Derivation of a collision operator from microscopic dynamics in the weak-coupling limit - application to magnetized plasma [1]

I. Kourakis

U.L.B. - Université Libre de Bruxelles
C.P. 231 Physique Statistique et Plasmas, Association Euratom - Etat Belge
boulevard du Triomphe, B-1050 Brussels, Belgium
and
Faculté des Sciences Apliquées, C.P. 165/81 Physique Générale
Avenue F.D.Roosevelt 49, B-1050 Brussels, Belgium
email: ikouraki@ulb.ac.be

Abstract

The rigorous derivation of a collision operator for a test-particle weakly coupled to a large heat-bath in thermal equilibrium, is presented, from first non-equilibrium statistical mechanical principles. Both subsystems are subject to an external force field. In principle, inter-particle interactions, assumed to be of long-range type and weak, are influenced by the existence of the field, which may strongly modify particle trajectories between collisions. The standard Liouville description leads to a Generalized Master Equation (GME), whose kernel has to be evaluated along the system's trajectories, taking into account the particular microscopic laws of motion corresponding to the dynamical problem in consideration. A Fokker-Planck-type equation is obtained in a 'markovian' approximation. Such an equation does not preserve the positivity of the distribution function. By applying techniques developed in the theory of quantum open systems, a correct Fokker-Planck equation is derived. Explicit expressions for the diffusion and drift coefficients, depending on the external field, are obtained.

The formalism is applied in the case of a charged particle moving in a uniform magnetic field against (and relaxing towards) a Maxwellian background plasma. By explicitly taking into account both field effects and collisions, a new (*cylindrical symmetric*) collision term is derived and discussed. In the absence of magnetic field, the well-known Landau limit is recovered as expected.

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1 Introduction

1. A number of works in Non-Equilibrium Statistical Mechanics have been devoted to the study of relaxation of a small subsystem close to (but not at) equilibrium 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 density function.

2. As a starting point one takes either the *BBGKY hierarchy* of equations for reduced distribution functions (rdf) or formal projection-operator methods. In a generic manner, both approaches rely on a *('non-markovian')* **generalized master equation** (GME), obtained in 2nd order in the interaction. It should be stressed that kernel of the GME has to be evaluated along the system's trajectories (see figure), since the particular microscopic laws of motion may *strongly modify the form of the collision operator*.

3. A *Fokker-Planck-type equation* is often derived from the GME as a "markovian" approximation. In general, such an equation does *not* preserve the positivity of the distribution function $f(\mathbf{x}, \mathbf{v}; t)$. This problem is in fact *generic* - regardless that is of the particular dynamical problem considered; it was first been pointed out in the theory of open quantum-mechanical systems and possible remedy to the situation was suggested [1]. An analytical procedure introduced therein [2], which essentially amounts to time-averaging with respect to free-particle motion, was recently tested in the magnetized plasma case and a modified plasma kinetic equation was obtained [3]. All coefficients in the equation are explicit functions of the dynamical variables $\{\mathbf{x}, \mathbf{v}\}$ *and* the external field; this fact suggests that the external field should *a priori* be explicitly taken into account when deriving a collision term, in one way or another.

4. This work aims in pointing out:
(i) the forementioned mathematical discrepancy which characterises a widely used kinetic evolution operator, once one takes into account inhomogeneity effects and
(ii) the necessity of explicitly taking into account the magnitude of the external force field (if such a field exists) when deriving analytic expressions for diffusion coefficients related to a specific system. In this paper, the problem is exposed in a general manner and then bed-tested in the case of a charged particle moving in a uniform magnetic field against a Maxwellian background.

Explicitly taking into account the details of single particle motion we have derived a Landau-type kinetic equation and pointed out the positivity (non-)preservation nuisance. Then, applying the forementioned averaging formalism a new kinetic equation is obtained and discussed. Analytic expressions for all coefficients are obtained.

