GENERAL PATH-INTEGRAL SUCCESSIVE-COLLISION SOLUTION OF THE BOUNDED DYNAMIC MULTI-SWARM PROBLEM

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The path-integral successive-collision method is extended and applied to the set of linear Boltzmann equations for a very general initial- and boundary-value multi-swarm problem allowing for volume production, reactive collisions, and various particle-surface interaction processes. The complete formal solution is given, and its convergence is inferred from a simple physical argument.

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The linearized Boltzmann equation has been widely used to describe the transport of particle swarms in prescribed fields and background media, such as neutrons in fissible material,[1] electrons in semiconductors,[2] or electrons and ions in weakly ionized gases.[3-8] These studies have two basic goals, namely (i) calculating transport coefficients (i.e., moments of the distribution functions), and/or (ii) finding the distribution functions themselves.

The present work is concerned with the second of these goals. We first formulate, in integro-differential form, a very general bounded and dynamic multi-swarm problem which, to our knowledge, includes all situations considered previously as special cases. The relevant linear Boltzmann equations are then cast into their path-integral forms, and their complete formal solution is derived by means of an appropriately extended version of the successive-collision iteration method.[2,4-7] This scheme is readily interpreted in physical terms, and its convergence is inferred from a simple physical argument.

Consider a fixed spatial domain $\mathcal{B}$ surrounded by the surface A as shown in Fig. 1, and assume that confined therein are n_σ particle swarms numbered by the swarm (or species) index σ $(\sigma = 1, \ldots, n_\sigma)$. Let species σ be characterized by the particle mass m^σ, the electric particle charge q^σ, and the velocity distribution function $f^\sigma(\mathbf{r}, \mathbf{v}, t)$. The swarm particles move in prescribed electromagnetic and gravitational fields $\mathbf{E}(\mathbf{r}, t), \mathbf{B}(\mathbf{r}, t)$, and $\mathbf{g}(\mathbf{r}, t)$, at the same time undergoing binary collisions with the molecules of a background gas having an arbitrary but given velocity distribution function. Allowing for volume production of swarm particles, the integro-differential linear Boltzmann equation may be written

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\frac{\partial}{\partial \mathbf{r}}+\mathbf{a}^\sigma\cdot\frac{\partial}{\partial \mathbf{v}}\right)f^\sigma=\gamma^\sigma+\sum_{\sigma'=1}^{n_\sigma}G^{\sigma\sigma'}-\nu^\sigma f^\sigma \tag{1}$$

where

$$\mathbf{a}^\sigma(\mathbf{r},\mathbf{v},t)=\frac{q^\sigma}{m^\sigma}\left[\mathbf{E}(\mathbf{r},t)+\frac{\mathbf{v}}{c}\times\mathbf{B}(\mathbf{r},t)\right]+\mathbf{g}(\mathbf{r},t)$$

is the acceleration, the source term $\gamma^\sigma(\mathbf{r},\mathbf{v},t)$ describes volume production,

$$G^{\sigma\sigma'}(\mathbf{r},\mathbf{v},t)=\int d^3\mathbf{v}'\,K^{\sigma\sigma'}(\mathbf{r},\mathbf{v}\leftarrow\mathbf{v}',t)\,f^{\sigma'}(\mathbf{r},\mathbf{v}',t)$$

describes the gain for species σ from collisions of species σ', and $\nu^\sigma(\mathbf{r},\mathbf{v},t)$ is the total collision frequency. The scattering kernel $K^{\sigma\sigma'}(\mathbf{r},\mathbf{v}\leftarrow\mathbf{v}',t)$ basically represents the probability for a species-σ' particle with pre-collision velocity $\mathbf{v}'$ to end up after collision as a species-σ particle with velocity $\mathbf{v}$. Any kind of collision, conservative or reactive, is admitted for which the G's and ν's remain finite.

