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Probabilistic Methods for Stationary Problems of Linear Transport Theory

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The steady state of a system of independent particles which undergo elastic collisions can be expressed in terms of the absorption probabilities of the associated Markov process. For the slab albedo problem, this representation enables the application of probabilistic methods to obtain explicit upper and lower bounds on the steady-state density. In particular, the bounds prove the $1/L$ decrease of the steady-state flux as a function of the slab width L (Fick's law).

KEY WORDS: Transport equation; absorption probabilities; slab albedo; Fick's law.

1. INTRODUCTION

Systems of independent particles which move by a combination of a steady free flow and a local scattering have been used as models for neutron diffusion in matter.[1] The purpose of this paper is to introduce some probabilistic methods which are helpful in the study of some such systems. We consider the particular case where a constant isotropic flux of particles is incident on one side of a slab, $\Lambda = \{(q_1, q_2, q_3) \in \mathbb{R}^3 | 0 \leqslant q_3 \leqslant L\}$, of a large thickness L. With time, a steady state is approached in which the incident flux and the loss due to particles leaving the slab are balanced. A simple probabilistic derivation is presented of the steady-state particle density and the steady-state net flux, to the leading orders in $1/L$.

Commonly,[1] such a particle dynamics is described by the one-speed transport equation (linear Boltzmann equation)

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\begin{aligned}
(\partial/\partial t)\psi(q,p,t) &= -p\cdot\nabla\psi(q,p,t) \\
&\quad + |p|\rho(q)\left\{\int_{S^2} d\Omega'\,\sigma_{|p|}(\Omega'\cdot\Omega)\psi(q,|p|\Omega',t) - \psi(q,p,t)\right\} \\
&\equiv (L\psi)(q,p,t) \qquad (1)
\end{aligned}
$$

Here, $\psi(q, p, t)$ is the density of the particles (in phase space) at the time t; $q \in \Lambda \subset \mathbb{R}^3$ is the position, and $p \in \mathbb{R}^3$ the velocity of a particle (we set the mass to one), $\Omega = p/|p| \in S^2$, and $d\Omega'$ is the normalized solid angle measure. We assume that the differential cross section $\sigma_{|p|}(\Omega'\cdot\Omega)\,d\Omega'$ comes from an interaction with static scatterers via a central potential and is therefore invariant under rotations. We let $\sigma_{|p|}$ be normalized to one,

$$\int d\Omega'\,\sigma_{|p|}(\Omega'\cdot\Omega) = \tfrac{1}{2}\int_{-1}^{1} du\,\sigma_{|p|}(u) = 1 \qquad (2)$$

so that $|p|\rho(q)$ is the collision rate.

To obtain the steady state one has to find a stationary solution of (1) with the boundary conditions which describe the incident flux. The quantities of most physical interest are then the spatial density in the steady state $\psi(q, p)$,

$$n(q) = \int dp\,\psi(q,p) \qquad (3)$$

and the steady-state flux

$$\mathbf{j}(q) = \int dp\,\mathbf{p}\psi(q,p) \qquad (4)$$

In fact, the above particle dynamics is proven[2] to be the low-density (Boltzmann–Grad) limit of the dynamics of the Lorentz gas, which is the motion of a mechanical particle through static scatterers randomly located in space. It was also shown[3] that for given incident flux the steady state of the Lorentz gas converges in the low-density limit to the stationary solution of (1).

We will use here a probabilistic method to obtain upper and lower bounds on the steady state, in particular, to derive the $1/L$ behavior of the steady flux (Fick's law). Usually, problems of this kind are studied by the method of singular eigenfunction expansions pioneered by Case[4] and described in detail in Ref. 1. The stationary solution is expanded in eigendistributions of L. The boundary conditions lead then to integral equations for the expansion coefficients. Unfortunately, even in the simplest cases, these integral equations are rather untractable.[5] In particular, the large-L behavior of the steady flux can be obtained only by a formal approximation. Instead, we first relate the steady state to hitting probabilities of the Markov process which describes the motion of the particles. These are then estimated using a certain martingale, which in physical terms has the following simple meaning.

