Open quantum dynamics via environmental monitoring

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Abstract. A general method is discussed to obtain Markovian master equations which describe the interaction with the environment in a microscopic and non-perturbative fashion. It is based on combining time-dependent scattering theory with the concept of continuous quantum measurements. The applications to the case of a Brownian point particle and to the case of a complex molecule, both in the presence of a gaseous environment, are outlined.

1. Introduction
Quite a number of contributions presented at the DICE2006 workshop were focused on possible extensions of standard quantum theory—be it to overcome the incompatibility of quantum theory and general relativity, or to understand the measurement process and our perception of the world as classical. When discussing these modifications of quantum theory, which often imply a violation of unitarity, it is important to keep in mind that their observability may be severely limited by environmental decoherence [1]. The latter occurs naturally within the framework of quantum theory if one accounts for the fact that all practically relevant quantum systems are in contact with some uncontrollable environment. Before interpreting the effects and judging the relevance of non-standard extensions it is therefore of great importance to have a full quantitative understanding of environmental decoherence.

In the present contribution I would like to discuss a new method to derive Markovian master equations for open quantum systems, which take into account the interaction with the environment in a microscopic and non-perturbative fashion [2, 3]. Such dynamic equations are a prerequisite for any faithful quantitative description of open quantum systems. In particular, it is well-known that phenomenological or perturbative master equations may fail by many orders of magnitude when applied to situations where the decoherence time is much shorter than the typical time scale of dissipation, even though they describe dissipation phenomena rather well, see e.g. [4].

In the standard approaches one starts out with an approximate total Hamiltonian for the system plus environment [5]. Then, various approximations are employed in the course of the derivation, one of which is often the Markov assumption. It implies that environmental correlations disperse fast, so that on a coarse-grained timescale the temporal change of the system state depends on the present state of the system, but not on its history. The starting point of the method presented here differs considerably from the standard methods. It is not based on an approximate “total” Hamiltonian of system plus environment. Rather, the environmental
coupling is described in an operational sense, by using scattering theory, which permits a non-perturbative description. In particular, this admits to take the Markov assumption as a premise, rather than having to introduce it ‘by hand’ in the course of the calculation.

The use and strength of the method will be exemplified by discussing the dynamics of two different quantum systems in the presence of an ideal, thermalized gas—a trapped molecule and a Brownian point particle. The corresponding master equations will be given in terms of the exact scattering amplitudes describing the interaction of the gas particle with the quantum system.

2. The monitoring approach
The present approach to the derivation of master equations is motivated by the observation that environmental decoherence, and Markovian open quantum dynamics in general, can be viewed as due to the information transfer from the system to the environment, see e.g. [4]. In accordance with this, we will picture the environment as consisting of (quasi-)particles, which serve to monitor the system continuously in terms of microscopic probes scattering off the system at random times. This point of view will be applicable whenever one can describe the interaction with the environment in terms of individual interaction events, and, of course, it suggests a formulation in terms of scattering theory. The Markov assumption is then easily incorporated from the outset by disregarding the change of the environmental state after each collision.

When setting up a dynamic equation, one would like to write the change of the system state in time as the infinitesimal rate of scatterings multiplied by its effect, i.e., by the state transformation due to an individual collision. However, not only the transformed state depends on the original system state, in general, but also the collision rate, so that this naive ansatz would yield a nonlinear equation. In order to account properly for the state dependence of the collision rate we will make use of the concept of continuous and generalized quantum measurements [6, 7, 8]. Specifically, and just for the sake of consistent bookkeeping of the probabilities, we shall assume that the system is surrounded by a hypothetical, minimally invasive transit detector,
which tells at any instant, and with a time resolution $\Delta t$, whether a probe particle has passed by and is going to scatter off the system, see Fig. 1.

2.1. The effect of continuous monitoring

Let us denote by $C$ the event that the transit detector triggers in the interval $(t; t + \Delta t)$ indicating that a collision is imminent. In general, the rate of collisions is then described by a positive operator $\Gamma$ acting in the the system-probe Hilbert space. Given the uncorrelated state $\rho_{\text{tot}} = \rho \otimes \rho_E$ it determines the probability of a collision to occur in a small time interval $\Delta t$,

$$\text{Prob (} C \text{ in } \Delta t | \rho \otimes \rho_E) = \Delta t \text{tr} (\Gamma [\rho \otimes \rho_E]).$$

(1)

Here $\rho_E$ is the stationary reduced single particle state of the environment. The microscopic definition of $\Gamma$ will in general involve the current density operator of the relative motion and a total scattering cross section, see below.

