Noise and damping from microscopic laws : a kinetic-theoretical classical test-particle approach

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1. Introduction

The relation of macroscopic random motion to microscopic particle dynamics has been a long standing problem. In a generic manner, fluctuations due to particle interactions (*collisions*) are modeled by a Fokker-Planck-type equation (FPE)(related to a Langevin-type equation of motion), which may either be derived intuitively, via physical phenomenology or, formally, through kinetic-theoretical arguments. In the latter framework, a number of works in Non-Equilibrium Statistical Mechanics have been devoted to the study of the relaxation of a small subsystem weakly interacting with a heat bath. A common aim of such studies is the derivation of a *kinetic equation*, describing the evolution in time of a phase-space probability density function. This is achieved by using either perturbation theory (typically a *BBGKY hierarchy* of equations for reduced distribution functions [1]) or formal theories for open systems (e.g. *projection-operator* methods [2]). In a generic manner, both approaches rely on a *generalized master equation* (GME) , obtained to 2nd order in the interaction. The kernel of the GME has to be evaluated along particle trajectories, so the influence of the field on microscopic laws of motion is expected to modify the form of the collision operator.

This work aims in discussing a general method for the rigorous derivation of a Fokker-Planck-type equation from microscopic dynamics, taking into account the existence of external force fields and interactions (possibly long-range) between particles. Explicit general expressions will be derived for diffusion and friction coefficients.

2. The model: Hamiltonian and equations of motion

We consider a test-particle (t.p.), say Σ, surrounded by (and weakly coupled to) a homogeneous reservoir R; $\mathbf{X} = (\mathbf{x}, \mathbf{v}) \equiv (\mathbf{x_\Sigma}(t), \mathbf{v_\Sigma}(t))$ and $\mathbf{X_R} \equiv \{\mathbf{X_j}\} = \{\mathbf{x_j}(t), \mathbf{v_j}(t), j = 1, 2, 3, ..., N\}$ will denote the coordinates of the test- ($\Sigma-$) and reservoir- ($R-$) particles. Both subsystems are subject to an external force field.

The *Hamiltonian* of the system is:

$$H = H_R + H_\Sigma + \lambda H_I \qquad (1)$$

where H_R (H_Σ) denotes the Hamiltonian of the reservoir (t.p.) alone:

$$H_R = \sum_{j=1}^{N} H_j + \sum_{j<n} \sum_{n=1}^{N} V_{jn}$$

where the single-particle Hamiltonian H_j ($j = 1, 2, ..., N, \Sigma$) takes into account the external field. H_I stands for the interaction (assumed to be weak: $\lambda \ll 1$) between Σ and R: $H_I = \sum_{n=1}^{N} V_{\Sigma n}$, where $V_{ij} \equiv V(|\mathbf{x_i} - \mathbf{x_j}|)$ $(i, j = 1, 2, ..., N, \Sigma)$ is a binary (possibly long-range, electrostatic) interaction potential.

The resulting *equations of motion* are:

$$\dot{\mathbf{x}} = \mathbf{v}\,, \qquad \dot{\mathbf{v}} = \mathbf{F_0}(\mathbf{x}, \mathbf{v}) + \lambda\, \mathbf{F_{int}}(\mathbf{x}, \mathbf{v}; \mathbf{X_R}; t) \qquad (2)$$

The force $\mathbf{F_0}$ is due to the external field. The *interaction* force $\mathbf{F_{int}}(\mathbf{x}, \mathbf{v}; \mathbf{X_R}; t) = -\frac{\partial}{\partial \mathbf{x}} \sum V(|\mathbf{x} - \mathbf{x_j}|)$ is actually the sum of interactions between $\Sigma-$ and $R-$ particles surrounding it; it represents a purely *random* process, as the reservoir is assumed to be in a homogeneous equilibrium state. In fact, $\mathbf{F_{int}}$ defines a zero-mean Gaussian process; furthermore, in many physical problems of interest, it comes out to be a *stationary* process, as the force correlations – see (12) – come out to be: $C_{ij}(t, t-\tau) = C_{ij}(\tau)$ [3].