The ensemble of particles initially at the specified position with a given velocity spreads due to random collisions. The total displacement of the ensemble center of mass, in the limit $t \to \infty$, is, however, finite and is given, as a function of the initial data, by the above-mentioned martingale. Its relation to the hitting probabilities is a consequence of the conservation law expressed by the optional stopping theorem.

In Section 2 we define the corresponding Markov process more precisely and show how its hitting probabilities can be used to express the steady state corresponding to a given incident flux. Since this connection is rather general, we will use less restrictive assumptions than those just mentioned. In Section 3 we consider the slab albedo problem and derive, using probabilistic methods, bounds on the steady-state density and the steady state flux.

Similar results may be obtained for more general (non-Markovian) one-particle dynamics. A sufficient condition for the $1/L$ decrease of the hitting probabilities for such systems is derived in Ref. 6 using a different probabilistic method.

2. STATIONARY STATES AND HITTING PROBABILITIES

The states of the system we shall discuss are described by measures μ on the one-particle phase space $\mathbb{X} = \mathbb{R}^d \times \mathbb{R}^d$. μ may represent the average density of particles of a fluid or the statistical distribution of each particle of the system.

The system's time evolution results from an independent motion of its particles. These move by a combination of the free flow

$$(q, p) \mapsto (q + pt, p) \qquad \forall \in (q, p) \in \mathbb{X}$$

and a local scattering occurring at the rate $\rho(q)$, $\sup \rho(q) < \infty$. Assuming independence of collisions, the one-particle time evolution is given by a Markov process for which the probability that, starting at (q, p), no collision occurs up to time t is $\exp[-\int_0^t ds\, |p| \rho(q + sp)]$. Given the initial momentum p, the scattered momentum is in dp' with probability $\sigma(dp'|p)$, $\int \sigma(dp'|p) = 1$, independent of the time of collision.

We shall assume that there is an invariant probability measure $h(dp)$ with respect to which σ is absolutely continuous and has the density $\sigma(p'|p)$, i.e.,

$$\sigma(dp'|p) = \sigma(p'|p) h(dp') \tag{5}$$

By the invariance of h

$$\int \sigma(p'|p) h(dp) = 1 \qquad \text{for} \quad h\text{-a.e. } p' \tag{6}$$

and by the normalization

$$\int \sigma(p'|p)h(dp') = 1 \qquad \forall p \in \mathbb{R}^d \tag{7}$$

Let m be the measure on $\mathbb{X}$:

$$m(dx) = l(dq)h(dp) \tag{8}$$

where $dx = dq\,dp$ and l is the Lebesque measure on $\mathbb{R}^d$. Then m is preserved by the above process independently of ρ.

It is convenient to introduce Γ, the space of paths whose points are piecewise continuous functions γ: $\mathbb{R} \to \mathbb{X}$. Each $\gamma(t)$ is a possible history of a particle. The initial state and the time evolution may be described by a measure on Γ. The conditional distribution of $\gamma(\cdot)$, given $\gamma(0)$, is described by the above process. Choosing the distribution of $\gamma(0)$ to be m, one obtains the time-invariant measure P on Γ.

The transition probabilities are defined by

$$P(\{\gamma \in \Gamma | \gamma(0) \in dx, \gamma(t) \in dy\}) = P_t(dy|x)m(dx) \qquad \text{for} \quad t \geqslant 0 \tag{9}$$

and (using the invariance of m) the transition probabilities $\tilde{P}_t(\cdot|\cdot)$ of the *time-reversed* process are defined by

$$P(\{\gamma \in \Gamma | \gamma(0) \in dx, \gamma(t) \in dy\}) = \tilde{P}_t(dx|y) \qquad \text{for} \quad t \leqslant 0 \tag{10}$$

i.e.,

$$P_t(dx|y)m(dy) = \tilde{P}_{-t}(dy|x)m(dx)$$

The time-reversed process is a combination of the flow $(q, p) \mapsto (q - tp, p)$ with scattering at the rate $\tilde{\rho}(q) = \rho(q)$ and the differential cross section $\tilde{\sigma}(p'|p) = \sigma(p|p')$.

