Invariant Imbedding and Neutron Transport Theory IV—Generalized Transport Theory

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1. Introduction. In a series of recent papers the principle of invariant imbedding has been utilized in the study of a variety of physical processes: radiative transfer [1, 2, 3, 4, 5], neutron transport [6, 7, 8, 9], random walk and scattering [10], and wave propagation [11, 12].

The aim of the present paper is to extend previous results and techniques so as to include an extensive category of transport processes involving deterministic and stochastic interactions and general geometries. Characteristic functions and probabilities as well as expected values (fluxes) are determined.

For intuitive reasons the reader may use neutron transport theory as a model, though we encase the problem in a more abstract setting in order to emphasize the common features of a number of particle processes. In this way we obtain an extensive generalization of the fundamental invariance principles of AMBARZUMIAN [13] and CHANDRASEKHAR [14].

In §§2–3 we present a rather general formulation of the flux or expected value problem. A single equation is developed which automatically accounts for different geometries, energy distributions, *etc.* This formula includes many of the problems considered in past work [1, 2, 6, 7, 8] and leads to new results. Some specializations are indicated in §4.

In §5 a particularly simple problem is investigated from a stochastic viewpoint. The resulting equation is analyzed and it is shown that the flux equation can be obtained from it. The last section deals with a general stochastic analysis. It is indicated that the results of §3 may be obtained by taking moments of the general stochastic equation.

2. Description of a Generalized Transport Process. Let a family of surfaces in n -dimensional space be characterized by a single continuous parameter $\eta \geq 0$. The surface corresponding to $\eta = 0$ (it may be a degenerate surface) will be considered a bounding surface, and the parametrization will be such that the region included between $\eta = 0$ and $\eta = \eta_1$ will be included by the region

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between $\eta = 0$ and $\eta = \eta_2 > \eta_1$. We shall not consider the topological properties of these surfaces and regions in detail and such ideas as outward and inward directions, area of a surface, *etc.* will be taken intuitively. The family of surfaces will be assumed to continuously partition all or part of the n -dimensional space into a set of strata.

For example, the family of surfaces might be the set of all spheres centered at the origin in three-dimensional space. Here η is r , and $\eta = 0$ is a degenerate bounding surface. Again, the family might be the set of all vertical lines, in the two-dimensional space, to the right of the vertical axis. In this case we can choose η to be x , and $x = 0$ is a non-degenerate bounding surface.

By a "particle" we shall understand a state vector S depending on the parameter η . The state vector may contain information regarding the direction of motion, energy, specific location on η and any other properties we may choose to designate the particle.

The stratum $(\eta, \eta + \Delta)$, $\Delta > 0$, will be assumed to contain a medium which transports particles. A particle passing through the stratum may engage in interactions of both a deterministic and a stochastic nature. The former will be proportional to Δ plus a term $o(\Delta)$; the latter will have *probability* proportional to Δ plus $o(\Delta)$. These interactions will have no effect on the transport medium but will be equivalent to a transformation on the state vector S , in some cases transforming it into two or more such vectors, in some cases annihilating it. Hence the movement of a particle within the medium between 0 and η can be thought of as a sequence of transformations on state vectors.

We shall now investigate the following problem. Let a particle specified by S impinge on η . What are the number and nature of the particles (state vectors) emergent from η after all time?* In some instances, what are the number and nature of particles emergent from $\eta = 0$ after all time? The former particles we shall call "reflected," the latter we call "transmitted." It is clear that in some cases, such as for the sphere mentioned above, the second problem is ill-posed. We shall investigate only the problem of reflection, leaving the formulas for transmission to the reader.

3. The Expected Value Equation. We begin by considering not the state vector itself, but its expected value. Consider a stream of particles, one per unit area per unit time, in state S , impinging upon the surface η . We ask for the expected number, or flux, of particles in state S' reflected per unit area per unit time. Denote this flux by $\psi(\eta, S, S')$. For the present discussion we shall assume that S and S' contain no information about the specific location on η . It is evident that this assumption imposes a strong symmetry requirement upon both the surface η and the impinging flux. (See, *e.g.*, [2].)

