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EXTENSION OF THE INVARIANT EMBEDDING METHOD FOR THE CALCULATION OF PARTICLE FLUCTUATIONS

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ABSTRACT

Invariant embedding theory is an alternative formulation of particle transport theory. So far the method has exclusively been used for calculating first moments, i.e. expectations. The present paper extends the method to treat fluctuations. A probability balance equation is derived in the traditional invariant embedding approach from which equations for the first and second order densities are derived. It is shown that only the equations for the first order densities are non-linear, while subsequent order densities obey linear equations. With the method, correlations between particles at two different energies and angles, or the higher moments of the emitted multiplicity distribution, such as the variance, from a target bombarded by incident particles can be determined. The approach is illustrated by a simple forward backward scattering model. The possibility of applying the method to finite sized slabs and spheres is also discussed.

Key Words: invariant embedding, fluctuations, sputtering, forward-backward model

1. INTRODUCTION

Invariant embedding theory is an alternative formulation of particle transport theory [1], [2]. Its most characteristic use is the calculation of the reflected radiation from a homogeneous semi-infinite medium. Its advantage is that it only needs to handle the energy and angle variable, but not the depth variable. In other words, in contrast to the traditional transport equation, the solution for the flux within the medium is not calculated in order to get the reflected flux. On the other hand the resulting equations are non-linear, at least for the first moment for which the method has been exclusively used so far.

However, in certain cases fluctuations in the reflected flux are of interest, such as the variance of the total number of sputtered particles from a bombarded medium in which an atomic collision process takes place. The objective of this paper is to give such an extension.

In the ordinary transport theory of particle fluctuations, usually a backward type transport master equation is used. This is because it operates on the initial co-ordinates, and can leave the final ones to represent a volume in phase space. The finite volume of phase space of terminal (detection) co-ordinates is essential in order to get non-trivial statistics (and a possibility to compare measurements with theory).

However, the invariant embedding approach operates both on the initial and on the final co-ordinates, i.e. one must have a point-like (infinitesimal) set of final co-ordinates. Hence a general equation for the probability distribution is not possible, only one-point, two-point etc. densities, from which the same order of moments (first, second etc.) can be calculated.

The application of the invariant embedding method for the first moment (one-point) distributions is well known, since all the applications so far treat such a case. In the derivation one constructs the reflected flux as the sum of the probabilities of the mutually exclusive events of a particle history with five different possibilities of having none, or at most one, collision in an infinitesimal layer added to a semi-infinite medium, in first order of the thickness of the layer.

This method is extended to obtain a general equation for the probability distribution, which is possible in the forward approach of stochastic transport [3]. We describe such a derivation in the next section. We also obtain two-point densities of the reflected flux in the case when branching on the collisions is accounted for, such as a projectile and recoil in an atomic collision cascade or in neutron induced fission. For obvious reasons the number of possibilities how the different particles (projectile and recoil) enter the material and get reflected becomes very much larger than in the case of one-point densities (in fact 16 different possibilities). This makes the resulting equations much more involved. On the other hand it is seen that, in contrast to the one-point density, the equation for the two-point densities is linear, although it contains products of one-point densities. In Section 3 we consider the applicability of the method to situations other than those involving semi-infinite plane geometries, viz., finite slabs and spheres. The method is then illustrated by considering a simple forward-backward scattering model describing atomic sputtering in Section 4.

2. EQUATION FOR THE NEUTRON DISTRIBUTION PROBABILITIES

We define $P_N(E_1,\Omega_1,E_2,\Omega_2,...E_N,\Omega_N;E_0,\Omega_0)$ as the probability that given one neutron incident with energy and direction E_0,Ω_0, N neutrons will emerge from the system one each in energy and solid angle elements $dE_1d\Omega_1$ around E_1,Ω_1, $dE_2d\Omega_2$ around E_2,Ω_2 and so on up to $dE_Nd\Omega_N$ around E_N,Ω_N. These functions are normalised as per the definition in our paper on forward stochastic transport theory [3]:

$$P_0+\int P_1(E_1,\Omega_1;E_0,\Omega_0)dE_1d\Omega_1+\frac{1}{2!}\int P_2(E_1,\Omega_1,E_2,\Omega_2;E_0,\Omega_0)dE_1d\Omega_1dE_2d\Omega_2 \\ +\frac{1}{3!}\int P_3(E_1,\Omega_1,E_2,\Omega_2,E_3,\Omega_3,;E_0,\Omega_0)dE_1d\Omega_1dE_2d\Omega_2dE_3d\Omega_3+.....=1 \quad (1)$$

The first and second order densities, and the probability generating functional (pgfl) are defined as follows:

$$f_1(E_1,\Omega_1;E_0,\Omega_0)=\sum_{N=1}^{\infty}\frac{1}{(N-1)!}\int P_N(E_1,\Omega_1,E_2,\Omega_2,...E_N,\Omega_N;E_0,\Omega_0)dE_2d\Omega_2....dE_Nd\Omega_N \quad (2)$$

$$\begin{aligned} &f_2(E_1,\Omega_1,E_2,\Omega_2;E_0,\Omega_0)\\ &=\sum_{N=2}^{\infty}\frac{1}{(N-2)!}\int P_N(E_1,\Omega_1,E_2,\Omega_2,...E_N,\Omega_N;E_0,\Omega_0)dE_3d\Omega_3....dE_Nd\Omega_N \end{aligned} \quad (3)$$

$$L([u];E_0,\Omega_0)=P_0+\sum_{N=1}^{\infty}\frac{1}{N!}\int P_N(E_1,\Omega_1,E_2,\Omega_2,...E_N,\Omega_N;E_0,\Omega_0)u(E_1,\Omega_1)....u(E_N,\Omega_N)dE_1d\Omega_1....dE_Nd\Omega_N \quad (4)$$