We will assume that the zeroth-order ('*free*') problem of motion (i.e. (2) for $\lambda = 0$) yields a known analytic solution in the form:

$$\mathbf{v}^{(0)}(t) = \mathbf{M}'(t)\, \mathbf{x} + \mathbf{N}'(t)\, \mathbf{v}$$

$$\mathbf{x}^{(0)}(t) = \mathbf{x} + \int_0^t dt'\, \mathbf{v}(t') = \mathbf{M}(t)\mathbf{x} + \mathbf{N}(t)\mathbf{v}$$

i.e.

$$\begin{pmatrix} \mathbf{x}^{(0)}(t) \\ \mathbf{v}^{(0)}(t) \end{pmatrix} = \begin{pmatrix} \mathbf{M}(t) & \mathbf{N}(t) \\ \mathbf{M}'(t) & \mathbf{N}'(t) \end{pmatrix} \begin{pmatrix} \mathbf{x} \\ \mathbf{v} \end{pmatrix} \equiv \mathbf{E} \begin{pmatrix} \mathbf{x} \\ \mathbf{v} \end{pmatrix}\,; \qquad (3)$$

the initial condition is: $\{\mathbf{x}^{(0)}(0), \mathbf{v}^{(0)}(0)\} = \{\mathbf{x}, \mathbf{v}\}$, i.e. $\mathbf{E}(0) = \mathbf{I}$. For a given dynamical problem in d dimensions ($d = 1, 2, 3$), the form of the $d \times d$ matrices $\{\mathbf{M}(t), \mathbf{N}(t)\}$ depends on the particular aspects of the dynamical problem taken into consideration. The $2d \times 2d$ matrix $\mathbf{E}(t)$ in (3) satisfies the *group property*: $\mathbf{E}(t)\mathbf{E}(t') = \mathbf{E}(t + t')$ $\quad \forall t, t' \in \Re$, implying $\mathbf{E}(-t) = \mathbf{E}^{-1}(t)$ (& algebraic relations for $\mathbf{M}, \mathbf{N}$). Dynamical systems obeying Eq. (3) include:

(i) *linear oscillator models*: $F^{(0)} = -m\omega^2 x$, so

$$\begin{pmatrix} x^{(0)}(t) \\ v^{(0)}(t) \end{pmatrix} = \begin{pmatrix} \cos\omega t & \omega^{-1}\sin\omega t \\ -\omega\sin\omega t & \cos\omega t \end{pmatrix} \begin{pmatrix} x(0) \\ v(0) \end{pmatrix} \equiv \mathbf{E}(t) \begin{pmatrix} x(0) \\ v(0) \end{pmatrix}.$$

(ii) *magnetized plasma* [3] (see §6. below), and

(iii) the *free motion (no-field-) limit* [a]: $\mathbf{F}^{(0)} = \mathbf{0}$ [cf. (2)] so

$$\{\mathbf{x}(t), \mathbf{v}(t)\} = \{\mathbf{x} + t\mathbf{v}, \mathbf{v}\}\,, \qquad \mathbf{v} = \text{cst.}$$

i.e. $M_{ij} = \delta_{ij}, N_{ij} = \delta_{ij}\, t$, and thus $M'_{ij} = 0, N'_{ij} = \delta_{ij}$.

[a] In the case of a central long-range interaction potential (e.g. gravitational or electrostatic interactions), this limit is known to yield the *Chandrasekhar* limit [4], describing stellar clusters, and the *Rosenbluth-MacDonald-Judd* limit [5] in electrostatic plasma, respectively.

3. Statistical formulation

Let $\rho = \rho(\{\mathbf{X}, \mathbf{X_R}\}; t)$ be the total *phase-space distribution function (d.f.)*, normalized to unity: $\int d\mathbf{X}\, \rho = 1$.

The *equation of continuity in phase space Γ* reads:

$$\frac{\partial \rho}{\partial t} + \mathbf{v_j} \frac{\partial \rho}{\partial \mathbf{x_j}} + \frac{\partial}{\partial \mathbf{v_j}} (\frac{1}{m} \mathbf{F_j} \rho) = 0 \qquad (4)$$

where a summation over j $(= 1, 2, 3, ..., N, \Sigma)$ is understood.

The method we follow consists in defining appropriate 's-body' ($s = 1, 2, 3, ...$) reduced distribution functions (rdf), among which the (1−body-) test-particle rdf: $f(\mathbf{x}, \mathbf{v}; t) = (I, \rho)_R \equiv \int_{\Gamma_R} d\mathbf{X_R}\, \rho$ (normalized to unity) and then appropriately integrating the total $((N+1)-$particle) Liouville equation (4) in order to obtain a system of coupled evolution equations for the rdfs.

This is rather standard procedure so details will be omitted here, since they can be found in the references[a].

