BENCHMARKING THE INVARIANT EMBEDDING METHOD AGAINST ANALYTICAL SOLUTIONS IN MODEL TRANSPORT PROBLEMS

by

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The purpose of this paper is to demonstrate the use of the invariant embedding method in a few model transport problems for which it is also possible to obtain an analytical solution. The use of the method is demonstrated in three different areas. The first is the calculation of the energy spectrum of sputtered particles from a scattering medium without absorption, where the multiplication (particle cascade) is generated by recoil production. Both constant and energy dependent cross-sections with a power law dependence were treated. The second application concerns the calculation of the path length distribution of reflected particles from a medium without multiplication. This is a relatively novel application, since the embedding equations do not resolve the depth variable. The third application concerns the demonstration that solutions in an infinite medium and in a half-space are interrelated through embedding-like integral equations, by the solution of which the flux reflected from a half-space can be reconstructed from solutions in an infinite medium or *vice versa*. In all cases, the invariant embedding method proved to be robust, fast, and monotonically converging to the exact solutions.

Key words: invariant embedding method, synthetic scattering kernel, sputtering spectrum, path length distribution

INTRODUCTION

Calculation of the flux reflected back from a bounded region or from a half-space induced by an incoming radiation is one of the basic tasks in transport theory. The need for such calculations arises frequently in nuclear engineering and related areas. In core calculations, the problem of calculating the exiting flux or current per unit incoming flux or current is known as the albedo factor; albedo was used in the past for approximating the effect of the reflector. Another case in core calculations is found in the application of the collision probability methods, where transmission and reflection of the fluxes between various regions appear explicitly in the calculations.

The largest relevance of calculating the reflected/exiting flux is in the field of charged particle transport, most notably atomic collision cascades including sputtering and electron reflection spectroscopy. The latter is a powerful method of material investigation, which consists of measuring the energy loss of reflected electrons or ions from a surface or an interface, by means of which one determines the material properties. In such cases, in order to be able to unfold the material properties from the measurements, *i. e.* to solve the inverse task, one needs to solve the direct task from theory, *i. e.* to calculate the energy loss characteristics of reflected ions or electrons by transport theory calculations for arbitrary materials.

Due to the nature of the problem (free surface boundary conditions), standard methods of reactor physics such as low-order P_n methods do not provide a solution with acceptable accuracy. In general,

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the integral forms of the transport equation, when solved by Neumann-series (collision number) expansion methods, are the most straightforward to tackle the problem of the free boundary. The invariant embedding equations are a special class of the integral transport equations, amenable to collision number expansion type iterative solutions [1-5]. They have, in addition, the advantage that they do not resolve the depth parameter, and hence the corresponding integrals have to be performed in fewer parameters. Despite the fact that the embedding equations are non-linear, in certain boundary condition problems the embedding technique lends the most effective way of numerical solutions. This quality of the embedding technique has been demonstrated in several papers recently, treating electron and positron backscattering from surfaces [6-9].

In addition to the above, some other advantageous properties of the embedding technique have been discovered relatively recently. One of these is the fact that with an ingenious trick, one can calculate the distribution of the path length that particles travel in the medium before being reflected back, with the invariant embedding equations [6]. This is slightly surprising, since the embedding technique does not resolve the depth variable, but only works with surface parameters. Another advantage comes from the recognition that the fluxes crossing the free surface of a semi-infinite medium and those crossing an imaginary surface inside an infinite medium can be related to each other by embedding-like integral equations [7]. Knowing the infinite medium solutions (which are much easier to obtain due to the absence of free surface boundary conditions), one can calculate the reflected fluxes from a half-space, or *vice versa*, by very fast converging iterative methods. These relationships between the infinite medium and bounded medium fluxes gave a further substantial increase of the usefulness of invariant embedding techniques.

The subject of the paper is the demonstration of the application of the invariant embedding method in the areas described above. For this purpose, we selected a very simple scattering model, originally suggested by Fermi [10-11] and developed further by Placzek, in which the particle directions are restricted to a movement along a one-dimensional straight line ("forward-backward scattering model"). Such kernels are also called synthetic scattering kernels. Both non-multiplying and multiplying media can be treated. The advantage of the simple scattering model is that for these cases, nontrivial analytic solutions can be obtained, and hence the correctness of the embedding solution can be verified.

Three different basic problem areas are treated in this paper. The first is the calculation of the energy spectrum of reflected (sputtered) particles from a multiplying medium when bombarded by a flux of monoenergetic particles of the same type. The second one concerns the calculation of the path length distribution of reflected particles from a medium without multiplication. Finally, we studied the technique of getting infinite medium results from those for a half-space by the method of solving the corresponding embedding-like integral equations, as suggested by Glazov [7]. The applicability of the embedding technique was tested by comparing the numerical solutions to analytic ones. In all cases the invariant embedding method proved to be robust, fast, and converged monotonically to the exact solutions.

DERIVATION OF THE INVARIANT EMBEDDING EQUATIONS

The detailed derivation of the invariant embedding equations is found in standard books and articles such as [1-5], hence we only give a very concise description. The main quantity of interest is the distribution of particles reflected/backscattered at the surface of the homogeneous semi-infinite material. Thus $Y\ (E_0, \vec{\Omega}_0, E, \vec{\Omega})\mathrm{d}E\mathrm{d}\vec{\Omega}$ denotes the probability in the first order of $\mathrm{d}E\mathrm{d}\vec{\Omega}$, that one particle will be emitted in the infinitesimal energy interval $(E, \mathrm{d}E)$ and outgoing direction interval $(\vec{\Omega}, \mathrm{d}\vec{\Omega})$, induced by one incoming particle with energy E_0 and an inward direction $\vec{\Omega}_0$. Due to the infinitesimal character of the phase space volume considered, this is equivalent with defining Y^- as the average number of particles crossing the surface with coordinates within $(E, \mathrm{d}E)$ and $(\vec{\Omega}, \mathrm{d}\vec{\Omega})$. The quantity Y^- (and likewise the transmitted flux, Y^+, to be defined later) will often be referred to as "fluxes" or "flux densities" (reflected or transmitted fluxes); although, to be correct, in the usual neutron transport theory sense these are normal components of the current vector, since they refer to the number of particles crossing the given surface.