The successive functional derivatives $\frac{\delta L}{\delta u(E_1,\Omega_1)},\frac{\delta^2 L}{\delta u(E_1,\Omega_1)\delta u(E_2,\Omega_2)}$ evaluated at $u=1$ give us the first and second order densities defined above. We note that the densities $f_1(E_1,\Omega_1;E_0,\Omega_0)$ and $f_2(E_1,\Omega_1,E_2,\Omega_2;E_0,\Omega_0)$ are defined such that $f_1(E_1,\Omega_1;E_0,\Omega_0)dE_1d\Omega_1$ and $f_2(E_1,\Omega_1,E_2,\Omega_2;E_0,\Omega_0)dE_1d\Omega_1dE_2d\Omega_2$ are the probabilities of getting respectively a neutron in the interval $dE_1d\Omega_1$ and of getting a neutron each in the intervals $dE_1d\Omega_1$ and $dE_2d\Omega_2$. However they are not probability distributions in the sense that integration over the variables E_1,Ω_1 or E_1,Ω_1 and E_2,Ω_2 does not give us unity, rather the expected number of neutrons emerging or the number of neutron pairs emerging. The singlet density $f_1(E_1,\Omega_1;E_0,\Omega_0)$ is not the angular flux emerging from the slab but can be related to the angular flux as follows: If instead of a single neutron incident on the slab, we have an incident angular flux $\delta(\Omega_0,E_0)$, then this means there is an incident current μ_0 where μ_0 is the component of Ω_0 normal to the slab. Hence the emerging angular flux will be given by $(\mu_0/\mu_1)f_1(E_1,\Omega_1;E_0,\Omega_0)$.

As an aside, we note that the forward stochastic transport theory formalism discussed in Ref. [3] based on the functions P_N, used in this paper, has considerable resemblance to derivations of the Boltzman equation via the BBKGY method in the kinetic theory of gases. However there are important differences. Apart from the fact that in the present formalism, there is a variable number of particles in the system due to various reactions and also due to movement in and out of the system volume, there is a difference in the way collisions are treated. They are treated probabilistically through phenomenological interaction cross sections rather than through the dynamics as in classical kinetic theory. Thus the starting point is a master equation for P_N rather than the Liouville equation. Secondly, since the particles collide only with the atoms of a medium in a given state but not with one another, the resulting master equation represents a linear process. As such instead of the BBKGY hierarchy of coupled equations for the densities,

which can be closed, say for the singlet density by assumptions such as molecular chaos, we obtain exact closed equations for densities of each order. The equation for the first order densities is the usual transport equation and is an exact consequence of the master equation for P_N.

The other function we need is the distribution function of the number of neutrons produced in a collision with the medium. This could be due to any reaction with the medium and the resulting function is a combination of the functions for each of these reactions weighted with the respective reaction probabilities. We call this function $\sigma_\nu(E_0,\Omega_0 \to E_1,\Omega_1,E_2,\Omega_2,...E_\nu,\Omega_\nu)$. The quantity $\sigma_\nu(E_0,\Omega_0 \to E_1,\Omega_1,E_2,\Omega_2,...E_\nu,\Omega_\nu)dE_1d\Omega_1....dE_\nu d\Omega_\nu$ represents the probability that ν neutrons are produced in a collision of a neutron having energy and direction variables (E_0,Ω_0) of which the first is in $dE_1d\Omega_1$ around E_1,Ω_1, the second is in $dE_2d\Omega_2$ around E_2,Ω_2 and so on. Associated with this there are the first and higher order densities defined below.

$$\rho_1(E_1,\Omega_1;E_0,\Omega_0)=\sum_{\nu=1}^{\infty}\nu\int\sigma_\nu(E_0,\Omega_0 \to E_1,\Omega_1,E_2,\Omega_2,...E_\nu,\Omega_\nu)dE_2d\Omega_2....dE_\nu d\Omega_\nu \qquad (5)$$

$$\rho_2(E_1,\Omega_1,E_2,\Omega_2;E_0,\Omega_0)=\sum_{\nu=2}^{\infty}\nu(\nu-1)\int\sigma_\nu(E_0,\Omega_0 \to E_1,\Omega_1,E_2,\Omega_2,...E_\nu,\Omega_\nu)dE_3d\Omega_3....dE_\nu d\Omega_\nu \quad (6)$$

For the invariant embedding formalism, we shall need a more general set of functions for the fission distribution which will be denoted as $\sigma_{\nu\mu}(E_0,\Omega_0 \to E_1,\Omega_1,E_2,\Omega_2,...E_\nu,\Omega_\nu;E_1',\Omega_1',E_2',\Omega_2',...E_\mu',\Omega_\mu')$. The difference between the un-primed and primed variables is that while the former refer to particles having outgoing directions, the latter refer to incoming directions with respect to the infinite medium vacuum interface. The generating functional of these functions is defined as follows:

$$L([u],[v];E_0,\Omega_0)=\sigma_{00}+\sum_{\nu,\mu=1}^{\infty}\int\sigma_{\nu\mu}(E_0,\Omega_0 \to E_1,\Omega_1,E_2,\Omega_2,...E_\nu,\Omega_\nu;E_1',\Omega_1',E_2',\Omega_2',...E_\mu',\Omega_\mu') \quad (7)$$
$$u(E_1,\Omega_1)....u(E_\nu,\Omega_\nu)\mathrm{v}(E_1',\Omega_1')....\mathrm{v}(E_\nu',\Omega_\nu')dE_1d\Omega_1....dE_\nu d\Omega_\nu dE_1'd\Omega_1'....dE_\mu'd\Omega_\mu'$$