In seek of an evolution equation for $f(t)$, the *BBGKY hierarchy* of equations can be truncated to 2nd order in λ. One obtains:

$$(\partial_t - L_0^{(\Sigma)})\, f(\mathbf{X}; t) = \lambda^2 \int d\mathbf{X_1}\, L_I\, g(\mathbf{X}, \mathbf{X_1}; t) + \mathcal{O}(\lambda^3)$$

$$(\partial_t - L_0^{(\Sigma)} - L_0^{(1)})\, g(\mathbf{X}, \mathbf{X_1}; t) = \lambda\, L_I\, F_1(\mathbf{X_1})\, f(\mathbf{X}) + \mathcal{O}(\lambda^2) \quad (5)$$

where $L_0^{(j)}$ $(j \in \{\Sigma, 1_R\})$ is the "free" Liouvillian (given the field):

$$L_0^{(j)} \cdot = -\mathbf{v_j} \frac{\partial \cdot}{\partial \mathbf{x_j}} - \frac{1}{m_j} \frac{\partial}{\partial \mathbf{v_j}} (\mathbf{F_0}\, \cdot) \qquad (6)$$

and $L_I \equiv L_{\Sigma 1}$ is the binary interaction operator:

$$L_I = -\mathbf{F_{int}}(|\mathbf{x} - \mathbf{x_1}|) \left(\frac{1}{m} \frac{\partial}{\partial \mathbf{v}} - \frac{1}{m_1} \frac{\partial}{\partial \mathbf{v_1}} \right). \qquad (7)$$

As obvious, $f = f(\mathbf{X}; t)$, $F_1(\mathbf{X_{1_R}})$ and $f_2(\mathbf{X}, \mathbf{X_1}; t)$ denote the $\Sigma-$1-body, $R-$1-body and $(1_R+\Sigma)-$2-body rdfs respectively and $g = g(\mathbf{X}, \mathbf{X_1}; t)$ is the 'two-body' $(1_R + \Sigma)$ correlation function: $g = f_2 - F_1\, f$. Note that the mean-field (*Vlasov*) term, in order λ^1, disappears for reasons of symmetry, since we assume the reservoir to be in a homogeneous equilibrium state $F_1 = n\, \phi_{eq}(\mathbf{v_1})$; $n = \frac{N}{V}$ is the reservoir particle density; obviously: $\partial F_1 / \partial t = L_0^{(1)}\, F_1 = 0$.

3.1 The Generalized Master Equation

Neglecting initial correlations, equations (5) lead to the *Non-Markovian* Generalized Master Equation:

$$\partial_t f - L_0\, f = n \int_0^t d\tau \int d\mathbf{x_1}\, d\mathbf{v_1}\, L_I\, U_0(\tau)\, L_I\, \phi_{eq}(\mathbf{v_1})\, f(\mathbf{x}, \mathbf{v}; t-\tau) \qquad (8)$$

$(f = f(\mathbf{x}, \mathbf{v}; t))$, where $L_0 \equiv L_0^{(\Sigma)}$ in the left-hand-side is the *"free"* Liouville operator defined in (6), L_I is the binary interaction Liouville operator $L_{\Sigma 1}$ (see (7)) and $U_0(\tau) = U_0^{(\Sigma)}(\tau)\, U_0^{(1)}(\tau)$ is an evolution operator (*propagator*) related to the formal solution of the "free" (collisionless) Liouville equation (e.g. (5a) for $\lambda = 0$): $f(t) = e^{L_0^{(j)} t}\, f(0) \equiv U_0^{(j)}(t)\, f(0)$ $(j \in \{\Sigma, 1\})$.

4. A 'quasi-Markovian' ($\Theta-$) approximation

A widely used 'markovian' assumption consists in:

(i) substituting with the zeroth-order solution

$$f(t - \tau) \approx e^{-L_0 \tau}\, f(t) \equiv U_0(-\tau)\, f(t)\,, \text{and}$$

(ii) evaluating the kernel asymptotically i.e. taking $t \to \infty$ in (8) .

Important comment:

the time-propagator $U(t)$ *does not* commute with Γ- gradients:

$$U_0^{(j)}(t) \frac{\partial}{\partial \mathbf{v_j}} U_0^{(j)}(-t) = \mathbf{N_j^T}(t) \frac{\partial}{\partial \mathbf{x_j}} + \mathbf{N_j'}^T(t) \frac{\partial}{\partial \mathbf{v_j}}. \qquad (9)$$

$(j = \Sigma,\ 1_R)$ A similar expression holds for the gradient $\frac{\partial}{\partial \mathbf{x}}$ [3]. Hence, the field should rigorously appear in the collision term.

