MICROSCOPIC THEORY FOR RANDOM PROCESSES IN WEAKLY - COUPLED OPEN SYSTEMS

IOANNIS KOURAKIS[†], ALKIS GRECOS[‡]

[†] *Institut für Theoretische Physik IV, Fakultät für Physik und Astronomie*
Ruhr–Universität Bochum, D–44780 Bochum, Germany
E-mail: ioannis@tp4.rub.de

[‡] *University of Thessaly, Euratom - Hellenic Republic Association*
Laboratory of Fluid Mechanics, Athinon Avenue - Pedion Areos
GR 383 34 Volos, Greece; E-mail: agrecos@mie.uth.gr

In order to relate macroscopic random motion (described e.g. by Langevin-type theories) to microscopic dynamics, we have undertaken the derivation of a Fokker-Planck-type equation from first microscopic principles. Both subsystems are subject to an external force field. Explicit expressions for the diffusion and drift coefficients are obtained, in terms of the field.

1. Introduction

The relation of macroscopic random motion to microscopic particle dynamics is 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 Langevin theory of random motion), which may either be derived intuitively, via phenomenology or, formally, through kinetic-theoretical arguments [1]. In the latter context, a number of works in Non-Equilibrium Statistical Mechanics have been devoted to the study of the relaxation of a small subsystem interacting with a large thermalized environment (heat bath). A common aim of such studies is the derivation of a *kinetic equation*, describing the evolution of a phase-space probability density function f. Assuming weak-interactions ($\lambda = E_{pot}/E_{cin} << 1$), this is achieved by using either perturbation theory in λ (typically a *BBGKY hierarchy* of equations for reduced distribution functions [2]) or formal theories for open systems (e.g. projection-operator methods [3], [4]). In a generic manner, both approaches rely on a *Generalized Master Equation* (*GME*), obtained in 2nd order in λ. The kernel of the *GME* is evaluated along particle trajectories, so external force fields enter the collision operator. Our aim here is to discuss a general method for the rigorous derivation of a *FP*-type equation from classical microscopic dynamics, with due account of external force fields and long-range interactions. For an analogous treatment in the quantum-mechanical case, see in [5].

2. The Model

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:

$$H = H_R + H_\Sigma + \lambda H_I \tag{1}$$

where H_R (H_Σ) denotes the Hamiltonian of the reservoir (t.p.) alone: $H_R = \sum_{j=1}^N H_j + \sum_{j<n}\sum_{n=1}^N V_{jn}$. The form of the single-particle Hamiltonian H_j should take 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 $V_{ij} \equiv V(|\mathbf{x_i} - \mathbf{x_j}|)$ is a binary-interaction (long-range e.g. Coulomb-type) potential. The resulting equations of motion for the test-particle are:

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

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 is a *random* process, as the reservoir is assumed to be in a homogeneous equilibrium state ($\mathbf{F_{int}}$ is actually a zero-mean Gaussian process).

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

$$\mathbf{v}^{(0)}(t) = \mathbf{M}'(t)\,\mathbf{x} + \mathbf{N}'(t)\,\mathbf{v}\,, \quad \mathbf{x}^{(0)}(t) = \mathbf{x} + \int_0^t d\tau\; \mathbf{v}(\tau) = \mathbf{M}(t)\mathbf{x} + \mathbf{N}(t)\mathbf{v} \tag{3}$$

with the initial condition $\{\mathbf{x},\mathbf{v}\} \equiv \{\mathbf{x}^{(0)}(0), \mathbf{v}^{(0)}(0)\}$ ($a' = da/dt$). Given a dynamical problem, the $d \times d$ matrices $\{\mathbf{M}(t), \mathbf{N}(t)\}$ ($d = 1, 2, 3$) express the action of the field on particle dynamics. For example, systems obeying (3) include:
(i) 1d linear oscillator chains: $F_0 = -m\,\omega^2\,x$ (*t.p.* mass m; frequency ω), where: $M(t) = \cos\omega t$, $N(t) = \omega^{-1}\,\sin\omega t$, (ii) magnetized plasma, where $\mathbf{F_0}$ is the Lorentz force: $\mathbf{F_0} = -\frac{q}{m}\mathbf{v} \times \mathbf{B}$ (q is *t.p.* charge) and: $M_{ij} = \delta_{ij}$ ($i, j = 1, 2, 3$); $\mathbf{N}'(t)$ is a rotation matrix (by an angle $\theta = \Omega t$; Ω is the cyclotron frequency $\Omega = qB/mc$) around the field $\mathbf{B}$ direction (and $\mathbf{N}(t) = \int_0^t \mathbf{N}'(t')\,dt'$) [6] and, of course, (iii) the free motion (no-field-) limit, where: $M_{ij} = \delta_{ij}$, $N_{ij}(t) = \delta_{ij}\,t$.