It is now important to note is that the information that a collision is going to take place changes our knowledge about the state, and therefore its description. Most generally, it is transformed by a generalized measurement transformation, i.e., a trace decreasing, completely positive map [6, 7]. At the same time, we have to take into consideration that the detector is not real, but is introduced here only for enabling us to account for the state dependence of the collision probability. It is therefore reasonable to take the detection process as efficient and minimally-invasive, so that it is described by a single operator which introduces no reversible back-action. The consistency requirement for measurement transformations then implies that after a (hypothetical) detector click, but prior to scattering, the normalized system-probe state must have the form

$$\mathcal{M} (\rho_{\text{tot}} | C) = \frac{\Gamma^{1/2} \rho_{\text{tot}} \Gamma^{1/2}}{\text{tr}(\Gamma \rho_{\text{tot}})}.$$  

(2)

This nonlinear transformation reflects our improved knowledge about the incoming two-particle wave packet, and it may be viewed as enhancing those parts which are heading towards a collision. Also the absence of a detection event during $\Delta t$ constitutes a measurement which changes the state. The corresponding probability must satisfy $\text{Prob (} \bar{C} \text{ in } \Delta t | \rho_{\text{tot}}) = 1 - \text{Prob (} C \text{ in } \Delta t | \rho_{\text{tot}})$, and the state conditioned on a null-event is given by

$$\mathcal{M} (\rho_{\text{tot}} | \bar{C}) = \frac{\rho_{\text{tot}} - \Delta t \Gamma^{1/2} \rho_{\text{tot}} \Gamma^{1/2}}{1 - \Delta t \text{tr}(\Gamma \rho_{\text{tot}})}.$$  

(3)

In fact, more general nonlinear transformations are conceivable, but this one is distinguished by the fact that it introduces no further operators.

The effect of a single collision is described by the two-particle S-matrix $S$. The unconditioned system-probe state after time $\Delta t$ can now be formed by taking into account that the detection outcomes are not really available. The infinitesimally evolved state is then given by the sum of the colliding state transformed by the S-matrix and the untransformed non-colliding one, weighted with their respective probabilities,

$$\rho_{\text{tot}} (\Delta t) = \text{Prob (} C \text{ in } \Delta t | \rho_{\text{tot}}) S \mathcal{M} (\rho_{\text{tot}} | C) S^\dagger + \text{Prob (} \bar{C} \text{ in } \Delta t | \rho_{\text{tot}}) \mathcal{M} (\rho_{\text{tot}} | \bar{C})$$

$$= S\Gamma^{1/2} \rho_{\text{tot}} \Gamma^{1/2} S^\dagger \Delta t + \rho_{\text{tot}} - \Gamma^{1/2} \rho_{\text{tot}} \Gamma^{1/2} \Delta t.$$  

(4)
2.2. Constructing a dynamic equation

In order to obtain a differential equation for the time evolution it is now convenient to split off the nontrivial part of the two-particle S-matrix, thus defining

$$T = i(\mathbb{I} - S).$$

(5)

This operator is proportional to the $T$-matrix of scattering theory (only) on the energy shell, and one finds that the unitarity of $S$ implies that it satisfies $i(T - T^\dagger) = -T^\dagger T$. Using this relation the differential quotient can be written as

$$\frac{\rho'(\Delta t) - \rho}{\Delta t} = T\Gamma^{1/2} \rho \Gamma^{1/2} T^\dagger - \frac{1}{2} T T^\dagger T \Gamma^{1/2} \rho \Gamma^{1/2} - \frac{1}{2} \Gamma^{1/2} \rho \Gamma^{1/2} T^\dagger T + \frac{i}{2} \left[ T + T^\dagger, \Gamma^{1/2} \rho \Gamma^{1/2} \right].$$

(6)

