantum Boltzmann equation [12] leads to a different expression of the coefficient D_{xx}, which is not just a function of η and T.

Concerning the comparison with the classical Brownian motion, the considered case of a constant scattering cross-section applies in the classical formulation to perfectly rigid spheres [32], and in that case the relevant classical scattering cross-section is the geometric one, $\sigma_{\text{tot}}^{\text{cl}} = \pi R^2$, with R radius of the sphere. We have just shown that the same friction coefficient appears for a constant scattering cross-section in the quantum case provided $R \gg \lambda_{\text{th}}^{\text{gas}}$, due to the fact that the forward scattering contribution then cancels out in the master-equation [33,34]. To see how the particular choice (15) of D_{xx} relates to the classical description it is now helpful to consider equation (13) in the Wigner-Weyl phase space formulation.

3.2 Phase space description

In view of the appearance of a quantum mechanically required "position-diffusion" term in the expression (13) it is of interest to follow the transition from quantum linear Boltzmann equation to quantum Fokker-Planck by means of the Wigner function [35], which despite the fact that it is not a proper probability density allows for a classical phase-space picture of the quantum dynamics. As usual, we denote the Wigner function associated to a statistical operator ρ as

$$W\left(\boldsymbol{X},\boldsymbol{P}\right) = \int \frac{\mathrm{d}\boldsymbol{K}}{\left(2\pi\hbar\right)^3} \mathrm{e}^{i\boldsymbol{X}\cdot\boldsymbol{K}/\hbar} \left\langle \boldsymbol{P} + \frac{\boldsymbol{K}}{2}|\rho|\boldsymbol{P} - \frac{\boldsymbol{K}}{2}\right\rangle. \tag{16}$$

Equation (11) then reads

$$\begin{aligned}
\frac{\partial}{\partial t}W\left(\boldsymbol{X},\boldsymbol{P}\right) ={}& n_{\mathrm{gas}}\frac{\sigma_{\mathrm{tot}}}{4\pi}\frac{m}{m_*^2}\int\frac{\mathrm{d}\boldsymbol{Q}}{Q}\int_{\boldsymbol{Q}^\perp}\mathrm{d}\boldsymbol{p}\,\mu_\beta\left(\boldsymbol{p}_{\perp\boldsymbol{Q}}+\frac{\boldsymbol{Q}}{2}\right)\int\frac{\mathrm{d}\boldsymbol{K}}{\left(2\pi\hbar\right)^3}\mathrm{e}^{i\boldsymbol{X}\cdot\boldsymbol{K}/\hbar} \\
&\times\left[\exp\left(-\beta\frac{\boldsymbol{Q}\cdot\left(\boldsymbol{P}-\boldsymbol{Q}\right)}{2M}\right)\left\langle\boldsymbol{P}-\boldsymbol{Q}+\frac{\boldsymbol{K}}{2}|\rho|\boldsymbol{P}-\boldsymbol{Q}-\frac{\boldsymbol{K}}{2}\right\rangle\right. \\
&\left.-\exp\left(-\beta\frac{\boldsymbol{Q}\cdot\left(\boldsymbol{P}+\boldsymbol{K}/2\right)}{2M}\right)\left\langle\boldsymbol{P}+\frac{\boldsymbol{K}}{2}|\rho|\boldsymbol{P}-\frac{\boldsymbol{K}}{2}\right\rangle\right. \\
&\left.-\exp\left(-\beta\frac{\boldsymbol{Q}\cdot\left(\boldsymbol{P}-\boldsymbol{K}/2\right)}{2M}\right)\left\langle\boldsymbol{P}+\frac{\boldsymbol{K}}{2}|\rho|\boldsymbol{P}-\frac{\boldsymbol{K}}{2}\right\rangle\right].
\end{aligned}$$

A closed equation for $W\left(\boldsymbol{X},\boldsymbol{P}\right)$ is obtained by inserting the inverse of (16),

$$\begin{aligned}
\frac{\partial}{\partial t}W\left(\boldsymbol{X},\boldsymbol{P}\right) ={}& n_{\mathrm{gas}}\frac{\sigma_{\mathrm{tot}}}{4\pi}\frac{m}{m_*^2}\int\frac{\mathrm{d}\boldsymbol{Q}}{Q}\int_{\boldsymbol{Q}^\perp}\mathrm{d}\boldsymbol{p}\,\mu_\beta\left(\boldsymbol{p}_{\perp\boldsymbol{Q}}+\frac{\boldsymbol{Q}}{2}\right) \\
&\times\left[\exp\left(-\beta\frac{\boldsymbol{Q}\cdot\left(\boldsymbol{P}-\boldsymbol{Q}\right)}{2M}\right)W\left(\boldsymbol{X},\boldsymbol{P}-\boldsymbol{Q}\right)\right. \\
&\left.-\exp\left(-\beta\frac{\boldsymbol{Q}\cdot\boldsymbol{P}}{2M}\right)\cosh\left(\frac{\beta\hbar}{4M}\boldsymbol{Q}\cdot\nabla_{\boldsymbol{X}}\right)W\left(\boldsymbol{X},\boldsymbol{P}\right)\right] \\
={}& n_{\mathrm{gas}}\frac{\sigma_{\mathrm{tot}}}{4\pi}\frac{m}{m_*^2}\int\frac{\mathrm{d}\boldsymbol{Q}}{Q}\int_{\boldsymbol{Q}^\perp}\mathrm{d}\boldsymbol{p}\,\mu_\beta\left(\boldsymbol{p}_{\perp\boldsymbol{Q}}+\frac{\boldsymbol{Q}}{2}\right) \\
&\times\left[\exp\left(-\boldsymbol{Q}\cdot\nabla_{\boldsymbol{P}}\right)-\cosh\left(\frac{\beta\hbar}{4M}\boldsymbol{Q}\cdot\nabla_{\boldsymbol{X}}\right)\right]\exp\left(-\beta\frac{\boldsymbol{Q}\cdot\boldsymbol{P}}{2M}\right)W\left(\boldsymbol{X},\boldsymbol{P}\right),
\end{aligned}$$

