Quantum position diffusion and its implications for the quantum linear Boltzmann equation

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We derive a quantum linear Boltzmann equation from first principles to describe collisional friction, diffusion, and decoherence in a unified framework. In doing so, we discover that the previously celebrated quantum contribution to position diffusion is not a true physical process, but rather an artifact of the use of a coarse-grained time scale necessary to derive Markovian dynamics.

I. INTRODUCTION

Well over a hundred years ago, Boltzmann derived the linear Boltzmann equation [1] to describe a tracer particle affected by molecules of a dilute gas. In more recent times, physicists became interested in quantum generalizations, which led to the well-established fields of collisional decoherence [2,3] as well as quantum Brownian motion [4,5], where the Brownian Boltzmann equation [1] to describe a tracer particle affected by molecules of a dilute gas. In more recent times, physicists became interested in quantum generalizations, which led to the linear Boltzmann equation (QLBE) [6] were developed to describe the interplay between collisional decoherence, friction, and diffusion. Not only is there a quantum description of friction and diffusion desirable, but it also sheds light on the nonclassical process of decoherence, which is believed to be of importance in the quantum classical transition. Furthermore, experimental observations [7] of the quantum nature and decoherence of large molecules have improved rapidly.

To fully appreciate the quantum discussion in this field, we state some well-known results of the classical theory [8]. On short time scales, the momentum of a particle initially at rest diffuses according to \( \Delta p^2 \propto t \), whereas the position variance behaves like \( \Delta x^2 \propto t^3 \). The reason is that an almost instantaneous collision of momentum changes the momentum but not the position of a particle. Only on a much larger scale, when the momentum distribution is close to thermal equilibrium, does the position diffuse according to \( \Delta x^2 \propto t \). Although for large classical particles one is more interested in time scales on which many collisions occur, in the study of decoherence of a quantum particle, the short time scales are of importance because no quantum behavior is observable after a large number of collisions.

Interestingly, microscopic derivations of QLBEs (which are all Markovian, i.e., they do not have memory) predict an additional quantum contribution to position diffusion (QPD) [6], acting already on the short time scale of momentum diffusion. Although such a process is impossible in classical dynamics as it derives from finite position jumps, the very same process is needed for a QLBE to be of the Lindblad form necessary for completely positive Markovian dynamics. Therefore QPD is currently believed to arise as a quantum effect accompanying collisional quantum friction [6]. In this article, we show the contrary. We find that QPD is not a real physical process, but results from using a coarse-grained time scale on which collisions appear to be instantaneous. Unproblematic in classical dynamics, where collision times of hard-core particles are indeed short, the assumption of instantaneous collisions has to be used with care in quantum dynamics, where collision times depend on the widths of the colliding wave packets.

Important contributions to QLBEs have been made in [9–12] and can be reviewed in [6]. Mostly, the analysis is based on using scattering theory to describe the effects of a single collision with a gas particle which is assumed to be in a momentum eigenstate. Unfortunately, such collisions with momentum eigenstates impose a major unphysical feature regarding decoherence. For simplicity we use one spatial dimension to point out our concern, but the three-dimensional case is along the same lines. Assume that before the collision, the tracer particle is in a superposition of two momentum eigenstates \( (|p\rangle + |p'\rangle)/\sqrt{2} \), whereas the colliding gas particle is in the state \( |p_g\rangle \). A collision will lead to

\[
\frac{1}{\sqrt{2}}(|\tilde{p}(p, p_g)\rangle \otimes |\tilde{p}_g(p, p_g)\rangle + e^{i\phi} |\tilde{p}(p', p_g)\rangle \otimes |\tilde{p}_g(p', p_g)\rangle)
\]

where \( \phi \) depends on the interaction potential, and the momenta after the collision are dictated by momentum and energy conservation:

\[
p = \frac{2mp_g + (m - m_g)p}{m + m_g}, \quad \tilde{p}_g = \frac{2m_p - (m - m_g)p_g}{m + m_g}.
\]

Because the gas particle’s momentum after the collision depends on the tracer particle’s momentum before the collision, it follows that after the collision, the two particles are entangled. In fact, \( \langle \tilde{p}_g(p, p_g)|\tilde{p}_g(p', p_g)\rangle = 0 \) for \( p \neq p' \), and tracing out the gas particle one then finds that all coherences between \( p \) and \( p' \) are lost in a single collision, no matter how small \( |p - p'| \). Furthermore, it follows from linearity that for a general incoming state of the tracer particle, the collision leads to a density matrix which is perfectly diagonal in the momentum representation. Therefore a well-localized state will be spread out infinitely after a single collision. In a three-dimensional collision, one finds that the tracer-particle density matrix will be perfectly diagonal only in the momentum component parallel to the momentum transfer, which was also discovered in [13] independently from the present authors.