From here it is easy to obtain a closed differential equation for $\rho$. We trace out the environment with $g = \rho \otimes \rho_E$, take the limit of continuous monitoring $\Delta t \to 0$, to arrive at [3]

$$\frac{d}{dt} \rho = \frac{i}{\hbar} [H, \rho] + \frac{i}{2} \text{Tr}_E \left( \left[T + T^\dagger, \Gamma^{1/2} [\rho \otimes \rho_E] \Gamma^{1/2} \right] \right) + \text{Tr}_E \left( \Gamma^{1/2} [\rho \otimes \rho_E] \Gamma^{1/2} T^\dagger T \right)$$

$$- \frac{1}{2} \text{Tr}_E \left( \Gamma^{1/2} T^\dagger T \Gamma^{1/2} [\rho \otimes \rho_E] \right) - \frac{1}{2} \text{Tr}_E \left( [\rho \otimes \rho_E] \Gamma^{1/2} T^\dagger T \Gamma^{1/2} \right).$$

(7)

The Markov approximation enters here by assuming the factorization $\rho \otimes \rho_E$ to be valid for all times. Note also that the generator $H$ of the free system evolution was added, thus switching from the interaction picture to the Schrödinger picture. The collision rate with its state dependence is incorporated by the operators $\Gamma^{1/2}$, while the operators $T$ describe the individual microscopic interaction process without approximation.

The discussion was very general, so far. However, to obtain concrete master equations system and environment have to be specified, along with the operators $\Gamma$ and $S$ describing their interaction. In the following applications, we will assume the environment to be an ideal Maxwell gas. Its single particle state

$$\rho_{\text{gas}} = \frac{\Lambda_{\text{th}}^3}{\Omega} \exp \left( -\beta \frac{p^2}{2m} \right)$$

is characterized by the inverse temperature $\beta$, the normalization volume $\Omega$, and the thermal de Broglie wave length $\Lambda_{\text{th}} = \sqrt{2\pi\hbar^2\beta/m}$.

3. Collisional decoherence of a discrete object

As a first concrete implementation of the monitoring approach, let us see how an immobile object with discrete internal states, such as the electronic, configuration, and rotation dynamics of a trapped molecule, gets affected by an environment of ideal gas particles. For example, such a master equation will describe how a possible superposition of configuration eigenstates of macromolecules decoheres into a mixture of robust configuration states, see Fig. [2].

The interaction between system and gas will be described in terms of the exact scattering amplitudes $f_{\alpha\alpha_0}(p,p_0)$ determined by the interaction potential. They describe the in general inelastic coupling between the internal energy eigenstates, which form a discrete basis of the system Hilbert space and are called *channels* in the language of scattering theory. The notation $|\alpha\rangle$ will be used in the following to indicate the system eigenstates of energy $E_\alpha$. In this channel basis, $\rho_{\alpha\beta} = \langle\alpha|\rho|\beta\rangle$, the equation of motion (7) takes on the form of a general discrete master equation of Lindblad type,

$$\dot{\rho}_{\alpha\beta} = -i\omega_{\alpha\beta} \rho_{\alpha\beta} + \sum_{\alpha_0\beta_0} \rho_{\alpha_0\beta_0} M_{\alpha\beta_0}^{\alpha_0\beta_0} - \frac{1}{2} \sum_{\alpha_0\gamma} \rho_{\alpha_0\beta} M_{\alpha\gamma}^{\alpha_0\gamma} - \frac{1}{2} \sum_{\beta_0\gamma} \rho_{\alpha\beta_0} M_{\gamma\gamma}^{\beta_0\gamma}.$$
Figure 2. Superpositions of different configuration states of a molecule will decohere into a mixture of configuration states, as a result of the interaction with a gaseous environment. The master equation (9) describes this process in a non-perturbative fashion.