We consider only atomic collisions with recoil production but no fission, $E_0 > E$, and $\vec{\Omega}_0 \cdot \vec{n} = \mu_0 > 0$ and $\vec{\Omega}\ \ \vec{n} = \mu < 0$, where $\vec{n}$ is an *inbound* normal vector at the surface; otherwise $Y^-\ \ 0$. This description does not need to specify whether the semi-infinite medium is filling the right or the left half-space, since it is invariant to the reflection of the system, a fact that will be made use of later. Irrespective of the absolute direction of the surface normal, one has that $Y\ (E_0, \vec{\Omega}_0, E, \vec{\Omega})\ \ 0$ if $\vec{\Omega}_0\ \ \vec{\Omega}\ \ 0$.

This circumstance will be important when we consider the case of an infinite medium, where we will have to consider impinging particles from two different half-spaces. For similar reasons, we will have to introduce the quantity $Y^-(E_0, \vec{\Omega}_0, E, \vec{\Omega})\mathrm{d}E\mathrm{d}\vec{\Omega}$ (the "transmitted flux") which will be non-zero for $\vec{\Omega}_0\ \ \vec{\Omega} > 0$. Trivially, for a semi-infinite medium, Y^+ would be equal to the in-

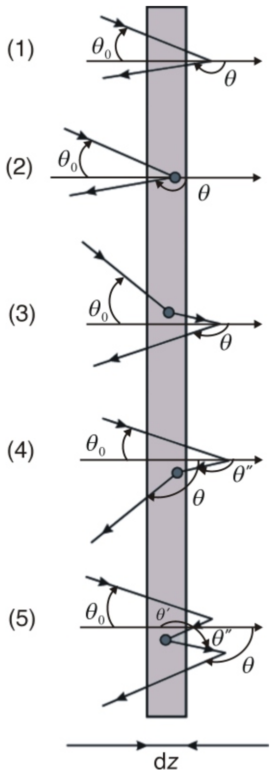

Figure 1. The five different interaction possibillities for zero and one collision in the added layer

coming source particle and therefore has no significance; it will only be non-trivial for the case of an infinite medium, where there will be a returning flux to the surface where the initial particle was started. This will be discussed in subsection on the analytical calculation in an infinite medium.

The derivation of the invariant embedding equation is based on considering an infinitesimal layer of thickness d*z* at the surface, in which the probability of multiple collisions can be neglected. Then the probability of backscattering can be formulated as the sum of the probabilities of five different mutually exclusive possible events having at most one collision in the layer either on the entry or on the leave of the particle. These possibilities can be listed as follows (see also fig. 1):

(1) No interaction in the layer on entering, reflection in the medium, no interaction in the layer on leaving;

(2) Interaction on entering with scattering outwards (backscattering from the layer);

(3) Interaction on entering with scattering inwards, reflection in the medium, no interaction in the layer on leaving;

(4) No interaction on entering, reflection in the material, interaction in the layer with scattering outwards;

(5) No interaction on entering, reflection in the medium, interaction on leaving with backscattering to the medium, reflection in the material, no interaction in the layer on leaving.

Adding up the expressions corresponding to the above terms, one arrives at the equation

$$\frac{\Sigma(E_0)}{\mu_0}\ \frac{\Sigma(E)}{|\mu|}\ Y\ \ (E_0,\vec{\Omega}_0,E,\vec{\Omega})$$

$$\frac{\Sigma(E_0)}{\mu}c(E_0)\mathrm{f}(E_0,\vec{\Omega}_0\qquad E,\vec{\Omega})$$

$$\frac{\Sigma(E_0)}{\mu_0}c(E_0)\ {}^{E_0}_{E\,\vec{\Omega}}\ \ \mathrm{f}(E_0,\vec{\Omega}_0\qquad E\ ,\vec{\Omega}\ )$$

$$Y\ \ (E\ ,\vec{\Omega}\ ,E,\vec{\Omega})\mathrm{d}E\ \mathrm{d}\vec{\Omega}$$

$$ {}^{E_0}_{E\,\Omega}\ \ \frac{\Sigma(E\ \ )}{|\mu\ \ |}c(E\ \ )Y\ \ (E_0,\vec{\Omega}_0,E\ \ ,\vec{\Omega}\ \ )$$

$$\mathrm{f}(E\ \ ,\vec{\Omega}\qquad E,\vec{\Omega})\mathrm{d}E\ \ \mathrm{d}\vec{\Omega}$$

$$+\ {}^{E_0}_{E\,\Omega}\ \ \frac{\Sigma(E\ \ )}{|\mu\ \ |}c(E\ \ )Y\ \ (E_0,\vec{\Omega}_0,E\ \ ,\vec{\Omega}\ \ )$$

$$ {}^{E}_{E\,\vec{\Omega}}\ \ \mathrm{f}(E\ \ ,\vec{\Omega}\qquad E\ ,\vec{\Omega}\ )$$

$$Y\ \ (E\ ,\vec{\Omega}\ ,E,\vec{\Omega})\mathrm{d}E\ \vec{\Omega}\ \mathrm{d}E\ \ \mathrm{d}\vec{\Omega} \qquad (1)$$

where (E) is the total macroscopic cross-section, $c(E)$ is the number of secondaries per collision, and $\mathrm{f}(E_0, \vec{\Omega}_0 \quad E, \vec{\Omega})$,), is the normalized scattering function. Since, for simplicity, only cases without absorption will be considered (with one exception in section on the path length distribution), c will be unity for a non-multiplying medium (*i. e.* for electron transport), and for the case of recoil production, we will have $c = 2$.

It is worth noting that due to the infinite extension of the semi-infinite material both with and without the infinitesimal layer (hence the term "invariant embedding"), the backscattering function $Y^{-}(E_0, \vec{\Omega}_0, E, \vec{\Omega})$ is the same on both sides of eq. (1).