This seemingly unphysical situation can be understood if the collision time is considered. As the collision time of two colliding wave packets depends on their width, it must be assumed to be infinity if the gas particle is in a nonlocalized momentum eigenstate. After an infinite time, it is not surprising...
that all momentum coherences disappear even if the interaction is only with a single gas particle.

One might wonder how others [9–12] were able to derive a QLBE to describe the tracer particle at finite times, without encountering the problem of infinite momentum decoherence in a single collision. For this purpose, we review Hornberger’s contribution [12] because it seems to be the most complete one. Due to momentum conservation, a two-particle collision reduces to a one-particle problem, where the transition operator $T$ with momentum matrix elements related to the scattering amplitude $\langle p_f | T | p_i \rangle = \delta(p_f^2 - p_i^2) f(p_f, p_i)/(\pi \hbar)$ is of importance. In particular, an expression of the form

$$X = \frac{(2\pi \hbar)^3}{\Omega} \langle p_f + q | T | p_i + q \rangle \langle p_i - q | T | p_f - q \rangle$$

appears behind an integral over the momentum transfer ($p_f - p_i$). Here, $\Omega \to \infty$ is a box-normalization volume which is taken to infinity. The diagonals of the tracer-particle density operator after the collision correspond to $q = 0$, whereas $q \neq 0$ describes coherences. For $q = 0$, this term contains an ill-defined square of the Dirac $\delta$ function and a physically motivated replacement rule

$$\frac{(2\pi \hbar)^3}{\Omega} |\langle p_f | T | p_i \rangle|^2 \to \delta\left(|p_f^2 - p_i^2|/2\right) \frac{|f(p_f, p_i)|^2}{\sigma(p_i)|p_f|}$$

is used. One should mention that for any representation of the $\delta$ function in terms of a series of functions, the square of the Dirac $\delta$ function goes to infinity. Hence, for $q = 0$, $X$ contains an infinite term divided by an infinite volume $\Omega$, justifying the use of a replacement rule to assign a finite value to the expression. On the contrary, for $q \neq 0$, the product of $\delta$ functions in Eq. (1) is well defined. In fact, using standard relations for Dirac $\delta$ functions,

$$X = \frac{\pi \hbar}{\Omega \sigma(p_i)|p_f|} \delta(p_i - p_f) \delta(|p_i - p_f|) q \times f(p_f + q, p_i + q) f^*(p_f - q, p_i - q)$$

is found, where $q = |q|$ and $p_{ij} = p$ projected on $q$. The product of $\delta$ functions encountered here is well defined and upon integration will lead to terms of finite value. Therefore, $X$ is now a term of finite value divided by an infinite volume $\Omega$ which can only result in zero. This confirms our earlier argument that momentum coherences vanish completely upon a single collision with a gas particle in a momentum eigenstate.

Diósi [9] and Vacchini [11] did not encounter this decoherence problem, because they assumed “quasidiagonality” of the density operator in momentum basis and only studied $q = 0$. Hornberger was on the right track in that he considered $q \neq 0$, but he substituted the square root of the replacement rule in Eq. (2) for $(p_f \pm q | T | p_i \pm q)$ in Eq. (1). This assigns a nonzero value to $X$, effectively bringing back the otherwise lost coherences of momentum states. The use of the replacement rule for a term which would otherwise vanish is not easily justified. Whether decoherence in momentum bases and the closely related QPD are correctly described by approaches of this kind is surely not certain.

Also, the use of nonlocalized momentum eigenstates for the gas particle seems physically problematic because of the resulting infinite collision time. First, any Markovian QLBE relies on the assumption of short collision times. Second, successive collisions are not independent of each other if the collision time is long compared to the inverse collision frequency, leading to the necessity of studying multiparticle collisions.

