

Quantum Master Equation of a Particle in a Gas Environment.

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Abstract. - The reduced dynamics of a Brownian particle is discussed in *single collision* approach valid typically in dilute-gas environments. Our main purpose is a consistent account of quantum friction caused by *local* environmental interactions. We derive a Lindblad master equation whose generators are calculated from the differential cross-section of single collisions between the Brownian and the gas particles, respectively. The existence of thermal equilibrium for the Brownian particle's state ρ is proved. Master equations proposed earlier are shown to be particular cases of our one.

In this letter we discuss the quantum counterpart of the classical Brownian motion. Instead of standard weak-interaction approach [1], a *single collision* mechanism will be assumed.

In the classical phenomenological theory, the momentum distribution $\rho(\mathbf{p})$ of a Brownian particle of mass M satisfies the Fokker-Planck equation [2]

$$\frac{d\rho(\mathbf{p})}{dt} = D_{pp} \nabla^2 \rho(\mathbf{p}) + \frac{\gamma}{M} \nabla(\mathbf{p}\rho(\mathbf{p})), \quad (1)$$

where D_{pp} is the coefficient of momentum diffusion and γ is the friction constant. In particular, $D_{pp} = k_B T \gamma$ if the environment is in equilibrium at temperature T . A naive quantum counterpart would be the following master equation [3]:

$$\frac{d\rho}{dt} = -D_{pp} [\mathbf{q}, [\mathbf{q}, \rho]] - i \frac{\gamma}{2M} [\mathbf{q}, \{\mathbf{p}, \rho\}], \quad (2)$$

where \mathbf{q} , \mathbf{p} denote the position and, respectively, the momentum *operators* in interaction picture. Equation (2), however, does not belong to the Lindblad class [4] and, consequently, may violate the positivity of the *density operator* ρ [5]. A complete dynamic analysis of the quantum Brownian motion in gas environment is thus needed.

Let us first consider a simple (frictionless) *classical* kinetic model. The momentum distribution of a Brownian particle, interacting with the particles of the environment,

satisfies the following kinetic equation:

$$\frac{d\varphi(\mathbf{p})}{dt} = n_0 \int dE d\Omega_i d\Omega_f k^2 \frac{d\sigma(\theta, E)}{d\Omega_f} \varphi^\alpha(\mathbf{k}_i) (\varphi(\mathbf{p} - \mathbf{k}_f) - \varphi(\mathbf{p})), \quad (3)$$

where n_0 is the density of environmental particles, φ^α is their momentum distribution; $d\sigma$ denotes the differential cross-section of their scattering on the Brownian particle, while $\mathbf{k}_f = \mathbf{k}_f - \mathbf{k}_i$ is the difference between the final and initial momenta of the scattered particle. Further symbols are used in a standard way and need no special explanation. Equation (3) is valid provided that: the typical scattering time is much smaller than the average period between subsequent collisions, the mass M of the Brownian particle is much bigger than the mass m of the environment particles, their interaction is spin independent, and the influence of the Brownian particle on the environment's momentum distribution φ^α can be ignored.

Looking for a master equation for the density operator φ , note that the classical equation (3) would govern the evolution of φ 's diagonal elements according to the substitution $\varphi(\mathbf{p}) = \langle \mathbf{p} | \varphi | \mathbf{p} \rangle$. For the off-diagonal part of φ , however, we have no evolution rule (cf. Pauli's master equation [6]). A natural extension [7] of the «Pauli» evolution equation (3) would be

$$\frac{d\varphi}{dt} = n_0 \int dE d\Omega_i d\Omega_f k^2 \frac{d\sigma(\theta, E)}{d\Omega_f} \varphi^\alpha(\mathbf{k}_i) (\exp[-i\mathbf{k}_f \mathbf{q}] \varphi \exp[i\mathbf{k}_f \mathbf{q}] - \varphi). \quad (4)$$

To understand friction, assume that the environment is in thermal equilibrium so that $\varphi^\alpha(\mathbf{k})$ is a symmetric function. If the Brownian particle moves with velocity \mathbf{p}/M then, in its co-moving system, it perceives an asymmetric distribution $\varphi^\alpha(\mathbf{k} - m\mathbf{p}/M)$ generating damping force.