Using the following notation for abbreviation

$$\frac{\Sigma(E_0)}{\mu_0}\ c(E_0)\ \mathrm{f}(E_0,\vec{\Omega}_0\qquad E,\vec{\Omega})$$
$$G(E_0,\vec{\Omega}_0,E,\vec{\Omega})$$

and

$$G(E_0,\vec{\Omega}_0,E\ ,\vec{\Omega}\ )\,Y\ \ (E\ ,\vec{\Omega}\ ,E,\vec{\Omega})\mathrm{d}E\ \mathrm{d}\vec{\Omega}$$
$$G\quad Y$$

the above general invariant embedding eq. (1) can be compactly written as

$$\frac{\Sigma(z,E_0)}{\mu_0} \quad \frac{\Sigma(z,E)}{|\mu|} \quad Y \;\; (E_0,\vec{\Omega}_0,E,\vec{\Omega})$$

$$G \;\; G \;\; Y \quad Y \quad G \;\; Y \quad G \;\; Y$$

$$(1 \;\; Y \;\;) \quad G \quad (1 \;\; Y \;\;) \tag{2}$$

This equation can be resolved into a set of iterative equations for the n-times collided particles, expressed explicitly in terms of integrals containing only lower order terms. That is, one has

$$Y \;\; (E_0,\vec{\Omega}_0,E,\vec{\Omega}) \quad \sum_{n\;1}^{\infty} Y_n \;\; (E_0,\vec{\Omega}_0,E,\vec{\Omega})$$

where Y_n stands for the reflected flux of exactly n-times collided particles. It is easily confirmed that the first term is given by

$$Y_1 \;\; (E_0,\vec{\Omega}_0,E,\vec{\Omega}) \quad \frac{\Sigma(z,E_0)}{\mu_0} \quad \frac{\Sigma(z,E)}{|\mu|}^{\;1}$$

$$G(E_0,\vec{\Omega}_0,E,\vec{\Omega}) \tag{3}$$

while the equations for the higher order terms are given as

$$Y_n \;\; (E_0,\vec{\Omega}_0,E,\vec{\Omega}) \quad \frac{\Sigma(z,E_0)}{\mu_0} \quad \frac{\Sigma(z,E)}{|\mu|}^{\;1}$$

$$G \quad Y_{n\;1} \quad Y_{n\;1} \quad G \sum_{m\;1}^{n\;2} Y_m \quad G \quad Y_{n\;m\;1} \tag{4}$$

The right hand side of the eq. (4) above contains only terms of order n – 1 or lower. This means that starting with n = 2, and using the Y_1 of eq. (3) on the right hand side, Y_2 can be calculated by a simple quadrature over the known functions, after which Y_1 and Y_2^- can be used on the right hand side to calculate Y_3, and so on to the higher orders. The procedure can be terminated when inclusion of more terms yields a smaller contribution than a pre-set error limit. This iterative scheme will be used throughout the paper for the numerical work.

THE SCATTERING MODEL

In this paper only cases when the bombarding particle is of the same type as the host material will be considered. This means that only scattering between particles of equal mass occurs. All calculations in this paper will be made by using a simple so called synthetic kernel, in which transport occurs along a straight line such that $\vec{\Omega}_z$ = cos θ μ can only take values ±1. A particle on collision can either continue or reverse, and in the case of recoil production, the same is valid to the recoil, independently on the direction in which the projectile leaves the collision site. This means that the conservation of energy and impulse is uncoupled, hence they are not conserved in the individual collisions, but only in an average over a large number of collisions. This corresponds to the "forward-backward" scattering model by Fermi. In the examples of the following sections this restriction is used everywhere in order to be able to compare the invariant embedding solutions with analytical calculations. In regard of the energy transfer, hard sphere scattering is also assumed, either with constant or power-law cross-sections.

Although the most obvious and customary way of accounting for the discrete available scattering angles is a Dirac-delta function representation such as in [11], this would lead to complications in the embedded formalism because there is one term where the scattering function stands alone, *i. e.* not under an integral sign. Hence it is simpler if the angular dependence of the scattering function is represented by Kronecker-delta functions, and the integrals with respect to the angular variable are replaced by summations.

According to the above, the normalized scattering function with hard sphere scattering between equal masses is given as

$$\mathrm{f}(E_0,\vec{\Omega}_0 \quad E,\vec{\Omega}) \quad \mathrm{f}(E_0,\mu_0 \quad E,\mu)$$

$$\frac{1}{2E_0}(\delta_{\mu_0,\mu} \quad \delta_{\mu_0,\;\mu}) \tag{5}$$

The case of no recoil production is then described by c = 1, and that of recoil production with c = 2. Using the above simplification, the embedding equation is written as:

$$Y \;\; (E_0,\mu_0,E,\mu)$$

$$\frac{\Sigma(E_0)}{\mu_0} \quad \frac{\Sigma(E)}{|\mu|}^{\;1} \quad \frac{\Sigma(E_0)}{\mu_0}\frac{c}{2E_0}(\delta_{\mu_0,\mu} \quad \delta_{\mu_0,-\mu})$$

$$\int_{E}^{E_0} \sum_{\mu\;\;1} \frac{\Sigma(E_0)}{\mu_0}\frac{c}{2E_0}(\delta_{\mu_0,\mu} \quad \delta_{\mu_0,\;\mu})$$

$$Y \;\; (E \;,\mu \;,E,\mu)\mathrm{d}E$$

$$\int_{E}^{E_0} \sum_{\mu\;\;1} Y \;\; (E_0,\mu_0,E \;\;,\mu \;\;)\frac{\Sigma(E \;\;)}{|\mu \;\;|}$$

$$\frac{c}{2E}(\delta_{\mu \;,\mu} \quad \delta_{\mu \;,\;\mu})\mathrm{d}E$$

$$\int_{E}^{E_0}\int_{E}^{E} \sum_{\mu\;\;1}\sum_{\mu\;\;1} Y \;\; (E_0,\mu_0,E \;\;,\mu \;\;)\frac{\Sigma(E \;\;)}{|\mu \;\;|}$$

$$\frac{c}{2E}(\delta_{\mu \;,\mu} \quad \delta_{\mu \;,\;\mu}) \;\; Y \;\; (E \;,\mu \;,E,\mu)\mathrm{d}E \;\; \mathrm{d}E$$