Now we are in a position to derive the equation for the probabilities $P_N(E_1,\Omega_1,E_2,\Omega_2,...E_N,\Omega_N;E_0,\Omega_0)$ or rather, $P_N(E_1,\mu_1,E_2,\mu_2,...E_N,\mu_N;E_0,\mu_0)$ since the normal component is the only relevant direction variable in this problem. Using the same arguments as before and omitting the indices from the function s_{nm}, we write down the following equation

$$
\begin{aligned}
&P_N(E_1,\mu_1,E_2,\mu_2,...E_N,\mu_N;E_0,\mu_0)\\
&=\left(1-\frac{\Sigma(E_0)dz}{\mu_0}\right)\left(1-\frac{\Sigma(E_1)dz}{|\mu_1|}\right)\left(1-\frac{\Sigma(E_2)dz}{|\mu_2|}\right).....\left(1-\frac{\Sigma(E_N)dz}{|\mu_N|}\right)P_N(E_1,\mu_1,E_2,\mu_2,...E_N,\mu_N;E_0,\mu_0)\\
&+\frac{\Sigma(E_0)dz}{\mu_0}\sum_{comb\{N,n_1,...n_\mu,\nu\}}\sum_{\nu,\mu}\sum_{\nu+n_1+...+n_\mu}\int\sigma(E_0,\mu_0\longrightarrow E_1,\mu_1,E_2,\mu_2,...E_\nu,\mu_\nu;E_1',\mu_1',E_2',\mu_2',...E_\mu',\mu_\mu')\\
&\times P_{n_1}(E_{\nu+1},\mu_{\nu+1},...E_{\nu+n_1},\mu_{\nu+n_1};E_1',\mu_1')P_{n_2}(E_{\nu+n_1+1},\mu_{\nu+n_1+1},...E_{\nu+n_1+n_2},\mu_{\nu+n_1+n_2};E_2',\mu_2')....\\
&P_{n_\mu}(E_{\nu+n_1+...+n_{\mu-1}+1},\mu_{\nu+n_1+...+n_{\mu-1}+1},...E_{\nu+n_1+...+n_\mu},\mu_{\nu+n_1+...+n_\mu};E_\mu',\mu_\mu')dE_1'd\mu_1'...dE_\mu'd\mu_\mu'\\
&+\sum_{comb\{N,n_1,...n_\mu,\nu,m\}}\sum_{\nu,\mu}\sum_{\nu+n_1+...+n_\mu}\int\frac{\Sigma(E)dz}{\mu}P_{m+1}(E_1,\mu_1,....,E_m,\mu_m,E,\mu;E_0,\mu_0)\\
&\text{x}\sigma(E,\mu\longrightarrow E_{m+1},\mu_{m+1},...,E_{m+\nu},\mu_{m+\nu};E_1',\mu_1',...,E_\mu',\mu_\mu')P_{n_1}(E_{m+\nu+1},\mu_{m+\nu+1},...E_{m+\nu+n_1},\mu_{m+\nu+n_1};E_1',\mu')\\
&\text{x}P_{n_2}(E_{m+\nu+n_1+1},\mu_{m+\nu+n_1+1},...E_{m+\nu+n_1+n_2},\mu_{m+\nu+n_1};E_2',\mu').....\\
&\text{x}P_{n_\mu}(E_{m+\nu+n_1+...+n_{\mu-1}+1},\mu_{m+\nu+n_1+...+n_{\mu-1}+1},...E_{m+\nu+n_1+...+n_\mu},\mu_{m+\nu+n_1+...+n_\mu};E_\mu',\mu_\mu')dEd\mu dE_1'd\mu_1'...dE_\mu'd\mu_\mu'
\end{aligned}
\tag{8}
$$

The summation over all combinations of the N sets of coordinates for the outgoing particles into the groups is indicated. Expanding out the product in the first term on the RHS of the above equation and retaining terms to the lowest order in dz, we get

$$
\begin{aligned}
&\left(\frac{\Sigma_0}{\mu_0}+\frac{\Sigma_1}{\mu_1}+\frac{\Sigma_2}{\mu_2}+...+\frac{\Sigma_N}{\mu_N}\right)P_N(E_1,\mu_1,E_2,\mu_2,...E_N,\mu_N;E_0,\mu_0)\\
&=\frac{\Sigma(E_0)}{\mu_0}\sum_{comb\{N,n_1,...n_\mu,\nu\}}\sum_{\nu,\mu}\sum_{\nu+n_1+...+n_\mu}\int\sigma(E_0,\mu_0\longrightarrow E_1,\mu_1,E_2,\mu_2,...E_\nu,\mu_\nu;E_1',\mu_1',E_2',\mu_2',...E_\mu',\mu_\mu')\\
&\times P_{n_1}(E_{\nu+1},\mu_{\nu+1},...E_{\nu+n_1},\mu_{\nu+n_1};E_1',\mu_1')P_{n_2}(E_{\nu+n_1+1},\mu_{\nu+n_1+1},...E_{\nu+n_1+n_2},\mu_{\nu+n_1+n_2};E_2',\mu_2')....\\
&P_{n_\mu}(E_{\nu+n_1+...+n_{\mu-1}+1},\mu_{\nu+n_1+...+n_{\mu-1}+1},...E_{\nu+n_1+...+n_\mu},\mu_{\nu+n_1+...+n_\mu};E_\mu',\mu_\mu')dE_1'd\mu_1'...dE_\mu'd\mu_\mu'\\
&+\sum_{comb\{N,n_1,...n_\mu,\nu,m\}}\sum_{\nu,\mu}\sum_{\nu+n_1+...+n_\mu}\int\frac{\Sigma(E)}{\mu}P_{m+1}(E_1,\mu_1,....,E_m,\mu_m,E,\mu;E_0,\mu_0)\\
&\sigma(E,\mu\longrightarrow E_{m+1},\mu_{m+1},...,E_{m+\nu},\mu_{m+\nu};E_1',\mu_1',...,E_\mu',\mu_\mu')P_{n_1}(E_{m+\nu+1},\mu_{m+\nu+1},...E_{m+\nu+n_1},\mu_{m+\nu+n_1};E_1',\mu')\\
&\text{x}P_{n_2}(E_{m+\nu+n_1+1},\mu_{m+\nu+n_1+1},...E_{m+\nu+n_1+n_2},\mu_{m+\nu+n_1};E_2',\mu').....\\
&\text{x}P_{n_\mu}(E_{m+\nu+n_1+...+n_{\mu-1}+1},\mu_{m+\nu+n_1+...+n_{\mu-1}+1},...E_{m+\nu+n_1+...+n_\mu},\mu_{m+\nu+n_1+...+n_\mu};E_\mu',\mu_\mu')dEd\mu dE_1'd\mu_1'...dE_\mu'd\mu_\mu'
\end{aligned}
\tag{9}
$$