Let the probability that a particle in state S passing through $(\eta, \eta \pm \Delta)$

* Sometimes the source will be given in particles per unit time, in which case we shall seek the number of particles emerging from η per unit time.

suffers a collision—the stochastic process—be given by $P(\eta, S)\Delta + o(\Delta)$. Let $T(\eta, S, S')$ be the average number of particles in state S' resulting from this interaction and transmitted to $\eta \pm \Delta$. Let $R(\eta, S, S')$ be the average number in state S' reflected back to η . Then, using the principle of invariant imbedding, [1], we find

$$\begin{aligned}
 \psi(\eta + \Delta, S, S') &= P(\eta, S)\Delta R(\eta, S, S') \\
 &+ P(\eta, S)\Delta \int_{S''} T(\eta, S, S'')\psi(\eta, S'', S') dS'' \\
 &+ [1 - P(\eta, S)\Delta]\psi(\eta, S, S')[1 - P(\eta, S')\Delta] \\
 (3.1) \quad &+ [1 - P(\eta, S)\Delta] \int_{S''} dS'' \psi(\eta, S, S'')\Delta P(\eta, S'') \left\{ T(\eta, S'', S') \right. \\
 &\quad \left. + \int_{S'''} R(\eta, S'', S''')\psi(\eta, S''', S') dS''' \right\} + o(\Delta).
 \end{aligned}$$

The first term on the right-hand side of this equation represents the contribution to the reflected flux from the neutrons which are reflected immediately from the slab of thickness Δ , and the second arises from the neutrons which fission in the slab, are reflected from the slab $[\eta, 0]$, and pass through the slab of thickness Δ . The third arises from the neutrons which do not fission in the slab $[\eta + \Delta, \eta]$, are reflected from the slab $[\eta, 0]$, and do not fission on the way out through the slab $[\eta + \Delta, \eta]$. The next term arises from those particles that do not fission on the way in, are reflected from the slab $[\eta, 0]$, and fission on the way out, giving rise to a direct contribution, or reenter the slab, where they are rereflected and then pass through the slab $[\eta + \Delta, \eta]$. All of the processes which have been neglected involve terms of at least Δ^2 , and are accounted for in the term $o(\Delta)$.

Here all the states on the right-hand side are taken at η , and the integration over states is symbolic. The transport equation resulting when $\Delta \rightarrow 0$ is then

$$\begin{aligned}
 \frac{\partial \psi}{\partial \eta} &= P(\eta, S)R(\eta, S, S') + P(\eta, S) \int_{S''} dS'' T(\eta, S, S'')\psi(\eta, S'', S') \\
 (3.2) \quad &- [P(\eta, S) + P(\eta, S')]\psi(\eta, S, S') \\
 &+ \int_{S''} dS'' \psi(\eta, S, S'')P(\eta, S'') \left\{ T(\eta, S'', S') \right. \\
 &\quad \left. + \int_{S'''} dS''' R(\eta, S'', S''')\psi(\eta, S''', S') \right\}.
 \end{aligned}$$

4. Some Examples. We shall now consider a few special cases, phrasing them in terms of neutron theory.

(I) A rod extending from 0 to x is made of a material which transports neutrons. The macroscopic cross section for collision is σ , a constant, and q neutrons

result on the average from such a collision, half going left, half right. One neutron per unit time enters the rod at x ; all velocities are the same and we wish to find the emergent flux $\psi(x)$.

Here $\eta = x$, and there is no necessity of specifying the state S since all neutrons may be considered in the same state. Further, $P = \sigma$, $R = T = \frac{1}{2}q$. The integrations in (3.2) become simple multiplications and we have

$$(4.1) \quad \begin{aligned} \frac{d\psi(x)}{dx} &= \frac{1}{2}\sigma q + \frac{1}{2}\sigma q\psi(x) - 2\sigma\psi(x) + \sigma\psi(x)(\frac{1}{2}q + \frac{1}{2}q\psi(x)) \\ &= \frac{1}{2}\sigma q + \sigma(q - 2)\psi(x) + \frac{1}{2}\sigma q\psi^2(x). \end{aligned}$$

The boundary condition is $\psi(0) = 0$.

In case $q = 2$ equation (4.1) reduces to

$$(4.2) \quad \frac{d\psi}{dx} = \sigma(1 + \psi^2),$$

a result previously found in [7, 8].

(II) The rod is situated as before, but now cross section and neutron production are energy dependent; neutrons are produced isotropically and we wish to find the emergent flux $\psi(x, E, E')$, due to one neutron of energy E per unit time impinging at x .

Here $\eta = x$ and $S = E$, the particle energy. Also $P = \sigma(E)$, $T = R = \frac{1}{2}q(E, E')$, where q is the total number of neutrons emerging at energy E' from a collision of one at energy E with a nucleus.