Here, the frequencies $\omega_{\alpha\beta} = [E_\alpha - E_\beta + (\varepsilon_\alpha - \varepsilon_\beta)]/\hbar$ involve energy shifts $\varepsilon_\alpha \in \mathbb{R}$, which are defined below. They describe the coherent modification of the system energies due to the presence of the environment analogous to the Lamb shift. More importantly, the incoherent dynamics effected by the environment is described by the set of complex rate coefficients

$$M^{\alpha\beta}_{\alpha\beta} = \langle \alpha | T \Gamma^{1/2} \left[ |\alpha_0\rangle \otimes \rho_{\text{gas}} \right] \Gamma^{1/2} T^\dagger |\beta\rangle.$$

(10)

Our main task is to calculate these quantities. As a first step we need to specify the rate operator $\Gamma$. It is naturally given in terms of the current density operator $j = n_{\text{gas}} p/m$ of the impinging gas particles multiplied by the channel-specific total scattering cross sections $\sigma(p, \alpha)$,

$$\Gamma = n_{\text{gas}} \sum_\alpha \Pi_\alpha \otimes \frac{|p|}{m} \sigma(p, \alpha),$$

(11)

with projectors $\Pi_\alpha = |\alpha\rangle \langle \alpha|$. For normalized and separable system-gas states the expectation value of $\Gamma$ thus yields the infinitesimal total collision probability—provided the motional state of the gas particle is a wave packet heading towards the origin. However, since (11) depends only on the modulus of the velocity $|p|/m$ it will yield a finite collision probability even if the particle is heading away from the origin. Hence, for (7) to make sense either the definition of $\Gamma$ should contain in addition a projection to the subset of incoming states, or the S-matrix should keep such a non-colliding state unaffected. The latter is not guaranteed in general, since even a purely outgoing wave packet, located far away from the origin, may get transformed by $S$ since the definition of the S-matrix involves a backward time-evolution [9].

3.1. A phase space-based calculation

In the following, we will explicitly disregard the outgoing states by using a non-diagonal decomposition of $\rho_{\text{gas}}$. As discussed in [10] the thermal gas state can be written as a phase space integration over projectors onto Gaussian states of minimum uncertainty,

$$|\psi_{r_0p_0}\rangle = \left(\frac{2\pi \hbar^2 \beta}{m}\right)^{3/4} \exp\left(-\frac{\beta (p - p_0)^2}{4m}\right) |r_0\rangle$$

(12)

characterized by an inverse temperature $\beta$ greater than the inverse gas temperature $\beta$. Denoting

the Maxwell-Boltzmann distribution corresponding to the temperature $\beta^{-1} = \beta^{-1} - \beta^{-1}$ by
\[ \mu(p_0) = \left(2\pi m/\hat{\beta}\right)^{-3/2} \exp(-\hat{\beta}p_0^2/(2m)) \] the state \((5)\) is represented as
\[
\rho_{\text{gas}} = \int dp_0 \hat{\mu}(p_0) \int d\mathbf{r}_0 \Omega |\psi_{\mathbf{r}_0 p_0}\rangle \langle \psi_{\mathbf{r}_0 p_0}|.
\] (13)
Inserting (13) into (10) yields the expression
\[
M_{\alpha\beta}^{\alpha_0\beta_0} = \int dp_0 \hat{\mu}(p_0) \int d\mathbf{r}_0 \Omega m_{\alpha\beta}^{\alpha_0\beta_0}(r_0, p_0)
\] (14)
with
\[
m_{\alpha\beta}^{\alpha_0\beta_0}(r_0, p_0) := \int dp \langle \alpha |(p|T\Gamma^{1/2}||\beta)\rangle \langle \psi_{\mathbf{r}_0 p_0}\rangle \langle \beta_0 |\psi_{\mathbf{r}_0 p_0}|\Gamma^{1/2}T^\dagger|\beta_0|\rangle |p\rangle.
\] (15)
Evidently, the phase space function \(m_{\alpha\beta}^{\alpha_0\beta_0}(r_0, p_0)\) gives the contribution of different phase space regions to the rate coefficient \(M_{\alpha\beta}^{\alpha_0\beta_0}\).