Equation (1) must be complemented by initial and boundary conditions. Let us assume that at the initial time t_i the swarm distributions are given everywhere as

$$f^\sigma(\mathbf{r},\mathbf{v},t=t_i)=f_i^\sigma(\mathbf{r},\mathbf{v})\,, \tag{2}$$

and that the relation between incoming and outgoing particles at the surface A is of the fairly general form

$$\begin{aligned} f_A^\sigma(\mathbf{r}_A,\mathbf{v}_{in},t)=&\,g_A^\sigma(\mathbf{r}_A,\mathbf{v}_{in},t)\\ &+\sum_{\sigma'=1}^{n_\sigma}\int d^3\mathbf{v}'_{out}\,b_A^{\sigma\sigma'}(\mathbf{r}_A,\mathbf{v}_{in}\leftarrow\mathbf{v}'_{out},t)\,f^{\sigma'}(\mathbf{r}_A,\mathbf{v}'_{out},t) \end{aligned} \tag{3}$$

where $\mathbf{r}_A$ is a "surface point" (i.e., a position still within $\mathcal{B}$ but infinitesimally close to A), $f_A^\sigma(\mathbf{r}_A,\mathbf{v}_{in},t)\equiv f^\sigma(\mathbf{r}_A,\mathbf{v}_{in},t)$ (which notation is convenient because $f_A^\sigma(\mathbf{r}_A,\mathbf{v}_{in},t)$ will be treated as an unknown), and $\mathbf{v}_{in}$ and $\mathbf{v}_{out}$ are inward and outward directed velocities, respectively, cf. Fig. 1. The (given) function $g_A^\sigma(\mathbf{r}_A, \mathbf{v}_{in}, t)$ describes externally controlled injection into $\mathfrak{B}$, while the "generalized- reflection" kernel $b_A^{\sigma\sigma'}(\mathbf{r}_A, \mathbf{v}_{in} \leftarrow \mathbf{v}'_{out}, t)$ basically represents the probability for a species-σ' particle hitting the surface A with velocity $\mathbf{v}'_{out}$ to be "re-injected" as a species-σ particle with velocity $\mathbf{v}_{in}$. Clearly, this model is capable of describing such processes as elastic or inelastic reflection, secondary emission, surface ionization and neutralization, or simply absorption of swarm particles.

Equations (1), (2) and (3) define a very general evolution problem for the functions $f_A^\sigma(\mathbf{r}_A, \mathbf{v}_{in}, t)$ and $f^\sigma(\mathbf{r}, \mathbf{v}, t)$, which we now cast into a path-integral form suitable for both general considerations and practical applications. As is well known, the operator

$$\frac{d_\sigma}{dt} \equiv \frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} + \mathbf{a}^\sigma \cdot \frac{\partial}{\partial \mathbf{v}} \tag{4}$$

appearing in (1) represents the time derivative associated with the motion of species-σ particles along their collisionless phase trajectories (free paths, characteristics). The species-σ characteristic through the point $[\mathbf{r}, \mathbf{v}, t]$, to be denoted by $[\hat{\mathbf{r}}^\sigma(\hat{t}), \hat{\mathbf{v}}^\sigma(\hat{t}), \hat{t}]$, can, in principle, always be calculated from the equations of motion $d\hat{\mathbf{r}}^\sigma/d\hat{t} = \hat{\mathbf{v}}^\sigma$ and $d\hat{\mathbf{v}}^\sigma/d\hat{t} = \hat{\mathbf{a}}^\sigma$, with $\hat{t} \leq t$ and the "final" conditions $\hat{\mathbf{r}}^\sigma(\hat{t} = t) = \mathbf{r}$, $\hat{\mathbf{v}}^\sigma(\hat{t} = t) = \mathbf{v}$. Of course, the symbol $\hat{\mathbf{a}}^\sigma$ introduced here is shorthand for $\mathbf{a}^\sigma(\hat{\mathbf{r}}^\sigma, \hat{\mathbf{v}}^\sigma, \hat{t})$, and analogous notations will be used for other quantities, too. With (4), formal integration of (1) along the species-σ characteristic through $[\mathbf{r}, \mathbf{v}, t]$ leads to