Applying (3.2) directly we get

$$(4.3) \quad \begin{aligned} \frac{d\psi}{dx}(x, E, E') &= \frac{1}{2}\sigma(E)q(E, E') \\ &+ \frac{1}{2}\sigma(E) \int_0^\infty q(E, E'')\psi(x, E'', E') dE'' - [\sigma(E) + \sigma(E')]\psi(x, E, E') \\ &+ \frac{1}{2} \int_0^\infty dE'' \psi(x, E, E'')\sigma(E'') \left\{ q(E'', E') \right. \\ &\quad \left. + \int_0^\infty dE''' q(E'', E''')\psi(x, E''', E') \right\}, \end{aligned}$$

$\psi(0, E, E') = 0$.

This should be compared with [8, Eq. (1.23)].

(III) An infinite cylinder is made of transport material, cross section $\sigma(r)$ dependent on the radial coordinate only; neutron production is energy independent and isotropic, q neutrons emerging from each collision. Angular coordinates as shown in Figure 1 are introduced to describe the neutron direction. A flux of one neutron per unit area per unit time impinges on the cylinder at angle (θ, φ) . Find the emergent flux $\psi(r, \mu, \varphi, \mu', \varphi')$, where $\mu = \cos \theta$.

FIGURE 1.

(For ingoing particles, θ is measured with respect to the inward normal.)

In this case $\eta = r$, $P = \sigma(r) (\csc \varphi)/\mu$, $T = R = q/4\pi$. The state S is now specified by the two direction coordinates (μ, φ) . The angle φ is independent of r , but μ is not. From Figure 2 we deduce

$$\sin \theta = \sqrt{1 - \mu^2} = \frac{b}{r}$$

so that

$$(4.4) \quad \frac{d\mu}{dr} = \frac{1 - \mu^2}{\mu r}.$$

(Note that this is an example of a *deterministic* change in state. The state (μ, φ) changes, as the neutron passes through Δ , in a completely determined manner.)

The resulting transport equation is

$$(4.5) \quad \begin{aligned} \frac{\partial \psi}{\partial r} + \frac{\partial \psi}{\partial \mu} \frac{1 - \mu^2}{\mu r} + \frac{\partial \psi}{\partial \mu'} \frac{1 - \mu'^2}{\mu' r} &= \frac{q\sigma(r) \csc \varphi}{4\pi\mu} \\ &+ \frac{q\sigma(r) \csc \varphi}{4\pi\mu} \int_0^\pi d\varphi'' \int_0^1 \psi(r, \mu'', \varphi'', \mu', \varphi') d\mu'' \\ &- \frac{\sigma(r)}{4\pi} \left[\frac{\csc \varphi}{\mu} + \frac{\csc \varphi'}{\mu'} \right] \psi(r, \mu, \varphi, \mu', \varphi') \\ &+ \frac{q\sigma(r)}{4\pi} \int_0^\pi d\varphi'' \int_0^1 d\mu'' \psi(r, \mu, \varphi, \mu'', \varphi'') \frac{\csc \varphi''}{\mu''} \\ &\cdot \left\{ 1 + \int_0^\pi d\varphi''' \int_0^1 d\mu''' \psi(r, \mu''', \varphi''', \mu', \varphi') \right\}, \end{aligned}$$

$$\psi(0, \mu, \varphi, \mu', \varphi') = 0.$$

It must be remarked that this formula does not agree with that in [2], where the φ -dependence was not considered.

FIGURE 2.

(IV) A sphere is composed of transport material, cross section $\sigma(\rho)$ dependent upon the radial coordinate ρ only. Neutron production is energy independent and isotropic. The angular coordinate α , $\cos \alpha = \nu$, is introduced as shown (Figure 3) and a conical flux of neutrons, direction ν , impinges uniformly on the surface of the sphere, one neutron per unit area per unit time. Find the emergent flux $\psi(\rho, \nu, \nu')$. (For ingoing particles, α is measured with respect to the inward normal.)

FIGURE 3.