Let now Λ be a domain in $\mathbb{R}^d$ whose boundary $\partial\Lambda$ is a finite union of smooth manifolds, e.g., a slab. We shall consider the situation in which there is a steady flux of particles into Λ through its boundary. The flux is described by a measure $\nu(dy)$ concentrated on $\Lambda \times \mathbb{R}^d$. Assuming that the particles that leave Λ are prevented from returning there, the time evolution is described by the map of measures on $\Lambda \times \mathbb{R}^d$, $\mu \to T_t\mu$,

$$(T_t\mu)(dx) = \int_{\Lambda \times \mathbb{R}^d} P_t'(dx|z)\,\mu(dz) + \int_0^t ds \int_{\Lambda \times \mathbb{R}^d} P_s'(dx|y)\,\nu(dy) \tag{11}$$

with the modified transition probabilities defined by

$$P_t'(dx|z)m(dz)$$
$$= P(\{\gamma \in \Gamma | \gamma(0) \in dz, \gamma(t) \in dx, \gamma(s) \in \Lambda \times \mathbb{R}^d \quad \forall s \in [0, t]\}) \tag{12}$$

If the initial measure is finite and if there is no trapping, i.e. for μ-a.e. $z \in \Lambda \times \mathbb{R}^d$

$$\lim_{t \to \infty} P_t'(\Lambda \times \mathbb{R}^d|z) = 0 \tag{13}$$

then T_t converges to the steady state $\bar{\mu}$

$$\bar{\mu}(dx) = \int_0^\infty ds \int_{\partial\Lambda \times \mathbb{R}^d} \nu(dy)\, P_s{}'(dx|y) \tag{14}$$

[(13) will not be satisfied for $z \in \Lambda \times \{0\}$.]

μ may also be expressed in terms of the hitting probabilities of the time-reversed process. This form is useful for our analysis. In order to introduce it we need some further notation.

Let us define a measure τ, which gives the flux into Λ in the invariant state m, as the solution of

$$\tau(dy) \int_0^t ds\, P_s{}'(dx|y) = P(B(t, dy, dx)) \tag{15}$$

for all $t \geqslant 0$, with

$$B(t, dx, dy) = \Big\{\gamma \in \Gamma | \gamma(0) \in dx \text{ and for some } s \in [0, t],$$
$$\bigcup_{t \in [0,s]} \{\gamma(-r)\} \subset \Lambda \times \mathbb{R}^d, \gamma(-s) \in dy \cap \partial\Lambda \times \mathbb{R}^d\Big\}$$

Equation (15) should be viewed as an equation for measures on the unintegrated variables.

That a solution to (15) for $t = t_1 > 0$ is also a solution for $t = t_1 + t_2$, $t_2 > 0$, follows directly from

$$\int_{\Lambda \times \mathbb{R}^d} P'_{t_2}(dx|z) P'_{t_1}(dz|y) = P'_{t_1+t_2}(dx|y) \tag{16}$$

which is implied by the Markov property, and from

$$\begin{aligned} &P(B(t_1 + t_2, dy, dx)) - P(B(t_1, dy, dx)) \\ &\quad = P\left(B(t_1 + t_2, dy, dx) \cap \left\{\delta \in \Gamma \,\middle|\, \bigcup_{r \in [0,t_1]} \{\gamma(r)\} \subset \Lambda \times \mathbb{R}^d\right\}\right) \\ &\quad = \int_{\Lambda \times \mathbb{R}^d} P(B(t_2, dy, dz)) P'_{t_1}(dx|z) \end{aligned} \tag{17}$$

The last equality results from conditioning on $\{\gamma(-t_1) = z\}$.

For the flow introduced above (15) can be solved by letting $t \to 0$. The solution is independent of ρ and is given in terms of the surface measure η and the inner normal $\hat{n}$ by

$$\tau(dq\, dp) = \eta(dq) h(dp) \max(0, \hat{n} \cdot p) \tag{18}$$

Next we define the time of the first exit and the exit distributions for the time-reversed process.

