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Monitoring approach to open quantum dynamics using scattering theory

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Abstract – It is shown how S-matrix theory and the concept of continuous quantum measurements can be combined to yield Markovian master equations which describe the environmental interaction non-perturbatively. The method is then applied to obtain the master equation for the effects of a gas on the internal dynamics of an immobile complex quantum system, such as a trapped molecule, in terms of the exact multi-channel scattering amplitudes.

Introduction. – A truism of quantum physics tells that no system is perfectly isolated and it is therefore not surprising that the study of open quantum systems is an ubiquitous theme of present-day quantum mechanics, see [1–4] and references therein. An important class of evolution equations for open systems are Markovian master equations. They imply that environmental correlations disperse fast, so that on a coarse-grained timescale the temporal change of the system state ρ depends on the present state of the system, but not on its history. From the strict point of view of an operationalist (who dismisses the notion of a "system" altogether and takes ρ as describing an equivalence class of preparations in the lab [5]) one may even argue that any valid differential equation for the time evolution of ρ must generate a completely positive dynamical semigroup [6] and must hence be Markovian.

Putting the pros and cons of Markovian *vs.* non-Markovian formulations aside, it is fair to say that a large class of open quantum systems is described appropriately by time-local master equations. At the same time, it is curious that the Markov property does not emerge naturally in standard microscopic derivations. Rather, one has to impose it "by hand", usually by interpreting some quantities as correlation functions, which must then be assumed to be δ-correlated. This may be still transparent in weak-coupling calculations such as the Bloch-Redfield approach [1], but tends to be awkward if a non-perturbative treatment of the interaction with the environment is needed.

In the present letter I would like to motivate and exemplify a general method of obtaining master equations which do incorporate the microscopic interactions in a non-perturbative fashion. It differs from the standard approaches in that it takes the Markov assumption not as an approximation in the course of the calculation, but as a premise, implemented before tracing out the environment. It will be applicable whenever the interaction with the environment can reasonably be described in terms of individual interaction events or "collisions", that is, if one can take the environment as consisting of independent (quasi)-particles which probe the system each at a time, in the sense that both the rate and the effect of an individual collision are separately physically meaningful and can be formulated microscopically. One may then implement the Markov requirement right from the outset by disregarding the change of the environmental state after each collision. This will be justified if the environment is sufficiently large and stationary, and in particular if many different environmental (quasi)-particles are involved so that each has much time to carry away and disperse its correlation with the system.

It is clear that the apparatus of time-dependent scattering theory [7] is predestined for this type of description. Its microscopically defined S-matrix maps from the incoming to the exact outgoing asymptotes of the system-environment state without a temporal evolution, and a partial trace over the scattered environment yields the system state after a single collision. One would like to write the temporal change of the system as the rate of collisions multiplied by this change due to an individual scattering. The great difficulty with this is that in general also the rate depends on the system state so that a naive implementation would yield a nonlinear equation. Below, I describe how this is circumvented by applying the concept of generalized and continuous measurements. The use and strength of the method is then demonstrated by deriving the master equation for the internal quantum dynamics of an immobile system affected by a gaseous environment in terms of the multichannel scattering amplitudes.

Monitoring approach. – My first aim is to argue that the system ρ evolves as $\partial_t \rho = (i\hbar)^{-1} [\mathsf{H}, \rho] + \mathcal{L}\rho$ with

$$\begin{aligned}\mathcal{L}\rho = {} & \frac{i}{2}\,\mathrm{Tr}_{\mathrm{env}}\left(\left[\mathsf{T}+\mathsf{T}^\dagger, \Gamma^{1/2}\left[\rho\otimes\rho_{\mathrm{env}}\right]\Gamma^{1/2}\right]\right)\\ & + \mathrm{Tr}_{\mathrm{env}}\left(\mathsf{T}\Gamma^{1/2}\left[\rho\otimes\rho_{\mathrm{env}}\right]\Gamma^{1/2}\mathsf{T}^\dagger\right)\\ & -\frac{1}{2}\,\mathrm{Tr}_{\mathrm{env}}\left(\Gamma^{1/2}\mathsf{T}^\dagger\mathsf{T}\Gamma^{1/2}\left[\rho\otimes\rho_{\mathrm{env}}\right]\right)\\ & -\frac{1}{2}\,\mathrm{Tr}_{\mathrm{env}}\left(\left[\rho\otimes\rho_{\mathrm{env}}\right]\Gamma^{1/2}\mathsf{T}^\dagger\mathsf{T}\Gamma^{1/2}\right). \end{aligned} \tag{1}$$