We perform the operation implied on the RHS of Eq. (4) to obtain the equation for the probability generating functional. The resulting equation is quite simply obtained but one or two points need be mentioned. The sum over all combinations after integration over the variables $E_1,\mu_1,.....E_N,\mu_N$ yields $\frac{N!}{n_1!.....n_\mu!}$ terms in the first sum and $\frac{N!}{n_1!.....n_\mu!m!}$ terms in the second sum. The final result is

$$\frac{\Sigma_0}{\mu_0}L([u];E_0,\mu_0)+\int\frac{\Sigma(E)}{\mu}u(E,\mu)\frac{\delta L([u];E_0,\mu_0)}{\delta u(E,\mu)}dEd\mu=\frac{\Sigma_0}{\mu_0}L_\sigma([u],[L([u];E',\mu')];E_0,\mu_0)$$
$$+\int\frac{\Sigma(E)}{\mu}\frac{\delta L([u];E_0,\mu_0)}{\delta u(E,\mu)}L_\sigma([u],[L([u];E',\mu')];E,\mu)dEd\mu \quad (10)$$

This equation can be used to derive equations for densities of any order by carrying out functional differentiation. The equations for the singlet and doublet densities read as follows

$$\left(\frac{\Sigma(E_0)}{\mu_0}+\frac{\Sigma(E_1)}{|\mu_1|}\right)f_1(E_1,\mu_1;E_0,\mu_0)=\frac{\Sigma_0}{\mu_0}\rho_1(E_1,\mu_1;E_0,\mu_0)$$
$$+\frac{\Sigma_0}{\mu_0}\int\rho_1(E',\mu';E_0,\mu_0)f_1(E_1,\mu_1;E',\mu')dE'd\mu'+\int\frac{\Sigma_f(E)}{|\mu|}f_1(E,\mu;E_0,\mu_0)\rho_1(E_1,\mu_1;E,\mu)dEd\mu \quad (11)$$
$$+\int\frac{\Sigma_f(E)}{|\mu|}f_1(E,\mu;E_0,\mu_0)\rho_1(E',\mu';E,\mu)f_1(E_1,\mu_1;E',\mu')dE'd\mu'dEd\mu$$

$$\left(\frac{\Sigma(E_0)}{\mu_0}+\frac{\Sigma(E_1)}{|\mu_1|}+\frac{\Sigma(E_2)}{|\mu_2|}\right)f_2(E_1,\mu_1,E_2,\mu_2;E_0,\mu_0)=\frac{\Sigma(E_0)}{\mu_0}\rho_2(E_1,\mu_1,E_2,\mu_2;E_0,\mu_0)$$
$$+\frac{\Sigma(E_0)}{\mu_0}\int\rho_2(E_1',\mu_1',E_2',\mu_2';E_0,\mu_0)f_1(E_1,\mu_1;E_1',\mu_1')f_1(E_2,\mu_2;E_2',\mu_2')dE_1'd\mu_1'dE_2'd\mu_2'$$
$$+\frac{\Sigma(E_0)}{\mu_0}\int\rho_2(E_1,\mu_1,E',\mu';E_0,\mu_0)f_1(E_2,\mu_2;E',\mu')dE'd\mu'$$
$$+\frac{\Sigma(E_0)}{\mu_0}\int\rho_2(E_2,\mu_2,E',\mu';E_0,\mu_0)f_1(E_1,\mu_1;E',\mu')dE'd\mu'$$
$$+\frac{\Sigma(E_0)}{\mu_0}\int\rho_1(E',\mu';E_0,\mu_0)f_2(E_1,\mu_1,E_2,\mu_2;E',\mu')dE'd\mu'$$
$$+\int\frac{\Sigma(E)}{\mu}f_1(E,\mu;E_0,\mu_0)\left[\begin{array}{l}\rho_2(E_1,\mu_1,E_2,\mu_2;E,\mu)\\+\int\rho_2(E_1',\mu_1',E_2',\mu_2';E,\mu)f_1(E_1,\mu_1;E_1',\mu_1')f_1(E_2,\mu_2;E_2',\mu_2')dE_1'd\mu_1'dE_2'd\mu_2'\end{array}\right]dEd\mu$$
$$+\int\frac{\Sigma(E)}{\mu}f_1(E,\mu;E_0,\mu_0)\left[\begin{array}{l}\int\rho_2(E_1,\mu_1,E',\mu';E,\mu)f_1(E_2,\mu_2;E',\mu')dE'd\mu'+\\\int\rho_2(E_2,\mu_2,E',\mu';E,\mu)f_1(E_1,\mu_1;E',\mu')dE'd\mu'+\\\int\rho_1(E_1',\mu';E',\mu')f_2(E_1,\mu_1,E_2,\mu_2;E_1',\mu_1')dE_1'd\mu_1'\end{array}\right]dEd\mu$$
$$+\int\frac{\Sigma(E)}{\mu}f_2(E_1,\mu_1,E,\mu;E_0,\mu_0)\left[\rho_1(E_2,\mu_2;E,\mu)+\int\rho_1(E',\mu';E,\mu)f_1(E_2,\mu_2;E',\mu')dE'd\mu'\right]dEd\mu$$
$$\int\frac{\Sigma(E)}{\mu}f_2(E,\mu,E_2,\mu_2;E_0,\mu_0)\left[\rho_1(E_1,\mu_1;E,\mu)+\int\rho_1(E',\mu';E,\mu)f_1(E_1,\mu_1;E',\mu')dE'd\mu'\right]dEd\mu$$

(12)