Definition 1. For

$$\gamma' \in \left\{\gamma \in \Gamma | \gamma(0) \in \Lambda \times \mathbb{R}_1{}^d, \bigcup_{s<0} \{\gamma(s)\} \not\subset \Lambda \times \mathbb{R}^d\right\}$$

the exit time is

$$t^*(\gamma') = \sup\{t \geqslant 0 | \gamma(s) \in \Lambda \times \mathbb{R}^d, \forall s \in (-t, 0)\} \tag{19}$$

Definition 2. For $0 \leqslant t \leqslant \infty$ the exit distributions for the time-reversed process are the measures $\tilde{e}(\cdot|x, t)$ defined for all $x \in \Lambda \times \mathbb{R}^d$ by

$$\tilde{e}(dy|x, t) = P(\{\gamma \in \Gamma | \gamma(0) \in dx, \gamma(-t^*) \in dy, t^*(\gamma) < t\}) \tag{20}$$

We write $\tilde{e}(dy|x) = \tilde{e}(dy|x, \infty)$. The exit distributions are useful for an expression of the steady-state $\bar{\mu}$ in situations in which the flux measure is absolutely continuous with respect to τ.

Proposition 1. If $\nu \ll \tau$, then $\bar{\mu} \ll m$ and its density $\psi = d\bar{\mu}/dm$ is given by

$$\psi(x) = \int_{\partial\Lambda \times \mathbb{R}^d} \tilde{e}(dy|x) \frac{d\nu}{d\tau}(y) \tag{21}$$

$$= E_x\left(\frac{d\nu}{d\tau}[\gamma(-t^*)]\right) \tag{22}$$

where E_x denotes the conditional expectation given that $\gamma(0) = x$.

Proof. Comparing (19) and (20) with (15), we obtain

$$\tau(dy) \int_0^t ds\, P_s'(dx|y) = m(dx)\tilde{e}(dy|x, t)$$

which, as $t \to \infty$, converges to

$$\tau(dy) \int_0^\infty ds\, P_s'(dx|y) = m(dx)\tilde{e}(dy|x) \tag{23}$$

Therefore, using Fubini's theorem for positive measures,

$$\begin{aligned}\bar{\mu}(dx) &= \int_0^\infty ds \int_{\partial\Lambda \times \mathbb{R}^d} \nu(dy) P_s'(dx|y) \\ &= \int_{\partial\Lambda \times \mathbb{R}^d} \tau(dy) \int_0^\infty ds\, P_s'(dx|y) \frac{d\nu}{d\tau}(y) \\ &= m(dx) \int_{\partial\Lambda \times \mathbb{R}^d} \tilde{e}(dy|x) \frac{d\nu}{d\tau}(y)\end{aligned}$$

proving (21). Equation (22) follows from the definition of $\tilde{e}$. ∎

3. STEADY-STATE DENSITY AND FLUX

We shall now return to the setting described in the introduction. The particles move in the slab $\Lambda = \{(q_1, q_2, q_3) \in \mathbb{R}^3, 0 \leqslant q_3 \leqslant L\}$. The scattering cross section is $\sigma_{|p|}(\Omega' \cdot \Omega)$ with the normalization (2). Because of the rotational invariance, (6) and (7) are satisfied if and only if h is a rotation-invariant probability measure. The collision rate is $|p|\rho(q)$ and it is further assumed that ρ is (a) horizontally homogeneous, i.e., $\rho(q) = \rho(q_3)$, (b) bounded above and below: $0 < a \leqslant p(q) < b < \infty$. (We could also accommodate other $|p|$ dependences of the collision rate.)

We consider an isotropic incident flux from below described by the flux measure ν on the boundary $\partial\Lambda \times \mathbb{R}^3$,

$$\begin{aligned} \nu(dg\, dp) &= dq_1\, dq_2\, h(dp) \max(0, p_3) && \text{on} \quad \{q_3 = 0\} \times \mathbb{R}^3 \\ \nu(dq\, dp) &= 0 && \text{on} \quad \{q_3 = L\} \times \mathbb{R}^3 \end{aligned} \tag{24}$$

By Proposition 1 the density of the steady state for these boundary conditions is given by

$$\psi(q, p) = \tilde{e}_-(q, p) \tag{25}$$

where

$$\tilde{e}_{(\mp)}(q, p) = \tilde{e}\left(\left\{q_3 = \underset{(L)}{0}\right\} \times \mathbb{R}^3 | q, p\right) \tag{26}$$

is the probability for the reversed process which starts at (q, p) to hit the plane $\{q_3 = 0\}$ ($\{q_3 = L\}$) before hitting the opposite one.