To resolve this matter of momentum decoherence as well as of QPD, we study in Sec. II a single collision in terms of localized gas states. Then a collision time can be precisely defined, and the low-density and high-temperature limit will be quantified by (collision time) $\times$ (collision rate) $\ll 1$. To examine a collision event time resolved, and to investigate under which conditions a complete collision of two wave packets occurs, we analytically solve the two-particle Schrödinger equation. This is in contrast to scattering calculations which postulate complete collisions of wave packets. Although solving Schrödinger’s equation requires more effort, the result will let us conclude that quantum collisions cannot contribute to QPD.

We will then go on to derive a QLBE in Sec. III. Here we will show how QPD arises naturally as a result of the Markovian approximation. In Sec. IV we apply our QLBE to equations of motion for expectation values. We conclude in Sec. V. To simplify the problem, we consider one spatial dimension and assume a hard-core interaction potential between gas and tracer particles. Our notations are as follows. Position and momentum operators are denoted with a hat, whereas wave function variables are primed. The index $g$ refers to gas particles.

II. THE COLLISION PROCESS AND ITS IMPLICATIONS FOR POSITION DIFFUSION

We will try to be quite detailed in the treatment of a single collision. The reason is that the properties of a single collision will be enough to make some statements about diffusion in processes which are made up of a large number of collisions. Furthermore, approximations used in the derivation of any QLBE might blur the true physics, and we feel that some issues are best made explicit before these approximations are done.

Before we go into the discussion of a single collision, we start with some important remarks about the density operator of a gas particle of an ideal Boltzmann gas in a thermal state. In particular, we wish to point out that there are many different convex decompositions

$$\rho_g = \int d\alpha \mu(\alpha) |\psi_g(\alpha)\rangle \langle \psi_g(\alpha)|$$

of such a thermal density operator. Here $\alpha$ is a finite set of parameters, $|\psi_g(\alpha)\rangle$ is a set of normalized gas-particle states (not necessarily orthogonal) spanning the Hilbert space of a gas particle, and $\mu(\alpha) \geq 0$ is the probability of the gas particle to be in the state $|\psi_g(\alpha)\rangle$. This freedom has some important consequences, one of which is that the notion of a collision time $t_c$, to be thought of roughly the time required for a wave packet of the tracer particle to cross the width of the wave packet of a gas particle (a more precise definition below), is not to be viewed as a physical parameter whose value is intrinsic to the gas, but rather a parameter whose value can be chosen to suit the needs of the analysis. But already here it is clear that momentum eigenstates which are often used in Eq. (4) are not appropriate to define a collision time.
A convex decomposition which is particularly useful for our purpose was given by Hornberger and Sipe [14]. In particular, they showed that the density operator of a thermal ideal-gas particle at temperature $T$ can be written in terms of Gaussian states, that is,

$$
\rho_g = \int \frac{dx_g}{L} \int dp_g \mu_{\sigma_g}(p_g) |x_g, p_g\rangle \langle x_g, p_g|,
$$

where $L$ is a normalization length and $|x, p\rangle$ denotes a Gaussian wave packet with position variance $\sigma'$:

$$
\langle x'|x,p\rangle = \frac{e^{-ix'p/2\hbar}}{\sqrt{\pi \sigma}} e^{ip\hbar(x-x')^2/2\sigma^2}. \tag{6}
$$

Hornberger and Sipe showed that Eq. (5) is valid if

$$
\mu_{\sigma_g}(p_g) = \frac{1}{\sqrt{2\pi m_g k_B T_{\sigma_g}}} e^{-p_g^2/2m_g k_B T_{\sigma_g}} \tag{7}
$$

and $T_{\sigma_g} = T - \frac{k^2}{2m_g \sigma_g^2}$. Note that the momentum distribution Eq. (7) is the Maxwell-Boltzmann distribution $\mu(p_g)$ for a one-dimensional ideal gas, but with the temperature $T$ replaced by the lower value $T_{\sigma_g}$. Therefore part of the thermal energy is in the distribution $\mu_{\sigma_g}(p_g)$ of the mean momenta of the states $|x_g, p_g\rangle_{\sigma_g}$, and another part in the momentum uncertainty of these states.

A. The collision of two Gaussian wave packets

It is the convex decomposition [Eq. (5)] that allows us to study a single collision with a thermal gas particle in terms of Gaussian wave packets. For now, we will leave the parameter $\sigma_g$ unspecified, but later we will take advantage of this free parameter and choose it for our convenience.