$$\begin{aligned} f^\sigma(\mathbf{r}, \mathbf{v}, t) =& f^\sigma(\hat{\mathbf{r}}_o^\sigma, \hat{\mathbf{v}}_o^\sigma, \hat{t}_o^\sigma) \exp[-\kappa^\sigma(\hat{t}_o^\sigma, t)] \\ &+ \int_{\hat{t}_o^\sigma}^{t} d\hat{t} \left[\sum_{\sigma'=1}^{n_\sigma} G^{\sigma\sigma'}(\hat{\mathbf{r}}^\sigma, \hat{\mathbf{v}}^\sigma, \hat{t}) + \gamma^\sigma(\hat{\mathbf{r}}^\sigma, \hat{\mathbf{v}}^\sigma, \hat{t}) \right] \exp[-\kappa^\sigma(\hat{t}, t)] \,, \end{aligned} \tag{5}$$

where $[\hat{\mathbf{r}}_o^\sigma = \hat{\mathbf{r}}^\sigma(\hat{t}_o^\sigma), \hat{\mathbf{v}}_o^\sigma = \hat{\mathbf{v}}^\sigma(\hat{t}_o^\sigma), \hat{t} = \hat{t}_o^\sigma]$ is the (suitably chosen) "origin" of the species-σ characteristic through $[\mathbf{r}, \mathbf{v}, t]$, and

$$\kappa^\sigma(\hat{t}_1, t) = \int_{\hat{t}_1}^{t} d\hat{t}\, \nu^\sigma(\hat{\mathbf{r}}^\sigma, \hat{\mathbf{v}}^\sigma, \hat{t})$$

is the "collisional relaxation exponent". In some cases — e.g., in time-independent problems—it may be convenient to re-write the path integrals by using one of the identities $d\hat{t} = |d\hat{\mathbf{r}}^\sigma| \,/\, |\hat{\mathbf{v}}^\sigma|$ and $d\hat{t} = |d\hat{\mathbf{v}}^\sigma| \,/\, |\dot{\hat{\mathbf{a}}}^\sigma|$.

Equation (5) represents the path-integral version of (1) and is readily interpreted in physical terms. As one proceeds along a characteristic, the memory of conditions at the origin is gradually wiped out by collisional loss (first term on the r.h.s.), while a new distribution builds up through both collisional gain and volume production, with more recent contributions being dominant (second term).

The species-σ characteristic passing through the point $[\mathbf{r}, \mathbf{v}, t]$ can either originate at an "initial" point $[\hat{\mathbf{r}}_i^\sigma \equiv \hat{\mathbf{r}}^\sigma(\hat{t} = t_i), \hat{\mathbf{v}}_i^\sigma \equiv \hat{\mathbf{v}}^\sigma(\hat{t} = t_i), \hat{t} = t_i]$, with $\hat{\mathbf{r}}_i^\sigma$ lying in the interior of $\mathcal{B}$, or at a surface point $[\hat{\mathbf{r}}_A^\sigma \equiv \hat{\mathbf{r}}^\sigma(\hat{t} = \hat{t}_A^\sigma), \hat{\mathbf{v}}_{in}^\sigma \equiv \hat{\mathbf{v}}^\sigma(\hat{t} = \hat{t}_A^\sigma), \hat{t} = \hat{t}_A^\sigma]$, with $t_i < \hat{t}_A^\sigma \leq t$. These trajectories, and the points through which they pass, will be referred to as "i-type" and "A-type", respectively, cf. the curves C_1 and C_2 in Fig. 1. For what follows it is convenient to introduce the unit-step functions $U_i^\sigma(\mathbf{r}, \mathbf{v}, t)$ (equals unity for i-type points, vanishes for A-type points) and $U_A^\sigma(\mathbf{r}, \mathbf{v}, t)$ (equals unity for A-type points, vanishes for i-type points).