4.1 The homogeneous case: $f = f(\mathbf{v}; t)$

For a spatially uniform system: $f = f(\mathbf{v}; t)$, combining (6), (7) and (9) into the kernel of the GME (8), we obtain the PDE

$$\frac{\partial f}{\partial t} + \frac{1}{m} \mathbf{F_0} \frac{\partial f}{\partial \mathbf{v}} = \frac{\partial}{\partial \mathbf{v}} \left(\mathbf{D} \frac{\partial f}{\partial \mathbf{v}} + \frac{m}{m_1} \mathbf{a} f \right) \qquad (10)$$

which takes the form of a 3d *Fokker-Planck-type equation (FPE)*:

$$\frac{\partial f}{\partial t} + \frac{1}{m} \mathbf{F_0} \frac{\partial f}{\partial \mathbf{v}} = -\frac{\partial}{\partial v_i} (\mathcal{F}_i\, f) + \frac{\partial^2}{\partial v_i\, \partial v_j} (D_{ij}\, f)\,. \qquad (11)$$

The vector F in the right-hand-side (*rhs*): $\mathcal{F}_i = (1 + \frac{m}{m_1}) \frac{\partial D_{ij}}{\partial v_j} \equiv -\frac{m}{m_1} a_j + \frac{\partial D_{ij}}{\partial v_j}$ represents the *dynamical friction* force suffered by the particle, due to interactions with its environment, and $\mathbf{D}$ is a (positive definite) *diffusion matrix* given by:

$$\mathbf{D} = \frac{n}{m^2} \int_0^\infty d\tau \int d\mathbf{x_1} \int d\mathbf{v_1}\, \phi_{eq}(\mathbf{v_1}) \mathbf{F_{int}}(|\mathbf{x}^{(0)} - \mathbf{x_1}^{(0)}|) \otimes \mathbf{F_{int}}(|\mathbf{x}^{(0)}(-\tau) - \mathbf{x_1}^{(0)}(-\tau)|)\, \mathbf{N'}^T(\tau)\,, \qquad (12)$$

[a] See e.g. in [1]; also, see in [3]b for details on the method as adapted to a test-particle problem.

or

$$D_{ij} = \frac{1}{m^2} \int_0^\infty d\tau\, C_{ik}(\mathbf{x}, \mathbf{v}; t, t - \tau)\, N'_{jk}(\tau)\,. \qquad (13)$$

C_{ik} are the force correlations (Kubo coefficients); cf. Eqs. (12, 13).

4.2 An *ill-defined* 6d Fokker-Planck equation

For $f = f(\mathbf{x}, \mathbf{v}; t)$, one obtains the (6+1)-variable PDE

$$\frac{\partial f}{\partial t} + \mathbf{v} \frac{\partial f}{\partial \mathbf{x}} + \frac{1}{m} \mathbf{F_0} \frac{\partial f}{\partial \mathbf{v}} = \frac{\partial}{\partial \mathbf{v}} \left(\mathbf{D} \frac{\partial f}{\partial \mathbf{v}} + \mathbf{G} \frac{\partial f}{\partial \mathbf{x}} + \frac{m}{m_1} \mathbf{a} f \right); \quad (14)$$

the form of $\mathbf{G}$ is obtained from rhs(12) upon $\mathbf{N}^T \to \mathbf{N}$.

Eq. (10) takes the form of a 6-dimensional *FPE*:

$$\frac{\partial f}{\partial t} + \mathbf{v} \frac{\partial f}{\partial \mathbf{x}} + \frac{1}{m} \mathbf{F_0} \frac{\partial f}{\partial \mathbf{v}} = -\frac{\partial}{\partial v_i} (\mathcal{F}_i^{(\Theta)}\, f) + \frac{\partial^2}{\partial v_i \partial v_j} (D_{ij}^{(\Theta)}\, f)\,. \quad (15)$$

Here, $\mathcal{F}_i^{(\Theta)}$ represents a 6d friction vector, and $\mathcal{D}_{ij}^{(\Theta)}$ is the matrix:

$$\mathcal{D}_{ij} = \begin{pmatrix} \mathbf{0}(t) & \frac{1}{2}\mathbf{G}^T(t) \\ \frac{1}{2}\mathbf{G}(t) & \mathbf{D}(t) \end{pmatrix}. \qquad (16)$$

Crucial remark: The diffusion matrix $\mathcal{D}_{ij}^{(\Theta)}$ is *not positive definite*; therefore, (10) determines an *ill-defined* kinetic operator: indeed, its action *does not preserve the positivity of the d.f. f*.