Here H is the Hamiltonian of the isolated system and ρ_{env} the reduced single-particle state of the environment. The operator T is the nontrivial part of the two-particle S-matrix $\mathsf{S} = \mathsf{I} + i\mathsf{T}$ describing the effect of a single collision between environmental particle and system. The rate of collisions is described by Γ, a positive operator in the total Hilbert space, which determines the probability of a collision to occur in a small time interval Δt,

$$\mathrm{Prob}\left(\mathrm{C}_{\Delta t}|\rho\right) = \Delta t\,\mathrm{tr}\left(\Gamma\left[\rho\otimes\rho_{\mathrm{env}}\right]\right). \tag{2}$$

Like the S-matrix, the operator Γ can in principle be characterized operationally in independent experiments. Its microscopic formulation will in general involve a total scattering cross-section and the current density operator of the relative motion (see below).

To motivate the time evolution (1) we picture the environment as monitoring the system continuously by sending probe particles which scatter off the system at random times. The state-dependent collision rate can now be incorporated into the dynamical description by assuming that the system is encased by a hypothetical, minimally invasive detector with time resolution Δt. It tells at any instant whether a probe particle has passed by and is going to scatter off the system.

The important point to note is that the information that a collision will take place changes our description of the impinging two-particle state. According to the theory of generalized measurements [5,8,9] the new state is the normalized image of a norm-decreasing completely positive map $\mathcal{M}(\cdot|\mathrm{C}_{\Delta t})$ in the total Hilbert space satisfying $\mathrm{tr}\left(\mathcal{M}(\varrho|\mathrm{C}_{\Delta t})\right) = \Delta t\,\mathrm{tr}\left(\Gamma\varrho\right)$. For an efficient [10] and minimally invasive detector it has the form

$$\mathcal{M}(\varrho|\mathrm{C}_{\Delta t}) = \Delta t\Gamma^{1/2}\varrho\Gamma^{1/2}. \tag{3}$$

The significance of this measurement transformation is to imprint our improved knowledge about the incoming two-particle wave packet, and it may be viewed as enhancing those parts which head towards a collision. In principle, an efficient measurement (which introduces no classical noise by mapping pure states to pure states) may be given by a more general operator, $\mathcal{M}(\varrho|\mathrm{C}_{\Delta t}) = \mathsf{M}_{\Delta t}\varrho\mathsf{M}_{\Delta t}^\dagger$ as long as it satisfies $\mathsf{M}_{\Delta t}^\dagger\mathsf{M}_{\Delta t} = \Delta t\Gamma$. The above "minimally invasive" choice of $\mathsf{M}_{\Delta t}$ is reasonable because a possible unitary part $\mathsf{U}_{\Delta t}$ in its general polar decomposition $\mathsf{M}_{\Delta t} = \mathsf{U}_{\Delta t}\Gamma^{1/2}\sqrt{\Delta t}$ would describe a reversible "back action" which has no physical justification in our case of a thought measurement invoked only to account for the state dependence of collision probabilities.

Also the absence of a detection event during Δt changes the state. The corresponding complementary map $\mathcal{M}(\cdot|\overline{\mathrm{C}}_{\Delta t})$ satisfies $\mathrm{tr}\left(\mathcal{M}(\varrho|\overline{\mathrm{C}}_{\Delta t})\right) = 1 - \Delta t\,\mathrm{tr}\left(\Gamma\varrho\right)$ and the Kraus representation with time-invariant operators reads $\mathcal{M}(\varrho|\overline{\mathrm{C}}_{\Delta t}) = \varrho - \Gamma^{1/2}\varrho\Gamma^{1/2}\Delta t$.