However, we need also to take into account that $Y^-(E', \mu', E, \mu)$ is only non-zero if $\mu' > 0$ and $\mu < 0$ as well as the fact that we can substitute $\mu_0 = 1$ and $\mu = -1$. Also, turning to constant cross-sections means that the cross-sections disappear from the equation, which in physical terms means that the reflected flux is invariant to a rescaling of the depth variable to the optical path. This will reduce the embedding equation to the final form

$$Y(E_0, E) = \frac{c}{4E_0} + \frac{c}{4E_0}\int_E^{E_0} Y(E', E)\mathrm{d}E' + c\int_E^{E_0} \frac{Y^-(E_0, E')}{4E'}\mathrm{d}E' + c\int_E^{E_0} \frac{Y(E_0, E')}{4E'}\int_E^{E'} Y(E'', E)\mathrm{d}E''\,\mathrm{d}E'$$

where

$$Y(E_0, E) = Y(E_0, \mu_0 = 1, E, \mu = -1)$$

SPUTTERING SPECTRUM FROM A SEMI-INFINITE MEDIUM

Constant cross-sections

Analytical solution

In the case of sputtering in an atomic collision cascade, recoil production is assumed on each scattering event; hence one has $c = 2$. Further, one can simplify the equations by rescaling the depth variable into units of the optical path ($\Sigma = 1$), which will have no influence on the sputtering spectrum at the surface. The ordinary transport equation reads as

$$\mu\frac{\partial Y(z, \mu, E)}{\partial z} + Y(z, \mu, E) = \int_E^{E_0} \frac{1}{E'}[Y(z, \mu, E') + Y(z, -\mu, E')]\mathrm{d}E' \tag{6}$$

with the boundary condition

$$Y(0, 1, E) = \delta(E - E_0)$$

which corresponds to one incoming particle on the surface with energy E_0 and direction $\mu = +1$. The searched quantity is $Y(0, -1, E)$, *i. e.* the outgoing flux at the surface. Rewriting the transport eq. (6) into the lethargy variable $u = \ln(E_0/E)$ gives

$$\mu\frac{\partial Y(z, \mu, u)}{\partial z} + Y(z, \mu, u) = \int_0^u [Y(z, \mu, u') + Y(z, -\mu, u')]\mathrm{d}u' \tag{7}$$

with the boundary condition in the form

$$Y(0, 1, u) = \frac{\delta(u)}{E_0} \tag{8}$$

The solution of this equation has been known for long [12-13] and it is given for the sputtered spectrum per unit energy interval as

$$Y(0, -1, u) = Y(0, u) = \frac{e^u}{E_0 u} I_1(u) \tag{9}$$

where I_1 is the modified Bessel function of the first order. This solution diverges with increasing lethargy, which expresses the fact that without a cut-off energy, or energy dissipation by binding energy, the number of recoils generated by a primary energetic particle diverges when the energy of the recoils tends to zero.

Invariant embedding solution

Using the iterative scheme described in eqs. (3) and (4), a numerical solution based on the invariant embedding technique can be obtained and the solution can be compared to the analytical solution. The calculations were performed by using a Matlab code. The results obtained with the use of the algorithm are shown in fig. 2. One can see that the iterations approach the analytical solution after some ten to fifteen iterations, as seen in fig. 2, where the first ten iterations are shown. It is also seen that the higher the lethargy or the E_0/E ratio, the more iterations are necessary for convergence, which is a consequence of the fact that the invariant embedding method uses a collision number expansion in the iterations, and the collision number increases with increasing lethargy.

Power law cross-sections

In the invariant embedding method the use of constant cross-sections can easily be abandoned

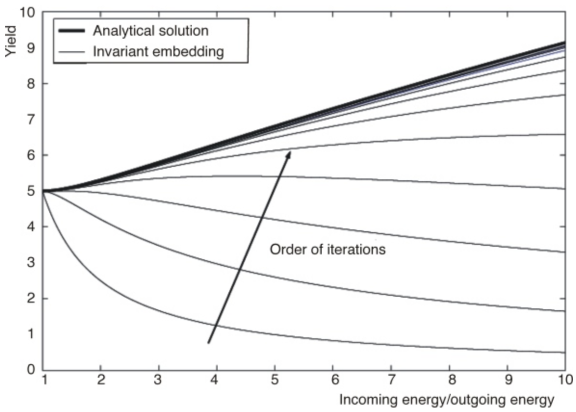

Figure 2. Sputtering spectrum with constant cross-sections

without any practical increase of difficulty of the solutions. This is not true for the analytic solutions of the ordinary transport equation which cannot be solved in a compact closed form for energy dependent cross-sections. For illustration, we show here the invariant embedding solutions for so called power law cross sections, commonly used in the theory of atomic collisions. These are given in the form [14]

$$\Sigma(E) \quad CE^{\;\;q} \tag{10}$$

where C is an arbitrary constant and q lies between zero and unity. For that case the invariant embedding equation – eq. (2), takes the form

$$Y\;(E_1, E_2)\quad \frac{1}{E_1^{\;\;q}\quad E_2^{\;\;q}}\;[(E_1^{\;(q\;\;1)}$$
$$E_1^{\;(q\;\;1)}\;{}_{E_2}^{E_1}\;Y\;(E\;, E_2)\mathrm{d}E$$
$${}_{E_2}^{E_1}\;E\;\;^{(q\;\;1)}Y\;(E_1, E\;)\mathrm{d}E$$
$${}_{E_2}^{E_1}\;E\;\;^{(q\;\;1)}Y\;(E_1, E\;)\;{}_{E_2}^{E}\;Y\;(E\;, E_2)\mathrm{d}E\;\mathrm{d}E\;)] \tag{11}$$

Here, E_1 stands for the energy of the incoming particle and E_2 for its post-collisional (outgoing) energy.