We therefore undertake this analysis by considering an initial state that approaches the product state

$$
|x_g, p_g\rangle_{\sigma_g} \otimes |x, p\rangle_{\sigma} \tag{8}
$$

in the limit of large separation; i.e., we assume negligible overlap of the two initial wave packets

$$
|x_g - x| \gg \sigma_g^2 + \sigma^2. \tag{9}
$$

As we are not interested in any details due to a complicated interaction potential, we use a simple hard-core interaction. In particular, we consider the two-particle Hamiltonian

$$
H = \frac{\hat{p}_g^2}{2m_g} + \frac{\hat{p}_x^2}{2m} + a\delta(\hat{x} - \hat{k}_g), \quad a \to \infty, \tag{10}
$$

where the interaction potential forbids any tunneling of the gas particle through the tracer particle. The two orthogonal sets of energy eigenstates in position space are

$$
\psi_{\hat{k}}^g(x'_g, x') = e^{i(x'_g + ax')} \sin(\hat{k}(x'_g - x')) \tag{11},
$$

$$
\psi_{\hat{k}}^k(x'_g, x') = e^{i(x'_g + ax')} \sin(\hat{k}|x'_g - x'|), \tag{12}
$$

with $\hat{k} \in \mathbb{R}$, $\hat{k} \in \mathbb{R}_+$, and $a = m_g/m$. The energies of these states are

$$
E(\hat{k}, \hat{k}) = \frac{(1 + \alpha)\hbar^2}{2m_g} (\hat{k}^2 + \alpha \hat{k}_g^2), \tag{13}
$$

and they also have a well-defined total momentum $p_{\text{tot}} = (1 + \alpha)\hbar \hat{k}$ as well as a squared relative velocity $v_{\text{rel}}^2 = (1/m_g + 1/m)^2 \hbar^2 k^2$.

It is important to note that we cannot directly use Eq. (8) as an initial state. The reason is that the two single-particle wave functions have a small but nonvanishing overlap which is not allowed by the hard-core interaction potential. Instead, we construct an initial two-particle state, expanded in terms of the energy eigenstates in Eqs. (11) and (12), which satisfies the boundary condition $\psi(t = 0, x_g, x = x_g) = 0$ required by the hard-core interaction, and which approaches Eq. (8) in the limit of Eq. (9). As the derivation is quite lengthy, we only present the result here. However, once the initial state is given, we will show below that it has indeed the required properties.

Our initial two-particle state is

$$
\psi(0, x'_g, x') = \frac{i}{\sqrt{2\pi}} \int_0^\infty dk \int_0^\infty d\tilde{k} \tilde{\psi}(0, \tilde{k}, \tilde{k}), \tag{14}
$$

with

$$
\tilde{\psi}(0, \tilde{k}, \tilde{k}) = \frac{(1 + \alpha)\sigma}{2\pi \sqrt{\alpha}} \left\{ \exp \left[ -\frac{(\tilde{k}^2 - (1 + \alpha)\sigma^2)}{2} \right] \left( e^{i\tilde{k}(x'_g - x')} \psi_{\tilde{k}}^g(x'_g, x') - e^{-i\tilde{k}(x'_g - x')} \psi_{\tilde{k}}^k(x'_g, x') \right) \right\}, \tag{15}
$$

where without loss of generality, we used the center-of-mass reference frame (i.e., $p = -p_g$ and $x = -\alpha x_g$) as well as $x_g < x$ and $p_g > p$ (the gas particle approaches the tracer particle from the left). Furthermore, we related the widths $a\sigma_g^2 = \sigma^2$ of the Gaussian wave packets to the relative mass of the colliding particles. This turns out to be the requirement for the two particles not being entangled after the collision (see also [15]), and therefore $|x, p\rangle_{\sigma}$ can be seen as the pointer bases [16] of a measurement performed by a gas particle in the state $|x_g, p_g\rangle_{\sigma_g}$.