We can now form the unconditioned system-probe state after time Δt by allowing for the fact that the detection outcomes are not really available. Thus, the infinitesimally evolved state is given by the mixture of the colliding state transformed by the S-matrix and the untransformed non-colliding one, weighted with the respective probabilities,

$$\begin{aligned}\varrho'(\Delta t) = {} & \mathrm{Prob}\left(\mathrm{C}_{\Delta t}|\rho\right)\mathsf{S}\frac{\mathcal{M}(\varrho|\mathrm{C}_{\Delta t})}{\mathrm{tr}\left(\mathcal{M}(\varrho|\mathrm{C}_{\Delta t})\right)}\mathsf{S}^\dagger\\ & + \mathrm{Prob}\left(\overline{\mathrm{C}}_{\Delta t}|\rho\right)\frac{\mathcal{M}(\varrho|\overline{\mathrm{C}}_{\Delta t})}{\mathrm{tr}\left(\mathcal{M}(\varrho|\overline{\mathrm{C}}_{\Delta t})\right)}\\ = {} & \mathsf{S}\Gamma^{1/2}\varrho\Gamma^{1/2}\mathsf{S}^\dagger\Delta t + \varrho - \Gamma^{1/2}\varrho\Gamma^{1/2}\Delta t. \end{aligned}$$

Using the unitarity of S, which implies $i(\mathsf{T} - \mathsf{T}^\dagger) = -\mathsf{T}^\dagger\mathsf{T}$, the differential quotient can be written as

$$\begin{aligned}\frac{\varrho'(\Delta t) - \varrho}{\Delta t} = {} & \mathsf{T}\Gamma^{1/2}\varrho\Gamma^{1/2}\mathsf{T}^\dagger - \frac{1}{2}\mathsf{T}^\dagger\mathsf{T}\Gamma^{1/2}\varrho\Gamma^{1/2}\\ & -\frac{1}{2}\Gamma^{1/2}\varrho\Gamma^{1/2}\mathsf{T}^\dagger\mathsf{T} + i\left[\mathrm{Re}\left(\mathsf{T}\right), \Gamma^{1/2}\varrho\Gamma^{1/2}\right]. \end{aligned}$$

One arrives at (1) by tracing out the environment with $\varrho = \rho\otimes\rho_{\mathrm{env}}$, taking the limit of continuous monitoring $\Delta t \to 0$, and adding the generator of the free system evolution. Thus, the collision rate with its state dependence is incorporated by the operators $\Gamma^{1/2}$ and they may be thought of, in a stochastic unravelling of the master equation [2,11–15], as serving to weight each trajectory with the rate before it scatters. The operators T describe the individual microscopic interaction process *without approximation*. Note also that (1) generates a dynamical semigroup by construction since $\mathcal{M}(\cdot|\mathrm{C}_{\Delta t})$ and $\mathcal{M}(\cdot|\overline{\mathrm{C}}_{\Delta t})$ are completely positive.

To judge whether the trace in (1) yields a useful master equation one has to specify system and environment. A first application of this general equation can already be found in the recent ref. [16], where it is used to describe the motion of a distinguished, freely moving point-particle in the presence of a gas. The above discussion thus serves to complete the derivation in [16], where a quantum version of the linear Boltzmann equation was obtained which displays all expected limiting properties. In the following, I will demonstrate the use and generality of eq. (1) by posing a complementary question, namely, how the the *internal* dynamics of an immobile system gets affected by an environment of structureless gas particles.

Application to an immobile system. – If the motional system degrees of freedom are disregarded, a single-particle S-matrix can be used to describe the (in general inelastic) interaction with the environmental particles. The resulting master equation should describe non-perturbatively both the coherent and the incoherent processes induced by this coupling. An example would be the collisional decay of molecular eigenstates into chiral configurations, or the phonon-induced decoherence of a quantum dot. For concreteness, the environment is assumed to be an ideal Maxwell gas of density n_{gas}, atomic mass m, and single-particle state $\rho_{\mathrm{env}} = \left(\lambda_{\mathrm{th}}^3/\Omega\right)\exp\left(-\beta \mathsf{p}^2/2m\right)$ with p the momentum operator, $\lambda_{\mathrm{th}} = \hbar\sqrt{2\pi\beta/m}$ the thermal wavelength, and Ω the normalization volume.