where cosh denotes the hyperbolic cosine. The equation can now be written more compactly as

$$\begin{aligned}
\frac{\partial}{\partial t}W\left(\boldsymbol{X},\boldsymbol{P}\right) ={}& n_{\mathrm{gas}}\frac{\sigma_{\mathrm{tot}}}{4\pi}\frac{m}{m_*^2}\int\frac{\mathrm{d}\boldsymbol{Q}}{Q}\int_{\boldsymbol{Q}^\perp}\mathrm{d}\boldsymbol{p}\,\mu_\beta\left(\boldsymbol{p}_{\perp\boldsymbol{Q}}+\frac{\boldsymbol{Q}}{2}\right) \\
&\times\left[\exp\left(-\boldsymbol{Q}\cdot\nabla_{\boldsymbol{P}}\right)-\cosh\left(\frac{\beta\hbar}{4M}\boldsymbol{Q}\cdot\nabla_{\boldsymbol{X}}\right)\right]\exp\left(-\beta\frac{\boldsymbol{Q}\cdot\boldsymbol{P}}{2M}\right)W\left(\boldsymbol{X},\boldsymbol{P}\right)
\end{aligned} \tag{17}$$

where we have used the unitary differential operators $\exp\left(-\boldsymbol{Q}\cdot\nabla_{\boldsymbol{P}}\right)$ and $\exp(\beta\hbar/\left(4M\right)\boldsymbol{Q}\cdot\nabla_{\boldsymbol{X}})$ effecting a shift in momentum and position, respectively, of the arguments of the Wigner function. As one can check, equation (17) differs from the corresponding classical expression of the linear Boltzmann equation [36] just by the hyperbolic cosine term, which in the classical case is replaced by unity, as one would obtain in the naive classical limit $\hbar \to 0$. An expansion up to second order of the exponential operators appearing in the kernel of (17) transforms the integro-differential equation for the Wigner function into a partial differential equation. It is the phase space representation of equation (13) and reads,

$$\frac{\partial}{\partial t}W\left(\boldsymbol{X},\boldsymbol{P}\right) = \eta\nabla_{\boldsymbol{P}}\cdot\left(\boldsymbol{P}W\left(\boldsymbol{X},\boldsymbol{P}\right)\right) + D_{pp}\Delta_{\boldsymbol{P}}W\left(\boldsymbol{X},\boldsymbol{P}\right) + D_{xx}\Delta_{\boldsymbol{X}}W\left(\boldsymbol{X},\boldsymbol{P}\right).$$

This is the quantum counterpart of the classical Fokker-Planck equation, for the time evolution of the probability density $f_{\mathrm{cl}}(\boldsymbol{X}, \boldsymbol{P})$ in phase-space,

$$\frac{\partial}{\partial t} f_{\mathrm{cl}}(\boldsymbol{X}, \boldsymbol{P}) = \eta \nabla_{\boldsymbol{P}} \cdot (\boldsymbol{P} f_{\mathrm{cl}}(\boldsymbol{X}, \boldsymbol{P})) + D_{pp} \Delta_{\boldsymbol{P}} f_{\mathrm{cl}}(\boldsymbol{X}, \boldsymbol{P}).$$

The quantum and the classical phase space equations for Brownian motion thus differ again by the appearance of a "position-diffusion" term, which is symmetric with respect to the regular diffusion term.

4 Diffusive limit in the Heisenberg picture

In the previous paragraphs we understood the quantum linear Boltzmann equation as a mapping $\mathcal{L}$ acting on the statistical operator, thus working in the Schrödinger picture. In the same spirit we considered its diffusive limit, which led to the quantum counterpart of the classical Fokker-Planck equation. In the following we will consider its adjoint mapping $\mathcal{L}^*$ for the time evolution of observables. It is defined through the relation

$$\mathrm{Tr}(\mathsf{A}\mathcal{L}\rho) = \mathrm{Tr}(\rho\mathcal{L}^*\mathsf{A}),$$

where the trace operation expresses the duality relation between the space of trace class operators, which contains the states given by statistical operators ρ, and its dual, the space of bounded operators A characterizing observables.