2 The model

We consider a test-particle (t.p.) 'Σ' surrounded by (and weakly coupled to) a homogeneous reservoir $R \equiv \{1, 2, ..., N\}$; $\mathbf{X} = (\mathbf{x}, \mathbf{v}) \equiv (\mathbf{x}_{\boldsymbol{\Sigma}}(t), \mathbf{v}_{\boldsymbol{\Sigma}}(t))$ and $\mathbf{X}_{\mathbf{R}} \equiv \{\mathbf{X}_{\mathbf{j}}\} = (\mathbf{x}_{\mathbf{j}}(t), \mathbf{v}_{\mathbf{j}}(t))$ will denote the coordinates of the test- ($\Sigma-$) and reservoir- ($R-$) particles respectively. In principle, the whole system is 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:

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

while H_I stands for the interaction (weak) between the two subsystems:

$$H_I = \sum_{n=1}^{N} V_{\Sigma n}$$

('tagged' by $\lambda \ll 1$). $V_{ij} \equiv V(|\mathbf{x_i} - \mathbf{x_j}|)$ $(i, j = 1, 2, ..., N, \Sigma)$ is a (typically long-range) binary-interaction 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 may be viewed as a *random* process, as the reservoir is assumed to be in equilibrium [2].

We will assume that the zeroth-order ('free') problem of motion (i.e. (2) for $\lambda = 0$) in d dimensions ($d = 1, 2, 3$) yields a known analytic solution in the form:

$$\begin{aligned} \mathbf{v}(t) &= \mathbf{M}'(t)\,\mathbf{x} + \mathbf{N}'(t)\,\mathbf{v} \\ \mathbf{x}(t) &= \mathbf{x} + \int_0^t dt'\; \mathbf{v}(t') = \mathbf{M}(t)\mathbf{x} + \mathbf{N}(t)\mathbf{v} \end{aligned}$$

i.e.

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

[3] with the initial condition $\{\mathbf{x}, \mathbf{v}\} \equiv \{\mathbf{x}^{(0)}(0), \mathbf{v}^{(0)}(0)\}$ (implying $\underline{\underline{\mathbf{E}}}(0) = \underline{\underline{\mathbf{I}}}$). The form of the $d \times d$ matrices $\{\underline{\underline{\mathbf{M}}}(t), \underline{\underline{\mathbf{N}}}(t)\}$ depends on the particular aspects of the dynamical problem taken into consideration; For the sake of clarity, a few explicit examples are given in the following.

[2] $\mathbf{F_{int}}$ actually comes out to be described by a stationary Gaussian process, determined by a vanishing mean-value.

[3] In a $d-$dimensional problem, $\{\mathbf{M}(t), \mathbf{N}(t)\}$ are $d \times d$ matrices whose form depends on the particular aspects of the dynamical problem taken into consideration; properly speaking, one has

$$\begin{pmatrix} M_{ij}(t) & N_{ij}(t) \\ M'_{ij}(t) & N'_{ij}(t) \end{pmatrix} = \begin{pmatrix} \frac{\partial x_i^{(0)}(t)}{\partial x_j} & \frac{\partial x_i^{(0)}(t)}{\partial v_j} \\ \frac{\partial v_i^{(0)}(t)}{\partial x_j} & \frac{\partial v_i^{(0)}(t)}{\partial v_j} \end{pmatrix}$$

(the derivatives are evaluated at the initial condition $\{\mathbf{x_0}, \mathbf{v_0}\}$) thus (3) may be viewed as a linearized (in x_j, v_j) solution of the - possibly nonlinear - 'free' (i.e. collisionless) motion problem.

2.1 Example 1: Free motion

$\mathbf{F}^{(0)} = \mathbf{0}$ (cf. (2)) so $\{x_i(t), v_i(t)\} = \{x_i + v_i t, v_i\}$ $(i = 1, \cdots, d)$ i.e. $M_{ij} = \delta_{ij}, N_{ij} = \delta_{ij}\, t$ (so $M'_{ij} = 0, N'_{ij}(t) = \delta_{ij}$).

2.2 Example 2: Harmonic oscillator in 1d

The force reads:

$$F^{(0)} = -m\omega_0^2 x$$

so the single-particle equation of motion ((2) for $\lambda = 0$) yields the solution (cf.(3)):

$$\begin{pmatrix} x^{(0)}(t) \\ v^{(0)}(t) \end{pmatrix} = \begin{pmatrix} \cos\omega_0 t & \omega_0^{-1}\sin\omega_0 t \\ -\omega_0 \sin\omega_0 t & \cos\omega_0 t \end{pmatrix} \begin{pmatrix} x \\ v \end{pmatrix} \equiv \mathbf{E}(t) \begin{pmatrix} x \\ v \end{pmatrix}$$

2.3 Example 3: Gyrating motion of a charged particle

[4] ... moving in a uniform magnetic field (along $\hat{z}$): $\mathbf{F}^{(0)}$ is now the Lorentz force:

$$\mathbf{F}_L = \frac{e_\alpha}{c}(\mathbf{v} \times \mathbf{B}) \equiv s\Omega m(\mathbf{v} \times \hat{\mathbf{z}})$$