In the language of scattering theory the free energy eigenstates of the non-motional degrees of freedom are called channels. In our case, they form a discrete basis of the system Hilbert space, and $|\alpha\rangle$ will be used to indicate internal (and possibly rotational), non-degenerate system eigenstates of energy E_α. In this channel basis, $\rho_{\alpha\beta} = \langle\alpha|\rho|\beta\rangle$, the equation of motion (1) takes on the form of a general master equation of Lindblad type,

$$\begin{aligned}\partial_t \rho_{\alpha\beta} \;=\; & \frac{E_\alpha + \varepsilon_\alpha - E_\beta - \varepsilon_\beta}{i\hbar}\rho_{\alpha\beta} + \sum_{\alpha_0\beta_0} \rho_{\alpha_0\beta_0}\, M_{\alpha\beta}^{\alpha_0\beta_0} \\ & -\frac{1}{2}\sum_{\alpha_0}\rho_{\alpha_0\beta}\,\sum_{\gamma} M_{\gamma\gamma}^{\alpha_0\alpha} - \frac{1}{2}\sum_{\beta_0}\rho_{\alpha\beta_0}\,\sum_{\gamma} M_{\gamma\gamma}^{\beta\beta_0}\end{aligned} \tag{4}$$

with energy shifts ε_α discussed below and rate coefficients

$$M_{\alpha\beta}^{\alpha_0\beta_0} = \langle\alpha|\,\mathrm{Tr}_{\mathrm{env}}\left(\mathsf{T}\Gamma^{1/2}\left[|\alpha_0\rangle\langle\beta_0|\otimes\rho_{\mathrm{env}}\right]\Gamma^{1/2}\mathsf{T}^\dagger\right)|\beta\rangle. \tag{5}$$

To calculate these complex quantities we need to specify the rate operator Γ. In the present case it is naturally given in terms of the current density operator $\mathsf{j} = n_{\mathrm{gas}}\mathsf{p}/m$ of the impinging gas particles and the channel-specific total scattering cross-sections $\sigma(\boldsymbol{p},\alpha)$,

$$\Gamma = \sum_\alpha |\alpha\rangle\langle\alpha|\otimes n_{\mathrm{gas}}\frac{|\mathsf{p}|}{m}\sigma\left(\mathsf{p},\alpha\right). \tag{6}$$

Defining the channel operator $\mathsf{c} = \sum_\alpha \alpha|\alpha\rangle\langle\alpha|$, one can thus write $\Gamma = |\mathsf{j}|\sigma\left(\mathsf{p},\mathsf{c}\right)$.

In principle, Γ must also involve a projection to the subspace of incoming wave packets, attributing zero collision probability to any wave packet located far off the scattering center and travelling away from it. This is important because such an outgoing state will not remain invariant under S. (It may be strongly transformed since the definition of S involves a backward evolution.) In practice, the microscopic definition of Γ is easier if one takes care of the projection separately. This is easily done if ρ_{env} admits a convex decomposition into incoming and outgoing states. Alternatively, one may dispense with the projection by modifying the definition of S so that outgoing wave packets are kept invariant (see below).

Let us now evaluate the rate coefficients $M_{\alpha\beta}^{\alpha_0\beta_0}$ by using a decomposition of ρ_{env} that permits to separate in- and out-wave packets. As shown in [17] the thermal gas state can be written as a phase space integration over projectors onto minimum uncertainty Gaussian states $|\psi_{\boldsymbol{r}_0\boldsymbol{p}_0}\rangle = \bar{\lambda}_{\mathrm{th}}^{3/2}\exp\left(-\bar{\beta}\left(\mathsf{p}-\boldsymbol{p}_0\right)^2/4m\right)|\boldsymbol{r}_0\rangle$ whose spatial extension $\bar{\lambda}_{\mathrm{th}} = \hbar\sqrt{2\pi\bar{\beta}/m}$ is determined by an inverse temperature $\bar{\beta} > \beta$,

$$\rho_{\mathrm{env}} = \int \mathrm{d}\boldsymbol{p}_0\hat{\mu}\left(\boldsymbol{p}_0\right)\int_\Omega \frac{\mathrm{d}\boldsymbol{r}_0}{\Omega}\,|\psi_{\boldsymbol{r}_0\boldsymbol{p}_0}\rangle\langle\psi_{\boldsymbol{r}_0\boldsymbol{p}_0}|. \tag{7}$$