5. A 'Markovian' ($\Phi-$) kinetic operator

We have considered, for *classical* systems, the Φ kinetic operator:

$$\Phi = \lim_{T \to \infty} \frac{1}{2T} \int_{-T}^{T} dt'\, U^{(0)}(t')\, \Theta\, U^{(0)}(-t') \qquad (17)$$

which was introduced in the theory of quantum open systems [6]. The construction of the Φ operator provides a well-defined FP kinetic equation in the 6d Γ-space $\{\mathbf{x}, \mathbf{v}\}$; cf. Eq. (15), setting $\Theta \to \Phi$ therein. In specific, the Φ operator:

– *preserves the norm and the positivity* of the d.f. f;

– satisfies an *H-theorem*, as can be proven analytically [3]b;

– accounts for *space diffusion* [a new feature; cf. (19) below].

6. A Markovian ($\Phi-$) plasma kinetic equation

To clarify our methodology, we have considered the motion of a test-particle (charge e_α, mass m_α, e.g. $\alpha = e, i, ...$) in a (uniform and stationary) magnetic field $\mathbf{B} = B\hat{z}$. $\mathbf{F}^{(0)}$ is the Lorentz force

$$\mathbf{F}_L = \frac{e_\alpha}{c} (\mathbf{v} \times \mathbf{B}) \equiv s_\alpha\, m_\alpha\, \Omega_\alpha\, (\mathbf{v} \times \hat{z})$$

where we defined: $\Omega_\alpha = |e_\alpha| B / (m_\alpha c)$ and $s_\alpha = e_\alpha / |e_\alpha| = \pm 1$.

The problem of motion: $\frac{d\mathbf{x}}{dt} = \mathbf{v}\,,\quad \frac{d\mathbf{v}}{dt} = \frac{e}{mc} (\mathbf{v} \times \mathbf{B})$ yields a well-known *helicoidal* solution, viz. Eq. (3) with $\mathbf{M} = \mathbf{I}, \mathbf{M}' = \mathbf{0}$ and

$$\mathbf{N}'^\alpha(t) = \mathbf{R}^\alpha(t) = \begin{pmatrix} \cos\Omega t & s\ \sin\Omega t & 0 \\ -s\ \sin\Omega t & \cos\Omega t & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\mathbf{N}^\alpha(t) = \int_0^t dt'\, \mathbf{R}^\alpha(t) = \Omega^{-1} \begin{pmatrix} \sin\Omega t & s\ (1 - \cos\Omega t) & 0 \\ s\ (\cos\Omega t - 1) & \sin\Omega t & 0 \\ 0 & 0 & \Omega t \end{pmatrix}. \qquad (18)$$

We have constructed the Θ and Φ F.P. equations for this model. The latter reads – for $f = f(\mathbf{x}, \mathbf{v}; t)$ –

$$\frac{\partial f}{\partial t} + \mathbf{v} \frac{\partial f}{\partial \mathbf{x}} + \frac{e}{mc} (\mathbf{v} \times \mathbf{B}) \frac{\partial f}{\partial \mathbf{v}} \equiv \Phi_2\, f(\mathbf{x}, \mathbf{v}; t)$$

$$\begin{aligned} = & \left[\left(\frac{\partial^2}{\partial v_x^2} + \frac{\partial^2}{\partial v_y^2} \right) \left[D_\perp(\mathbf{v}) f \right] + \frac{\partial^2}{\partial v_z^2} [D_\parallel(\mathbf{v}) f] \right. \\ & + 2\, s\, \Omega^{-1} \left[\frac{\partial^2}{\partial v_x \partial y} - \frac{\partial^2}{\partial v_y \partial x} \right] \left[D_\perp(\mathbf{v}) f \right] + \frac{\partial^2}{\partial z \partial v_z} [D_\parallel^{(VX)}(\mathbf{v}) f] \\ & + \Omega^{-2} \left[Q(\mathbf{v}) + D_\perp(\mathbf{v}) \right] \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) f + \frac{\partial^2}{\partial z^2} [D_\parallel^{(XX)} f] \\ & - \frac{\partial}{\partial v_x} \left[\mathcal{F}_x(\mathbf{v})\, f \right] - \frac{\partial}{\partial v_y} \left[\mathcal{F}_y(\mathbf{v})\, f \right] - \frac{\partial}{\partial v_z} \left[\mathcal{F}_z(\mathbf{v})\, f \right] \\ & + s\, \Omega^{-1}\, \mathcal{F}_y(\mathbf{v}) \frac{\partial}{\partial x} f - s\, \Omega^{-1}\, \mathcal{F}_x(\mathbf{v}) \frac{\partial}{\partial y} f\,; \end{aligned} \qquad (19)$$

— the *blue* terms (homogeneous part) coincide (Θ vs. Φ);

— the *red* terms (non-uniform part) are new in Φ;

— the terms in *magenta* present infinities, due to resonance with the continuum spectrum of free motion ($\parallel$ **B** part) (details in [3]b).

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