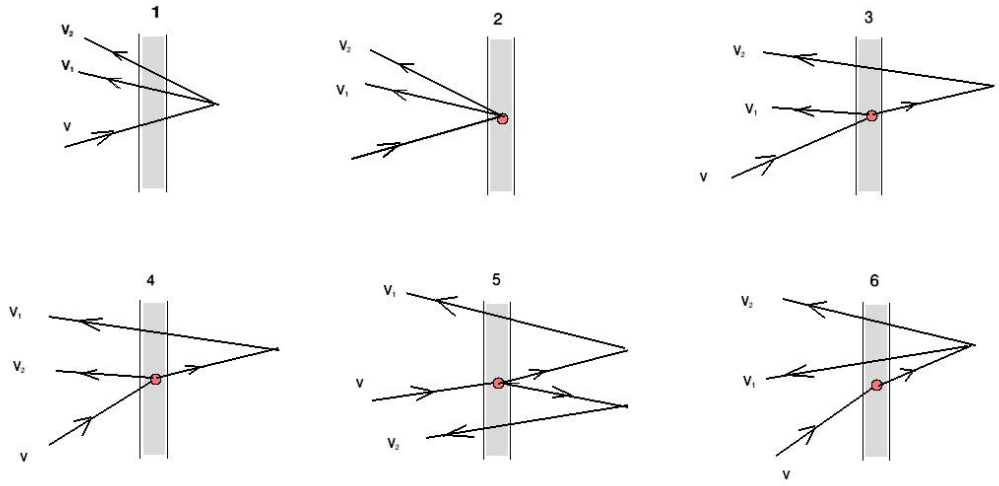

Figure 1. The first few terms in the possibilities for backscattering with branching.

The first four terms correspond to the production of doublets in a collision of the incoming neutron in the first infinitesimal layer of the medium with:

- both going out in the required coordinate intervals;
- both going in followed by each producing a singlet in the required coordinate intervals;
- one going out in the required coordinate interval and the other going in followed by production of a singlet in the required coordinate intervals; there are two such terms.

The fifth term corresponds to production of a singlet going in followed by a doublet going out in the required coordinate intervals. The first five terms are graphically illustrated on Figs 1a – 1e.

The next five terms refer to the possibility of no collision of the incoming neutron in the outer infinitesimal layer but the return of a singlet which collides in the outer infinitesimal layer, and the last four terms correspond to the return of a doublet, one of which collides in the outer infinitesimal layer.

Two interesting observation regarding Eqs. (11) and (12) are worth mentioning. The first is that the equations for each order of densities are closed, like in Ref. [3], but unlike the BBKGY hierarchy in the kinetic theory. The second is that while the equation for the singlet density [Eq.(11)] is non-linear, the one for the doublet density [Eq. (12)] is linear in the doublet density variable. Eq. (12) can be solved numerically with a similar collision number expansion as is usual for the first moment equation [4]. This procedure will be illustrated in the paper for a simple forward-backward scattering model.

3. FINITE SLABS AND SPHERES

Invariant embedding theory to yield the reflected flux (or singlet density) from finite slabs and spheres has been discussed by Bellman et al (1960) We have shown [5] that it is possible to extend our theory to derive equations for the probability generating functional and higher order densities. For finite slabs these equations can be solved by the usual discrete ordinates (DS_n) method. For one velocity transport problems the discretisation in the angle variable gives a system of $n^2/4$ ordinary differential equations with the thickness (z) of the slab as the independent variable. The problem is an initial value problem with the reflected densities being zero for $z=0$ and should be easily solvable with an ODE solver. The advantage of the method over conventional transport theory methods is that that the quantity of interest is obtainable as a function of the slab thickness in a single run. For the case of $n=2$, there is a single equation for densities of any order. The first of these is quadratically nonlinear but the rest are linear. Analytical solutions to these equations for the singlet and doublet densities are possible and we write these down below. In the S_2 approximation, there are two directions viz., $\mu = \pm 0.57735$ with $w=1$ for both. The equation for the singlet density becomes

$$\frac{2|\mu|}{c}\frac{df_1}{dz} = f_1^2 + (2-4/c)f_1 + 1 \tag{13}$$

where c is the mean number of secondaries. The solutions for $c<1$ and $c>1$ are respectively

$$f_1 + 1 - \frac{2}{c} = \frac{2\sqrt{1-c}}{c}\tanh\left(\frac{cz}{2|\mu|} + \tanh^{-1}\left(\frac{1-2/c}{2\sqrt{1-c}}\right)\right) \tag{14}$$

$$f_1 + 1 - \frac{2}{c} = \frac{2\sqrt{c-1}}{c}\tan\left(\frac{cz}{2|\mu|} + \tan^{-1}\left(\frac{1-2/c}{2\sqrt{c-1}}\right)\right) \tag{15}$$

Eq. (15) can be used to estimate the critical thickness since the reflected density is expected to go to infinity as criticality is approached. The equation for the doublet density is

$$\frac{2|\mu|}{c}\frac{df_2}{dz} - 3\left(f_1 + 1 - \frac{2}{c}\right)f_2 = \frac{\overline{c(c-1)}}{2c}(1+f_1)^3 \tag{16}$$

where $\overline{c(c-1)}$ is the second factorial moment of the number of secondaries. This is a linear differential equation and the solution can be reduced to quadrature by substituting the expressions for f_1. For $c>1$ we have

$$f_2 = \frac{\overline{c(c-1)}}{c^2\cos^{3a}(cz/2|\mu| + \beta)}\int_0^{cz/2|\mu|}(1+\sqrt{c-1}\tan(\xi+\beta))^3\cos^{3a}(\xi+\beta)d\xi \tag{17}$$

where $a = 2\sqrt{c-1}/c$ and $\beta = \tan^{-1}\left(\frac{1-2/c}{2\sqrt{c-1}}\right)$. We can obtain a similar expression for $c<1$ with the hyperbolic tangent and cosine functions. While an analytical expression can be written down, we do not display the result as it is rather complicated. A numerical evaluation of the integral is however fairly straightforward.