The quantitative solutions are shown in fig. 3. Since no analytical solutions are available, we cannot compare the embedding solutions with the exact results. In this case, we can only make a quantitative comparison with Monte-Carlo calculations of the total sputtering yield, published by Conrad and Urbassek [14].The results displayed in fig. 3 show that the sputtering spectra and hence also the integrals of the sputtering spectra (sputtering yields) decrease monotonically and uniformly in E_0/E with the increasing value of q. In fig. 3 the cases $q = 0$, $q = 0.5$, and $q = 1$ are shown. When $q = 0$, the solution is identical with the solution for the energy independent cross-sections, as it should be. The above trends are in accordance with the findings published in [14], where the same tendency was found for the sputtering yield, as a function of the power law exponent q. Compared with the Monte-Carlo method used in [14] for the same task, the invariant embedding method is much faster for the same accuracy than the Monte-Carlo calculations.

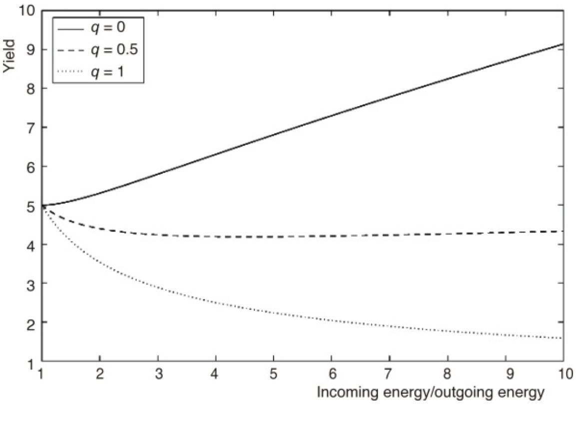

Figure 3. Sputtering spectrum from three different power law cross-sections $\quad = CE^{-q}$

PATH LENGTH DISTRIBUTION

The path length distribution is interesting for the reflection of injected particles from a non-multiplying medium, such as the electron reflection from solids. The distribution of the particles with respect to the total path length traveled in an energy-independent description has been frequently used to calculate the energy loss of the reflected electrons just below the elastic peak, by convoluting the path length distribution with the energy loss function [6].

Analytical calculation

Since in this (and only this) section we consider an energy-independent case (one-speed description), notations on energy will be omitted. The scattering kernel thus has the form

$$f(\mu \quad \mu\;)\;\; \frac{1}{2}(a\,\delta_{\mu,\mu}\quad b\,\delta_{\mu,\;\mu}\;) \tag{12}$$

where a and b describe the forward and backward scattering probabilities. Here, and only in this section, we maintain the possibility of anisotropic scattering which prevails when $a \quad b$, and the possibility of absorption, when $a + b < 1$. Further, since there is no recoil production, we shall have $c = 1$ in the non-absorbing case, and allow also for $c < 1$ to account for absorption.

Although the path length variable is usually not operated on in the ordinary transport equation, one can make use of the fact that in one-speed case with a constant particle speed v, the path length variable R is equal to $R = vt$ and hence the time dependent transport equation can be used for calculation of the dependence of the reflected flux on R. The modified transport equation reads as [15]

$$\frac{\partial Y(z, \mu, R)}{\partial R}\quad \mu\frac{\partial Y(z, \mu, R)}{\partial z}\quad Y(z, \mu, R)$$
$$aY(z, \mu, R)\quad bY(z, \;\;\mu, R)$$
$$\delta(z)\,\delta(R)\,\delta_{\mu,\;1} \tag{13}$$

where the last term on the right hand side represents the source particle. Since the source particle is explicitly written in the equation, it does not show up in the boundary conditions:

$$Y(z \quad 0, \mu \quad 1, R) \quad 0 \tag{14}$$

$$Y(z, \mu \quad 1, R \quad 0) \quad 0 \tag{15}$$

whereas the reflected flux $Y(z = 0, \mu = -1, R)$ is unknown and has to be determined from the solution. This problem can also be solved in a closed analytical form, and the solution reads as

$$Q(R) \quad Y \quad (0, R) \quad \frac{e^{(a \quad 1)R}}{R} I_1(bR) \tag{16}$$

which, when there is no absorption present (*i. e.* when $a + b = 1$), reduces to

$$Y \quad (0, R) \quad \frac{e^{\quad bR}}{R} I_1(bR) \tag{17}$$

This is the analytical solution to which we shall compare the invariant embedding results.

Path length distribution using invariant embedding

In a recent publication, by finding an analogy between the generating function of the full path length distribution form of the embedding equation and the ordinary embedding one, Vicanek [6] has constructed an embedding solution to the path length distribution in a very ingenious way. The essence of the method is the following (for details, refer to [6]). With the usual arguments, one can derive an embedding-like equation for the path length distribution $Q(R)$ of eq. (16) as

$$\frac{1}{\mu_0} \quad \frac{1}{|\mu|} \quad \frac{\partial}{\partial R} \quad 1 \;\; Q(R)$$

$$\delta(R)G \quad G \quad Q(R) \quad Q(R) \quad G$$

$$Q(R \;)GQ(R \quad R \;)\mathrm{d}R$$

Then the solution of the above equation can be given as

$$Q(R) \quad \sum_{n \quad 1}^{\infty} Y_n \, Q_n(R) \tag{18}$$

where

$$Q_n(R) \quad \frac{R^{n \quad 1}}{(n \quad 1)!} e^{\quad R} \tag{19}$$

The $Q_n(R)$ are the path length distributions of the particles that have suffered n elastic collisions before leaving the medium. The quantities Y_n^-, on the other hand, are calculated as the collision number expansion coefficients of the total reflected flux Y^-. This latter is defined by the energy independent form of the embedding equation with the forward-backward scattering kernel in the form

$$(Y \quad)^2 \quad 2Y \quad 1 \quad 0 \tag{20}$$

where $Y \quad Y \;(\mu_0, \mu) \quad Y \;(\;\; 1, \;\; 1)$. This equation has the trivial solution

$$Y \quad 1; \quad \text{hence} \quad \sum_{n \quad 1}^{\infty} Y_n \quad 1$$

expressing the fact that in a purely scattering infinite half-space, the reflected flux is equal to the incoming flux, which is unity. However, for the invariant embedding type path length distribution we need the expansion coefficients Y_n *i. e.* the contributions of the n-times collided particles to the total reflection coefficient. These can easily be determined recursively in the way described in connection with eq. (4), in this case purely through algebraic summations, without integration. Knowing the Y_n the path length distribution can easily be calculated via eqs. (18) and (19).

