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A collision kinetic operator from microscopic dynamics in the presence of external fields

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1. Introduction

A plethora of works in Non-Equilibrium Statistical Mechanics have been devoted to the study of the kinetic behaviour of large ensembles of interacting particles, in an attempt to relate the macroscopic properties of a system to the microscopic dynamics of its constituent particles. A common aim of such theories is the derivation of a *kinetic equation,* describing the evolution in time of a single-particle distribution function (d.f.) in phase-space (i.e. a function $f(\mathrm{x}, \mathrm{V}; t)$ of particle position and velocity).
Certain studies rely on a phenomenological description of particle collisions (mostly related to *stochastic* mathematical theories) while others adopt a more rigorous (kinetic-) theoretical approach, by taking as a starting point either a hierarchy of coupled equations for reduced p-body (p = 1, 2, 3, ...) distribution functions or formal projection-operator methods [Balescu 1997].
The generic form of a kinetic equation is:

$$\frac{\partial f}{\partial t} + \mathrm{v}\frac{\partial f}{\partial \mathrm{x}} + m^{-1}\mathrm{F}\frac{\partial f}{\partial \mathrm{v}} = C\{f\}$$

where x and v denote particle position and velocity variables, respectively, F denotes the total force exerced on the particle. The *collision term* C in the right-hand-side *(rhs)* accounts for particle interactions; it first appeared in the original Boltzmann equation and has ever since been a controversial subject in literature, since it is related to the *irreversible* character of dynamics of matter.

A point that should be made is the following. Particle interactions are in principle influenced by the physical parameters of the system (e.g. temperature, density) *and* the existence of an external force field, since the latter may strongly modify particle trajectories between collisions. The collision term is *a priori* expected to depend on all these parameters and should bear a form which takes into account, in particular, the exact effect of the external field on particle dynamics. Curiously enough, the latter is simply absent from most kinetic equations widely used in literature, such as the celebrated Fokker-Planck equation (FPE) (derived from stochastic calculus) [Risken 1989], the Landau equation and the Balescu-Lenard-Guernsey equation, both derived in the case of particles interacting through weak long-range (e.g. electrostatic or gravitational) interactions [Balescu 1997] or, finally, variations of the latter, meant to take into account the field in the zeroth-order Liouville part, i.e. the left-hand-side *(lhs)* of the equation, but not in the collision term (see e.g. in [Balescu 1988]).

In the above framework, a case study of particular interest among statistical physicists consists of the relaxation of a small system towards thermal equilibrium under the influence a large heat-bath (thermostat). Both sub-systems may interact with one another and also with an external field (if one is present). In earlier work of ours we have undertaken a study of such a system, consisting of a charged test-particle moving against a thermalized background (plasma) [Kourakis 1999, 2000]. Starting from first microscopic principles, a markovian FPE-type kinetic equation was derived and analytical expressions for the coefficients were obtained. Emphasis was made on the magnetic field dependence of the collision integral, as well as the effect of non space-uniformity of the d.f. $f(\mathrm{x}, \mathrm{v}; t)$. This new equation was thus suggested as a basis for the study of plasma kinetic properties (as compared, that is, to the standard (unmagnetized) Landau description). The general formalism introduced in order to obtain those results may be applied in any specific weakly-coupled N-body system, subject to an external field. The scope of this paper is to outline this method, present a set of exact computable expressions for the diffusion coefficients and actually point out their dependence on, among other parameters, the external field.

2. The model

We consider a test-particle (t.p.) Σ surrounded by (and *weakly* interacting with[1]) a homogeneous background reservoir (N particles) assumed in equilibrium. The weak interaction assumption implies a low ratio of average potential to kinetic energy of the particle; this condition, which is indeed fulfilled in a variety of real systems e.g. high-temperature plasmas, stellar clusters etc., is technically' necessary to obtain an evolution equation for the 1-particle d.f. by truncating the full N-particle Liouville, equation (see e.g. [Balescu 1997]).
The whole system is subject to an external field.
The equations of motion for the t.p. read:

$$\frac{d\mathrm{x}}{dt} = \mathrm{v} \quad ; \quad \frac{d\mathrm{v}}{dt} = \mathrm{F}^0(\mathrm{x},\mathrm{v}) + \lambda \mathrm{F}_{\mathrm{int}}(\mathrm{x},\mathrm{v},\mathrm{X}_R\,;\mathrm{t}) \tag{1}$$

where $X = (x, v) = (x\Sigma, v\Sigma)$ and $X_R = \{X_j\} = (x_j, v_j)$ ($j = 1,2,...,N$) denote the coordinates of the test- and reservoir (R) particles respectively. The force $F^{(O)}$ is due to the external field. The *interaction* force $F_{int}(x, v; X_R; t)$ $= -\frac{\partial}{\partial \mathrm{x}}\sum V(|\mathrm{x}-\mathrm{x}_j|)$ ('tagged' by λ), represents the sum of random interactions between Σ and the heat bath.

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

$$\mathrm{v}^{(O)}(t) = \mathrm{M}'(t)x + \mathrm{N}'(t)\mathrm{v}$$

$$\mathrm{x}^{(0)}(t) = \mathrm{x} + \int_0^t dt'\,\mathrm{v}(t') = \mathrm{M}(t)\mathrm{x} + \mathrm{N}(t)\mathrm{v} \tag{2}$$

with the initial condition $\{x, v\} \equiv \{x^{(O)}(0), v^{(O)}(0)\}$. The form of the d x d matrices $\{M(t), N(t)\}$ depends on the particular aspects of the dynamical problem taken into consideration and thus, definitely, on the external field. For the sake of clarity, a few explicit examples are given in the following.

2.1. Example 1: Free motion

in the absence of external field, $F^{(O)} = O$ in (1), so $x(t) = x+vt$, $v(t) = v = const.$ i.e. $M_{ij} = \delta_{ij}, N_{ij} = \delta_{ij} t$ (so $M'_{ij} = 0, N'_{ij} = \delta_{ij}$; $i,j = 1,\ldots,d$)

2.1. Example 2: *Harmonic Ostillator in 1 dimension*

The force reads:

$$F^{(o)} = - m\omega^2 \chi$$

and the solution to the single-particle equation of motion (1) reads:

$$x^{(0)}(t) = x \cos \omega t + v\, \omega^{-1} \sin \omega t, \quad v^{(0)}(t) = - x\omega \sin \omega t + v \cos \omega t$$

which can be readily cast in the form of (2).

2.3. Example 3: Gyrating motion of a charged particle

Consider a charged particle (mass m, charge q) moving in a uniform magnetic field (along the z-axis); $F^{(O)}$ is now the Lorentz force: $F_L = q$ (v x B); the well-known (helicoidal) solution is exactly of the form of (2) where $N'(t)$ is a rotation matrix:

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

and $N(t) = \int_0^t dt^2 \quad R(t')$; Ω is the *gyroscopic* frequency $\Omega = qB/m$.

3. Kinetic description

The test-particle's reduced distribution function is $\int(\mathrm{x},\mathrm{v};t)=(I,\rho)_R\equiv\int r_R d\mathrm{X}_\mathrm{R}\rho$, where $\rho=\rho(\{\mathrm{X},\mathrm{X}_\mathrm{R}\};t)$ denotes the *total* phase-space d.f., which is normalized to unity: $\int dX\rho = 1$. Assuming interactions to be weak ($\lambda \ll 1$)and neglecting initial correlations, *f* is found to obey a *Non-Markovian Generalized Master Equation:*

$$\frac{\partial f}{\partial t}+\mathrm{v}\frac{\partial f}{\partial \mathrm{x}}+m^{-1}\mathrm{F}^{(0)}\frac{\partial f}{\partial \mathrm{v}}=+\lambda^{2n}\int_0^t dr\int d\mathrm{x}_1 d\mathrm{v}_1 L_i U^{(0)}(r)L_{\Sigma 1}\phi_{eq}(\mathrm{v}_1)\int(\mathrm{x},\mathrm{v};t-r) \tag{3}$$

Where we use terminology and notions of Statistical Mechanics and details can be found in relative textbooks; see for instance in [Balescu 1997].