Using the form (2)–(3) of $\mathcal{L}$ this leads to the explicit identification

$$\mathcal{L}^*\mathsf{A} = \int \mathrm{d}\boldsymbol{Q} \int_{\boldsymbol{Q}^\perp} \mathrm{d}\boldsymbol{p} \left[L^\dagger(\boldsymbol{p}, \mathsf{P}; \boldsymbol{Q}) \, \mathrm{e}^{-i\boldsymbol{Q}\cdot\mathsf{X}/\hbar} \mathsf{A} \mathrm{e}^{i\boldsymbol{Q}\cdot\mathsf{X}/\hbar} L(\boldsymbol{p}, \mathsf{P}; \boldsymbol{Q}) - \frac{1}{2} \left\{ L^\dagger(\boldsymbol{p}, \mathsf{P}; \boldsymbol{Q}) L(\boldsymbol{p}, \mathsf{P}; \boldsymbol{Q}), \mathsf{A} \right\} \right]. \tag{18}$$

The full differential equation for the time evolution of an Heisenberg operator A_t is thus given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathsf{A}_t = \frac{1}{i\hbar}\left[\mathsf{A}_t, \frac{\mathsf{P}^2}{2M}\right] + \int \mathrm{d}\boldsymbol{Q} \int_{\boldsymbol{Q}^\perp} \mathrm{d}\boldsymbol{p} \left[L^\dagger(\boldsymbol{p}, \mathsf{P}; \boldsymbol{Q}) \, \mathrm{e}^{-i\boldsymbol{Q}\cdot\mathsf{X}/\hbar} \mathsf{A}_t \mathrm{e}^{i\boldsymbol{Q}\cdot\mathsf{X}/\hbar} L(\boldsymbol{p}, \mathsf{P}; \boldsymbol{Q}) \right.$$
$$\left. - \frac{1}{2}\left\{ L^\dagger(\boldsymbol{p}, \mathsf{P}; \boldsymbol{Q}) L(\boldsymbol{p}, \mathsf{P}; \boldsymbol{Q}), \mathsf{A}_t \right\} \right].$$

We will take the Heisenberg operator to coincide with the corresponding Schrödinger observable at $t = 0$, i.e., $\mathsf{A}_0 = \mathsf{A}$.

An important class of Schrödinger picture observables are those which are only functions of the momentum operator, $\mathsf{A} = A(\mathsf{P})$. The equation of motion in the Heisenberg picture then simplifies considerably,

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathsf{A}_t = \int \mathrm{d}\boldsymbol{Q} \int_{\boldsymbol{Q}^\perp} \mathrm{d}\boldsymbol{p} \, |L(\boldsymbol{p}, \mathsf{P}; \boldsymbol{Q})|^2 \left[\mathrm{e}^{-i\boldsymbol{Q}\cdot\mathsf{X}/\hbar} \mathsf{A}_t \mathrm{e}^{i\boldsymbol{Q}\cdot\mathsf{X}/\hbar} - \mathsf{A}_t \right].$$

Note that $\mathcal{L}$, and equivalently $\mathcal{L}^*$, is covariant under translations [22] in the sense that

$$\mathcal{L}\left[\mathrm{e}^{-i\boldsymbol{b}\cdot\mathsf{P}/\hbar} \rho \mathrm{e}^{i\boldsymbol{b}\cdot\mathsf{P}/\hbar} \right] = \mathrm{e}^{-i\boldsymbol{b}\cdot\mathsf{P}/\hbar} \mathcal{L}[\rho] \, \mathrm{e}^{i\boldsymbol{b}\cdot\mathsf{P}/\hbar}.$$

It follows that the algebra generated by the momentum operator is left invariant. Consequently, $\mathsf{A}_0 = A_0(\mathsf{P})$ implies $\mathsf{A}_t = A_t(\mathsf{P})$ for $t > 0$ and therefore $[\mathsf{A}_t, \mathsf{P}] = 0$. In particular, recalling the definition of the quantum and the classical in-rates in (6) and (7), respectively, we find that observables given by a function of momentum obey

$$\frac{\mathrm{d}}{\mathrm{d}t}A_t(\mathsf{P}) = \int \mathrm{d}\boldsymbol{Q} M_{\mathrm{in}}^{\mathrm{cl}}(\mathsf{P} + \boldsymbol{Q}; \boldsymbol{Q}) \left[\mathrm{e}^{-i\boldsymbol{Q}\cdot\mathsf{X}/\hbar} A_t(\mathsf{P}) \mathrm{e}^{i\boldsymbol{Q}\cdot\mathsf{X}/\hbar} - A_t(\mathsf{P}) \right]$$
$$= \int \mathrm{d}\boldsymbol{Q} M_{\mathrm{in}}^{\mathrm{cl}}(\mathsf{P} + \boldsymbol{Q}; \boldsymbol{Q}) \left[A_t(\mathsf{P} + \boldsymbol{Q}) - A_t(\mathsf{P}) \right],$$

in strict analogy with the classical formulation.