The time evolution is now easily achieved by multiplying the integrand of Eq. (14) by $e^{-i\tilde{k}\hat{k}_g\hat{x}_g/\hbar}$. After straightforward integration, we find

$$
\psi(t, x'_g, x') = -\frac{\sigma \sqrt{\alpha}}{\sqrt{\pi}} \left( \frac{m_g + m}{m} \right) \exp \left[ \frac{i(x_g p_g + xp)}{2\hbar} \right] \times \exp \left[ \frac{-(\frac{1+\alpha}{\alpha})\sigma^2 (x + \frac{p}{m})^2 - (x + \alpha x_g)^2 (\sigma^2 - \frac{\hbar^2}{m})}{(\sigma^2 + \frac{\hbar^2}{m})} \right] \times \exp \left[ \frac{-(x'_g - x)^2 (x - \frac{p}{m})^2 + i(\frac{\sigma^2}{\hbar^2} - \frac{\hbar^2}{m})}{(\sigma^2 + \frac{\hbar^2}{m})} \right] - \exp \left[ \frac{-(x'_g - x)^2 (x + \frac{p}{m})^2 + i(\frac{\sigma^2}{\hbar^2} - \frac{\hbar^2}{m})}{(\sigma^2 + \frac{\hbar^2}{m})} \right] \tag{15}
$$

for $x'_g < x'$, and $\psi(t, x'_g, x') = 0$ otherwise. At time $t = 0$, the first term in the curly brackets is the dominant one. If relation (9) holds, then we can neglect the second term and...
Eq. (15) becomes the position representation of the desired initial state (8) as promised earlier. If the particles’ relative velocity is large compared to their velocity uncertainty

$$|p| \gg \sqrt{\frac{1}{1 + \alpha^2} \frac{h}{\sigma_g}},$$

(16)

then we can neglect the first term sufficiently long after the collision. In this case, Eq. (15) is the position representation of the remarkably simple product state

$$U_g(t)|-x, -p⟩_g \otimes U(t)|-x, -p⟩_σ,$$

(17)

where $U(t)$ is the free particle evolution operator. That is, sufficiently long after the collision the two colliding particles are again in a product state, despite being entangled during the collision process. This nonentangled final state is a direct consequence of the way we related the width of the two Gaussian wave packets, i.e., $m_g \sigma_g^2 = m \sigma^2$. From relations (9) and (16) we can also see that the parameter $\sigma_g$ has to be bound from below and above.

Relation (16) is actually quite intuitive, because if it were not satisfied, the wave packets would spread faster than the velocity of their center, and part of the wave packets would move away from the center of mass of the two particles. The result would be an incomplete collision even for $t \to \infty$, and a collision time could not be well defined. On the other hand, if relation (16) is satisfied, we can use Eq. (15) to finally give a precise definition of the collision time

$$t_c = \sqrt{\frac{8}{1 + \alpha^2}} \frac{m_g}{|p|}$$

(18)

as the time it takes from the first term in the curly brackets to dominate, to the second term to dominate.

At this point, we are in the position to discuss the appearance of position and momentum “jumps” during the collision process. In the first term of Eq. (15), the tracer-particle momentum is localized around $p$, and in the second term around $-p$. During the collision, the first term decreases continuously while the second term increases. As there is never any momentum distribution well between $p$ and $-p$, this process accounts for momentum “jumps” (although the jump is not instantaneous), and if these occur at random we are led to momentum diffusion. In fact, already the energy eigenstates (11) and (12) show that the absolute relative velocity of the gas and tracer particle is a constant of motion. Therefore, in the collision, the eigenvalues for the relative velocity can swap their sign but not change continuously. An example of the momentum probability distribution

$$p(t, p') = \int dx' |\psi(t, x'_g, p')|^2,$$

$$\psi(t, x'_g, p') = \frac{1}{\sqrt{2\pi\hbar}} \int dx e^{-i p' x'/\hbar} \psi(t, x'_g, x')$$

is plotted in Fig. 1(b).

The situation is different in position space, because during the collision ($x + \frac{p}{m_g} \approx 0$) both terms of Eq. (15) are located at the same position. To be more precise, we take a look at the position probability distribution $p(t, x') = \int dx'_g |\psi(t, x'_g, x')|^2$

$$\psi(t, x'_g, x') = \frac{1}{\sqrt{2\pi\hbar}} \int dx e^{-i p x'/\hbar} \psi(t, x'_g, x')$$

is plotted in Fig. 1(a).

This apparent contradiction can, however, be resolved by taking into account that any Markovian master equation is only valid on a coarse-grained time scale $\delta$ which has to be large compared to the collision time $t_c$, such that a collision
can be considered as an instantaneous event. During a time interval \( \delta \), a collision does not only change the momentum distribution, but also significantly influences the position distribution, as indicated by the arrow in Fig. 2. That is, looking only at a coarse-grained time grid, a collision results in apparent position jumps, therefore leading to fictitious position diffusion.