It may be more convenient to think in terms of the given process rather than the time-reversed one. Denoting its exit distribution by $\tilde{e}_{(\pm)}(q, p)$ we have, due to the time-reversal symmetry of the motion,

$$\tilde{e}_{(\pm)}(q, p) = \tilde{e}_{(\pm)}(q, -p) \tag{27}$$

However, in order to keep the origin of terms clear, we shall continue to use the time-reversed process.

The key observation for our estimates of $\tilde{e}_{(\pm)}$ is that the time-reversed process has a convenient martingale, namely: For all $t \leqslant 0$

$$E_x(f(\gamma(t))) = f(x) \tag{28}$$

$$f(q, p) = q_3\bar{\rho}(q_3) - \alpha(|p|)p_3/|p| \tag{29}$$

with

$$\bar{\rho}(q_3) \equiv (1/q_3) \int_0^{q_3} dz\, \rho(z) \tag{30}$$

and

$$\alpha(|p|) = \left[1 - \tfrac{1}{2} \int_{-1}^{1} du\, u\sigma_{|p|}(u)\right]^{-1} \tag{31}$$

Clearly $E_x(|f(\sigma(t))|) \leqslant c_1(x) + c_2(x)t$, with appropriate $c_1(x), c_2(x) < \infty$, and (28) holds since f is a solution of

$$-p\cdot\nabla f(q,p) + |p|\rho(q) \times \left\{\int d\Omega'\, \sigma_{|p|}(\Omega'\cdot\Omega) f(q, |p|\Omega') - f(q,p)\right\} = 0 \tag{32}$$

In the case of a constant collision rate ρ, $-\rho^{-1}\alpha(|p|)p_3/|p|$ is the expected drift in the q_3 direction for particles with initial momentum p, which move by the time-reversed process. For purely backward scattering $\alpha(|p|) = \frac{1}{2}$ and for purely forward scattering $\alpha(|p|) = \infty$. Since by assumption the differential cross section is absolutely continuous with respect to $d\Omega$, $\frac{1}{2} < \alpha(|p|) < \infty$.

Our main result is as follows:

Theorem. For the above-defined system the steady-state density, given by (21), satisfies

$$\left|\psi(q,p) - \left(1 - \frac{\bar\rho(q_3)}{\bar\rho(L)}\frac{q_3}{L}\right)\right| \leqslant \frac{1}{L}\frac{2\alpha(|p|)}{\bar\rho(L)} \tag{33}$$

The steady state flux $\mathbf{j}(q)$, given by (4), points in the 3-direction and is independent of q, $\mathbf{j}(q) \equiv (0,0,j)$ and j satisfies

$$\frac{1}{L}\int h(dp)\frac{|p|\alpha(|p|)}{3\bar\rho(L)} \leqslant j \leqslant \frac{1}{L}\int h(dp)\frac{|p|\alpha(|p|)}{3[\bar\rho(L) - 2\alpha(|p|)/L]} \tag{34}$$

In particular, for a constant collision rate, $\rho(q) \equiv \rho$, we find that

$$\lim_{L\to\infty} Lj_L = (1/\rho)\int h(dp)\, 1/3|p|\alpha(|p|) \tag{35}$$

where j_L denotes the flux for a slab of height L. Thus, Fick's law of diffusion is valid for the linear transport (Boltzmann) equation.

To apply the optional stopping theorem we prove the following:

Proposition 2. For all $x \in \Lambda \times \mathbb{R}^d$, $P_x(\{t^* = \infty\}) = 0$.