With these preparations, Eq. (5) can be re-written in more detail as follows:

$$
\begin{aligned}
f^\sigma = U_i^\sigma &\left\{ \hat{f}_i^\sigma \exp[-\kappa^\sigma(t_i,t)] + \int_{t_i}^{t} d\hat{t} \left[\sum_{\sigma'=1}^{n_\sigma} \hat{G}^{\sigma\sigma'} + \hat{\gamma}^\sigma \right] \exp[-\kappa^\sigma(\hat{t},t)] \right\} \\
+ U_A^\sigma &\left\{ \hat{f}_A^\sigma \exp[-\kappa^\sigma(\hat{t}_A^\sigma,t)] + \int_{\hat{t}_A^\sigma}^{t} d\hat{t} \left[\sum_{\sigma'=1}^{n_\sigma} \hat{G}^{\sigma\sigma'} + \hat{\gamma}^\sigma \right] \exp[-\kappa^\sigma(\hat{t},t)] \right\}
\end{aligned}
\tag{6}
$$

where $\hat{f}_i^\sigma = f^\sigma(\hat{\mathbf{r}}_i^\sigma, \hat{\mathbf{v}}_i^\sigma, t_i)$ and $\hat{f}_A^\sigma = f^\sigma(\hat{\mathbf{r}}_A^\sigma, \hat{\mathbf{v}}_{in}^\sigma, \hat{t}_A^\sigma)$. This integral equation is very convenient in that it explicitly accounts for the mixed initial- and boundary-value character of the problem. It has to be solved simultaneously with the boundary condition (3), which also becomes an integral equation for $f_A^\sigma(\mathbf{r}_A, \mathbf{v}_{in}, t)$ and $f^\sigma(\mathbf{r}, \mathbf{v}, t)$ when $f^{\sigma'}(\mathbf{r}_A, \mathbf{v}'_{out}, t)$ on the r.h.s. is re-expressed in terms of these functions via (6).

We now solve Eqs. (3) and (6) formally using the method of successive collisions.[2,4–7] To this end we decompose the two unknown distribution functions in the form

$$
f_A^\sigma(\mathbf{r}_A, \mathbf{v}_{in}, t) = \sum_{\nu=0}^{\infty} f_{A,\nu}^\sigma(\mathbf{r}_A, \mathbf{v}_{in}, t) \tag{7a}
$$

$$
f^\sigma(\mathbf{r}, \mathbf{v}, t) = \sum_{\nu=0}^{\infty} f_\nu^\sigma(\mathbf{r}, \mathbf{v}, t) \tag{7b}
$$

where the "partial distribution functions" $f_{A,\nu}^\sigma$ and f_ν^σ are the distribution functions of the "class-(σ,ν)" particles, by which we mean those species-σ particles that have suffered exactly ν generalized collisions since their first appearance in the system. By definition, a swarm particle suffers a "generalized collision" either when it collides with a background-gas molecule, or when it hits the surface A. By "first appearance" of a swarm particle we mean either its presence within $\mathcal{B}$ at $t = t_i$, its creation by volume production at some $t > t_i$, or its injection through the surface at some $t > t_i$. Classes with $\nu = 0$ are populated by these first-appearance mechanisms, whereas classes with $\nu \geq 1$ gain their particles from classes with $\nu - 1$ through generalized collision processes. Every class (σ, ν) loses particles through generalized collision processes, and if the latter are non-destructive, these particles go into classes with $\nu + 1$. According to this philosophy, the partial distribution functions must clearly satisfy the equations

$$f^{\sigma}_{A,0}(\mathbf{r}_A, \mathbf{v}_{in}, t) = g^{\sigma}_{A}(\mathbf{r}_A, \mathbf{v}_{in}, t) \tag{8a}$$

$$\begin{aligned} f^{\sigma}_0 = U^{\sigma}_i &\left\{ \hat{f}^{\sigma}_i \exp[-\kappa^{\sigma}(t_i, t)] + \int_{t_i}^{t} d\hat{t}\, \hat{\gamma}^{\sigma} \exp[-\kappa^{\sigma}(\hat{t}, t)] \right\} \\ + U^{\sigma}_A &\left\{ \hat{g}^{\sigma}_A \exp[-\kappa^{\sigma}(\hat{t}^{\sigma}_A, t)] + \int_{\hat{t}^{\sigma}_A}^{t} d\hat{t}\, \hat{\gamma}^{\sigma} \exp[-\kappa^{\sigma}(\hat{t}, t)] \right\} \end{aligned} \tag{8b}$$