(Ω is the gyroscopic frequency $\Omega^\alpha \equiv \frac{|e_\alpha| B}{m_\alpha c}$ and $s = \frac{e_\alpha}{|e_\alpha|} = \pm 1$); the well-known (helicoidal) solution reads:

$$\begin{pmatrix} \mathbf{x}^{(0)}(t) \\ \mathbf{v}^{(0)}(t) \end{pmatrix} = \begin{pmatrix} \mathbf{I} & \mathbf{N}(t) \\ \mathbf{0} & \mathbf{R}(t) \end{pmatrix} \begin{pmatrix} \mathbf{x} \\ \mathbf{v} \end{pmatrix} \equiv \mathbf{E}(t) \begin{pmatrix} \mathbf{x} \\ \mathbf{v} \end{pmatrix} \tag{4}$$

where

$$\mathbf{R}^\alpha(t) = \begin{pmatrix} \cos\Omega t & s\ \sin\Omega t & 0 \\ -s\ \sin\Omega t & \cos\Omega t & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\mathbf{N}^\alpha(t) = \int_0^t dt'\ \underline{\underline{\mathbf{R}}}^\alpha(t) = \Omega^{-1} \begin{pmatrix} \sin\Omega t & s\ (1 - \cos\Omega t) & 0 \\ s\ (\cos\Omega t - 1) & \sin\Omega t & 0 \\ 0 & 0 & \Omega t \end{pmatrix} \tag{5}$$

2.4 Group properties

Notice that 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

$$\mathbf{E}(-t) = \mathbf{E}^{-1}(t)$$

[4](particle species $\alpha \in \{e, i, ...\}$, mass m_α, charge e_α)

as well as a number of relations for the $d \times d$ sub-matrices; in particular, if $\mathbf{M}(t) = \mathbf{I}$ as in cases in §2.1, §2.3, we have:

$$\mathbf{N}'(t)\,\mathbf{N}'(t') \;=\; \mathbf{N}'(t+t') \quad , \qquad \mathbf{N}(t') + \mathbf{N}(t)\mathbf{N}'(t') \;=\; \mathbf{N}(t+t') \qquad \forall t, t' \in \Re$$

thus, setting $t' = -t$:

$$\mathbf{N'}^{-1}(t) \;=\; \mathbf{N}'(-t) \quad , \qquad \mathbf{N}(-t) \;=\; -\mathbf{N}(t)\mathbf{N}'(-t) \neq \mathbf{N}^{-1}(t) \qquad \forall t \in \Re$$

3 Statistical formulation

The test-particle's reduced distribution function is $f(\mathbf{x}, \mathbf{v}; t) \;=\; (I,\, \rho)_R \;\equiv\; \int_{\Gamma_R} d\mathbf{X_R}\, \rho$, where $\rho = \rho(\{\mathbf{X}, \mathbf{X_R}\}; t)$ ($F = F(\mathbf{X_R})$) denotes the total (reservoir) phase-space distribution function (d.f.), which is normalized to unity: $\int d\mathbf{X}\, \rho = 1 \;\; (\int d\mathbf{X_R}\, F = 1)$.

The equation of continuity in phase space reads:

$$\frac{\partial \rho}{\partial t} + \mathbf{v_j}\frac{\partial \rho}{\partial \mathbf{x_j}} + \frac{\partial}{\partial \mathbf{v_j}}(\frac{1}{m}\,\mathbf{F_j}\,\rho) \;=\; 0 \tag{6}$$

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

3.1 Reduction of the Liouville equation - BBGKY hierarchy

The standard procedure consists in defining appropriate 's-body' reduced distribution functions (rdf), among which the (1−body-) test-particle rdf:

$$f(\mathbf{x}, \mathbf{v}; t) = (I,\, \rho)_R \equiv \int_{\Gamma_R} d\mathbf{X_R}\, \rho$$

and then appropriately integrating the $N-$particle Liouville equation in order to obtain a hierarchy of coupled equations of evolution of the rdf's. This is more or less a standard procedure [4] and details will be omitted here. In order to obtain an equation of evolution for $f(t)$, the *BBGKY hierarchy* of equations thus obtained can be truncated to 2nd order in λ by assuming interactions to be weak (i.e. $\lambda \ll 1$). One thus obtains the system:

$$\begin{aligned} (\partial_t - L_0^\Sigma)\, f(\mathbf{X}; t) &= \lambda^2 \int d\mathbf{X_1}\, L_I\, g(\mathbf{X}, \mathbf{X_1}; t) \,+ \mathcal{O}(\lambda^3) \\ (\partial_t - L_0^\Sigma - L_0^1)\, g(\mathbf{X}, \mathbf{X_1}; t) &= \lambda\, L_I\, F_1(\mathbf{X_1})\, f(\mathbf{X}) + \mathcal{O}(\lambda^2) \end{aligned} \tag{7}$$

where L_0^j is the "free" Liouvillian *in* the field:

$$L_0^j \cdot \;=\; -\mathbf{v_j}\,\frac{\partial\, \cdot}{\partial \mathbf{x_j}} - \frac{1}{m_j}\,\frac{\partial}{\partial \mathbf{v_j}}\,(\mathbf{F_0}\,\cdot\,) \tag{8}$$

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

$$L_{ij} = -\mathbf{F_{int}}(|\mathbf{x_i} - \mathbf{x_j}|)\left(\frac{1}{m_i}\frac{\partial}{\partial \mathbf{v_i}} - \frac{1}{m_j}\frac{\partial}{\partial \mathbf{v_j}}\right) \tag{9}$$

($i, j \in \{\Sigma, 1_R^{\alpha'}\}$). As obvious, $f = f(\mathbf{X}^\alpha; t)$, $F_1(\mathbf{X}_{1_R^{\alpha'}})$ and $f_2(\mathbf{X}^\alpha, \mathbf{X_1}^{\alpha'}; t)$ denote the $\Sigma-1$-body, $R-1$-body and $(1_R^{\alpha'} + \Sigma^\alpha)-2$-body rdf's respectively and $g = g(\mathbf{X}^\alpha, \mathbf{X_1}^{\alpha'}; t)$ is the 'two-body' $(1_R^{\alpha'} + \Sigma^\alpha)$ correlation function:

$$g(\mathbf{X}, \mathbf{X_1}; t) = f_2(\mathbf{X}^\alpha, \mathbf{X_1}^{\alpha'}; t) - F(\mathbf{X_1}^{\alpha'}) f(\mathbf{X}^\alpha; t)$$

Note that the mean-field *(Vlasov)* term, in order λ^1, disappears since we have assumed the reservoir to be in a homogeneous equilibrium state $F = n_{\alpha'} \phi_{eq}^{\alpha'}(\mathbf{v_1})$.

3.2 Solution of the problem in λ^0

Formal solution of the "free" (collisionless) Liouville equation:

$$f(t) = e^{L_0 t} f(0) \equiv U^{(0)}(t) f(0)$$

Note that:

$$U(t) f(\mathbf{x}, \mathbf{v}) \equiv U(t) f(\mathbf{x}, \mathbf{v}; 0) = f(\mathbf{x}, \mathbf{v}; t) = f(\mathbf{x}(-t), \mathbf{v}(-t); 0) \equiv f(\mathbf{x}(-t), \mathbf{v}(-t)) \tag{10}$$

(actually a consequence of Liouville's theorem) [5].

(Most) important for the following: The influence of the propagator on any function of the dynamical variables $\{\mathbf{x}, \mathbf{v}\}$ has to be evaluated *by taking into account the external field.* Note that, in fact, $U(t)$ *does not* commute with Γ-space gradients $\frac{\partial}{\partial \mathbf{v}}$, $\frac{\partial}{\partial \mathbf{x}}$; in general, by applying the principle of (10), one may show that [6] :

$$\underline{\mathbf{D}}_{\mathbf{V_i}}(t) \equiv U^{(0)}(t) \frac{\partial}{\partial \mathbf{v_i}} U^{(0)}(-t) \;=\; \underline{\underline{\mathbf{N_i}}}^{\mathbf{T}}(t)\, \frac{\partial}{\partial \mathbf{x_i}} + \underline{\underline{\mathbf{N'_i}}}^{\mathbf{T}}(t)\, \frac{\partial}{\partial \mathbf{v_i}} \qquad i = \Sigma,\ 1^R \tag{11}$$

3.3 The Generalized Master Equation

By assuming the interactions to be weak, the BBGKY hierarchy of equations is truncated to 2nd order in λ; by neglecting initial correlations, f is found to obey a Non-Markovian Generalized Master Equation (G.M.E.):

$$\partial_t f(\mathbf{x}, \mathbf{v}; t) = L_0 f(\mathbf{x}, \mathbf{v}; t) + \lambda^2 n \int_0^t d\tau \int d\mathbf{x_1}\, d\mathbf{v_1}\, L_I\, U^{(0)}(\tau)\, L_{\Sigma 1}\, \phi_{eq}(\mathbf{v_1})\, f(\mathbf{x}, \mathbf{v}; t - \tau) \tag{12}$$