Here $\hat{\mu}(\boldsymbol{p}_0) = (2\pi m/\hat{\beta})^{-3/2}\exp(-\hat{\beta}\boldsymbol{p}_0^2/2m)$ is the Maxwell-Boltzmann distribution corresponding to the temperature $\hat{\beta}^{-1} = \beta^{-1} - \bar{\beta}^{-1}$, so that by setting a $\bar{\beta}$ one splits up the gas temperature β^{-1} into a part determining the localization of the $|\psi_{\boldsymbol{r}_0\boldsymbol{p}_0}\rangle$ and a part characterizing their motion. We choose $\bar{\beta}$ large and take eventually the limit $\bar{\beta}\to\infty$, $\hat{\beta}\to\beta$ of very extended wave packets so that $\hat{\mu}$ approaches the original Maxwell-Boltzmann distribution μ. Inserting (7) into (5) yields

$$M_{\alpha\beta}^{\alpha_0\beta_0} = \int \mathrm{d}\boldsymbol{p}_0\hat{\mu}\left(\boldsymbol{p}_0\right)\int_\Omega \frac{\mathrm{d}\boldsymbol{r}_0}{\Omega}\, m_{\alpha\beta}^{\alpha_0\beta_0}\left(\boldsymbol{r}_0,\boldsymbol{p}_0\right). \tag{8}$$

Here the phase space function

$$\begin{aligned}m_{\alpha\beta}^{\alpha_0\beta_0}\left(\boldsymbol{r}_0,\boldsymbol{p}_0\right) := \int \mathrm{d}\boldsymbol{p}\,&\langle\alpha|\langle\boldsymbol{p}|\mathsf{T}\Gamma^{1/2}|\alpha_0\rangle|\psi_{\boldsymbol{r}_0\boldsymbol{p}_0}\rangle \\ &\times\langle\beta_0|\langle\psi_{\boldsymbol{r}_0\boldsymbol{p}_0}|\Gamma^{1/2}\mathsf{T}^\dagger|\beta\rangle|\boldsymbol{p}\rangle\end{aligned} \tag{9}$$

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 (8) it is natural to confine this spatial average at fixed $\boldsymbol{p}_0$ to a cylinder pointing in the direction of $\boldsymbol{p}_0$, whose longitudinal support $\Lambda_{\boldsymbol{p}_0}$ vanishes at outgoing positions and whose transverse base area is given by an average cross-section $\Sigma_{\boldsymbol{p}_0}$. In terms of the longitudinal and transverse positions $\boldsymbol{r}_{\|\boldsymbol{p}_0} := (\boldsymbol{r}\cdot\boldsymbol{p}_0)\,\boldsymbol{p}_0/p_0^2$ and $\boldsymbol{r}_{\perp\boldsymbol{p}_0} = \boldsymbol{r} - \boldsymbol{r}_{\|\boldsymbol{p}_0}$ we have

$$M_{\alpha\beta}^{\alpha_0\beta_0} = \int \mathrm{d}\boldsymbol{p}_0\,\hat{\mu}(\boldsymbol{p}_0)\int_{\Lambda_{\boldsymbol{p}_0}}\frac{\mathrm{d}\boldsymbol{r}_{\|\boldsymbol{p}_0}}{\Lambda_{\boldsymbol{p}_0}}\int_{\Sigma_{\boldsymbol{p}_0}}\frac{\mathrm{d}\boldsymbol{r}_{\perp\boldsymbol{p}_0}}{\Sigma_{\boldsymbol{p}_0}} \times m_{\alpha\beta}^{\alpha_0\beta_0}\left(\boldsymbol{r}_{\|\boldsymbol{p}_0}+\boldsymbol{r}_{\perp\boldsymbol{p}_0},\boldsymbol{p}_0\right). \tag{10}$$

In order to evaluate $m_{\alpha\beta}^{\alpha_0\beta_0}$, insert momentum resolutions of unity between the T and Γ operators in (9) and use the representation [7]

$$\langle\alpha_f|\langle\boldsymbol{p}_f|\mathsf{T}|\alpha_i\rangle|\boldsymbol{p}_i\rangle = \frac{f_{\alpha_f\alpha_i}\left(\boldsymbol{p}_f,\boldsymbol{p}_i\right)}{2\pi\hbar m}\,\delta\left(E_{p_f\alpha_f}-E_{p_i\alpha_i}\right) \tag{11}$$

in terms of the multi-channel scattering amplitude and total energies $E_{p\alpha} = p^2/2m + E_\alpha$. By transforming the new integration variables to mid-points and chords, one obtains a Gaussian function which approaches, for large $\bar{\beta}$, a δ-function in the midpoints. Integrating out the latter one finds that the combination of the δ-functions from (11) confine the chord integration to a plane perpendicular to $\boldsymbol{p}_0$. Integrating out the parallel component leads to the factor $\exp\left(-\bar{\beta}m\left(E_\alpha - E_{\alpha_0} - E_\beta + E_{\beta_0}\right)^2/8p_0^2\right)$ which, again for large $\bar{\beta}$, can be replaced by

$$\chi_{\alpha\beta}^{\alpha_0\beta_0} := \begin{cases} 1, \text{ if } E_\alpha - E_{\alpha_0} = E_\beta - E_{\beta_0},\\ 0, \text{ otherwise.}\end{cases}$$