We now focus on the time evolution of the expectation values of momentum and kinetic energy, $A(\mathsf{P}) = \mathsf{P}$ and $A(\mathsf{P}) = \mathsf{P}^2/(2M)$, respectively. We shall first obtain the explicit dynamic equations and then the limiting form corresponding to the diffusive limit. Starting from the expression for the time evolution of expectation values,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \mathsf{A}\rangle_{\rho_t} := \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Tr}\,(\mathsf{A}\rho_t) = \mathrm{Tr}\,(\mathsf{A}\mathcal{L}\rho_t) = \mathrm{Tr}\,(\rho_t\mathcal{L}^*\mathsf{A}),\tag{19}$$

we can now exploit the fact that functions of the momentum operator are mapped by $\mathcal{L}^*$ to functions of the momentum operator. Specifically, it is convenient to first evaluate

$$\mathcal{L}^*\,[A(\mathsf{P})] = \int \mathrm{d}\boldsymbol{Q}\, M_{\mathrm{in}}^{\mathrm{cl}}(\boldsymbol{P}+\boldsymbol{Q};\boldsymbol{Q})\,[A(\boldsymbol{P}+\boldsymbol{Q}) - A(\mathsf{P})],\tag{20}$$

which can be easily dealt with as an equation for $\mathbb{C}$-numbers, by working in the momentum basis. Moreover, assuming that the scattering cross-section is invariant under parity transformations the scattering rate (7) satisfies

$$\begin{aligned}M_{\mathrm{in}}^{\mathrm{cl}}(\boldsymbol{P}+\boldsymbol{Q};\boldsymbol{P}) &\equiv M_{\mathrm{in}}^{\mathrm{cl}}(\boldsymbol{P}\to\boldsymbol{P}+\boldsymbol{Q})\\ &= M_{\mathrm{in}}^{\mathrm{cl}}(-\boldsymbol{P}\to-\boldsymbol{P}-\boldsymbol{Q})\\ &\equiv M_{\mathrm{in}}^{\mathrm{cl}}(-\boldsymbol{P}-\boldsymbol{Q};-\boldsymbol{Q}),\end{aligned}\tag{21}$$

so that the operator $\mathcal{L}^*\,[A(\mathsf{P})]$ has the same parity as $A(\mathsf{P})$. According to our convention momentum or energy transfers are positive when the test particle gains momentum or energy. The fact that $M_{\mathrm{in}}^{\mathrm{cl}}$ is positive thus ensures the obvious physical requirement that the change of momentum is positive when the momentum transfer is positive, and likewise that a positive energy transfer increases the energy. In fact, for $A(\boldsymbol{P}) = \boldsymbol{P}$ the quantity $[A(\boldsymbol{P}+\boldsymbol{Q}) - A(\boldsymbol{P})]$ is simply the momentum transfer in the single collision, while for $A(\boldsymbol{P}) = P^2/(2M)$ the quantity $[A(\boldsymbol{P}+\boldsymbol{Q}) - A(\boldsymbol{P})]$ is the energy transfer $E(\boldsymbol{Q},\boldsymbol{P}) = (\boldsymbol{P}+\boldsymbol{Q})^2/(2M) - P^2/(2M)$ in a single collision with momentum gain $\boldsymbol{Q}$.

Let us first write the explicit expression for $M_{\mathrm{in}}^{\mathrm{cl}}(\boldsymbol{P}+\boldsymbol{Q};\boldsymbol{P})$ for a gas described by the Maxwell-Boltzmann distribution (5):

$$\begin{aligned}M_{\mathrm{in}}^{\mathrm{cl}}(\boldsymbol{P}+\boldsymbol{Q};\boldsymbol{Q}) &= \frac{n_{\mathrm{gas}}m}{m_*^2 Q}\int_{\boldsymbol{Q}^\perp}\mathrm{d}\boldsymbol{p}\,\mu_\beta\left(\boldsymbol{p}_{\perp\boldsymbol{Q}}+\frac{m}{m_*}\frac{\boldsymbol{Q}}{2}+\frac{m}{M}\boldsymbol{P}_{\parallel\boldsymbol{Q}}\right)\\ &\quad\times\sigma\left(\mathrm{rel}\,(\boldsymbol{p}_{\perp\boldsymbol{Q}},\boldsymbol{P}_{\perp\boldsymbol{Q}})-\frac{\boldsymbol{Q}}{2},\mathrm{rel}\,(\boldsymbol{p}_{\perp\boldsymbol{Q}},\boldsymbol{P}_{\perp\boldsymbol{Q}})+\frac{\boldsymbol{Q}}{2}\right).\end{aligned}\tag{22}$$

Inserting this into equation (20) invites the more compact notation

$$\tilde\sigma(\boldsymbol{P}_{\perp\boldsymbol{Q}},\boldsymbol{Q}) \equiv \int_{\boldsymbol{Q}^\perp}\mathrm{d}\boldsymbol{p}\,\mu_\beta(\boldsymbol{p}_{\perp\boldsymbol{Q}})\,\sigma\left(\mathrm{rel}\,(\boldsymbol{p}_{\perp\boldsymbol{Q}},\boldsymbol{P}_{\perp\boldsymbol{Q}})-\frac{\boldsymbol{Q}}{2},\mathrm{rel}\,(\boldsymbol{p}_{\perp\boldsymbol{Q}},\boldsymbol{P}_{\perp\boldsymbol{Q}})+\frac{\boldsymbol{Q}}{2}\right),\tag{23}$$

so that we can write

$$\begin{aligned}\mathcal{L}^*\,[A(\mathsf{P})] = \frac{n_{\mathrm{gas}}}{m_*^2}\sqrt{\frac{\beta m}{2\pi}}\int\frac{\mathrm{d}\boldsymbol{Q}}{Q}\tilde\sigma(\mathsf{P}_\perp,\boldsymbol{Q})\exp\left(-\beta\frac{mQ^2}{8m_*^2}-\beta\frac{m\mathsf{P}_{\parallel\boldsymbol{Q}}^2}{2M^2}-\beta\frac{m\boldsymbol{Q}\cdot\mathsf{P}}{2Mm_*}\right)\\ \times[A(\mathsf{P}+\boldsymbol{Q})-A(\mathsf{P})].\end{aligned}\tag{24}$$