We start from the unitary dynamics of the density operator $\varphi^{\mathcal{L} + \mathcal{E}}$ corresponding to the Brownian particle (\mathcal{L}) plus the environment (\mathcal{E}) coupled to each other. In an interaction picture, a single collision between the Brownian and an environmental particle transforms the initial state $\varphi_i^{\mathcal{L} + \mathcal{E}}$ into the final one $\varphi_f^{\mathcal{L} + \mathcal{E}}$ via the unitary scattering operator S :

$$\varphi_f^{\mathcal{L} + \mathcal{E}} = S \varphi_i^{\mathcal{L} + \mathcal{E}} S^\dagger. \quad (5)$$

Let us introduce the transition operator T by $S = 1 + iT$. From the unitarity of S , we obtain $T^\dagger T = i(T^\dagger - T)$. Then eq. (5) yields [8]

$$\Delta\varphi^{\mathcal{L} + \mathcal{E}} \equiv \varphi_f^{\mathcal{L} + \mathcal{E}} - \varphi_i^{\mathcal{L} + \mathcal{E}} = \frac{i}{2} [T + T^\dagger, \varphi_i^{\mathcal{L} + \mathcal{E}}] + T \varphi_i^{\mathcal{L} + \mathcal{E}} T^\dagger - \frac{1}{2} \{T^\dagger T, \varphi_i^{\mathcal{L} + \mathcal{E}}\}. \quad (6)$$

The change $\Delta\varphi$ of the Brownian particle's density operator is given by the trace of eq. (6) over the environmental degrees of freedom. We shall approximate $d\varphi/dt$ by

$$\frac{\Delta\varphi}{\Delta t} = \frac{1}{\Delta t} \text{tr}_{\mathcal{E}} \Delta\varphi^{\mathcal{L} + \mathcal{E}}, \quad (7)$$

where Δt , considered longer than the typical collision time, is the period spanned by the initial and final states according to eq. (5).

Consider the standard form of the transition operator for the (spin-independent) scattering of the environmental particle on the Brownian one, with initial laboratory

momenta \mathbf{k}_i and \mathbf{p}_i , respectively:

$$T = \frac{1}{2\pi m^*} \int d\mathbf{p}_i d\mathbf{k}_i d\mathbf{k}_f f(\mathbf{k}_f^*, \mathbf{k}_i^*) \delta(E_{\mathbf{k}_f} - E_{\mathbf{k}_f^*}) |\mathbf{p}_i - \mathbf{k}_{\bar{n}}, \mathbf{k}_f\rangle \langle \mathbf{p}_i, \mathbf{k}_i|. \quad (8)$$

This equation is valid in the laboratory system though c.m.s. quantities (marked by stars) appear in it: $M^* = M + m$, $m^* = mM/M^*$, $\mathbf{k}_i^* = (M/M^*)\mathbf{k}_i - (m/M^*)\mathbf{p}_i$, and $\mathbf{k}_f^* = \mathbf{k}_f - (m/M^*)(\mathbf{k}_i + \mathbf{p}_i)$. The c.m.s. scattering amplitude has been denoted by f .

Let us assume now the form $\rho_i \otimes \rho^G$, for $\rho_i^{\ell+G}$. Let the environment's state ρ^G be stationary, representing n_0 uncorrelated identical particles per unite volume, with the same momentum distribution $\rho^G(\mathbf{k})$ for each. (Assume Boltzmann statistics, for simplicity.) Let us substitute eq. (8) into eq. (6) and single out the second term on the r.h.s.:

$$\text{tr}_G(T\rho_i \otimes \rho^G T^\dagger) = \frac{2\pi n_0}{m^{*2}} \int \int d\mathbf{p}_i d\mathbf{p}'_i d\mathbf{k}_i d\mathbf{k}_f \rho^G(\mathbf{k}_i) \cdot f(\mathbf{k}_f^*, \mathbf{k}_i^*) \delta(E_{\mathbf{k}_f^*} - E_{\mathbf{k}_f}) |\mathbf{p}_i - \mathbf{k}_{\bar{n}}\rangle \langle \mathbf{p}_i | \rho | \mathbf{p}'_i \rangle \langle \mathbf{p}'_i - \mathbf{k}_{\bar{n}} | f^*(\mathbf{k}_f^{*'}, \mathbf{k}_i^{*'}) \delta(E_{\mathbf{k}_f^{*'}} - E_{\mathbf{k}_f^*}). \quad (9)$$