Energy dependent problems involving slowing down can be handled similarly by the usual multi-group method as a sequence of one velocity problems. The general energy dependent problem, is however expected to be much more involved. A similar treatment of the problem in spherical geometry should be possible in principle though practical details would require more careful consideration. This more or less exhausts the practical utility of the method and extension to multi-dimensional problems does not seem to be practical.

4. ATOMIC SPUTTERING MODEL

So far we have considered applications to neutron transport. There are other areas where transport theory and consequently invariant embedding theory are applicable, some of which were mentioned in the introduction. One of these is atomic sputtering and has been studied fairly extensively [6,7]. In this section we consider a simple model of atomic sputtering studied in Ref. [8]. The model is essentially a forward-backward scattering model with the difference that instead of fission based multiplication of particles, we have multiplication of a cascade due to displacements of atoms from their sites by an incoming energetic particle. The displaced particles acquire energy to continue the cascade in addition to the incoming particle. Some of the particles are emitted from the surface and the number of particles, the energy distribution and variance of the number of particles are quantities of interest. The model is described by the following single scattering function σ_2, all others being zero

$$\sigma_2(x_0 \to x_1, x_2) = \frac{\delta(E_0 - E_1 - E_2)}{4E_0}\left[\delta(\mu_0 - \mu_1) + \delta(\mu_0 + \mu_1)\right]\left[\delta(\mu_0 - \mu_2) + \delta(\mu_0 + \mu_2)\right] \quad (18)$$

The atomic displacement energy is assumed to be the same as the surface barrier energy and hence there is no loss of energy in the collisions, only during escape, which can be treated by cutting off escaping particles having energies lower than the surface barrier. The first delta function ensures overall energy conservation while the others imply equal probabilities for production of the two particles, the projectile (subscript 1) and the recoil (subscript 2), respectively, in forward and backward directions. While the total collision cross section is assumed to be independent of energy, energy dependent treatment is required due to the requirement of quantities of interest mentioned above.

We suppose that the incident particle has $\mu = 1$ and the emitted particles have $\mu = -1$. For this reason, as well as due to the fact that the solution of the singlet density equation is analytically obtainable in the lethargy variable, we transform both our equations to lethargy variables $u = \ln\frac{E_0}{E}$. Though the doublet density equation is not solvable analytically, we find that

numerically it is closed on a rectangular grid in lethargy. Moreover the variation of the densities with lethargy is smoother. In the energy variable, most of the density is concentrated around E=0. We note that in terms of the lethargy variable Eq. (18) becomes

$$\sigma_2(x \to x_1, x_2) = \frac{\delta(E_0(\mathrm{e}^{-u} - \mathrm{e}^{-u_1} - \mathrm{e}^{-u_2})}{4E_0\mathrm{e}^{-u}} E_0^2 \mathrm{e}^{-u_1}\mathrm{e}^{-u_2} \left[\delta(\mu_0 - \mu_1) + \delta(\mu_0 + \mu_1)\right]\left[\delta(\mu_0 - \mu_2) + \delta(\mu_0 + \mu_2)\right] \quad (19)$$

The corresponding ρ functions are given by

$$\rho_1(u_1)du_1 = \mathrm{e}^{(u-u_1)}du_1 \quad (20)$$

$$\rho_2(u_1,u_2)du_1du_2 = \frac{\delta(E_0(\mathrm{e}^{-u} - \mathrm{e}^{-u_1} - \mathrm{e}^{-u_2})}{2E_0\mathrm{e}^{-u}} E_0^2 \mathrm{e}^{-u_1}\mathrm{e}^{-u_2} du_1du_2 \quad (21)$$

Substituting these equations in Eqs. (11) and (12), we obtain the following equations for the first and second order densities:

$$\begin{aligned} 2f_1(u_1;0) &= \exp(-u_1) + \int_0^{u_1} \exp(-u) f_1(u_1;u)du + \int_0^{u_1} \exp(u-u_1) f_1(u;0)du \\ &+ \int_0^{u_1} f_1(u_1;u')du' \int_0^{u'} \exp(u-u') f_1(u;0)du \end{aligned} \quad (22)$$

$$\begin{aligned} 3f_2(u_1,u_2;0) &= \frac{\delta[1-\mathrm{e}^{-u_1}-\mathrm{e}^{-u_2}]}{2}\mathrm{e}^{-u_1}\,\mathrm{e}^{-u_2} + \frac{1}{2}\mathrm{e}^{-u_1} f_1(u_2;-\ln(1-\mathrm{e}^{-u_1})) + \frac{1}{2}\mathrm{e}^{-u_2}\, f_1(u_1;-\ln(1-\mathrm{e}^{-u_2})) \\ &+ \frac{\mathrm{e}^{-u}\,\mathrm{e}^{-u_2}\, f_1(-\ln(\mathrm{e}^{-u_1}+\mathrm{e}^{-u_2});0)}{2(\mathrm{e}^{-u_1}+\mathrm{e}^{-u_2})^2} + \int_{-\ln(1-\mathrm{e}^{-u_2})}^{u_1} \mathrm{e}^{-u_1} f_1(u_1;u) f_1(u_2;-\ln(1-\mathrm{e}^{-u}))du \\ &+ \int_{-\ln(1-\mathrm{e}^{-u_1})}^{u_2} \frac{f_1(-\ln(\mathrm{e}^{-u_1}+\mathrm{e}^{-u});0) f_1(u_2;u)\mathrm{e}^{-u_1}\,\mathrm{e}^{-u}\,du}{2(\mathrm{e}^{-u_1}+\mathrm{e}^{-u})^2} + \int_{-\ln(1-\mathrm{e}^{-u_2})}^{u_1} \frac{f_1(-\ln(\mathrm{e}^{-u_2}+\mathrm{e}^{-u});0) f_1(u_1;u)\mathrm{e}^{-u_2}\,\mathrm{e}^{-u}\,du}{2(\mathrm{e}^{-u_2}+\mathrm{e}^{-u})^2} \\ &+ \int_{-\ln(1-\mathrm{e}^{-u_1})}^{u_2} \int_{-\ln(1-\mathrm{e}^{-u_2'})}^{u_1} \frac{f_1(-\ln(\mathrm{e}^{-u_1'}+\mathrm{e}^{-u_2'});0) f_1(u_1;u_1') f_1(u_2;u_2')\mathrm{e}^{-u_1'}\,\mathrm{e}^{-u_2'}\,du_1'du_2'}{2(\mathrm{e}^{-u_1'}+\mathrm{e}^{-u_2'})^2} \\ &+ \int_0^{-\ln(\mathrm{e}^{-u_1}+\mathrm{e}^{-u_2})} \mathrm{e}^{-u}\, f_2(u_1,u_2;u)du + \int_{-\ln(1-\mathrm{e}^{-u_2})}^{u_1} \mathrm{e}^{u-u_1}\, f_2(u,u_2;0)du + \int_{-\ln(1-\mathrm{e}^{-u_1})}^{u_2} \mathrm{e}^{u-u_2}\, f_2(u_1,u;0)du \\ &\int_0^{-\ln(\mathrm{e}^{-u_1}+\mathrm{e}^{-u_2})} du\,\mathrm{e}^{-u}\, f_2(u_1,u_2;u) \int_0^{u} \mathrm{e}^{u'}\, f_1(u';0)du' + \int_{-\ln(1-\mathrm{e}^{-u_2})}^{u_1} du\,\mathrm{e}^{u}\, f_2(u,u_2;0) \int_u^{u_1} \mathrm{e}^{-u'}\, f_1(u_1;u')du' \\ &+ \int_{-\ln(1-\mathrm{e}^{-u_1})}^{u_2} du\,\mathrm{e}^{u}\, f_2(u_1,u;0) \int_u^{u_2} \mathrm{e}^{-u'}\, f_1(u_2;u')du' \end{aligned} \quad (23)$$