3. Statistical Formulation - a 'Quasi-Markovian' Approximation

Let $\rho = \rho(\{\mathbf{X},\mathbf{X_R}\};t)$ be the total phase-space distribution function (*d.f.*), normalized as $\int d\mathbf{X}\,\rho = 1$. The equation of continuity in phase space Γ reads:

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

(a summation over particles j is understood. Defining appropriate 's-body' ($s = 1, 2, 3, ...$) reduced distribution functions (*rdf*), among which the *t.p.* *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 Liouville equation (4), we obtain a *BBGKY hierarchy* of coupled evolution equations for the *rdf*s (details in [2], [6]). Truncating to λ^2, one obtains:

$$(\partial_t - L_0^{(\Sigma)})\,f(\mathbf{X};t) = \lambda^2 \int d\mathbf{X_1}\,L_I\,g(\mathbf{X},\mathbf{X_1};t) + \mathcal{O}(\lambda^3)$$
$$(\partial_t - L_0^{(\Sigma)} - L_0^{(1)})\,g(\mathbf{X},\mathbf{X_1};t) = \lambda\,L_I\,F_1(\mathbf{X_1})\,f(\mathbf{X}) + \mathcal{O}(\lambda^2) \tag{5}$$

where $L_0^{(j)}$ ($j \in \{\Sigma, 1_R\}$) is the zeroth-order ("free") Liouvillian in the presence of the field:

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

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

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

As obvious, $f = f(\mathbf{X}; t)$, $F_1(\mathbf{X_{1_R}})$ and $f_2(\mathbf{X}, \mathbf{X_1}; t)$ denote the Σ–1-body, R–1-body and $(1_R + \Sigma)$–2-body *rdf*s respectively and $g = g(\mathbf{X}, \mathbf{X_1}; t)$ is the 'two-body' $(1_R + \Sigma)$ correlation function: $g = f_2 - F_1 f$ (i.e. $g = 0$ for uncorrelated particles). We have assumed 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: $\partial F_1 / \partial t = L_0^{(1)} F_1 = 0$), so the mean-field *(Vlasov)* term disappears for reasons of symmetry.

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

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

The *"free"* Liouville operator $L_0 \equiv L_0^{(\Sigma)}$ is defined in (6), and L_I in (7); $U_0(\tau) = U_0^{(\Sigma)}(\tau)\, U_0^{(1)}(\tau)$ is the evolution operator (*propagator*) related to the formal solution of the "free" Liouville equation (i.e. (5a) for $\lambda = 0$): $f(t) = e^{L_0^{(j)} t} f(0) \equiv U_0^{(j)}(t)\, f(0)$ ($j \in \{\Sigma, 1\}$). Note the non-Markovian character (non-locality) of (8).

A widely used 'markovian' assumption consists in assuming that $f(t - \tau) \approx e^{-L_0 \tau}$ $f(t) \equiv U_0(-\tau)\, f(t)$, and then taking $t \to \infty$. It should be noted here, that the time-propagator $U(t)$ *does not* permute with Γ-space gradients $\frac{\partial}{\partial \mathbf{v}}, \frac{\partial}{\partial \mathbf{x}}$; indeed, one rigorously obtains the expression: $U_0^{(j)}(t) \frac{\partial}{\partial \mathbf{v_j}} U_0^{(j)}(-t) = \mathbf{N_j}^T(t)\, \frac{\partial}{\partial \mathbf{x_j}} + \mathbf{N_j'}^T(t)\, \frac{\partial}{\partial \mathbf{v_j}}$ ($j = \Sigma,\ 1_R$; superscript T denotes the transposed matrix); a similar expressions holds for the space gradient $\frac{\partial}{\partial \mathbf{x}}$. The field therefore generically (and inevitably) enters a rigorously derived collision term via the matrices $\mathbf{N}, \mathbf{N}'$.