This permits now to restrict the calculation to incoming wave packets. Since the \(m_{\alpha\beta}^{\alpha_0\beta_0}\) are averaged over all available positions in (14) it is natural to confine this spatial average at fixed \(p_0\) to a cylinder pointing in the direction of \(p_0\), whose longitudinal support \(\Lambda_{p_0}\) vanishes at outgoing positions. Its transverse base area is given by an average cross section \(\Sigma_{p_0}\). In order to evaluate the phase space function (15), one inserts momentum resolutions of unity between the \(T\) and \(\Gamma\) operators and notes the representation \(9\)
\[
\langle \alpha_f |(p_f|T|\alpha_i)\rangle |p_i\rangle = \frac{\rho_{\alpha_f\alpha_i}(p_f, p_i)}{2\pi\hbar m} \delta \left(E_{p\alpha_f} - E_{p\alpha_i}\right)
\] (16)
in terms of the multi-channel scattering amplitude and total energies \(E_{p\alpha} = p^2/2m + E_{\alpha}\). In the calculation one chooses \(\hat{\beta}\) large and eventually takes the limit \(\hat{\beta} \rightarrow \infty, \hat{\beta} \rightarrow \beta\) of very extended wave packets so that \(\hat{\mu}\) approaches the original Maxwell-Boltzmann distribution \(\mu\). In this limit the dependence on \(\Lambda_{p_0}\) and \(\Sigma_{p_0}\) drops out provided one identifies \(\Sigma_{p_0}\) with the geometric mean of the total cross sections of the involved channels. One obtains \(3\)
\[
M_{\alpha\beta}^{\alpha_0\beta_0} = \chi_{\alpha\beta}^{\alpha_0\beta_0} \frac{n_{\text{gas}}}{m^2} \int dp \, dp_0 \mu(p_0) f_{\alpha\alpha_0}(p, p_0) f_{\beta\beta_0}^*(p, p_0) \delta \left(\frac{p^2 - p_0^2}{2m} + E_{\alpha} - E_{\alpha_0}\right)
\] (17)
with the Kronecker-like factor \(\chi_{\alpha\beta}^{\alpha_0\beta_0}\), which is equal to one if \(E_{\alpha} - E_{\alpha_0} = E_{\beta} - E_{\beta_0}\) and zero otherwise. Moreover, the energy shifts are determined the real parts of the forward scattering amplitude,
\[
\epsilon_{\alpha} = -2\pi\hbar^2 n_{\text{gas}}/m \int dp_0 \mu(p_0) \text{Re} \left[f_{\alpha\alpha}(p_0, p_0)\right].
\] (18)
For the special case of factorizing interactions, \(H_{\text{int}} = A \otimes B_E\), and for times large compared to all system time scales this result can be obtained rigorously \(11\), by means of a “low density limit” scaling method \(12\) \(5\). As discussed in \(3\), limiting forms of \(9\) display the expected dynamics. On the diagonal, it reduces to a rate equation, where the total inelastic cross sections determine the transition rates, while in the case of elastic scattering the coherences decay exponentially.
3.2. An equivalent approach

It is worth noting that the result (17) for the rate coefficients \( M_{\alpha\beta}^{\alpha_0\beta_0} \) can as well be obtained in a more direct, while less obvious way, if the diagonal momentum representation of \( \rho_{\text{env}} \) is used instead of (13). In this case, the improper eigenstates \( |p\rangle \) have a meaning beyond their use as convenient basis states for the expansion of the incoming state. Rather, each momentum state in \( \rho_{\text{env}} \) must be viewed as representing the limiting form of a normalized wave packet. It is therefore necessarily restricted to a discrete set defined by the corresponding volume-normalized states \( |\tilde{p}\rangle \). The problem is then that the application of \( S \) to these spatially extended states leads to the unwanted transformation also of its “outgoing components”. As a consequence, the resulting expression for \( M_{\alpha\beta}^{\alpha_0\beta_0} \) involving

\[
\frac{(2\pi\hbar)^3}{\Omega} \langle \alpha p_1 | T_0 | \alpha_0 p_0 \rangle \langle \beta_0 p_0 | T_0^\dagger | \beta p_1 \rangle
\]  

(19)

is ill-defined since it contains the square of the \( \delta \)-functions in (16) and the normalization volume \( \Omega \).