Observe that the coherent uncertainties of the gas particles' c.m.s. momenta are much less than the coherent uncertainty of the Brownian particle's momentum, since $|\mathbf{k}_i^{*'} - \mathbf{k}_i^*| = |\mathbf{k}_f^{*'} - \mathbf{k}_f^*| = (m/M^*)|\mathbf{p}'_i - \mathbf{p}_i|$. If $(m/M^*)|\mathbf{p}'_i - \mathbf{p}_i|$ is small the following substitution on the r.h.s. of eq. (9) allows a good approximation:

$$\rho^G(\mathbf{k}_i) \rightarrow \sqrt{\rho^G(\mathbf{k}_i)} \sqrt{\rho^G(\mathbf{k}'_i)}, \quad (10)$$

with $\mathbf{k}'_i \equiv \mathbf{k}_i^* + (m/M)(\mathbf{p}'_i + \mathbf{k}_f^*)$. Now, let us change the integration variables $d\mathbf{k}_i$, $d\mathbf{k}_f$ for $d\mathbf{k}_i^*$, $d\mathbf{k}_f^*$, respectively. Then, apply an approximation again: let the momenta $\mathbf{k}_i^{*'}$, $\mathbf{k}_f^{*'}$ be identified with \mathbf{k}_i^* , \mathbf{k}_f^* , respectively. One obtains

$$\text{tr}_G(T\rho \otimes \rho^G T^\dagger) = \frac{2\pi n_0}{m^{*2}} \left(\frac{M^*}{M}\right)^3 \int \int d\mathbf{p}_i d\mathbf{p}'_i d\mathbf{k}_i^* d\mathbf{k}_f^* |f(\mathbf{k}_f^*, \mathbf{k}_i^*)|^2 \cdot [\delta(E_{\mathbf{k}_f^*} - E_{\mathbf{k}_f^*})]^2 \sqrt{\rho^G(\mathbf{k}_i)} \sqrt{\rho^G(\mathbf{k}'_i)} |\mathbf{p}_i - \mathbf{k}_{\bar{n}}\rangle \langle \mathbf{p}_i | \rho | \mathbf{p}'_i \rangle \langle \mathbf{p}'_i - \mathbf{k}_{\bar{n}}|. \quad (11)$$

This approximation is justified, similarly to the former step (10), if $(m/M^*)|\mathbf{p}'_i - \mathbf{p}_i|$ is small enough (cf. footnote⁽¹⁾). One can rewrite eq. (11) in operator form:

$$\text{tr}_G(T\rho \otimes \rho^G T^\dagger) = \frac{2\pi n_0}{m^{*2}} \left(\frac{M^*}{M}\right)^3 \int \int d\mathbf{k}_i^* d\mathbf{k}_f^* |f(\mathbf{k}_f^*, \mathbf{k}_i^*)|^2 \cdot [\delta(E_{\mathbf{k}_f^*} - E_{\mathbf{k}_f^*})]^2 \sqrt{\rho^G(\mathbf{k}_i)} \exp[-i\mathbf{k}_{\bar{n}}^* \mathbf{q}] \rho \exp[i\mathbf{k}_{\bar{n}}^* \mathbf{q}] \sqrt{\rho^G(\mathbf{k}_i)}, \quad (12)$$

where $\mathbf{k}_i = \mathbf{k}_i^* + (m/M)(\mathbf{p} + \mathbf{k}_f^*)$. Taking the usual approximation $\delta(E)|_{E=0} \sim \Delta t/2\pi$, eq. (12)