for $\nu = 0$, and

$$f^{\sigma}_{A,\nu}(\mathbf{r}_A, \mathbf{v}_{in}, t) = \sum_{\sigma'=1}^{n_\sigma} \int d^3 v'_{out}\, b^{\sigma\sigma'}_{A}(\mathbf{r}_A, \mathbf{v}_{in} \leftarrow \mathbf{v}'_{out}, t)\, f^{\sigma'}_{\nu-1}(\mathbf{r}_A, \mathbf{v}'_{out}, t) \tag{9a}$$

$$\begin{aligned} f^{\sigma}_{\nu} = U^{\sigma}_i &\int_{t_i}^{t} d\hat{t} \left[\sum_{\sigma'=1}^{n_\sigma} \hat{G}^{\sigma\sigma'}_{\nu-1} \right] \exp[-\kappa^{\sigma}(\hat{t}, t)] \\ + U^{\sigma}_A &\left\{ \hat{f}^{\sigma}_{A,\nu} \exp[-\kappa^{\sigma}(\hat{t}^{\sigma}_A, t)] + \int_{\hat{t}^{\sigma}_A}^{t} d\hat{t} \left[\sum_{\sigma'=1}^{n_\sigma} \hat{G}^{\sigma\sigma'}_{\nu-1} \right] \exp[-\kappa^{\sigma}(\hat{t}, t)] \right\} \end{aligned} \tag{9b}$$

for $\nu \geq 1$, where

$$G^{\sigma\sigma'}_{\nu-1} = \int d^3 v'\, K^{\sigma\sigma'}(\mathbf{r}, \mathbf{v} \leftarrow \mathbf{v}', t)\, f^{\sigma'}_{\nu-1}(\mathbf{r}, \mathbf{v}', t)\,. \tag{10}$$

Equations (8a,b) yield explicit expressions for $f^{\sigma}_{A,0}$ and f^{σ}_0, whence $G^{\sigma\sigma'}_0$ can be calculated via (10). Using these results in (9a,b) and (10), one successively finds $f^{\sigma}_{A,1}$, f^{σ}_1 and $G^{\sigma\sigma'}_1$, which in turn can be inserted into (9a,b) and (10) to yield $f^{\sigma}_{A,2}$, f^{σ}_2 and $G^{\sigma\sigma'}_2$, etc. Thus, Eqs. (7)–(10) define a closed iteration scheme, which yields the formal solution to our swarm problem and can be seen to converge as follows.

In a specific application, the number of partial distribution functions that must be retained in (7a,b) for a meaningful approximation to the exact distribution functions increases with the number of generalized collisions a typical swarm particle can undergo. E.g., in a situation where there are hardly any swarm particles having undergone more than three generalized collisions, one may safely neglect in (7a,b) all $f^{\sigma}_{A,\nu}$'s and f^{σ}_{ν}'s with say $\nu \geq 5$. This indicates that the method of successive collisions may become computationally expensive in problems where the particles have to be traced through many collisions. However, for finite evolution times ($t - t_i < \infty$) the scheme (7)–(10) is always bound to converge, and since it can handle non-standard (e.g., strongly non-equilibrium) situations in a natural way,[6-7] it may well provide a suitable basis for attacking swarm problems which because of their complexity have hardly been looked at as yet. As an example we may mention swarm behavior near walls, which is important but needs further consideration.[8]

In conclusion, recent studies[5-7] and the present work have contributed towards making the path-integral successive-collision method a practicable tool of transport theory, which seems suitable for attacking more complex swarm problems than hitherto considered.

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Figure Captions

FIG. 1. Two-dimensional visualization of swarm-problem geometry.