This is by no means a quantum feature, as also classical dynamics lead to position diffusion if they are derived using a coarse grained time scale. In particular Smoluchowski [17] used the damping time as coarse grained time scale to derive Brownian motion, one of the most fundamental diffusion processes in nature. However, in classical dynamics it is very much accepted that position diffusion results from a coarse graining time approximation and is not apparent on short time scales. In fact, if the interaction between gas and tracer particle is of the hard core type, it is possible to derive classical Markovian dynamics without using a coarse grained time approximation [8]. The resulting Fokker-Planck equation for the phase space probability distribution (also known as the Kramers equation) then exhibits momentum diffusion, but not position diffusion.

The wave nature of quantum particles forbids instantaneous collisions even for hard core interaction potentials, and therefore the introduction of a time coarse graining approximation is necessary to derive Markovian quantum dynamics. For the same reason as for classical calculations, the coarse-graineded time scale then leads to position diffusion on the short time scales. But again, it has to be realized that this contribution to position diffusion is not a physical process, even if any possible QLBE would indicate so.

### III. DERIVATION OF THE QUANTUM LINEAR BOLTZMANN EQUATION

The purpose of deriving a QLBE is twofold. First, this equation can be used to describe all physical aspects of a tracer particle in a dilute gas, including the understanding of decoherence induced by the colliding gas particles. Second, as stated above, we want to show how QPD naturally arises as a result of the Markovian approximation.

#### A. The collision of a tracer particle in a general state with a gas particle

A first step toward a QLBE is the transformation of a general density operator due to a single collision. To this end, we note that the calculation in the center-of-mass reference frame in Sec. II A is easily generalized to a general reference frame by using the unitary Glauber displacement operator \( \hat{D}(x, p) = e^{i(x \cdot \vec{x} - \hat{p} \cdot \vec{p})/\hbar} \). The result is

\[
|x_g, p_g\rangle_\sigma \otimes |x, p\rangle_\sigma \xrightarrow{\text{scattering}} U_{g}(t)|\tilde{x}_g, \tilde{p}_g\rangle_\sigma \otimes U(t)|\tilde{x}, \tilde{p}\rangle_\sigma ,
\]

where positions and momenta after the collision relate to the initial values by the same relations as in a classical collision [noting that \( U(t) \) shifts the position by \( \tilde{\tilde{p}}t/m \)]:

\[
\begin{align*}
\tilde{x}_g &= \frac{2x - (1 - \alpha)x_g}{1 + \alpha}, & \tilde{p}_g &= \frac{2p + (1 - \alpha)p_g}{1 + \alpha}, \\
\tilde{\tilde{p}} &= \frac{2p}{1 + \alpha}.
\end{align*}
\]

The transformation of a general tracer-particle-density matrix (not necessarily a Gaussian wave packet) due to a collision with a gas particle in the state \( |x_g, p_g\rangle_\sigma \) can be written in terms of Kraus operators as

\[
\rho(t) = \int \int d\tilde{x}d\tilde{p} U(t)K_{x, p_\sigma}(\tilde{x}, \tilde{p})\rho(0)K_{x, p_\sigma}^\dagger(\tilde{x}, \tilde{p})U(t) .
\]

The derivation of the Kraus operators

\[
K_{x, p_\sigma}(\tilde{x}, \tilde{p}) = \hat{D}_x \left[ \frac{2\alpha}{1 + \alpha}(x - \tilde{x}), \frac{2}{1 + \alpha}(p - \alpha \tilde{p}) \right] \sqrt{\pi}(\tilde{x}, \tilde{p}),
\]

\[
\hat{\pi} = \int \int \frac{dx dp}{2\pi\hbar} w(x, p) |\tilde{x} + x, \tilde{p} + p\rangle_\sigma \langle \tilde{x} + x, \tilde{p} + p|,
\]

\[
w(x, p) = \frac{2\alpha}{\pi \hbar (1 - \alpha)^2} \exp \left[ -\frac{2\alpha}{(1 - \alpha)^2} \left( \frac{x^2}{\sigma^2} + \frac{\sigma^2p^2}{\hbar^2} \right) \right].
\]

is quite technical and will be omitted here. Instead we note that the reader can check the correctness of our Krauss operators by applying the transformation (23) to Gaussian states and comparing the result to Eq. (20). Indeed, because Gaussian states form an over-complete set of states, an operator transformation is uniquely defined by its action on the set \( \{ |x, p\rangle_\sigma \} \).