The resulting expression is independent of $\boldsymbol{r}_{\|\boldsymbol{p}_0}$,

$$\begin{aligned} m_{\alpha\beta}^{\alpha_0\beta_0}(\boldsymbol{r}_0,\boldsymbol{p}_0) = {}& \chi_{\alpha\beta}^{\alpha_0\beta_0}\frac{n_{\text{gas}}}{m^2}\int\mathrm{d}\boldsymbol{p}\int\frac{\mathrm{d}\tilde{\boldsymbol{p}}_{\perp\boldsymbol{p}_0}}{(2\pi\hbar)^2} \\ &\times\exp\left(-\bar{\beta}\frac{\tilde{\boldsymbol{p}}_{\perp\boldsymbol{p}_0}^2}{8m} - i\frac{\boldsymbol{r}_{0,\perp\boldsymbol{p}_0}\cdot\tilde{\boldsymbol{p}}_{\perp\boldsymbol{p}_0}}{\hbar}\right) \\ &\times f_{\alpha\alpha_0}\left(\boldsymbol{p},\boldsymbol{p}_0^+\right)f_{\beta\beta_0}^*\left(\boldsymbol{p},\boldsymbol{p}_0^-\right) \\ &\times\delta\left(\frac{\boldsymbol{p}^2-\left(\boldsymbol{p}_0^+\right)^2}{2m}+E_\alpha-E_{\alpha_0}\right) \\ &\times\sqrt{\left(1+\frac{\tilde{\boldsymbol{p}}_{\perp\boldsymbol{p}_0}^2}{4p_0^2}\right)\sigma\left(\boldsymbol{p}_0^+,\alpha_0\right)\sigma\left(\boldsymbol{p}_0^-,\beta_0\right)} \end{aligned}$$

with $\boldsymbol{p}_0^\pm := \boldsymbol{p}_0 \pm \tilde{\boldsymbol{p}}_{\perp\boldsymbol{p}_0}/2$. The $\boldsymbol{r}_{\|\boldsymbol{p}_0}$-integration in (10) yields an approximate two-dimensional δ-function in $\tilde{\boldsymbol{p}}_{\perp\boldsymbol{p}_0}$ so that we obtain

$$M_{\alpha\beta}^{\alpha_0\beta_0} = \chi_{\alpha\beta}^{\alpha_0\beta_0}\frac{n_{\text{gas}}}{m^2}\int\mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{p}_0\mu(\boldsymbol{p}_0)\,f_{\alpha\alpha_0}(\boldsymbol{p},\boldsymbol{p}_0) \times f_{\beta\beta_0}^*(\boldsymbol{p},\boldsymbol{p}_0)\,\delta\left(\frac{\boldsymbol{p}^2-\boldsymbol{p}_0^2}{2m}+E_\alpha-E_{\alpha_0}\right), \tag{12}$$

provided we identify the average cross-section of (10) with the geometric mean of the total cross-sections of the involved channels, *i.e.*, $\Sigma_{\boldsymbol{p}_0} = \sqrt{\sigma(\boldsymbol{p}_0;\alpha_0)\,\sigma(\boldsymbol{p}_0;\beta_0)}$. Moreover, the final limit $\bar{\beta}\to\infty$ replaced $\hat{\mu}$ by μ in (12).

With the same method one shows that the first term in (1) merely modifies the unitary evolution. Its effect is to shift the system energies from E_α to $E_\alpha + \varepsilon_\alpha$ by a thermal average of the "forward scattering amplitudes",

$$\varepsilon_\alpha = -2\pi\hbar^2\frac{n_{\text{gas}}}{m}\int\mathrm{d}\boldsymbol{p}_0\mu(\boldsymbol{p}_0)\,\mathrm{Re}\left[f_{\alpha\alpha}(\boldsymbol{p}_0,\boldsymbol{p}_0)\right]. \tag{13}$$

It is reassuring that the explicit expressions (12) and (13) can be shown to be equivalent to the more abstract master equation by Dümcke [18], obtained in a "low-density limit" scaling approach [1,6,19] for the special case of a factorizing interaction potential, $\mathsf{V}_{\text{tot}} = \mathsf{A}\otimes\mathsf{B}_{\text{env}}$, and for times large compared to all system time scales. The present approach thus generalizes this result to arbitrary interaction potentials (satisfying asymptotic completeness) and to arbitrary times as long as they are greater than the duration of a single collision.