The equation for the singlet density can be solved analytically. Writing $f_1(u_1;0) = \exp(-u_1)g(u_1)$, we get

$$2g(u_1) = 1 + 2\int_0^{u_1} g(u)du + \int_0^{u_1} g(u')du' \int_0^{u_1-u'} g(u)du \tag{24}$$

Differentiating w.r.t. u_1 we get

$$2g'(u_1) = 2g(u_1) + \int_0^{u_1} g(u')g(u_1-u')du' \tag{25}$$

Laplace transformation yields us the following quadratic equation if we remember that $g(0) = 1/2$:

$$\bar{g}^2(s) - 2(s-1)\bar{g}(s) + 1 = 0 \tag{26}$$

The solution is

$$\bar{g}(s) = (s-1) \pm \sqrt{(s-1)^2 - 1} \tag{27}$$

The solution with the negative sign for the square root is a proper Laplace transform for which the inverse can be written down with a little algebra and Laplace transform tables to finally yield

$$g(u) = \frac{\exp(u_1)I_1(u_1)}{u_1} \tag{28}$$

Hence the solution for the singlet density can be written down as

$$f_1(u_1;0) = \frac{I_1(u_1)}{u_1} \tag{29}$$

4.1. Numerical solution of the doublet density equation

The doublet density equation is not amenable to analytical solution. In what follows, we sketch a method for numerical solution. On making the substitution

$$\varphi_2(u_1,u_2;0) = 3f_2(u_1,u_2;0) - \frac{\delta[1-e^{-u_1}-e^{-u_2}]}{2}e^{-u_1}e^{-u_2} \tag{30}$$

for eliminating the delta function, and carrying out the simpler integrations, we get the final form of the integral equation for the doublet density as

$$\varphi_2(u_1,u_2) = S(u_1,u_2) + \int_0^{-\ln(e^{-u_1}+e^{-u_2})} \frac{1}{3}\varphi_2(u_1-u,u_2-u)\big(I_0(u)-I_1(u)\big)du$$
$$+ \int_0^{u_1+\ln(1-e^{-u_2})} \frac{1}{3}\varphi_2(u_1-u,u_2)\big(I_0(u)-I_1(u)\big)du + \int_0^{u_2+\ln(1-e^{-u_1})} \frac{1}{3}\varphi_2(u_1,u_2-u)\big(I_0(u)-I_1(u)\big)du, \quad (31)$$

where $S(u_1,u_2)$ is a source term, composed of singlet density functions as

$$S(u_1,u_2) = \frac{e^{-(u_1+u_2)}}{6(e^{-u_1}+e^{-u_2})^2}\Big(I_0[-\ln(e^{-u_1}+e^{-u_2})] - I_1[-\ln(e^{-u_1}+e^{-u_2})] + 3f_1(-\ln(e^{-u_1}+e^{-u_2});0)\Big)$$
$$+ \frac{e^{-u_1}}{6}\Big(I_0[u_2+\ln(1-e^{-u_1})]\Big) - \Big(I_0[u_2+\ln(1-e^{-u_1})] + 3f_1(u_2+\ln(1-e^{-u_1});0)\Big)$$
$$+ \frac{e^{-u_2}}{6}\Big(I_0[u_1+\ln(1-e^{-u_2})]\Big) - \Big(I_0[u_1+\ln(1-e^{-u_2})] + 3f_1(u_1+\ln(1-e^{-u_2});0)\Big)$$
$$+ \int_{-\ln(1-e^{-u_2})}^{u_1} e^{-u} f_1(u_1-u;0) f_1(u_2+\ln(1-e^{-u});0)du$$
$$+ \int_0^{-\ln(e^{-u_1}+e^{-u_2})} \Big(f_1(u_2+\ln(e^{-u}-e^{-u_1});0)e^{-u_1} + f_1(u_1+\ln(e^{-u}-e^{-u_2});0)e^{-u_2}\Big) f_1(u;0)e^{u}du$$
$$+ \int_0^{-\ln(e^{-u_1}+e^{-u_2})} f_1(u;0)e^{u}du \int_{-\ln(e^{-u}-e^{-u_1})}^{u_2} f_1(u_2-u';0) f_1(u_1+\ln(e^{-u}-e^{-u'});0)e^{-u'}du' \quad (32)$$

for $\exp(-u_1)+\exp(-u_2)<1$, and zero otherwise.