Remember that $f=f(\mathrm{x},\mathrm{v};t)$, $\phi_{eq}=\phi_{eq}(v_1)$ respectively denote the distribution functions of the test-particle and one *(any)* particle from the (homogeneous) reservoir; $n = N/V$ is the particle density; $U^{(O)}(t)$ denotes the evolution operator ('propagator') involved in the formal solution of the zeroth-order Liouville equation: $f(t) \approx e^{Lot} f(0) \equiv U^{(0)}(t) f(0)$ finally, L_l is the binary interaction Liouville operator:

$$L_l=-\mathrm{F}_{\mathrm{int}}(r)\left(\frac{1}{m}\frac{\partial}{\partial \mathrm{v}}-\frac{1}{m_1}\frac{\partial}{\partial \mathrm{v}_1}\right)$$

where ($r = |\mathrm{r}| \equiv |\mathrm{x}-\mathrm{x}_1|$)

Notice that the mean-field (Vlasov) term, obtained in λ^1 , has disappeared in the *lhs,* for reasons of symmetry (since the reservoir has been taken to be uniform).

The above master equation is *Non-Markovian* (non-local in time), since the value of $f(t)$ depends on its whole history, i.e. through $f(t-r)$. A traditional 'markovianization' method consists in substituting with the zeroth-order solution, i.e. assuming: $f(t-r)\approx e^{-L_0 r}f(t)\equiv U^{(0)}(-r)f(t)$, and then evaluating the kernel asymptotically i.e. taking the upper integration limit t to be ∞. This is a more or less standard procedure, leading to time-independent coefficients.

3.1. Homogeneous systems

For a *homogeneous* system , equation (3) thus takes the form of a (linear) 2nd-order parabolic partial derivative equation in velocity space [Kourakis 2002b]:

$$\frac{\partial f}{\partial t} + m^{-1}\mathrm{F}^{(0)}\frac{\partial f}{\partial \mathrm{v}} = -\frac{\partial}{\partial v_i}(F_i f) + \frac{\partial^2}{\partial v_i \partial v_j}(D_{ij} f) \qquad (4)$$

This equation provides the *generic* form of the Fokker-Planck-type kinetic equation obtained for *any* particular dynamical system. The *diffusion matrix* D in it can be explicitly evaluated by making use of the Fourier transform of the interaction potential $V_{(\mathrm{r})}$ and the zeroth-order trajectory presented above:

$$D_{ij} = \frac{n}{m^2}(2\pi)^3 \int_0^t d\tau \int d\mathrm{v}_1 \phi_{eq}(\mathrm{v}_1) \int d\mathrm{k}\, e^{i\mathrm{k}\Delta r(r)} k_i k_m V_k^2 N_{jm}(\tau) \qquad (5)$$

(one is mostly interested in the asymptotic limit i.e.).t$\rightarrow \infty$ The exponential: Δr = r(t - τ)can be exactly computed by making use of the solution (2) of the problem of motion; in the case where M = I (e.g. the first and third of the examples mentioned above), it simplifies to:

$$\Delta \mathrm{r}\,(\tau) = \mathrm{N}\,(\tau)\mathrm{v} - \mathrm{N1}\,(\tau)\mathrm{v}_1$$

Note the explicit appearance of the external force field (through the N, N' matrices). The drift vector F_i represents a mechanism of *dynamical friction* acting on the particle, due to collisions; it is given by:

$$F_i = (1 + \frac{m}{m_1})\frac{\partial D_{ij}}{\partial v_j} \qquad (6)$$

3.2. Inhomogeneous systems

For a spatially *inhomogeneous* system, i.e. if $f = f(\mathrm{x}, \mathrm{v}; t)$, the above markovian approximation may lead to erroneous results, as argued in the past [Tzanakis 1987], [Grecos 1988]; we shall not go into details in the limited space provided here. See details in [Kourakis 2002b]. Let us only mention that, adopting an alternative markovianization procedure developed in the past in the context of open systems [Davies 1974], [Van-Kampen 1992], one obtains a correct generalization of (4) which accounts for diffusion in real (position) space as well velocity space. For instance, in the case of magnetized plasma (see §2.3) we have obtained [Kourakis 1999]:

$$\frac{\partial f}{\partial t}+\mathrm{v}\frac{\partial f}{\partial x}+\frac{e}{mc}(\mathrm{vxB})\frac{\partial f}{\partial \mathrm{v}}=\left(\frac{\partial^2}{\partial v_x^2}+\frac{\partial^2}{\partial v_y^2}\right)[D(\mathrm{v})f]+\frac{\partial^2}{\partial v_x^2}[D\,(\mathrm{v})f]$$

$$+2\Omega^{-1}\left[\frac{\partial^2}{\partial v_x \partial y}-\frac{\partial^2}{\partial v_y \partial x}\right][D_\perp(\mathrm{v})f]+\Omega^{-2}\left[D^{(xx)}_\perp(\mathrm{v})\right]\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)f$$

$$-\frac{\partial}{\partial v_x}[F_x(\mathrm{v})f]-\frac{\partial}{\partial v_y}[F_y(\mathrm{v})f]-\frac{\partial}{\partial v_z}[F_z(\mathrm{v})f]+\Omega^{-1}F_y(\mathrm{v})\frac{\partial}{\partial x}f-\Omega^{-1}F_x(\mathrm{v})\frac{\partial}{\partial y}f \tag{7}$$

As an additional paradigm, considering the case of a chain of linear oscillators (see §2.2 above) we have obtained:

$$\frac{\partial f}{\partial t}+v\frac{\partial f}{\partial x}-\omega_0^2 x\frac{\partial f}{\partial v}=\frac{\partial^2}{\partial v^2}[D_{VV}(v)f]+\frac{\partial^2}{\partial v\partial x}[D_{VX}(v)f]+\frac{\partial^2}{\partial x^2}[D_{XX}(v)f]$$

$$-\frac{\partial}{\partial v}[F_v(v)f]-\frac{\partial}{\partial x}[F_x(v)f] \tag{8}$$

All coefficients have been explicitly computed and will be reported elsewhere [Kourakis 2002c]; they are omitted here for brevity.

4. Application to an electrostatic plasma.

Let us consider the case of a large ensemble of charged particles (plasma), interacting through (long- range) electrostatic interactions. This is a widely studied physical system, so a few comments relating the point we want to make, here, to previous work are definitely imposed.

In the general kinetic-theoretical framework, this system is most often described by the celebrated LANDAU kinetic equation, derived in 1936 for *unmagnetized* plasma (i.e. in *no* field) [Balescu 1963]. In the presence of external fields, and namely for a uniform magnetic field (cf. §2.3), a field-dependent collision term was later elaborated by a number of studies, e.g. -to mention only a few -[Rostoker 1961] in the early 60's, and also [Haggerty 1967], [Schram 1969], [Montgomery 1974] and [Ghendrih 1987] more recently. Notice, however, that these studies have always focused on the *space-homogeneous* case, either deliberately omitting or neglecting (through physical arguments e.g. [Ghendrih 1987]) the space inhomogeneity of the distribution function. It should also be noted that these studies have treated the complete (intrinsically nonlinear) kinetic problem, whereas our scope here was limited to the study of a test-particle problem (as described above), in order to examine collisional relaxation phenomena and their dependence on physical parameters. One thus expects to gain in analytical tractability (since the background equilibrium state is assumed to be known; see above), thus inevitably somewhat losing in generality and validity range (yet not in rigor).

Focusing on the test-particle problem, *unmagnetized* plasma obeys a linearized Landau equation of the form of (4) (cancelling the force in the *lhs* and evaluating the *rhs* according to §2.1); this system has been extensively studied in the past, so details can be found in literature. It is well-known to exhibit a diffusive behaviour in velocity space and diffusion coefficients are found to decrease with velocity (see figure 1). Since the value of the diffusion coefficient is related to the inverse of the relaxation time T_R (i.e. the time the particle takes to relax towards thermal equilibrium [Montgomery 1963]), we see that faster particles take longer to relax. Furthermore, a force of dynamical friction is exerced on the particle, its magnitude depending on its velocity: $F_i = -\eta\ (v) v_i$. In figures la, and b we have depicted this behaviour, relying on the analytical data presented in [Balescu 1963] .