Here $\eta = \rho$, $P = \sigma(\rho)/\nu$, $T = R = q/4\pi$. The state S is specified by ν and $d\nu/d\rho = (1 - \nu^2)/\nu\rho$, similar to (4.4). The transport equation is

$$\begin{aligned}
 (4.6) \quad & \frac{\partial \psi}{\partial \rho} + \frac{1 - \nu^2}{\nu \rho} \frac{\partial \psi}{\partial \nu} + \frac{1 - \nu'^2}{\nu' \rho} \frac{\partial \psi}{\partial \nu'} = \frac{q\sigma(\rho)}{4\pi\nu} + \frac{q\sigma(\rho)}{2\nu} \int_0^1 \psi(\rho, \nu'', \nu') d\nu'' \\
 & - \sigma(\rho) \left(\frac{1}{\nu} + \frac{1}{\nu'} \right) \psi(\rho, \nu, \nu') \\
 & + \frac{q}{2} \sigma(\rho) \int_0^1 d\nu'' \frac{\psi(\rho, \nu, \nu'')}{\nu''} \left\{ 1 + 2\pi \int_0^1 \psi(\rho, \nu''', \nu') d\nu''' \right\}.
 \end{aligned}$$

5. A Simple Stochastic Case. Before attempting to write down a general stochastic functional equation, we consider a simple example, the first of §4. We assume, for further simplicity, that in a collision *exactly* two neutrons emerge, one going right, one left, so that $q = 2$. We let one neutron enter the bar at time zero.

Let $\{U^{(i)}(x)\}$, $i = 1, 2, 3, \dots$, be a sequence of random variables denoting

the number of neutrons reflected from the bar in all time. Let $\{F^{(i)}(\Delta)\}$, $i = 1, 2, 3, \dots$, be another sequence of random variables with

$$F^{(i)}(\Delta) = \begin{cases} 1 & \text{if a collision occurs in a segment of length } \Delta, \\ 0 & \text{otherwise.} \end{cases}$$

FIGURE 4.

Then, using the invariant imbedding principle, we have

$$(5.1) \quad \begin{aligned} U^{(1)}(x) &= F^{(1)}(\Delta) \{1 + U^{(2)}(x - \Delta)\} \\ &+ (1 - F^{(1)}(\Delta)) \sum_{i=4}^{U^{(3)}(x-\Delta)+4} \{1 + F^{(i)}(\Delta) U^{(i)}(x - \Delta)\} + w(x, \Delta), \end{aligned}$$

where $\text{Prob}\{w(x, \Delta) \neq 0\} = o(\Delta)$.

Let us interpret this equation. The superscripts in themselves have no significance and serve merely to distinguish one random variable from another. Notice that if the initiating particle makes a collision in passing from x to $x - \Delta$ (Figure 4), the second term of (5.1) is zero while the first gives just the number of particles emergent from $x - \Delta$ —namely, the one immediately out due to the collision in $(x - \Delta, x)$ plus the random number $U^{(2)}$ due to the left moving neutron acting as a source particle for the rod $(0, x - \Delta)$. If there is no initial interaction in the interval $(x - \Delta, x)$, then the first term of (5.1) is zero, and the second term counts. Of the random number $U^{(3)}(x - \Delta)$ of neutrons emerging from $x - \Delta$ some make no collisions in $(x - \Delta, x)$ and hence contribute only one to the sum. Others make a collision in $(x - \Delta, x)$ giving not only an immediate right travelling particle, but also a random number $U^{(i)}(x - \Delta)$ reflected from $(0, x - \Delta)$. The fact that all other processes are “unlikely” is included in the term w .

We now introduce the generating function

$$(5.2) \quad u(x, t) = E\{t^{U(x)}\}.$$

Then, using the properties of the generating function [15, Chapter 11] and writing $\text{Prob}\{F^{(1)} = (\Delta) = 1\} = \sigma\Delta + o(\Delta)$, we find, after careful calculation with (5.1),

$$(5.3) \quad \begin{aligned} u(x, t) &= \sigma\Delta tu(x - \Delta, t) \\ &+ (1 - \sigma\Delta)u(x - \Delta, (1 - \sigma\Delta)t + \sigma\Delta tu(x - \Delta, t)) + o(\Delta) \\ &= \sigma\Delta tu(x, t) + (1 - \sigma\Delta)[u(x - \Delta, t) \\ &+ u_t(x - \Delta, t)(-\sigma\Delta t + \sigma\Delta tu)] + o(\Delta). \end{aligned}$$

This leads at once to the partial differential equation

$$(5.4) \quad u_x = -\sigma u + \sigma t u - \sigma t u_t + \sigma t u u_t.$$

This is precisely the equation derived in [6] using quite different methods, and from it may be obtained the usual flux equations for the rod case.*

6. A Basic Stochastic Functional Equation. We shall now derive a basic stochastic functional equation applicable to the generalized situations described in §2. We introduce appropriate random variables.