We now proceed to evaluate this expression explicitly for the case of the momentum and the kinetic energy observable, by considering the special case of a constant scattering cross-section, $\left|f(\boldsymbol{p}_f,\boldsymbol{p}_i)\right|^2 = \sigma_{\mathrm{tot}}/4\pi$, as in section 3. In the momentum case, $A(\mathsf{P}) = \mathsf{P}$, it is advantageous to rescale by the reference value Mv_β, where $v_\beta = p_\beta/m = \sqrt{2/(\beta m)}$ is the most probable velocity of the gas particles.

$$\begin{aligned}\mathcal{L}^*\left[\frac{\mathsf{P}}{Mv_\beta}\right] = \frac{n_{\mathrm{gas}}}{\sqrt{\pi}m_*^2 v_\beta^2 M}\frac{\sigma_{\mathrm{tot}}}{4\pi}\int\mathrm{d}\boldsymbol{Q}\frac{\boldsymbol{Q}}{Q}\exp\left(-\beta\frac{mQ^2}{8m_*^2}-\beta\frac{m\mathsf{P}_{\parallel\boldsymbol{Q}}^2}{2M^2}-\beta\frac{m\boldsymbol{Q}\cdot\mathsf{P}}{2Mm_*}\right)\\ \equiv I_1.\end{aligned}\tag{25}$$

Similarly, for the kinetic energy $A(\mathsf{P}) = \mathsf{P}^2/(2M)$ the expression (24) leads to

$$\mathcal{L}^* \left[\frac{1}{2M} \left(\frac{\mathsf{P}}{Mv_\beta} \right)^2 \right] = \frac{n_{\text{gas}}}{\sqrt{\pi} m_*^2 v_\beta^3 M^2} \frac{\sigma_{\text{tot}}}{4\pi} \int \frac{\mathrm{d}\boldsymbol{Q}}{Q} \exp \left(-\beta \frac{mQ^2}{8m_*^2} - \beta \frac{m\mathsf{P}_{\|\boldsymbol{Q}}^2}{2M^2} - \beta \frac{m\boldsymbol{Q} \cdot \mathsf{P}}{2Mm_*} \right)$$
$$\times \left[\frac{Q^2}{2M} + \frac{\mathsf{P} \cdot \boldsymbol{Q}}{M} \right] \equiv I_2. \tag{26}$$

The evaluation of I_1 and I_2 is most easily done by focussing on their functional expression, thus determining them as functions of the dimensionless variable

$$\boldsymbol{U} = \frac{\boldsymbol{P}}{Mv_\beta} = \frac{\boldsymbol{V}}{v_\beta},$$

and carrying out the integration over the scaled momentum transfer $\boldsymbol{K}$

$$\boldsymbol{K} = \frac{\boldsymbol{Q}}{m_* v_\beta}.$$

From the right hand side of (25) we have

$$I_1(\boldsymbol{U}) = n_{\text{gas}} \frac{\sigma_{\text{tot}}}{4\pi} \frac{v_\beta}{\sqrt{\pi}} \frac{m_*}{M} \int \mathrm{d}\boldsymbol{K} \frac{\boldsymbol{K}}{K} \exp \left(-K^2 \left(\frac{1}{2} + \frac{\boldsymbol{U} \cdot \boldsymbol{K}}{K^2} \right)^2 \right), \tag{27}$$

and writing

$$\boldsymbol{K} = \boldsymbol{K}_{\|\boldsymbol{U}} + \boldsymbol{K}_{\perp\boldsymbol{U}}$$

one finds that only $\boldsymbol{K}_{\|\boldsymbol{U}}$, i.e., the component parallel to $\boldsymbol{U}$, contributes to (27). We are thus left with

$$I_1(\boldsymbol{U}) = n_{\text{gas}} \frac{\sigma_{\text{tot}}}{4\pi} \frac{v_\beta}{\sqrt{\pi}} \frac{m_*}{M} \int \mathrm{d}\boldsymbol{K} \frac{\boldsymbol{K}_{\|\boldsymbol{U}}}{K} \exp \left(-K^2 \left(\frac{1}{2} + \frac{\boldsymbol{U} \cdot \boldsymbol{K}}{K^2} \right)^2 \right).$$