Remember that $f = f_1^\alpha(\mathbf{x}, \mathbf{v})$, $F_1^{\alpha'}(\mathbf{x_1}, \mathbf{v_1})$ $(= \phi(\mathbf{v_1})$ here) denote the distributions functions of the test-particle and one (*any*) particle from the reservoir; $n = \frac{N}{V}$ is the particle density; finally $L_0 \equiv L_\Sigma^{(0)}$ is the *"free"* Liouville operator defined previously (see (8)) and L_I is the binary interaction Liouville operator $L_{\Sigma 1}$ (cf. (9)).

[5]See about the propagator formalism in [4], [5].

[6]cf. [5]; note that $\underline{\mathbf{D}}_{\mathbf{V_i}}(0) = \frac{\partial}{\partial \mathbf{v_i}}$, $\underline{\mathbf{D}}_{\mathbf{X_i}}(0) = \frac{\partial}{\partial \mathbf{x_i}}$).

4 A 'quasi-Markovian' approximation - the $\Theta-$operator

The standard 'markovianization' method consists in substituting with the zeroth-order solution, i.e. assuming that $f(t-\tau) \approx e^{-L_0\tau} f(t) \equiv U^{(0)}(-\tau)\, f(t)$, and then evaluating the kernel asymptotically i.e. taking the upper integration limit t to be ∞, one obtains the *quasi-markovian master equation*:

$$\begin{aligned}
\partial_t f(\mathbf{X};t) &= L_0 f(\mathbf{X};t) \\
&\quad + n \int_0^\infty d\tau \int_\Gamma d\mathbf{X_1}\; L'_{\Sigma 1}\, U^{(0)}(\tau)\; L'_{\Sigma 1}\, U^{(0)}(-\tau)\; \phi_{eq}(\mathbf{X_1})\; f(\mathbf{X};t) \\
&= L_0 f(\mathbf{X}) + \int_0^\infty d\tau\, \mathcal{K}(\tau)\, f(\mathbf{X}) \quad \equiv \quad \Theta_2(t)\, f
\end{aligned} \tag{13}$$

4.1 "Quasi-markovian" Fokker-Planck equation

By explicitly recalling definitions (8), (9) and then using (10), (11) to evaluate the kernel in (13), we obtain an equation of the form:

$$\frac{\partial f}{\partial t} + \mathbf{v}\frac{\partial f}{\partial \mathbf{x}} + \frac{1}{m}\mathbf{F_{ext}}\frac{\partial f}{\partial \mathbf{v}} = \frac{\partial}{\partial \mathbf{v}}[\mathbf{A}(\mathbf{x},\mathbf{v})\frac{\partial}{\partial \mathbf{v}} + \mathbf{G}(\mathbf{x},\mathbf{v})\frac{\partial}{\partial \mathbf{x}} + \mu\, \mathbf{a}(\mathbf{x},\mathbf{v})]\, f \tag{14}$$

($f = f(\mathbf{x},\mathbf{v};t)$; $\mu \equiv m/m_1^{\alpha'}$). After an algebraic manipulation, (14) takes the form of a 6-d *'diffusion' equation*:

$$\frac{\partial f}{\partial t} + \mathbf{v}\frac{\partial f}{\partial \mathbf{x}} + \frac{1}{m}\mathbf{F_{ext}}\frac{\partial f}{\partial \mathbf{v}} = -\frac{\partial}{\partial \mathbf{q}}(\underline{\mathcal{F}}^{\Theta}\, f) + \frac{\partial}{\partial \mathbf{q}}\frac{\partial}{\partial \mathbf{q}} : (\underline{\underline{\mathbf{D}}}^{\Theta}\, f) \tag{14-bis}$$

where $q \equiv (\mathbf{x},\mathbf{v})$. The 6x6 *diffusion matrix* is:

$$\underline{\underline{\mathbf{D}}}^{\Theta}(\mathbf{x},\mathbf{v}) = \begin{pmatrix} \underline{\underline{\mathbf{0}}} & \frac{1}{2}\underline{\underline{\mathbf{G}}}^{\mathbf{T}} \\ \frac{1}{2}\underline{\underline{\mathbf{G}}} & \underline{\underline{\mathbf{A}}} \end{pmatrix} \tag{15}$$

and the 6-d [7] vector $\mathcal{F}^{\Theta}$ reads: $\mathcal{F}^{\Theta} = (\mathbf{0},\mathbf{F})^T$.