Proof. Since ρ is bounded, a particle which at time $t = 0$ is in Λ undergoes an infinite, but locally finite, number of collisions in the time $(-\infty, 0)$. Let us denote by $t_1 > t_2 > \cdots$ the times and by $q_1, q_2,\ldots$ the positions of these collisions. Let

$$A_n = \{\gamma \in \Gamma | \gamma(0) = (q,p),\quad q_1,\ldots,q_n \in \Lambda\}$$

Since p is bounded and $|p|$ is absolutely continuous, it follows, using the Markov property and a geometric argument, that for some $\epsilon > 0$

$$P_x(A_{n+1}|A_n) \leqslant 1 - \epsilon \tag{36}$$

independent of n. However, $A_{n+1} \subset A_n$ and thus

$$P_x(A_n) = P_x(A_1)P_x(A_2|A_1) \cdots P_x(A_n|A_{n-1}) \leqslant C(1-\epsilon)^n \tag{37}$$

Therefore

$$P_x(\{t^* = \infty\}) = P_x(\{\alpha(-t) \in \Lambda \times \mathbb{R}^3, \quad \forall t \geqslant 0\})$$
$$= P_x\left(\bigcap_{n \geq 1} A_n\right) = 0$$

Proof of the Theorem. We have $E_x(|f(\alpha(t^*))|) < \infty$ and

$$\liminf_t \int_{\{t^* > t\}} |f(\alpha(t))| \, dP_x \leqslant \liminf_t cP_x(\{t^* > t\}) = 0 \tag{38}$$

by Proposition 2 and since f is bounded on $\Lambda \times \mathbb{R}^3$. Therefore, sufficient conditions for the optional stopping theorem (Ref. 7, Theorem 14.12) are met. It implies

$$f(x) = E_x(f(\gamma(t^*)) \tag{39}$$

for all $x \in \Lambda \times \mathbb{R}^3$. Here $\gamma(t^*)$ is the exit point on the boundary $\partial\Lambda \times \mathbb{R}^3$ for the time-reversed process. Conveniently enough, $\bar{\rho}(\alpha(t^*)) = \in\{0, \bar{\rho}(L)\}$ and we obtain

$$q_3\bar{\rho}(q_3) - \alpha(|p|)p_3/|p| = L\bar{\rho}(L)e_+(q, p) \tag{40}$$

Since by (25) and Proposition 2

$$\psi(q, p) = 1 - \tilde{e}_+(q, p) \tag{41}$$

claim (33) follows from (40).

By the symmetry and the conservation of mass, $\mathbf{j}(q) = (0, 0, j)$. Evaluating the flux at $q = 0$ by inserting (41) in (4), we obtain

$$j = \int h(dp) \, p_3\tilde{e}_+(0, -p) \tag{42}$$

[$\tilde{e}_+(0, -p) = 0$ for $p_3 < 0$]. Read differently, $h(dp)p_3$ is the incident flux and $\tilde{e}_+(0, p) = \tilde{e}_+(0, -p)$ the fraction of it that leaves through the upper boundary $\{q_3 = L\}$.

Let $j(v)$ be the steady flux for $h_v(dp) = (1/4\pi v^2) \int \delta(|p| - v) \, dp$. Then $j = \int h(dp)j(|p|)$. Integrating (40) with $h_v(dp)$ leads to

$$L\bar{\rho}(L)j(v) = \tfrac{1}{3}v\alpha(v) + \alpha(v) \int h_v(dp) \, p_3\tilde{E}_{q,p}(p_3(\gamma(t^*))/|p|) \tag{43}$$

In terms of the exit distributions

$$\int h_v(dp) \, p_3\tilde{E}_{q,p}(p_3(\gamma(t^*))/|p|)$$
$$= \int h_v(dp) \, p_3(p_3'/|p'|)\tilde{e}(\{q_3 = 0\} \times dp'|q, p)$$
$$- \int h_v(dp) \, p_3(-p_3'/|p'|)\tilde{e}(\{q_3 = L\} \times dp'|q, p) \tag{44}$$

The first term is the steady flux corresponding to an incident flux measure density $p_3/|p|$ from below, whereas the second term is minus the steady flux corresponding to an incident flux measure density $-p_3/|p|$ from above. By symmetry both terms are equal. Therefore, using again constancy of the flux,

$$\begin{aligned} 0 &\leqslant \int h_v(dp)\, p_3 \tilde{E}_{q,p}(p_3(\gamma(t^*))/|p|) \\ &= 2\int h_v(dp)\, p_3(p_3'/|p|)\tilde{e}(\{q_3 = 0\} \times dp'|L, p) \\ &\leqslant 2\int h_v(dp)\, p_3 \tilde{e}_-(L, p) = 2j(v) \end{aligned} \tag{45}$$

Combining (43) with (45) yields (34). ■

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