However, we will outline the major steps of the derivation of the Kraus operators, because it reveals some interesting physical interpretation about a measurement which the gas particle performs on the tracer particle. To this end, we imagine that a generalized measurement (see, e.g., [16] for a good introduction to positive operator valued measures or POVM) on the gas particle is performed at time \( t \), which is assumed to be after the collision took place. As this procedure should serve as the best possible indirect measurement of the tracer-particle state, Eq. (20) suggests using \( \hat{\pi}_{x, p} = \frac{1}{\pi \hbar} U_{g}(t)|\tilde{x}_g, \tilde{p}_g\rangle_\sigma \langle \tilde{x}_g, \tilde{p}_g|U_{g}^\dagger(t) \) as effect operators describing the simultaneous position-momentum measurement on the gas particle. The theory of indirect measurements [18] then leads to \( \hat{\pi}_{\tilde{x}, \tilde{p}} \) as in Eq. (24) for the effect operators acting on the tracer-particle state.
The Kraus operators are found by the requirement

\[ K_{xg,pg} (\tilde{x}, \tilde{p}) = A_{xg,pg} (\tilde{x}, \tilde{p}) \sqrt{\pi (\tilde{x}, \tilde{p})}, \]

where \( A_{xg,pg} (\tilde{x}, \tilde{p}) \) is a unitary operator which may depend on the measurement outcome \((\tilde{x}, \tilde{p})\) as well as on the state \((x_g, p_g)\) of the gas particle which is used for the measurement. Next we determined \( \sqrt{\pi (\tilde{x}, \tilde{p})} |x, p \rangle_\sigma \), which leads to an unnormalized Gaussian wave packet. A consistency requirement that the action of the Kraus operators on \(|x, p \rangle_\sigma \) must yield a state proportional to \(|\tilde{x}, \tilde{p} \rangle_\sigma \) is then imposed. This shows that \( A_{xg,pg} (\tilde{x}, \tilde{p}) \) is given by the displacement operator as in Eq. (24).

This measurement interpretation of a collision process was first put forward in the phenomenological work of Barnett and Cresser [10]. For such an interpretation to be valid, it is necessary that the tracer and gas particles do not interact anymore when the measurement is performed on the latter. Then the measurement procedure (without readout) does not influence the tracer-particle state, and therefore the transformation in Eq. (23) is correct whether or not such a measurement on the gas particle is actually realized. Hence, one may say the gas particle performs a measurement on the tracer particle.

B. The quantum linear Boltzmann equation

Using the results from a single collision, we can now go on and derive a master equation for a tracer particle experiencing random collisions with gas particles. In Eq. (23), we assumed that the tracer particle collides with the gas particle. However, that will not always be the case, e.g., if the two particles move away from each other or if they are too far apart. Therefore, as a first step, we have to determine whether during a time interval \( \delta \) the tracer particle actually collides with a gas particle, given the latter is in the state \(|x_g, p_g \rangle \). For this purpose we assume

\[ \delta \gg \tau_e, \quad (25) \]

which enables us to neglect partial or uncompleted collisions and to use classical trajectories. It follows that the two particles collide if \((x, p)\) is within the phase-space region \( S_\delta (x_g, p_g) = \{(x, p) | 0 < x - x_g \leq \frac{\mu \delta x}{m - \mu p/m} < \delta \} \), shown in Fig. 3(a). Therefore we have to project the tracer-particle density operator onto \( S_\delta (x_g, p_g) \) before applying the transformation (23). Of course, phase-space projections do not exist in quantum mechanics, but as long as (25) is satisfied we can use the approximate projection operator [see Fig. 3(b)]

\[ \Gamma_\delta (x_g, p_g) = \int_{S_\delta (x_g, p_g)} \frac{dx dp}{2\pi \hbar} |x, p \rangle_\sigma \langle x, p|. \quad (26) \]

The action of this operator can be visualized in Fig. 3(b).