Now let us switch on a uniform external magnetic field. We saw that this case is described by the (linear) kinetic equation (7), where coefficients are explicit functions of particle velocity and the field [Kourakis et al. 2000]. A numerical study, based on formulae (5), (6) (as applied to the dynamical problem in §2.3) reveals a similar qualitative behaviour versus velocity, with a clear (yet rather not dramatic) dependence on the magnitude of the magnetic field. Rigorously speaking, as we already mentioned, this is only true for the homogeneous case i.e. equation (4); see, for instance, §37 in [Balescu 1963] and references made to the original works therein. Expressions are too lengthy to provide here, yet details can be

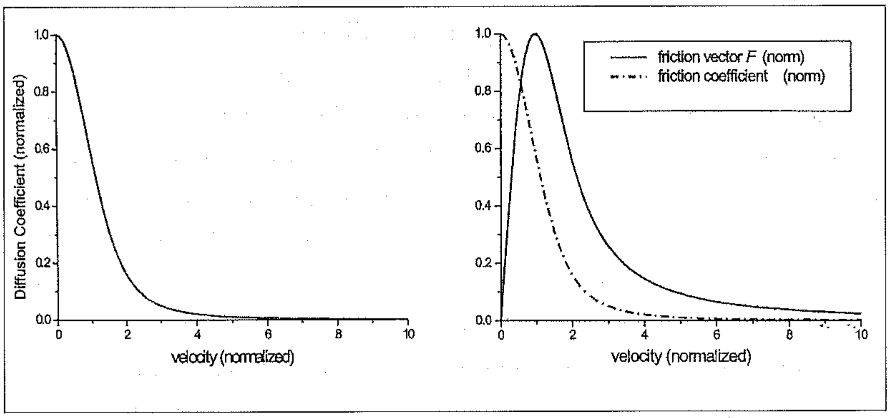

Figure 1: (a) Diffusion coefficient (normalized) and (b) the norm of the drift vector $F_i = -\eta\ (v)v_i$ and the dynamical friction coefficient $\eta(v)$ (normalized), versus particle velocity v (normalized over the thermal velocity) for an electrostatic plasma in no external field (analytical data taken from [Balescu 1963]).

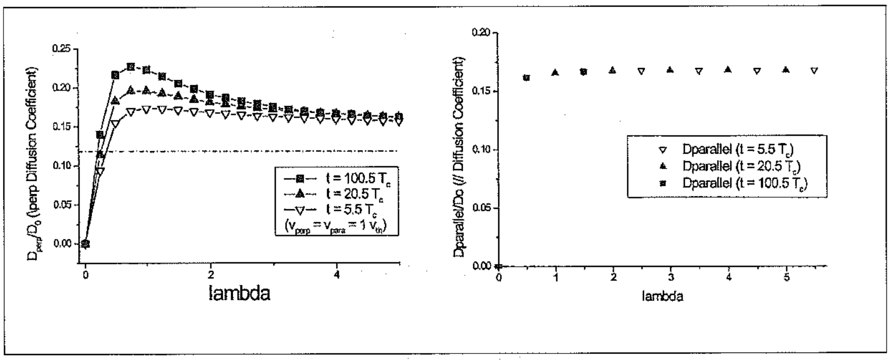

Figure 2: (a) The perpendicular diffusion coefficient $D_\perp$ and (b) its $\|$ -counterpart plotted against λ (~1/B), at different instants of t (cf. (5)). $D_\perp$ slightly increases in time, yet only around $\lambda \approx 1$(i.e.$\rho_L \approx r_D$, above which it practically remains constant. The field-dependence is smoothed out, as $D_\perp$. approaches the asymptotic value for $\Omega \rightarrow 0$ (dash-dot line).$D_{\|}$, on the contrary, comes out to be independent of the field; this is reasonable, since Lorentz forces do not modify dynamics parallel to the magnetic field. In the plot we have considered a temperature of T = 10KeV and a particle density of n = 1020m-3, implying: λ = 4.531/B (B expressed in Tesla) (according to definitions in [Kourakis2002a]).