(1) To formulate the correct conditions, let us introduce the quantum uncertainty Δp of the Brownian particle's momentum: let $\langle \mathbf{p}' | \rho | \mathbf{p} \rangle \approx 0$ if $|\mathbf{p}' - \mathbf{p}| \gg \Delta p$. The steps (10), (11) are justified approximations provided $\Delta k \equiv (m/M)\Delta p$ is so small that the variations of both the distribution ρ^G and the scattering amplitude f can be ignored when their arguments are varied by $\sim \Delta k$.

takes the following form:

$$\frac{1}{\Delta t} \text{tr}_{\rho} (T_{\rho} \otimes \rho^{\rho} T^{\dagger}) = \frac{n_0}{m^{*2}} \left(\frac{M^*}{M} \right)^3 \iint d\mathbf{k}_i^* d\mathbf{k}_f^* \delta(E_{k_i^*} - E_{k_f^*}) |f(\mathbf{k}_f^*, \mathbf{k}_i^*)|^2 V_{k_i^* k_f^*} \rho V_{k_i^* k_f^*}^{\dagger}, \quad (13)$$

with

$$V_{k_i^* k_f^*} = \sqrt{\rho^{\rho} \left(\mathbf{k}_i^* + \frac{m}{M} (\mathbf{p} + \mathbf{k}_f^*) \right)} \exp[-i\mathbf{k}_{\text{ff}}^* \mathbf{q}]. \quad (14)$$

By now, all preparations have been done for calculating the rate $d\rho/dt$ which we shall approximate by $\Delta\rho/\Delta t$ (7). Consider the r.h.s. of eq. (6). The contribution of its first term will be neglected (that can be justified in dilute gases), the contribution of the second one has been given by eq. (13), and the third term's yield would also be given by a properly altered form of eq. (13). Invoking eq. (7), too, all these lead to the following equation:

$$\frac{d\rho}{dt} = \frac{n_0}{m^{*2}} \left(\frac{M^*}{M} \right)^3 \iint d\mathbf{k}_i^* d\mathbf{k}_f^* \delta(E_{k_i^*} - E_{k_f^*}) |f(\mathbf{k}_f^*, \mathbf{k}_i^*)|^2 \cdot \left(V_{k_i^* k_f^*} \rho V_{k_i^* k_f^*}^{\dagger} - \frac{1}{2} \{V_{k_i^* k_f^*}^{\dagger} V_{k_i^* k_f^*}, \rho\} \right). \quad (15)$$

An equivalent equation can be given in terms of the c.m.s. differential cross-section $d\sigma/d\Omega = |f|^2$ as follows:

$$\frac{d\rho}{dt} = n_0 \left(\frac{M^*}{M} \right)^3 \int dE^* d\Omega_i^* d\Omega_f^* k^{*2} \frac{d\sigma(\theta^*, E^*)}{d\Omega_f^*} \left(V_{k_i^* k_f^*} \rho V_{k_i^* k_f^*}^{\dagger} - \frac{1}{2} \{V_{k_i^* k_f^*}^{\dagger} V_{k_i^* k_f^*}, \rho\} \right). \quad (16)$$

This is the central result of our letter: a quantum master equation of Lindblad form [4] with Lindblad generators $V_{k_i^* k_f^*}$, describing the fluctuational-frictional evolution of the Brownian particle's density operator ρ , valid at time scales longer than the typical collision time. We shall prove the existence of thermal equilibrium for the stationary solutions.

The master equation (16) preserves translation invariance: density operators which are diagonal in momentum representation will remain diagonal. Equation (16) implies the following closed equation for translation-invariant states:

$$\frac{d\rho(\mathbf{p})}{dt} = n_0 \left(\frac{M^*}{M} \right)^3 \int dE^* d\Omega_i^* d\Omega_f^* k^{*2} \frac{d\sigma(\theta^*, E^*)}{d\Omega_f^*} \cdot \left(\rho^{\rho} \left(\frac{M^*}{M} \mathbf{k}_i^* + \frac{m}{M} (\mathbf{p} - \mathbf{k}_{\text{ff}}^*) \right) \rho(\mathbf{p} - \mathbf{k}_{\text{ff}}^*) - \rho^{\rho} \left(\frac{M^*}{M} \mathbf{k}_i^* + \frac{m}{M} \mathbf{p} \right) \rho(\mathbf{p}) \right), \quad (17)$$