This can be healed by the second option mentioned above, the formal modification of the operator \( S \), such that it keeps outgoing components invariant. In the continuous basis of improper states the unitarity of \( S \) is expressed by the optical theorem, which quantifies the diffraction limitation of the scattering probability. Since diffraction cannot be accommodated in the discrete basis, the requirement of probability current conservation must be incorporated additionally in any consistent modification of \( S \), which serves to define a normalized transition matrix for the “scattering” into the different “leads” characterized by the discrete \( |\tilde{p}\rangle \). The point is now that this normalization condition can again be viewed in the continuous basis of improper states, and thus provides a simple rule how to form a well-defined expression [10]. Its multichannel version is to replace (19) by

\[
\frac{\chi_{\alpha\beta}^{\alpha_0\beta_0}}{p_0 m} \frac{f_{\alpha\alpha_0}(p,p_0)}{\sqrt{\sigma(p_0,\alpha_0)}} \frac{f_{\beta\beta_0}^*(p,p_0)}{\sigma(p_0,\beta_0)} \delta \left( \frac{p^2 - p_0^2}{2m} + E_\alpha - E_{\alpha_0} \right).
\]  

(20)

The appearance of the cross sections in the denominator is here a direct consequence of the normalization requirement for the probability current. By using this replacement one obtains the result (17) immediately from (10) for any momentum diagonal \( \rho_{\text{env}} \).

It should be mentioned that the problem of squared delta functions can also be circumvented, as discussed in [13, 14], by appealing to the Fermi golden rule when one writes down the dynamic equation. This way one leaves the realm of (time-dependent) scattering theory [9], since one needs to speak about the “elapsed time” during the scattering process. Effectively, the “interaction Hamiltonian” of the dynamic description is thus identified with the off-shell T-matrix, a step which is valid (only) in second-order perturbation theory. It should be noted that the form of such a Born approximation to the master equation can differ from the non-perturbative result, as demonstrated in the following section.

4. Collisional decoherence of a Brownian particle

As a second, nontrivial application of the monitoring approach, let us consider how the motional state of a single Brownian particle is affected by a gaseous environment. In analogy to the classical case, the corresponding master equation may be called a linear quantum Boltzmann equation. Here the term “linear” refers to the fact that the equation for the single Brownian particle is linear (the particle is not interacting with itself), and should not be confused with the “linearized”, i.e., perturbative description of the reduced single particle state a self-interacting gas. The resulting equation will describe, on equal footing, both the short-time decoherence
behavior, i.e. the rapid “localization” of a spatial superposition state into a mixture, and the long-time dissipative behavior, i.e. the gradual thermalization of the Brownian particle.

Let us denote by $M$ and $m$ the masses of the Brownian and the gas particle, and the reduced mass by $m_*$. Since a collision affects only the relative coordinates we denote the single particle S-matrix by $S_0 = \mathbb{I} + i T_0$. Moreover, it is convenient to denote the relative momentum by

$$\text{rel}(p, P) := \frac{m_*}{m} p - \frac{m_*}{M} P.$$  \hspace{1cm} (21)

Like above, the first step in obtaining the master equation is to specify the rate operator. In classical mechanics, the rate is determined by the modulus of the relative current density

$$j_\text{rel}(p, P) = \frac{n_{\text{gas}} |\text{rel}(p, P)|}{m_*} \times \frac{\sigma(p_{\text{in}})}{2 \pi \hbar}.$$  \hspace{1cm} (22)

and, indeed, for normalized and separable particle-gas states the expectation value of this operator yields the collision rate experienced by the Brownian particle. Like above, the definition (22) does not yet include the projection to the subspace of incoming particle-gas wave packets.

4.1. Calculation in the momentum diagonal basis

Inserting the diagonal momentum representation of the gas state (8) into (7) we find that the equation of motion for the Brownian particle in momentum representation,

$$\partial_t \rho(P, P') = \langle P | \rho | P' \rangle,$$

takes the form

$$\partial_t \rho(P, P') = \int dQ M_\text{in}(P, P'; Q) \rho(P - Q, P' - Q) - \frac{1}{2} \left[ M^\text{clout}_\text{in}(P) + M^\text{clout}_\text{out}(P') \right] \rho(P, P').$$  \hspace{1cm} (23)

In particular, there is no contribution of the second term in (7), since the gas density is uniform. Equation (23) is specified by the complex rate function [2]

$$M_\text{in}(P, P'; Q) = \frac{n_{\text{gas}}}{m_*} \int dp_0 \mu(p_0) \sqrt{\frac{|p_i + q|}{|p_i - q|}} \frac{\sigma(p_i + q)}{\sigma(p_i - q)} \frac{(2\pi\hbar)^3}{\Omega} \langle p_f + q | T_0 | p_i + q \rangle \langle p_i - q | T_0^\dagger | p_f - q \rangle.$$  \hspace{1cm} (24)