Let

$$(6.1) \quad U(S, S', \eta) = \begin{array}{l} \text{random number of particles in state } S' \text{ reflected from } \eta \\ \text{over all time due to an initial particle in state } S \text{ imping-} \\ \text{ing on } \eta \text{ at time zero. (} S \text{ and } S' \text{ may now include infor-} \\ \text{mation as to the specific location on } \eta \text{.)} \end{array}$$

$$(6.2) \quad r(S, \eta) = \begin{cases} 1 & \text{if the particle in state } S \text{ is involved in an interaction in} \\ & \text{the stratum } (\eta - \Delta, \eta), \\ 0 & \text{otherwise.} \end{cases}$$

$$(6.3) \quad Z(S; S'_1, S'_2, \dots, S'_k; \eta) = \begin{cases} 1 & \text{if the result of an interaction of a} \\ & \text{particle in state } S \text{ with the medium} \\ & \text{is to produce } k \text{ particles in state } S'_1, \\ & S'_2, \dots, S'_k, k = 1, 2, 3, \dots, \\ 0 & \text{otherwise.} \end{cases}$$

By the stochastic variables $U^{(i)}$, $r^{(i)}$, $Z^{(i)}$ we shall mean respectively any of a denumerable set of variables with the properties described above. Different superscripts will serve merely to distinguish different random variables, and sometimes they will be omitted.

Also, let $Q(S, \eta)$ denote the deterministic change in state caused by passage through the stratum $(\eta - \Delta, \eta)$.

Finally, we assume that only a finite set of states S is possible. This permits us to use characteristic functions rather than characteristic functionals, and considerably simplifies the discussion.

At the risk of being somewhat redundant, we now discuss the random physical processes which occur. A particle in state S incident on the surface η enters the stratum $(\eta - \Delta, \eta)$. There it may undergo a deterministic transformation, converting it from state S to state $Q(S, \eta)$. In addition, it may undergo a stochastic change (collision) producing a random number of particles in a random set of states. Each of these particles acts independently of the others and may emerge from η or be incident upon $\eta - \Delta$. In the latter case the particle is a "source" particle on $\eta - \Delta$, resulting in a random number of particles in a

* It was first pointed out to us by T. E. HARRIS that the functional equation approach could be applied directly to the generating function.

random set of states eventually emerging from $\eta - \Delta$. Each of these reflected particles may undergo deterministic and stochastic transformations in $(\eta - \Delta, \eta)$. Some emerge from η and are counted, others return as source particles into $\eta - \Delta$ and must be followed out again. No processes need be traced to order higher than Δ —that is, to more than one collision in $(\eta - \Delta, \eta)$.

Enumerating these events mathematically, we arrive at the functional equation

$$\begin{aligned}
 U(S, S', \eta) = & r(S, \eta) \sum_{\{S_{i'}'\}} Z(S; S'_1, S'_2, \dots, S'_k; \eta) \\
 & \cdot \left[\sum_{i=1}^k U^{(i)}(S'_i, S', \eta - \Delta) \right] + (1 - r(S, \eta)) \sum_{i=1}^n (1 - r^{(i)}(S', \eta)) \\
 (6.4) \quad & + (1 - r(S, \eta)) \sum_{S_m'} \left[\sum_{i=1}^{n'} \left[r^{(i)}(S'_m, \eta) \left\{ \sum_{\{S_{i''}'\}} Z^{(i)}(S'_m; S''_i, \dots, S''_k; \eta) \right. \right. \right. \\
 & \left. \left. \left. \cdot \sum_{p=1}^k U^{(p)}(S''_p, \bar{S}', \eta - \Delta) \right\} \right] \right] + w(S, S', \eta)
 \end{aligned}$$

where

$$n = U(Q(S, \eta), S', \eta - \Delta),$$

$$n' = U(Q(S, \eta), S'_m, \eta - \Delta),$$

$$\bar{S} \text{ is such that } S' = Q(\bar{S}', \eta),$$

and $w(S, S', \eta)$ is the contribution from events that have probability $o(\Delta)$. The symbol $\{S_i\}$ means all the subsets of the set of states.

Proceeding as in §5 it is now theoretically possible to derive the flux equation of §3 by taking expected values of (6.4). It is likely that the direct approach of §3 is really simpler. However, the basic stochastic equation (6.4) seems of considerable theoretical interest and could well be used for computational purposes.

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