The quantitative results from the invariant embedding calculations were compared with the analytical results. Three cases were selected for the comparison of the analytical and invariant embedding solutions, with varying degrees of absorption: no absorption, weak absorption, and strong absorption (fig. 4). It can be seen in the fig. 4 that, especially when absorption is present, only a few of these coefficients are needed for convergence, and as few as the first two Y_1^- and Y_2^- are sufficient for the case of strong absorption. Without absorption, more coefficients are needed for convergence, hence in fig. 4a and fig. 4b only every third iteration is shown for clarity. One can note the decrease in number of coefficients with the increase of absorption. The accuracy obtained in the individual iterations for the three cases are shown in tabs. 1-3 below.

Table 1. No absorption

Path length R	Analytical value	Iterations	Relative deviation
1	0.1564	6	$9.6907\ 10^{-5}$
2	0.1040	9	$3.5542\ 10^{-5}$
3	0.0730	11	$4.8046\ 10^{-5}$
4	0.0538	13	$4.8975\ 10^{-5}$
5	0.0413	15	$4.3560\ 10^{-5}$
6	0.0328	17	$3.5817\ 10^{-5}$
7	0.0268	18	$8.3710\ 10^{-5}$
8	0.0223	20	$6.0753\ 10^{-5}$
9	0.0190	22	$4.3373\ 10^{-5}$
10	0.0164	23	$7.9678\ 10^{-5}$

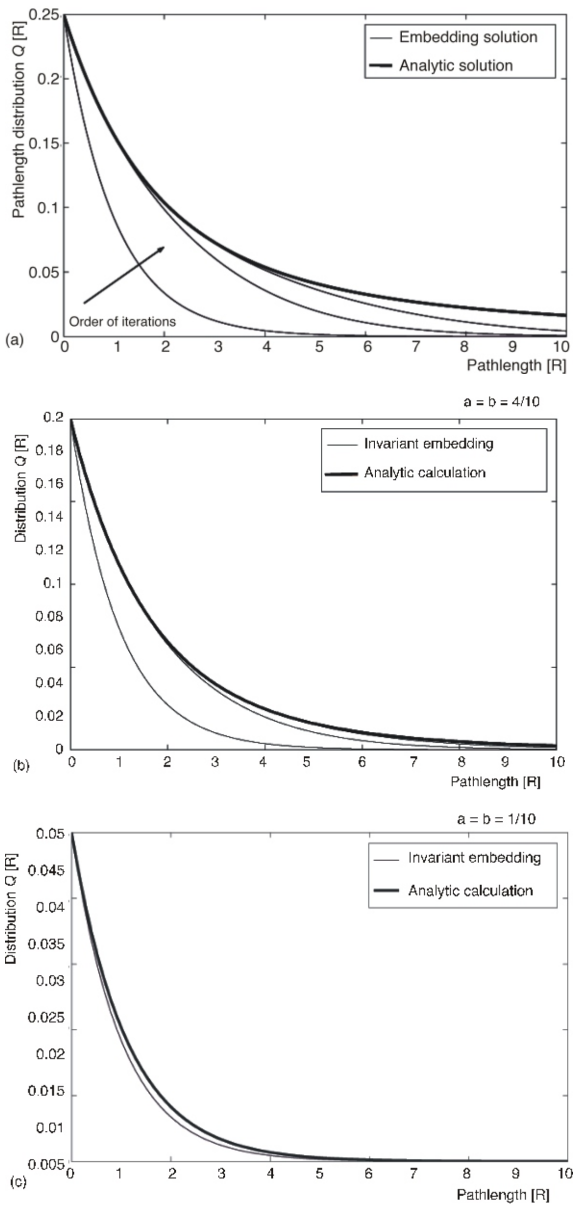

Figure 4 Path length distributions in three cases with varying degree of absorption: (a) no absorption, (b) week absorption, and (c) strong absorption

Table 2. Moderate absorption, a = b = 4/10

Path length R	Analytical value	Iterations	Relative deviation
1	0.1120	6	2.7663 10^{-5}
2	0.0652	8	3.8659 10^{-5}
3	0.0394	10	3.0571 10^{-5}
4	0.0246	11	8.6933 10^{-5}
5	0.0158	13	4.8975 10^{-5}
6	0.0105	14	9.4659 10^{-5}
7	0.0071	16	4.9523 10^{-5}
8	0.0049	17	8.0502 10^{-5}
9	0.0034	19	4.1214 10^{-5}
10	0.0024	20	6.0753 10^{-5}

Table 3. Strong absorption, a = b = 1/10

Path length R	Analytical value	Iterations	Relative deviation
1	0.0204	4	1.0204 10^{-5}
2	0.0083	5	9.4707$\cdot 10^{-6}$
3	0.0034	5	6.6541$\cdot 10^{-5}$
4	0.0014	6	2.7663$\cdot 10^{-5}$
5	5.7299 10^{-4}	6	9.6907 10^{-5}
6	2.3614 10^{-4}	7	3.7253 10^{-5}
7	9.7555 10^{-5}	7	9.9949 10^{-5}
8	4.0396 10^{-5}	8	3.8659 10^{-5}
9	1.6766 10^{-5}	8	8.9882 10^{-5}
10	6.9746 10^{-5}	9	3.5542 10^{-5}

RELATIONSHIP BETWEEN THE SOLUTIONS IN A HALF-SPACE AND IN AN INFINITE MEDIUM

It is possible to reconstruct the solution in a half-space medium from the solution in an infinite medium and *vice versa* [7]. The reflection problem in an infinite medium is defined by the current of particles leaving an imaginary surface at $z = 0$ into the negative direction, induced by one incoming particle starting at the surface into the positive z-direction. In this case, the reflected flux is not only due to recoiled particles generated exclusively by the initial particle, since now the particles emitted can be back-scattered from the other half-space and reenter the domain $z > 0$, thereby creating more recoils which will add to the reflected flux into the half-space $z < 0$.