For a spatially uniform system: $f = f(\mathbf{v};\, t)$ eqs. (6), (7) and (8) lead to the *Fokker-Planck-type equation*:

$$\frac{\partial f}{\partial t} + \frac{1}{m} \mathbf{F_0} \frac{\partial f}{\partial \mathbf{v}} = -\frac{\partial}{\partial v_i} (\mathcal{F}_i\, f) + \frac{\partial^2}{\partial v_i\, \partial v_j} (D_{ij}\, f) \tag{9}$$

where the vector $\mathcal{F}_i = (1 + \frac{m}{m_1}) \frac{\partial D_{ij}}{\partial v_j}$ 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:

$$\mathbf{D} = \frac{1}{m^2} \int_0^{t \to \infty} d\tau\, \mathbf{C}(t, t - \tau)\, \mathbf{N'}^T(\tau) \tag{10}$$

where

$$\mathbf{C} = n \int d\mathbf{x_1} \int d\mathbf{v_1}\, \phi_{eq}(\mathbf{v_1}) \mathbf{F_{int}}(|\mathbf{x}^{(0)} - \mathbf{x_1}^{(0)}|) \otimes \mathbf{F_{int}}(|\mathbf{x}^{(0)}(-\tau) - \mathbf{x_1}^{(0)}(-\tau)|) \tag{11}$$

denotes the correlation matrix $C_{ij} = \langle F_{int,i}(t)\, F_{int,j}(t - \tau) \rangle_R$; (11) becomes:

$$C_{ij} = \frac{n}{m^2} (2\pi)^d \int d\mathbf{v_1}\, \phi_{eq}(\mathbf{v_1}) \int d\mathbf{k}\, e^{i\mathbf{k}\, \mathbf{\Delta r}}\, k_i\, k_j\, \tilde{V}_k^2 \tag{12}$$

where $\tilde{V}_k$ denotes the Fourier transform of $V(r)$. The exponential: $\mathbf{\Delta r} = \mathbf{r}(t) - \mathbf{r}(t-\tau)$ (where $\mathbf{r} = \mathbf{x}^{(0)} - \mathbf{x_1}^{(0)}$) can be computed by (3); if $\mathbf{M} = \mathbf{I}$, in particular, $\mathbf{\Delta r}(\tau) = \mathbf{N}(\tau)(\mathbf{v}^{(0)} - \mathbf{v_1}^{(0)})$; the process is then *stationary*: $C_{ij} = C_{ij}(\tau)$ [6].

It should be noted, for rigor, that the kinetic operator defined above does not define a semi-group [1]. In the general case: $f = f(\mathbf{x}, \mathbf{v}; t)$, one obtains a modified *FPE*, describing diffusion in the full $2d$-dimensional $\Gamma-$space $\{\mathbf{x}, \mathbf{v}\}$; however, the associated $2d \times 2d$ diffusion matrix is *not* positive definite, so positivity preservation of the *d.f.* f *is not guaranteed.* This problem was first pointed out in the theory of open quantum mechanical systems (see e.g. [3, 5], [7]). An alternative treatment was suggested as possible remedy in [7] and later formulated with respect to certain *classical* systems of interest [4, 6]. Summarizing those results, not reported here for lack of space, evaluating the action of the operator: $\mathcal{A}_{t'} \cdot = \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} dt'\, U^{(0)}(-t') \cdot U^{(0)}(t')$ on the "quasi-Markovian" operator defined above results in a modified, $2d-$variable Fokker-Planck equation, which contains the a spatial diffusion operator (previously absent); the associated diffusion matrix *is* now positive definite.

In conclusion, we have suggested a derivation, of the Fokker-Planck equation (9) from a kinetic perspective. Relations (10) - (12) for coefficients should be 'tailor-cut' to the specific system one is interested in. Diffusion coefficients are thus related to force correlations in agreement with phenomenological stochastic theories. The interaction mechanism, with account of the field, is an intrinsic part of the formalism here, and is not plainly represented by *ad hoc* assumptions on the nature of the process (e.g. white noise or else). Furthermore, the external force field appears explicitly in correlation functions C_{ij} and diffusion - drift coefficients (i.e. relaxation scales).

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[†] On leave from: U.L.B. - Université Libre de Bruxelles, Faculté des Sciences Apliquées - C.P. 165/81 Physique Générale, Avenue F. D. Roosevelt 49, B-1050 Brussels, Belgium.

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