By multiplying this operator with the probability of finding a gas particle in the state \(|x_g, p_g \rangle_\sigma \), we define the collision probability operator

\[ P_\delta (x_g, p_g) = n_g \mu (p_g) \Gamma_\delta (x_g, p_g), \quad (27) \]

where \( n_g \) is the gas number density. In fact, the expectation value \( \text{Tr} [\rho P_\delta (x_g, p_g)] \) gives the probability of a collision of the tracer particle and a gas particle described by \(|x_g, p_g \rangle_\sigma \). We also define \( P_\delta = \int dx dp P_\delta (x_g, p_g) \) corresponding to the total collision probability. In Eq. (27) we used the Maxwell-Boltzmann distribution \( \mu (p_g) \) rather than \( \mu (p_g) \) from the convex decomposition of the gas density operator of Eq. (5). The reason is that relation (16) has to be satisfied for most states of the thermal gas which requires \( \sigma_g \gg \frac{\hbar}{\sqrt{m_\mu k_B T}} \) which in turn leads to \( T_{\mu \sigma} \approx T \).

To find the density operator for the tracer particle at time \( \delta \), quantum trajectory theory [19] suggests multiplying each Kraus operator by the square root of the probability operator. We use the low-density assumption

\[ \text{Tr} (\rho P_\delta) \ll 1 \quad (28) \]

to neglect two or more collisions during \( \delta \) and find

\[ \rho (\delta) = U (\delta) \int_0^\infty \int_0^\infty dx dp \tilde{p} [K_{xg,pg} (\tilde{x}, \tilde{p}) \times \rho (0)] U (\delta) \]

\[ + \sqrt{1 - P_\delta} \rho (0) \sqrt{1 - P_\delta} U (\delta). \quad (29) \]

The integration is over all gas-particle states \( x_g \) and \( p_g \), as well as over all possible "measurement outcomes" \( \tilde{x} \) and \( \tilde{p} \). The last term accounts for the possibility that during \( \delta \) no collision occurs.

Next we use Eq. (29) and homogeneity in time to construct a differential equation according to which \( \rho (t) \) approximately evolves. To this end, we take the interaction picture \( \rho_{\text{int}} (t) = U (t) \rho (t) U (t) \) and define \( L_\delta [\rho_{\text{int}} (0)] = \frac{\partial}{\partial t} \rho_{\text{int}} (0) \). The structure of \( L_\delta \) is easily obtained from Eq. (29) and \( \sqrt{1 - P_\delta} \approx 1 - P_\delta /2 \). At this point, the usual approach to a master equation is to take the limit \( \delta \to 0 \) in \( L_\delta \). However, this limit is not allowed in \( \Gamma_\delta (x_g, p_g) \) as then uncompleted collisions are not negligible. We will therefore keep \( \delta \) as a small but finite parameter in \( L_\delta \). We could now identify \( \frac{\partial}{\partial t} \rho_{\text{int}} (0) \approx L_\delta [\rho_{\text{int}} (0)] \), but this would eventually lead to errors of first order in \( \delta \). We

\[ \text{This relation can be relaxed if the tracer particle moves faster than an average gas particle.} \]
can reduce errors due to finite \( \delta \) to second order by noting that for any smooth function \( f(\delta)/f(0) \),
\[
\frac{\rho_{\text{int}}(t)}{\delta} = \frac{1}{2} \left[ R \rho(t) + \rho(R) \right]
\] + \int \int \int \, dx_g dp_g \, d\tilde{\rho} \left[ U \left( \frac{\delta}{2} \right) K_{xg,pg}(\tilde{x}, \tilde{p}) \right.
\times \sqrt{R}(x_g, p_g)U^\dagger \left( \frac{\delta}{2} \right) \rho(t)U \left( \frac{\delta}{2} \right) \sqrt{R}(x_g, p_g)
\times K^\dagger_{xg,pg}(\tilde{x}, \tilde{p})U \left( \frac{\delta}{2} \right),
\] (31)
where the free evolution operators arise by virtue of Eq. (30) and partially counteract unphysical effects due to finite \( \delta \) in \( \Gamma_{\delta}(x_g, p_g) \). Furthermore, \( R = P_\delta/\delta \) and \( R_\delta(x_g, p_g) = P_\delta(x_g, p_g) / \delta \) are rate operators corresponding to collision rates. Note that \( R \) depends only on physical parameters such as density and temperature, but not on the coarse-graining time \( \delta \). It is therefore a measurable physical quantity. In fact, one can show that
\[
R = n_g \left[ \sqrt{2k_B T} \right] \exp \left( - \frac{m_p \delta^2}{2k_B T m^2} \right) + \rho \right] \, m \right] \, m \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \right] \r...