In the demonstration of the method, we shall now reconstruct the infinite-medium solution from the half-space one, since the latter was already determined in the previous section. However, to check the correctness of the reconstruction procedure, here we need also an analytical result with which the invariant embedding result will be checked.

Analytical calculation in an infinite medium

The starting equation is identical with that in the semi-infinite medium, eq. (7):

$$\mu \frac{\partial Y(z,\mu,u)}{\partial z} \quad Y(z,\mu,u) \quad \int_0^u [Y(z,\mu,u) \quad Y(z, \quad \mu,u)]\mathrm{d}u \quad \frac{\delta(u)}{E_0}\delta_{\mu,\ 1}\delta(z) \tag{21}$$

The difference is that now the solution is sought for $-\infty < z < \infty$; also, the source particle was included into the equation instead of treating it as an interface condition. Indeed, in an infinite medium, there will be more particles crossing the surface $z = 0$ into the positive direction than just the source particle. The only boundary condition we have now is that

$$Y(z, \mu, u) \quad \infty \text{ for } z \qquad \infty$$

The task is to calculate the quantity

$$Y_\infty(u) \quad Y(0, \mu \qquad 1, u)$$

which is the probability density (in energy units) of the particle crossing the surface at $z = 0$ in an infinite medium, with lethargy u, into the opposite direction as that of the initial starting particle which induced the cascade, and which was injected at the same surface.

This problem can also be solved analytically. The solution for the total reflected flux at $z = 0$ in an infinite medium is obtained as

$$Y \quad (u) \quad \frac{e^u I_0(u)}{2E_0} \tag{22}$$

The solution in a semi-infinite medium is known from before – eq. (9), as

$$Y_{1/2}(u) \quad \frac{e^u I_1(u)}{E_0 u} \tag{23}$$

The asymptotic properties of Y_∞ and $Y_{1/2}$ for small u values are the same:

$$\lim_{u \quad 0} Y_{1/2} \quad \frac{1}{2E_0} \tag{24}$$

$$\lim_{u \quad 0} Y_\infty \quad \frac{1}{2E_0} \tag{25}$$

This means that for small lethargies (incoming energy and outgoing energy are close to each other) the functions for the semi-infinite and the infinite medium are identical. This is understandable, since there is a very small probability for a sputtered particle with small lethargy to have crossed the plane $z = 0$ more than once in the infinite medium case. The asymptotic properties for large lethargies are, on the other hand, quite different:

$$\lim_{u \quad \infty} Y_{1/2} \quad \frac{e^{2u}}{E_0 u \sqrt{2\pi u}} \quad O(1/u)$$

$$\lim_{u \quad \infty} Y_\infty \quad \frac{e^{2u}}{2E_0 \sqrt{2\pi u}} \quad O(1/u)$$

The sputtering spectrum diverges faster for an infinite medium than for the semi-infinite one. This can be physically understood, since while a particle that leaves the semi-infinite medium never returns, in the infinite medium it can return and induce further scattering reactions and further sputtered particles into the left half-space.

Relationship between the semi-infinite and infinite medium solutions

Consider two cases in parallel: a homogenous semi-infinite medium for $z \quad 0$, and an infinite medium of the same material properties. Let us induce cascades in both media by one impinging particle into the positive z direction at $z = 0$ and follow the fluxes that cross the surface at $z = 0$. Then let us use the following notations:

$Y_{1/2}^-(E_0, E)$ – the reflected flux in a semi-infinite medium,
$Y_\infty^-(E_0, E)$ – all outgoing passages in the infinite medium (reflected flux), and
– $Y_\infty(E_0, E)$ – all ingoing passages *except the initial particle* in the infinite medium ("transmitted" flux).

Here, $Y_\infty^-(E_0, E)$ is the total reflected flux through the surface in a direction that is opposite to that of the incoming particle, whereas $Y_\infty(E_0, E)$ is the total flux crossing the surface into the same direction as the incoming particle, but *excluding* the initial particle. Due to the symmetry of the infinite medium, these two quantities will be the same irrespective of in which direction the original particle starts, as long as the signs are meant with respect to the direction of the source particle.

It follows then that $Y_\infty^-(E_0, E)$ can be expressed as the sum over the flux that does not return and an integral over the transmitted flux in an infinite medium as

$$Y_\infty(E_0, E) \quad Y_{1/2}(E_0, E)$$
$$\int_0^{E_0} Y_\infty(E_0, E') \, Y_{1/2}(E', E)\mathrm{d}E' \tag{26}$$

Likewise, for $Y_\infty(E_0, E)$ one will have

$$Y_\infty(E_0, E) \quad \int_0^{E_0} Y_{1/2}(E_0, E') \, Y_\infty(E', E)\mathrm{d}E' \tag{27}$$

Introducing the following notation

$$A \quad B \qquad A(E_0, E')B(E', E)\mathrm{d}E' \tag{28}$$

eqs. (26) and (27) can be written as

$$Y_\infty \quad Y_{1/2} \quad Y_{1/2} \quad Y_\infty \tag{29}$$

$$Y_\infty \quad Y_{1/2} \quad Y_\infty \tag{30}$$

Define now the symmetrised and antisymmetrised fluxes as

$$S(E_0, E) \quad Y_\infty (E_0, E) \quad Y_\infty (E_0, E) \qquad (31)$$

$$A(E_0, E) \quad Y_\infty (E_0, E) - Y_\infty (E_0, E) \qquad (32)$$

where S describes all passages through $z = 0$ (total or scalar flux in reactor physics terminology), except the initial particle and A describes the net current through the surface, except the initial particle.