4.2 Coefficients

$$\left\{ \begin{array}{c} \underline{\underline{\mathbf{A}}}(\mathbf{x},\mathbf{v}) \\ \underline{\underline{\mathbf{G}}}(\mathbf{x},\mathbf{v}) \end{array} \right\} = \frac{n}{m^2}\int_0^\infty d\tau \int d\mathbf{x_1} \int d\mathbf{v_1}\, \phi_{eq}(\mathbf{v_1})$$
$$\mathbf{F_{int}}(|\mathbf{x}-\mathbf{x_1}|) \otimes \mathbf{F_{int}}(|\mathbf{x}(-\tau)-\mathbf{x_1}(-\tau)|) \left\{ \begin{array}{c} \underline{\underline{\mathbf{N}}}'^{\mathbf{T}}(\tau) \\ \underline{\underline{\mathbf{N}}}^{\mathbf{T}}(\tau) \end{array} \right\}$$

[7] i.e. in a 3-d problem; in the general - d-dimensional - case, read '$2d-$' ('$d-$') instead of '$6-$' ('$3-$').

$$
\begin{aligned}
&= \frac{n}{m^2}\int_0^\infty d\tau\, \underline{\underline{\mathbf{C}}}(\mathbf{x},\mathbf{v};t,t-\tau) \left\{ \begin{array}{c} \underline{\underline{\mathbf{N}}}'^{\mathbf{T}}(\tau) \\ \underline{\underline{\mathbf{N}}}^{\mathbf{T}}(\tau) \end{array} \right\} \\
\underline{\mathbf{a}}(\mathbf{x},\mathbf{v}) &= -\frac{n}{m^2}\int_0^\infty d\tau \int d\mathbf{x_1} \int d\mathbf{v_1}\, \phi_{eq}(\mathbf{v_1}) \\
&\qquad \mathbf{F_{int}}(|\mathbf{x}-\mathbf{x_1}|) \otimes \mathbf{F_{int}}(|\mathbf{x}(-\tau)-\mathbf{x_1}(-\tau)|)\, \underline{\underline{\mathbf{N}}}'^{\mathbf{T}}_{\mathbf{1}}(\tau)\, \frac{\partial\phi(\mathbf{v_1})}{\partial\mathbf{v_1}} \\
&= -\frac{n}{m^2}\int_0^\infty d\tau\, \underline{\mathbf{d}}(\mathbf{x},\mathbf{v};t,t-\tau) \qquad (16)
\end{aligned}
$$

Remark: Explicit appearance of the correlation function in the diffusion coefficients, explicit dependence on the external force field through the $\mathbf{N}(t), \mathbf{N}'(t)$ matrices *and* - implicitly - through $\mathbf{F_{int}}$.

4.3 The positivity issue

A kinetic equation should possess a number of properties; namely, it should preserve (i) the reality, (ii) the normalization and (iii) the positivity of the (probability) distribution function. Furthermore, (iv) an H-theorem should be satisfied.

In order for the probability distribution to be positive at any instant t under the action of an evolution operator e.g. $\Theta(t)$, the diffusion matrix $\underline{\underline{\mathbf{D}}}$ should be positive definite, i.e. one should have, for any $\mathbf{a} \in \Re^6$:

$$
(\mathbf{a}, \underline{\underline{\mathbf{D}}}\mathbf{a}) = \mathbf{a}^T \underline{\underline{\mathbf{D}}}\mathbf{a} = \mathbf{a}^T \underline{\underline{\mathbf{D}}}^{SYM}\mathbf{a} \,\geq\, 0
$$

This criterion is definitely *not* satisfied here (note that $det\, \underline{\underline{\mathbf{D}}}^{\Theta} = -(det \underline{\underline{\mathbf{C}}})^2 \leq 0$).

As a consequense,

the Quasi-Markovian F.P. equation (14) *does not guarantee preservation of the positivity* of the probability d.f. f.

Comments:

1. The problem of positivity preservation has not been noticed in the past as the effect of spatial inhomogeneity of the plasma on the collision term has always been neglected, through one argument or another, or even plainly omitted [8].