found in [Kourakis 2002a]. Let us only point out that the magnitude of all coefficients in (7) comes out to depend on a dimensionless parameter related to the Larmor radius to Debye length ratio, say $\lambda \sim \rho_L / r_D$ i.e. qualitatively speaking, to the relative magnitude of the gyration to interaction mechanisms (as intuitively expected). The *Debye sphere* delimits the range of electrostatic interactions when taking into account charge screening; see e.g. [Balescu 1963]. Tracing the dependence of the $D_\perp$ coefficient, for instance, on the magnitude of the field *B* (via $\lambda \sim 1 / B$) (see fig. 2), we see that it is more important around $\rho_L \approx r_D$ and practically disappears for lower values of the field (since particle trajectories in that parameter range are less curved within a Debye radius -so the field is less important -as more or less assumed in most studies) .

En résumé, as a *priori* expected, the field modifies the value of the diffusion coefficients (it actually seems to favor relaxation, since it lowers the value of the characteristic relaxation time $\tau_R \sim 1 / D$ (Montgomery 1964]; cf. figure 2), yet only in the region where ρ_L is comparable to or slightly greater than r_D; beyond that value, the influence of the field is rather unimportant, as was in fact suggested by previous studies.

5. Conclusion

In conclusion, we saw that the Fokker-Planck-type collision term describing a weakly-coupled *N* -body system depends on external fields that may be present. Special attention should therefore be paid to the rigorous derivation of the kinetic equation, in order to take due account of the field as well as spatial inhomogeneity effects.

References

Balescu Radu, 1963: *Statistical Mechanics of Charged Particles,* Interscience Publishers.

Balescu Radu, 1988: *Transport Processes in Plasmas,* vol. 1, North - Holland.

Balescu Radu, 1997: *Statistical Dynamics,* Imperial College Press.

Montgomery D.C. & Tidman D.A., 1963: *Plasma Kinetic Theory,* McGraw-Hill Inc.

Risken Rannes, 1989: *The Fokker-Planck Equation,* Springer-Verlag.

Van Kampen N. G., 1992: *Stochastic Processes in Physics and Chemistry,* North-Holland.

Articles:

Davies E.B., 1974: Comm. Math. Physics 3991.

Ghendrih P., 1987: PhD Thesis, Université de Paris-Sud (Orsay).

Grecos A.P. & C. Tzanakis: 1988, Physica A 151, 61-89; also, a series of papers: (i) Physica A 256, 87-111, (ii) *idem,* 112-128 and references therein.

Raggerty M.J., 1967: Phys. Fluids vol. 10 no.(10) 2199.

Kourakis I., 1999: Plasma Phys. Control. Fusion 41, pp. 587 -594.

Kourakis I., D. Carati & B. Weyssow, 2000: Proceedings of the ICPP 2000/ APS-DPP Conference, Québec 2000, pp. 49 -52. Kourakis I., 2002:

(a) *«Relaxation times for Magnetized Plasmas -a parametric study»,* Proc. 29th EPS Conf. Plasma Phys. & Contr. Fusion, P4.008 (to appear in Europhysics Conference Abstracts);

(b) *«Kinetic Theory of Transport Processes in Magnetized Plasmas»,* PhD thesis, Université Libre de Bruxelles (in preparation);

(c) *'Derivation and properties of a kinetic equation for one-dimensional gases'* (in preparation). Montgomery D.C. & D.A. Tidman, 1964: *Plasma Kinetic Theory,* McGraw-Hill.

Montgomery D.C., Turner L., Joyce G.: 1974, Phys. Fluids 17 (5) 954.

Rostoker N., 1960: Phys. Fluids 3 (6)922.

Schram P.P.J.M., 1969: Physica 45 165.

Tzanakis C., 1987: *«On the Kinetic Theory of Test -Particles Weakly Coupled to Large Equilibrium Systems»,* PhD thesis, Université Libre de Bruxelles.