Here $p_i := \text{rel}(p_0, \frac{P + P'}{2} - Q)$ and $p_f := p_i - Q$ were introduced as functions of $p_0$. Moreover, $q := \text{rel}(0, \frac{P - P'}{2})$. The rate function (24) defines also

$$M^\text{clout}_\text{out}(P) = \int dQ M^\text{in}_\text{in}(P + Q, P + Q; Q),$$  \hspace{1cm} (25)

which will turn out to be the rate in the classical linear Boltzmann equation of a particle with momentum $P$ to be scattered by the gas into a different direction or velocity. The remaining difficulty is to evaluate the function (24). Like in the previous section, our use of a diagonal representation of the normalized gas state leads to an ill-defined expression involving a square of delta-functions and the normalization volume, which can be traced back to the unwanted transformation of the outgoing parts of the normalized state,

$$\frac{(2\pi\hbar)^3}{\Omega} \langle p_f + q | T_0 | p_i + q \rangle \langle p_i - q | T_0^\dagger | p_f - q \rangle g(q).$$  \hspace{1cm} (26)
Like above, it can be argued that any consistent modification of the S-matrix, i.e., of \( T_0 \), which keeps the outgoing parts invariant must necessarily transform (20) into

\[
\delta \left( \frac{P_f^2 - P_i^2}{2} \right) f \left( P_f + q, \frac{P_i + q}{2} \right) \sqrt{\frac{\sigma}{|P_i + q|}} g \left( \frac{P_i - q}{2} \right) \cdot
\]

Here, we denote, for given \( q \neq 0 \) the parallel contribution of a vector \( P \) by \( P_{\| q} = (P \cdot q) q/q^2 \) and the perpendicular one by \( P_{\perp q} = P - P_{\| q} \). These projections manifestly guarantee the conservation of energy in the two scattering amplitudes individually. As discussed in [2], this treatment leads directly to

\[
M_{\text{in}}(P, P'; Q) = \int_{Q^\perp} dKL(K, P - Q; Q) L^*(K, P' - Q; Q)
\]

with

\[
L(K, P; Q) = \sqrt{\frac{\mu}{Qm^2}} K Q + \left( 1 + \frac{m}{M} \right) \frac{Q}{2} + \frac{m}{M} P_{\| q} \right)^{1/2} \times f \left( \text{rel} (K_{\perp q}, P_{\perp q}) - \frac{Q}{2}, \text{rel} (K_{\perp q}, P_{\perp q}) + \frac{Q}{2} \right).
\]

The integration in (28) is over the plane \( Q^\perp = \{K \in \mathbb{R}^3 : K \cdot Q = 0\} \) perpendicular to the momentum transfer \( Q \). Clearly, the function \( L \) contains all the details of the collisional interaction with the gas. It involves the elastic scattering amplitude \( f(\rho_{\text{out}}, \rho_{\text{in}}) \), the momentum distribution function \( \mu(p) \) of the gas, and its number density \( n_{\text{gas}} \).

### 4.2. Operator form of the quantum linear Boltzmann equation

The particular form (23) with (28) and (29) admits the master equation to be written in a representation-independent fashion. One finds the form [2]

\[
\partial_t \rho = \frac{1}{\hbar} [H, \rho] + \int dQ \int_{Q^\perp} dK \left\{ L_{Q, K} \rho L_{Q, K}^\dagger - \frac{1}{2} \rho L_{Q, K}^\dagger L_{Q, K} - \frac{1}{2} L_{Q, K}^\dagger \rho L_{Q, K} \right\}
\]

with the Lindblad operators \( L_{Q, K} \) defined by

\[
L_{Q, K} = e^{iQ \cdot X / \hbar} L(K, P; Q).
\]

Here, the position and the momentum operator of the Brownian particle are denoted by \( X \) and \( P \), respectively. Reassuringly, this form of the master equation is in agreement with the general structure of a translation-invariant and completely positive master equation, as characterized by Holevo [15], see the discussion in [16, 17]. Moreover, on the momentum diagonal it reduces to the classical linear Boltzmann equation for the momentum distribution function.