Taking now the direction of $\boldsymbol{U}$ as the polar axis and denoting by ξ the cosine of the angle between $\boldsymbol{K}$ and $\boldsymbol{U}$ we have to evaluate

$$I_1(\boldsymbol{U}) = n_{\text{gas}} \frac{\sigma_{\text{tot}}}{4\pi} \frac{v_\beta}{\sqrt{\pi}} \frac{m_*}{M} 2\pi \frac{\boldsymbol{U}}{U} \int_0^{+\infty} \mathrm{d}K K^2 \int_{-1}^{+1} \mathrm{d}\xi\, \xi \mathrm{e}^{-(K/2+U\xi)^2}$$
$$= -n_{\text{gas}} \frac{\sigma_{\text{tot}}}{4\pi} \sqrt{\frac{8\pi}{m\beta}} \frac{m_*}{M} \frac{\boldsymbol{U}}{U} \int_0^{+\infty} \mathrm{d}K K^2 \mathrm{e}^{-K^2/4} \tag{28}$$
$$\times \left\{ \frac{\sqrt{\pi}K}{4U^2} \mathrm{e}^{K^2/4} \left[\mathrm{erf} \left(\frac{K}{2} + U \right) - \mathrm{erf} \left(\frac{K}{2} - U \right) \right] - \frac{\mathrm{e}^{-U^2}}{U^2} \sinh(UK) \right\}$$
$$= -n_{\text{gas}} \frac{\sigma_{\text{tot}}}{4\pi} \sqrt{\frac{8\pi}{m\beta}} \frac{m_*}{M} \frac{\boldsymbol{U}}{U^2} \left\{ [1 + 2U^2] \mathrm{e}^{-U^2} - [1 - 4U^2 - 4U^4] \frac{\sqrt{\pi}}{2} \frac{\mathrm{erf}(U)}{U} \right\}.$$

Here, $\mathrm{erf}(x) = 2\pi^{-\frac{1}{2}} \int_0^x \exp\left(-t^2\right) \mathrm{d}t$ denotes the error function. The expression (28) can be further simplified and expressed more compactly by means of the confluent hypergeometric function $_1F_1$, in particular by using the known expression of $_1F_1(\alpha, \gamma; z)$ for indexes $\alpha = -1/2$ and $\gamma = 5/2$ [37],

$$_1F_1 \left(-\frac{1}{2}, \frac{5}{2}; -U^2 \right) = \frac{3}{16} \frac{1}{U^2} \left\{ [1 + 2U^2] \mathrm{e}^{-U^2} - [1 - 4U^2 - 4U^4] \frac{\sqrt{\pi}}{2} \frac{\mathrm{erf}(U)}{U} \right\}. \tag{29}$$

This way (28) finally becomes

$$I_1\left(\boldsymbol{U}\right) = -n_{\text{gas}}\frac{\sigma_{\text{tot}}}{4\pi}\frac{16}{3}\sqrt{\frac{8\pi}{m\beta}}\frac{m_*}{M}\boldsymbol{U}{}_1F_1\left(-\frac{1}{2},\frac{5}{2};-U^2\right),\tag{30}$$

with ${}_1F_1\left(-\frac{1}{2},\frac{5}{2};-U^2\right)$ a positive, monotonically increasing function.

For the rescaled kinetic energy one has to consider the r.h.s. of (26), so that the function I_2 is given by

$$I_2\left(U^2\right) = 2n_{\text{gas}}\frac{\sigma_{\text{tot}}}{4\pi}\frac{v_\beta}{\sqrt{\pi}}\frac{m_*}{M}\int \mathrm{d}\boldsymbol{K}\exp\left(-K^2\left(\frac{1}{2}+\frac{\boldsymbol{U}\cdot\boldsymbol{K}}{K^2}\right)^2\right)\left[\frac{1}{2}\frac{m_*}{M}K+\frac{\boldsymbol{U}\cdot\boldsymbol{K}}{K}\right].$$

As before, we take the direction of $\boldsymbol{U}$ as polar axis and denote by ξ the cosine of the angle between $\boldsymbol{K}$ and $\boldsymbol{U}$. This way,

$$\begin{aligned}
I_2\left(U^2\right) &= 2n_{\text{gas}}\frac{\sigma_{\text{tot}}}{4\pi}\sqrt{\frac{8\pi}{m\beta}}\frac{m_*}{M}\int_0^{+\infty}\mathrm{d}KK^2\int_{-1}^{+1}\mathrm{d}\xi\,\mathrm{e}^{-(K/2+U\xi)^2}\left[\frac{1}{2}\frac{m_*}{M}K+U\xi\right]\\
&= -2n_{\text{gas}}\frac{\sigma_{\text{tot}}}{4\pi}\sqrt{\frac{8\pi}{m\beta}}\frac{m_*}{M}\int_0^{+\infty}\mathrm{d}KK^2\mathrm{e}^{-K^2/4}\\
&\quad\times\left\{\left(1-\frac{m_*}{M}\right)\frac{\sqrt{\pi}K}{4U}\mathrm{e}^{-K^2/4}\left[\mathrm{erf}\left(\frac{K}{2}+U\right)-\mathrm{erf}\left(\frac{K}{2}-U\right)\right]-\frac{\mathrm{e}^{-U^2}}{U}\sinh(UK)\right\}\\
&= -2n_{\text{gas}}\frac{\sigma_{\text{tot}}}{4\pi}\sqrt{\frac{8\pi}{m\beta}}\frac{m_*}{M}\left\{\left[1+2U^2\right]\mathrm{e}^{-U^2}-\left[1-4U^4-4U^2\right]\frac{\sqrt{\pi}}{2}\frac{\mathrm{erf}(U)}{U}\right.\\
&\quad\left.-\frac{m_*}{M}\left(\left[5+2U^2\right]\mathrm{e}^{-U^2}+\left[3+12U^2+4U^4\right]\frac{\sqrt{\pi}}{2}\frac{\mathrm{erf}\left(U\right)}{U}\right)\right\}.
\end{aligned}$$