2. In fact, inhomogeneity effects in the collision term have been considered in certain works, yet the second (inhomogeneity) term in the RHS of eq.(14) has always been neglected - often by assuming on physical grounds that it is negligible - or even plainly omitted.

3. The existence of the problem was however pointed out in [6] where the authors used formal operator methods to show that the problem was due to the very construction of the kinetic equation and actually suggested possible “therapy” (mainly for systems with a discrete spectrum of the zeroth-order Liouville operator). That point of view is the formal basis of the analysis that follows.

[8] This problem does *a priori* not arise in the homogeneous case.

5 Towards a Markovian kinetic equation - the $\Phi-$operator

In search for a correct markovian approximation, we have considered an evolution operator which was first suggested by E.B.Davies in the theory of open quantum systems [1], [2] [9], and was later re-formulated with respect to classical systems [6] [10]. It essentially amounts to considering the averaging operation:

$$\mathcal{A}_{t'} \cdot \, = \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} dt' \, U^{(0)}(-t') \, \cdot \, U^{(0)}(t') \tag{17}$$

which is applied to the *rhs* of eq.(14).

In the following, we shall explicitly construct (and compare) the $\Theta-$ and $\Phi-$ operators (defined by (14) and (17) respectively) in two typical cases of interest.

6 Case of interest: 3d magnetized plasma

Let us consider the case of a charged particle moving in a uniform magnetic field against a Maxwellian background plasma (cf. §2.3).

6.1 The homogeneous case

In the homogeneous case i.e. $f = f(\mathbf{v}; t)$, both operators coincide. The kinetic equation obtained is of the form [3]:

$$\begin{aligned} \frac{\partial f}{\partial t} + \frac{e}{mc}\,(\mathbf{v}\times\mathbf{B})\,\frac{\partial f}{\partial \mathbf{v}} = & \Big[\Big(\frac{\partial^2}{\partial v_x^2} + \frac{\partial^2}{\partial v_y^2}\Big)\Big[D_\perp(\mathbf{v}) f\Big] + \frac{\partial^2}{\partial v_z^2}[D_\parallel(\mathbf{v}) f] \\ & - \frac{\partial}{\partial v_x}\Big[\mathcal{F}_x(\mathbf{v})\, f\Big] - \frac{\partial}{\partial v_y}\Big[\mathcal{F}_y(\mathbf{v})\, f\Big] - \frac{\partial}{\partial v_z}\Big[\mathcal{F}_z(\mathbf{v})\, f\Big] \end{aligned} \tag{18}$$

The explicit form of the coefficients in (18) is presented in [3], [8] (provided in the Appendix); it will be omitted here. Eq. (18) is in agreement with earlier works [10].

Note that all coefficients are functions of $\mathbf{v}$ (actually of $\{v_\perp, v_\parallel\}$) only.

[9] The $\Phi-$operator appears as *'Davies' device'* in the quantum case in [2]; however, curiously enough, the classical case is not adressed therein.

[10] The implementation of this operator seems to be well defined for classical subsystems possessing a *discrete* spectrum of eigenvalues of the corresponding Liouville operator. Yet, this is not the case for free particle motion (cf. §2.1 above); indeed, coefficients obtained through the $\Phi-$ operator appear to be ill-defined. In the case of helicoidal motion in a magnetic field (cf. §2.3), it was therefore expected (and indeed verified) that such a problem would arise in the z-direction, as the magnetic field does not confine motion along z (the Lorentz force yields no component along the field). In the following section §5.2, we shall therefore only consider distribution functions which do not depend on z (actually looking into the plane $\perp$ $\mathbf{B}$).

6.2 The general (inhomogeneous) case

In the general case, i.e. $f = f(\mathbf{x}, \mathbf{v}; t)$, the change is dramatic; The $\Phi-$operator yields the equation:

$$\frac{\partial f}{\partial t} + \mathbf{v}\frac{\partial f}{\partial \mathbf{x}} + \frac{e}{mc}(\mathbf{v}\times\mathbf{B})\frac{\partial f}{\partial \mathbf{v}} = \Big[\Big(\frac{\partial^2}{\partial v_x^2} + \frac{\partial^2}{\partial v_y^2}\Big)\Big[D_\perp(\mathbf{v})f\Big] + \frac{\partial^2}{\partial v_z^2}[D_\parallel(\mathbf{v})f]$$
$$+2\, s\, \Omega^{-1}\Big[\frac{\partial^2}{\partial v_x \partial y} - \frac{\partial^2}{\partial v_y \partial x}\Big]\Big[D_\perp(\mathbf{v})f\Big]$$
$$+\,\Omega^{-2}\,[D_\perp^{(XX)}(\mathbf{v})](\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2})f$$
$$-\frac{\partial}{\partial v_x}\Big[\mathcal{F}_x(\mathbf{v})\,f\Big] - \frac{\partial}{\partial v_y}\Big[\mathcal{F}_y(\mathbf{v})\,f\Big] - \frac{\partial}{\partial v_z}\Big[\mathcal{F}_z(\mathbf{v})\,f\Big]$$
$$+\,s\,\Omega^{-1}\,\mathcal{F}_y(\mathbf{v})\,\frac{\partial}{\partial x}\,f - \,s\,\Omega^{-1}\,\mathcal{F}_x(\mathbf{v})\,\frac{\partial}{\partial y}\,f \qquad (19)$$

whereas in the case of the $\Theta-$ operator, typically of the form of (14), the 3rd (space-diffusion) and 5th lines are missing, where the 2nd line (cross-V-X term) is strongly modified [3].

Notice that the collision term (RHS) in the above equation, as well as (18), is *cylindrical symmetric*; this fact reflects the intrinsic symmetry of the problem, due to the external field. If we switch the latter off, the well-known (*spherical symmetric*) Landau collision term [4] is recovered (readily obtained by substituting from the expressions in §2.1 (free-motion limit) for the dynamic matrices $\mathbf{M}(t), \mathbf{N}(t)$ in the formulae for the coefficients in §4.2).

7 Note added in proof: a 1d lattice of linear oscillators

Let us consider the case of a chain of linear oscillators (cf. §2.1).

Equation (14) together with definitions in §4 lead to:

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} - \omega_0^2\, x\,\frac{\partial f}{\partial v} = \frac{\partial^2}{\partial v^2}\Big[D_{VV}^{(\Theta)}(v)f\Big] + \frac{\partial^2}{\partial v \partial x}\Big[D_{VX}^{(\Theta)}(v)f\Big] - \frac{\partial}{\partial v}\Big[\mathcal{F}_V^{(\theta)}(v)\,f\Big] \qquad (20)$$

where $f = f(x, v; t)$. It can be checked that the solution of equation (20) is ill-defined, since the second-order diffusion matrix is not positive-definite (cf. §4.3) [11]. It is interesting to see that this problem does not arise in the homogeneous case (i.e. if $f = f(v)$), since the second term in each side cancels and the diffusion coefficient D_{VV} is a positive quantity.

By applying the $\Phi-$ operator, we obtain the equation:

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} - \omega_0^2\, x\,\frac{\partial f}{\partial v} = \frac{\partial^2}{\partial v^2}\Big[D_{VV}^{(\Phi)}(v)f\Big] + \frac{\partial^2}{\partial v \partial x}\Big[D_{VX}^{(\Phi)}(v)f\Big] + \frac{\partial^2}{\partial x^2}\Big[D_{XX}^{(\Phi)}(v)f\Big]$$
$$-\frac{\partial}{\partial v}\Big[\mathcal{F}_V^{(\Phi)}(v)\,f\Big] - \frac{\partial}{\partial x}\Big[\mathcal{F}_X^{(\Phi)}(v)\,f\Big] \qquad (21)$$

[11] This point can be illustrated quite elegantly - yet not so rigorously - by assuming for a while that all coefficients are constant $\in \Re_+$. Contrary to the correct FPE without cross-velocity-position derivative (i.e. for $D_{VX} = 0$) this equation has no solution. Indeed, as one may check analytically, the corresponding Green's function develops a singularity at some instant of time.

Note the space-diffusion term in the RHS.

All coefficients in this paragraph have been explicitly computed and will be reported elsewhere [7]; nevertheless, they were omitted here for brevity.

8 Conclusion

In conclusion, we have reported two (linear) kinetic evolution operators and presented the corresponding Fokker-Planck-type kinetic equations, obtained to second order in the (weak) interaction.

We have pointed out:
(i) that the widely used collision operator defined by (13), does *not* preserve the positivity of the distribution function $f(\mathbf{x}, \mathbf{v}; t)$ once one takes into account inhomogeneity effects
and
(ii) the necessity of explicitly taking into account the influence of the external force field (if such a field exists) on particle trajectories when deriving analytic expressions for diffusion coefficients related to a specific system.

Finally, the formalism has been applied in the case of magnetized plasma, where a new collision term was presented and discussed.

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Appendix

(provided below - see in the end of this poster)

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