Equation (30) should be viewed as a full quantum version of the linear Boltzmann equation. Although its representation independent operator form (29)-(31) might appear complicated at first sight, it has in fact a rather suggestive interpretation when viewed in the momentum representation (23). To see this let us define as a possible two-particle momentum trajectory \( (P_{\text{in}}, \rho_{\text{in}}) \rightarrow (P_{\text{out}}, \rho_{\text{out}}) \) any combination of initial and final momenta of the Brownian and the gas particle, respectively. The allowed two-particle trajectories are those which conserve the total momentum end energy. The in-rate (28) in the momentum representation (23) can now be understood as the integral over the scattering amplitudes of all allowed pairs of two-particle trajectories, which end at \( P \) and \( P' \), respectively, and correspond to the common momentum exchange \( Q \), cf. Fig 3. The integration measure, i.e., the weight of the pairs of trajectories, is simply given by the distribution in the gas, as restricted by the choice of \( P \), \( P' \), and \( Q \), and by the requirement of energy and momentum conservation.
Figure 3. A pictorial view of the pairs of “two-particle trajectories” entering the in-rate with \(28\). For a given pair of final Brownian particle momenta, \(P\) and \(P'\), and for given common momentum exchange \(Q\), there are many different pairs of \((\xi, \xi')\) of initial gas momenta which are consistent with the conservation of energy and total momentum. The integral in \(28\) covers them all and weights them according to their distribution in the gas.

4.3. Relation to previous results

A master equation very similar to the monitoring result \(29\)-(31) was proposed, on a slightly more heuristic basis, in 1995 by Diósi [13]. In the present notation his equation is given by \(30\) and \(31\) provided the functions \(L(K, P; Q)\) are replaced by

\[
L_{\text{Diósi}}(K, P; Q) = \sqrt{\frac{m_{\text{gas}} m}{Q m_s^*}} \mu \left( K + \left(1 + \frac{m}{M}\right) \frac{Q}{2} + \frac{m}{M} P \right)^{1/2} f \left( \frac{m_s K - Q}{2}, \frac{m}{m_s} K + \frac{Q}{2} \right).
\]

(32)

The main difference with respect to the present result \(31\) is that the arguments of the scattering amplitude do not depend on \(P\). This implies that the complex rate function \(M_{\text{in}}\) is determined by the differential cross section \(d\sigma/d\Omega = |f|^2\), rather the individual complex scattering amplitudes of the collision trajectories. This indicates that it does not incorporate the non-parallel pairs of trajectories, \(\xi \neq \xi'\), though, a priori, one would expect them to contribute to the rate as well. On the diagonal, i.e., for \(P = P'\), Diósi’s equation coincides with the present result \(29\)-(31); however they differ in the “Brownian limit” of small momentum transfers, thus predicting different coefficients for the corresponding Fokker-Planck equation.

Related and more recent works can be found in [18, 19]. The most relevant development for our case is the theory by Vacchini [20, 21], which uses the van Hove expression for macroscopic scattering to relate the two-point correlation function of the gas with the collision kernel, a treatment which is valid in the weak-coupling limit. It turns out that his equation coincides with the limiting form of the present result if one replaces the scattering amplitude in \(29\) by its Born approximation \(f_B\). The reason is that \(f_B\) depends only on the difference of the momenta so that the \(P\)- and \(K\)-dependence of the scattering amplitude vanishes in this limit. Incidentally, this shows that the non-perturbative form of the master equation cannot be specified by a weak coupling calculation alone. In particular, it is not obtained by simply replacing the Born approximation of the scattering amplitude with the exact one.

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 present result \(29\)-(31) reduces in this limit to the proper master equation for collisional decoherence [10], which was recently tested experimentally [22, 23].

5. Conclusions

In summary, I presented a general method of incorporating proper time-dependent scattering theory into the dynamic description of open quantum systems. Its derivation is based on the theory of generalized and continuous measurements and it yields completely positive master
equations, which account for the environmental interaction in a non-perturbative fashion. When applied to either the case of an immobile, complex object or the case of a Brownian point particle, it provides a detailed and realistic account of the dissipation and decoherence effects induced by the presence of a gaseous environment.

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