Also this expression can be written much more compactly by exploiting again (29), as well as the known expression of ${}_1F_1\left(-\frac{1}{2},\frac{3}{2};-U^2\right)$, as given in [37], and the functional relations between confluent hypergeometric functions with different indexes [38]. This yields

$$_1F_1\left(-\frac{3}{2},\frac{3}{2};-U^2\right) = \frac{1}{8}\left\{\left[5+2U^2\right]\mathrm{e}^{-U^2}+\left[3+12U^2+4U^4\right]\frac{\sqrt{\pi}}{2}\frac{\mathrm{erf}\left(U\right)}{U}\right\},\tag{31}$$

and therefore

$$I_2\left(U^2\right) = -2n_{\text{gas}}\frac{\sigma_{\text{tot}}}{4\pi}\frac{16}{3}\sqrt{\frac{8\pi}{m\beta}}\frac{m_*}{M}\left\{U^2{}_1F_1\left(-\frac{1}{2},\frac{5}{2};-U^2\right)-\frac{3}{2}\frac{m_*}{M}{}_1F_1\left(-\frac{3}{2},\frac{3}{2};-U^2\right)\right\},\tag{32}$$

with both ${}_1F_1\left(-\frac{1}{2},\frac{5}{2};-U^2\right)$ and ${}_1F_1\left(-\frac{3}{2},\frac{3}{2};-U^2\right)$ positive and monotonically increasing functions.

Finally, coming back to the operator expression with the original variables (25)–(26) the time evolution of the momentum expectation values satisfies, according to (19),

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\mathsf{P}\rangle_{\rho_t} = -n_{\text{gas}}\frac{\sigma_{\text{tot}}}{4\pi}\frac{16}{3}\sqrt{\frac{8\pi}{m\beta}}\frac{m_*}{M}\left\langle\mathsf{P}{}_1F_1\left(-\frac{1}{2},\frac{5}{2};-\left(\frac{\mathsf{P}}{Mv_\beta}\right)^2\right)\right\rangle_{\rho_t}.\tag{33}$$

Similarly, we have for the kinetic energy $\mathsf{E}=\mathsf{P}^2/\left(2M\right)$

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\langle\mathsf{E}\rangle_{\rho_t} = &-2n_{\text{gas}}\frac{\sigma_{\text{tot}}}{4\pi}\frac{16}{3}\sqrt{\frac{8\pi}{m\beta}}\frac{m_*}{M}\\
&\times\left\langle{}_1F_1\left(-\frac{1}{2},\frac{5}{2};-\beta\mathsf{E}\frac{m}{M}\right)\mathsf{E}-\frac{3}{2\beta}\frac{m_*}{m}{}_1F_1\left(-\frac{3}{2},\frac{3}{2};-\beta\mathsf{E}\frac{m}{M}\right)\right\rangle_{\rho_t}.
\end{aligned}\tag{34}$$

From this it is immediately clear that in general there is no closed evolution equation for either the first or the second moment of the momentum operator, $\langle \mathsf{P} \rangle_{\rho_t}$ or $\langle \mathsf{P}^2 \rangle_{\rho_t}$, since due to the presence of the confluent hypergeometric functions moments of arbitrary high order are involved in the equation.

However, the equations do get closed in the limit of a very massive test particle close to thermal equilibrium, since in this case the velocity $\boldsymbol{V} = \boldsymbol{P}/M$ of the test particle is much smaller than the typical velocity v_β of the gas particles. Thus using $\boldsymbol{V}/v_\beta \ll 1$ and $m/M \ll 1$ in (33) and (34) the confluent hypergeometric functions are replaced by unity, since $_1F_1(\alpha, \gamma; 0) = 1$, and the reduced mass m_* is replaced by m. This leads to

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \mathsf{P} \rangle_{\rho_t} = -n_{\text{gas}} \frac{\sigma_{\text{tot}}}{4\pi} \frac{32}{3M} \sqrt{\frac{2\pi m}{\beta}} \langle \mathsf{P} \rangle_{\rho_t} = -\eta \langle \mathsf{P} \rangle_{\rho_t}$$

which describes velocity-proportional friction with coefficient η leading to the expected exponential relaxation to a mean momentum equal to zero. Similarly,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \mathsf{E} \rangle_{\rho_t} = -2n_{\text{gas}} \frac{\sigma_{\text{tot}}}{4\pi} \frac{32}{3M} \sqrt{\frac{2\pi m}{\beta}} \left(\langle \mathsf{E} \rangle_{\rho_t} - \frac{3}{2\beta} \right) = -2\eta \left(\langle \mathsf{E} \rangle_{\rho_t} - \frac{3}{2\beta} \right)$$

shows that the mean kinetic energy relaxes exponentially to the equipartition value $3/2k_{\text{B}}T$. The relaxation rate

$$\eta = \frac{16}{3} n_{\text{gas}} \sigma_{\text{tot}} \sqrt{\frac{m k_{\text{B}} T}{2\pi M^2}},$$

is equal to the result (12) obtained in section 3 for the considered case of a constant scattering cross-section.