Now $f_1(u)$ is already known and $f_2(u_1,u_2)$ was calculated by a numerical solution of Eq.(31). As already mentioned earlier the equation is closed in two variables if we introduce a rectangular mesh grid in the lethargy variable. This is illustrated in Fig. 2. The integrals in this equation were replaced by a trapezoidal integration formula and the various source terms were evaluated by calculation of the functions involved or by single or double numerical quadrature. The resulting system of linear equations was solved by a simple iteration strategy in which the first guess is the sum of all the source terms.

As an application of the method, the ratio of the variance to the mean of the yield of sputtered particles was calculated as a function of lethargy. This quantity is related to the first and second factorial moments of the distribution of the number of emitted particles. These can be calculated by a quadrature of the one- and two-point distributions as follows.

$$M_1 = \int_0^{U_d} f_1(u)du \quad (33)$$

$$M_2 = \int_0^{U_d}\int_0^{U_d} f_2(u_1,u_2)du_1du_2 \quad (34)$$

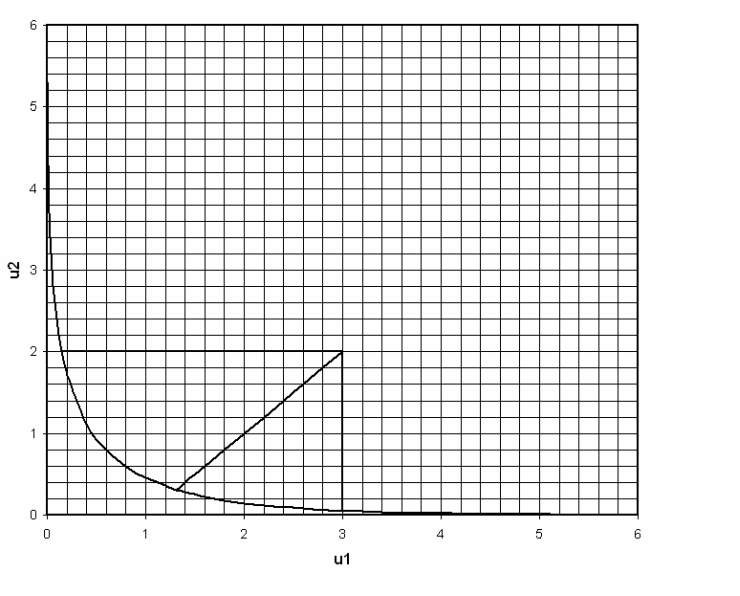

Figure 2. The rectangular grid used for solving Eq. (31) in the lethargy variables u_1 and u_2. The curve represents the equation exp(-u1)+exp(-u2)=1. The three straight lines represent the lines on which the three integrals in Eq. (31) are evaluated by trapezoidal rule for calculating $\varphi_2(u_1,u_2)$ on the point (3,2). By closure we mean that the lines lie along the grid points on which we are calculating $\varphi_2(u_1,u_2)$. Below and on the curve $\varphi_2(u_1,u_2)$ is zero.

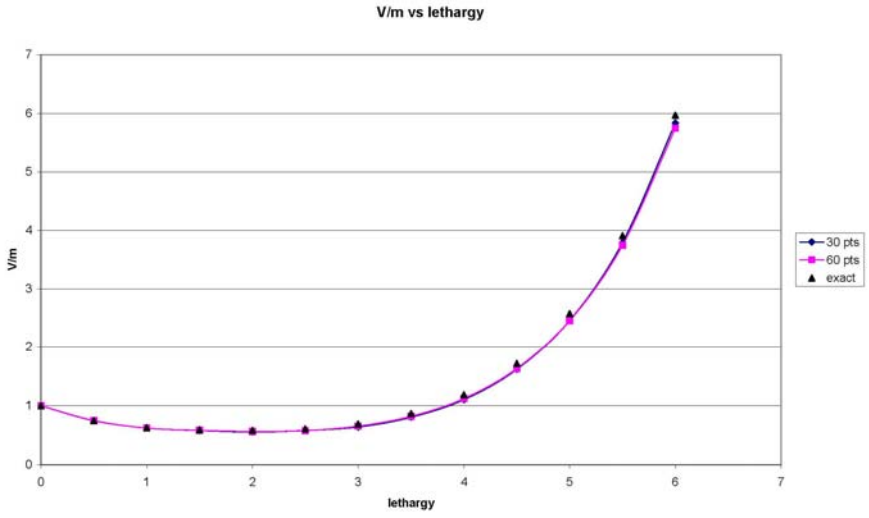

Figure 3. The dependence of the variance to mean on the lethargy in the simple one-dimensional scattering model, by invariant embedding and transport theory methods.

where M_1 and M_2 are the first and second factorial moments, respectively, and $U_d = \log E_0 / E_d$ is the maximum lethargy at which a particle having initial energy E_0 can cause a sputtered particle to be ejected.

Fig. 3 shows the results of the invariant embedding for the dependence of the variance to mean as a function of lethargy. Also shown alongside these are (by points marked as "exact") the variance to mean values calculated by [8] using transport theory and verified with Monte-Carlo results. As is seen, there is a generally good agreement between the invariant embedding and the transport calculations, but slight deviations are also visible, especially for high lethargy values. The exact reason for this slight discrepancy is not fully clear, but presumably it is a result of the inaccuracy of the numerical scheme used in the calculations of the embedding results.

5. CONCLUSIONS

An extension of the invariant embedding method to calculate higher order moments of the distribution of the reflected particles is given. The numerical results are in good agreement with alternative calculations in the field. It is expected that the method will find more applications when fluctuations in the reflected flux are of interest. Apart from the traditional problem of refection from a semi-infinite slab, the method can be profitably employed for treatment of one dimensional problems involving finite slabs and spheres.

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