where, as before, the normalized distribution $\rho(\mathbf{p})$ is defined by $\rho(\mathbf{p}) = \text{const}(\mathbf{p} | \rho | \mathbf{p})$. At the same time, this equation can be considered the extension of the classical kinetic equation (3) including friction this time. To find the stationary solution of the quantum master equation (16) is easy. Since it must be translation invariant, its diagonal will be subjected to the classical equation (17). Invoking the symmetry of $d\sigma$ for \mathbf{k}_i^* , \mathbf{k}_f^* interchanged, the condition for $d\rho/dt = 0$ can be the following:

$$\rho^{\rho}(\mathbf{k}_i) \rho(\mathbf{p}_i) = \rho^{\rho}(\mathbf{k}_f) \rho(\mathbf{p}_f), \quad (18)$$

i.e. one obtains the *detailed balance* condition. It has very important consequences. Assume that the environment is in thermal equilibrium at temperature T , with Boltzmann distribution $\rho^{\mathcal{G}}(k) = \text{const} \exp[-\beta E]$, where $\beta \equiv 1/k_B T$. Then eq. (18) implies that the stationary state ρ of the Brownian particle will be the thermal-equilibrium state $\text{const} \exp[-\beta p^2/2M]$ in both classical and quantum cases.

As an important special case, we consider a heavy Brownian particle in dilute Boltzmann gas. In this limiting case $m/M \rightarrow 0$ but mp/Mk is finite. Then eq. (16) yields

$$\frac{d\rho}{dt} = n_0 \int dE d\Omega_i d\Omega_f k^2 \frac{d\sigma(\theta, E)}{d\Omega_f} \rho^{\mathcal{G}}(k_i) \left(V_{k_f k_i, \rho} V_{k_f k_i}^\dagger - \frac{1}{2} \{ V_{k_f k_i}^\dagger V_{k_f k_i}, \rho \} \right). \quad (19)$$

The Lindblad generators (14) will reduce to the form

$$V_{k_f k_i} = \left(1 - \frac{\beta}{2M} \mathbf{k}_i \mathbf{p} \right) \exp[-i \mathbf{k}_f \mathbf{q}] \quad (20)$$

found phenomenologically by Gallis [9].

Also Dekker's proposal [10] is recovered by our eqs. (19), (20) in the limit when the coherent extension of the Brownian particle and/or the transferred momentum $|\mathbf{k}_f|$ in single collisions are small enough. Then $\exp[-i \mathbf{k}_f \mathbf{q}]$ on the r.h.s. of eq. (20) is approximated by $1 - i \mathbf{k}_f \mathbf{q}$ and, neglecting terms of order of $q^2 p^2$, eq. (19) can be written as follows:

$$\frac{d\rho}{dt} = -D_{pp}[\mathbf{q}, [\mathbf{q}, \rho]] - D_{qq}[\mathbf{p}, [\mathbf{p}, \rho]] - i \frac{\gamma}{2M} [\mathbf{q}, \{\mathbf{p}, \rho\}], \quad (21)$$

with $\gamma = \beta D_{pp}$ and with diffusion parameters expressed as

$$D_{pp} = \frac{2}{3} n_0 \int dE d\Omega_i d\Omega_f k^4 \frac{d\sigma(\theta, E)}{d\Omega_f} \rho^{\mathcal{G}}(k_i) \sin^2 \frac{\theta}{2}, \quad (22)$$

$$D_{qq} = \frac{1}{6} n_0 \left(\frac{\beta}{2M} \right)^2 \int dE d\Omega_i d\Omega_f k^4 \frac{d\sigma(\theta, E)}{d\Omega_f} \rho^{\mathcal{G}}(k_i). \quad (23)$$

Our result differs from the naive quantum master equation (2) by the additional term of *position diffusion* which is absent in the classical Fokker-Planck equation (1), nonetheless without which no mathematically consistent (*i.e.* Lindblad) quantum master equation would be written down (cf. ref. [11]).

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