5 Conclusions

In conclusion, we discussed how the "diffusive limit" of the quantum version of the linear Boltzmann equation yields the master equation for quantum Brownian motion, and provides a microscopic formulation of the relaxation and diffusion constants. In particular, we saw that this procedure leads naturally to the *minimal extension* required to turn the Caldeira-Leggett master equation into Lindblad form. The approximations invoked in this limit could be physically justified by using both the operator and the Wigner-Weyl formulation of quantum mechanics in the Schrödinger picture, while the Heisenberg picture provided a dynamic description of the relaxation behaviour. Still, a mathematically more rigorous treatment of the diffusive limit is clearly desirable, together with an extension of the obtained results to the case of an arbitrary scattering cross-section.

References

1. A.O. Caldeira, A.J. Leggett, Physica A **121**, 587 (1983)
2. R.P. Feynman, F.L. Vernon, Ann. Phys. (NY) **24**, 118 (1963)
3. F. Haake, R. Reibold, Phys. Rev. A **32**, 2462 (1985)
4. H. Grabert, P. Schramm, G. Ingold, Phys. Rev. **168**, 115 (1988)
5. W.G. Unruh, W.H. Zurek, Phys. Rev. D **40**, 1071 (1989)
6. B.L. Hu, J.P. Paz, Y. Zhang, Phys. Rev. D **45**, 2843 (1992)
7. A. Tameshtit, J. Sipe, Phys. Rev. Lett. **77**, 2600 (1996)
8. See e.g., K. Hornberger, *Introduction to Decoherence Theory*, eprint quant-ph/0612118

9. H.-P. Breuer, F. Petruccione, *The Theory of Open Quantum Systems* (Oxford University Press, Oxford, 2002)
10. A. Săndulescu, H. Scutaru, Ann. Phys. (NY) **173**, 277 (1987)
11. L. Diósi, Europhys. Lett. **22**, 1 (1993)
12. L. Diósi, Europhys. Lett. **30**, 63 (1995)
13. J. Halliwell, A. Zoupas, Phys. Rev. D **52**, 7294 (1995)
14. S.M. Barnett, J.D. Cresser, Phys. Rev. A **72**, 022107 (2005)
15. C. Cercignani, *Theory and Application of the Boltzmann Equation* (Scottisch Academic Press, Edinburgh, 1975)
16. B. Vacchini, Phys. Rev. Lett. **84**, 1374 (2000)
17. K. Hornberger, Phys. Rev. Lett. **97**, 060601 (2006)
18. E. Joos, H.D. Zeh, Z. Phys. B: Condens. Matter **59**, 223 (1985)
19. M.R. Gallis, G.N. Fleming, Phys. Rev. A **42**, 38 (1990)
20. K. Hornberger, J.E. Sipe, Phys. Rev. A **68**, 012105 (2003)
21. B. Vacchini, Phys. Rev. E **63**, 066115 (2001)
22. B. Vacchini, J. Math. Phys. **42**, 4291 (2001)
23. P.J. Dodd, J.J. Halliwell, Phys. Rev. D **67**, 105018 (2003)
24. K. Hornberger, Europhys. Lett. **77**, 50007 (2007)
25. A.S. Holevo, J. Math. Phys. **37**, 1812 (1996)
26. F. Petruccione, B. Vacchini, Phys. Rev. E **71**, 046134 (2005)
27. B. Vacchini, Phys. Rev. Lett. **95**, 230402 (2005)
28. K. Hornberger, J.E. Sipe, M. Arndt, Phys. Rev. A **70**, 053608 (2004)
29. K. Hornberger, S. Uttenthaler, B. Brezger, L. Hackermüller, M. Arndt, A. Zeilinger, Phys. Rev. Lett. **90**, 160401 (2003)
30. L. Hackermüller, K. Hornberger, B. Brezger, A. Zeilinger, M. Arndt, Appl. Phys. B **77**, 781 (2003)
31. M. Arndt, K. Hornberger, A. Zeilinger, Phys. World **18**, 35 (2005)
32. C.S.W. Chang, G.E. Uhlenbeck, *The Kinetic Theory of Gases*, in *Studies in Statistical Mechanics*, Vol. 5, edited by J.D. Boer (North-Holland, Amsterdam, 1970)
33. L.I. Schiff, *Quantum Mechanics*, 3rd edn. (McGraw-Hill, New York, 1968)
34. S.L. Adler, J. Phys. A: Math. Gen. **39**, 14067 (2006)
35. B. Vacchini, Phys. Rev. E **66**, 027107 (2002)
36. M.M.R. Williams, *The Slowing Down and Thermalization of Neutrons* (North-Holland, Amsterdam, 1966)
37. See e.g., http://functions.wolfram.com
38. I.S. Gradshteyn, I.M. Ryzhik, *Table of Integrals, Series and Products* (Academic Press, 1965)