Inserting eqs. (26) and (27) into eqs. (31) and (32) the following relationships are readily derived:

$$S \quad Y_{1/2} \quad Y_{1/2} \quad S \qquad (33)$$

$$A \quad Y_{1/2} \quad Y_{1/2} \quad A \qquad (34)$$

Equations (31) and (32) give

$$Y_\infty \quad \frac{S \quad A}{2} \qquad (35)$$

From eqs. (33) and (34) the solutions to S and A can be expressed in the form of a Neumann series expansion that contains nothing more than integrals over $Y_{1/2}$:

$$S \quad Y_{1/2} \quad Y_{1/2} \quad Y_{1/2} \quad Y_{1/2} \quad Y_{1/2} \quad Y_{1/2} \quad \ldots (36)$$

$$A \quad Y_{1/2} \quad Y_{1/2} \quad Y_{1/2} \quad Y_{1/2} \quad Y_{1/2} \quad Y_{1/2} \quad \ldots (37)$$

Combining eqs. (35), (36) and (37) gives the solution for the infinite medium as

$$Y_\infty \quad \frac{1}{2}(Y_{1/2} \quad Y_{1/2} \quad Y_{1/2} \quad Y_{1/2}$$
$$Y_{1/2} \quad Y_{1/2} \quad Y_{1/2} \quad Y_{1/2} \quad Y_{1/2} \quad \ldots) \qquad (38)$$

In many cases, the infinite medium solution is easier to calculate, since the associated boundary conditions (no divergence at infinity) are much simpler than the free surface boundary conditions of a half-space. Using the same procedure but expressing $Y_{1/2}$ instead of Y_∞ one can just as easily express the half-space solutions as functions of the infinite medium solutions in Neumann series expansions similar to eq. (38) as iterated integrals over Y_∞.

The method of reconstructing the solutions in an infinite medium from those in a half-space were also tested quantitatively and checked up with the analytical solutions in the infinite medium. Equation (38) was calculated in iterations as follows:

$$Y^-_{1,\infty} \quad \frac{1}{2} Y^-_{1/2}$$

$$Y^-_{2,\infty} \quad \frac{1}{2}(Y^-_{1/2} \quad Y^-_{1/2} * Y^-_{1/2} * Y^-_{1/2})$$

$$Y^-_{3,\infty} \quad \frac{1}{2}(Y^-_{1/2} \quad Y^-_{1/2} * Y^-_{1/2} * Y^-_{1/2}$$
$$Y^-_{1/2} * Y^-_{1/2} * Y^-_{1/2} * Y^-_{1/2} * Y^-_{1/2})$$

and so forth.

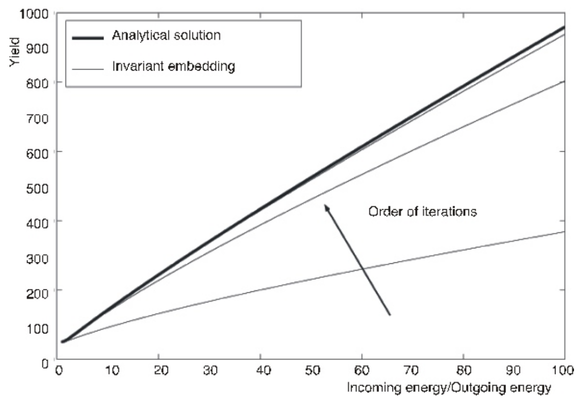

Figure 5. Calculating the solutions in an infinite medium from those in a half space

As fig. 5 shows, the solution converges very rapidly to the analytical result. It is not necessary to include more than three or four terms. The rapid convergence is due to the fact that the involved integral eqs. (26) and (27) are linear equations of the Fredholm type in contrast to the ordinary embedding equations which are non-linear and hence possess less advantageous convergence properties.

CONCLUSIONS

The main purpose of this paper was to demonstrate the application of the invariant embedding method in simple model cases where the technique is transparent and can be compared to known analytical solutions. Hence we believe that the cases shown here will help those who could have use of this powerful method in their own applications to get a hands-on training with the algorithm. As the simple examples show, the application of the embedding method is straightforward and it has good and stable convergence properties. Needless to say, the technique is just as straightforward to be applied to the real energy- and angle-dependent cross-sections and hence to realistic problems. Some of the potentials of this so far less favoured or recognized method will be described in a coming review article where the potentials of obtaining solutions through the infinite medium reformulation of the embedding equations will also be demonstrated [16].

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Малин ВАЛБЕРГ, Имре ПАЖИТ

СТАНДАРДИЗОВАЊЕ МЕТОДЕ ИНВАРИЈАНТНОГ УЛАГАЊА ПОСРЕДСТВОМ АНАЛИТИЧКИХ РЕШЕЊА МОДЕЛОВАНОГ ТРАНСПОРТА

Циљ рада је да прикаже употребу методе инваријантног улагања на неколико примера моделованог транспорта за које је такође могуће добити аналитичка решења. Коришћење методе приказано је у три различите области. Прва је прорачун енергетског спектра распрашених честица из расејавајуће средине без апсорпције у којој је мултипликација (честична каскада) настала услед узмаклих честица. Разматрани су пресеци за судар независни од енергије, и енергетски зависни у виду степене функције. Друга примена тиче се прорачуна расподеле пређеног пута честица рефлектованих од неумножавајуће средине. Ово је релативно необична примена, утолико што једначине улагања не дају решење променљиве по дубини. Трећа примена показује да су решења у бесконачној средини и у полупростору међусобно повезана посредством интегралних једначина сличних инваријантним, чијим се решавањем рефлектовани флукс од полупростора може реконструисати из решења за бесконачну средину, и обрнуто. У свим случајевима, брзом и монотоном конвергенцијом ка егзактном решењу потврђена је поузданост методе инваријантног улагања.

Кључне речи: метода инваријантног улагања, синтетична функција расејања, спектар распрашених честица, расподела пређеног пута