It is worth noting that the $M_{\alpha\beta}^{\alpha_0\beta_0}$ can as well be obtained in a more direct, while less solid way if the *diagonal* momentum representation of ρ_{env} is used instead of (7). A projection to the incoming wave packets is then hard to implement and, as discussed above, the application of S to improper momentum states leads to the unwanted transformation also of its "outgoing components". As a consequence, the resulting expression for $M_{\alpha\beta}^{\alpha_0\beta_0}$ is ill-defined, involving the square of the δ-functions in (11) and the normalization volume Ω. This can be healed by noting that any consistent modification of S which keeps outgoing wave packets invariant must conserve the probability current. This condition provides a simple rule how to form a well-defined expression [17,20], whose multichannel version yields the result (12) immediately for any momentum diagonal ρ_{env}.

The expression for the rate coefficients can be rewritten, for isotropic μ, in terms of an average over the velocity distribution $\nu(v) = 4\pi m^3 v^2\mu(mv)$ and angular integrations, which bring about the velocity $v_{\text{out}} = \sqrt{v^2 - 2(E_\alpha - E_{\alpha_0})/m}$ of the gas particle after a possibly inelastic collision. For rotationally invariant scattering amplitudes, $f_{\alpha\alpha_0}\left(\cos(\boldsymbol{p},\boldsymbol{p}_0);E = p_0^2/2m\right)$, we have

$$M_{\alpha\beta}^{\alpha_0\beta_0} = \chi_{\alpha\beta}^{\alpha_0\beta_0}\int_0^\infty\mathrm{d}v\,\nu(v)\,n_{\text{gas}}v_{\text{out}}2\pi\int_{-1}^1\mathrm{d}(\cos\theta) \times f_{\alpha\alpha_0}\left(\cos\theta;\frac{m}{2}v^2\right)f_{\beta\beta_0}^*\left(\cos\theta;\frac{m}{2}v^2\right). \tag{14}$$

This shows that limiting cases of (4) display the expected dynamics. For the populations $\rho_{\alpha\alpha}$ it reduces to a rate equation where the total cross sections $\sigma_{\alpha\alpha_0}\left(\frac{m}{2}v^2\right)$ for scattering from channel α_0 to α determine the transition rates, $M_{\alpha\alpha}^{\alpha_0\alpha_0} = \int\mathrm{d}v\,\nu(v)\,n_{\text{gas}}v_{\text{out}}\sigma_{\alpha\alpha_0}$. In the case of purely elastic scattering, on the other hand, *i.e.*, $M_{\alpha\beta}^{\alpha_0\beta_0} = M_{\alpha\beta}^{\alpha\beta}\delta_{\alpha\alpha_0}\delta_{\beta\beta_0}$, the coherences decay exponentially, $\partial_t|\rho_{\alpha\beta}| = -\gamma_{\alpha\beta}^{\text{elastic}}|\rho_{\alpha\beta}|$, with a rate determined by a *difference* of scattering amplitudes,

$$\gamma_{\alpha\beta}^{\mathrm{elastic}} = \pi \int \mathrm{d}v\, \nu\,(v)\, n_{\mathrm{gas}} v_{\mathrm{out}} \int_{-1}^{1} \mathrm{d}\,(\cos\theta) \times \left| f_{\alpha\alpha}\left(\cos\theta; \frac{m}{2}v^2\right) - f_{\beta\beta}\left(\cos\theta; \frac{m}{2}v^2\right) \right|^2 . \quad (15)$$

It shows clearly that the more coherence is lost, in this case, the better the scattering environment can distinguish between system states $|\alpha\rangle$ and $|\beta\rangle$.

Conclusions. – In conclusion, a general method of incorporating formal scattering theory into the dynamic description of open quantum systems was presented. Based on the theory of generalized measurements, it yields completely positive master equations which account for the environmental interaction in a non-perturbative fashion. When applied to an immobile system in the presence of a gas, it provides a detailed and realistic account of the interplay between coherent system dynamics and the (possibly much faster) incoherent effects of the environment.

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