Nuclear Mathematical and Computational Sciences: A Century in Review, A Century Anew
Gatlinburg, Tennessee, April 6-11, 2003, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2003)

INTEGRAL EQUATION FORMULATION OF A MIXED DIFFUSION-JUMP MODEL OF ELASTIC SCATTERING

R. B. Cruise
University Information Technology Services
Indiana University
2711 E. 10^{th} Street, Bloomington, IN 47408
rcruise@indiana.edu

L. S. Papiez
Department of Radiation Oncology
Indiana University School of Medicine
535 Barnhill Drive, RT-041, Indianapolis, IN 46202
lpapiez@iupui.edu

ABSTRACT

The model of elastic scattering as a mixed diffusion-jump stochastic process is developed in [1]. In the model a particle trajectory is the realization of a compound stochastic process. A Brownian motion on the unit sphere in momentum space modeling soft collisions is occasionally interrupted by hard collisions of a given angular distribution. These hard collisions are distributed Poisson-like along the particle track. The objective is to obtain an approximation of the probability density associated with this mixed process that is suited to fast numerical solution. However, in the case where backscattering may be substantial, the computational complexity of the model and the form of an efficient solution algorithm are uncertain. Here we continue development of the model by treating the equation of motion as a Schrödinger-like equation with an interaction term. We then identify the Green function, and the solution assumes the form of a standard Fredholm type 2 integral equation. In this standard formulation we are able to estimate computational complexity and employ off-the-shelf solution algorithms. Using Monte Carlo integral equation solution algorithms we are able to implement standard variance-reduction techniques. Furthermore, the integral equation formulation offers additional insight into both the physical and mathematical aspects of the model. The additional physical insight is detailed in Section 3 in which the integral equation is directly derived from physical arguments about incoming and outgoing particles at a collision center. The additional mathematical insight is substantiated at the end of Section 2 in which the model developed in [1] is interpreted as an infinite Born series of single scattering events. The practicality of the approach is being tested and will be the subject of a forthcoming publication.

Key Words: multiple scattering, phase space evolution, particle transport

1. INTRODUCTION

The key aspects of the mixed diffusion-jump model of elastic scattering developed in [1] are summarized as follows. The diffusion process is a Brownian motion on the unit sphere in momentum space modeling soft elastic collisions, while the jump process is a compound Poisson process on the unit sphere in momentum space modeling hard elastic collisions. The particle evolution is modeled as a stochastic process $(\Omega(t), r(t))$ where $\Omega(t) \equiv \mathbf{k}/k$ is the diffusion-jump process on the unit sphere in momentum space, and where $r(t) = \int_0^t \Omega(t')dt'$ is the coordinate-space position. Beginning with phenomenologically justified probabilistic assumptions, the equation of motion for the probability density $f(t,\Omega,r)$ of the stochastic process $(\Omega(t),r(t))$ can be derived [1]:

$$\left[\frac{\partial}{\partial t} \;+\; \Omega\cdot\nabla_r \;-\; \frac{D}{2}\Delta_\Omega\right] f(t,\Omega,r) \;\;=\;\; \lambda \int_S d\tilde{\Omega}\; p(\tilde{\Omega})\; \left[f(t,\Omega-\tilde{\Omega},r) \;-\; f(t,\Omega,r)\right] \tag{1}$$

where D is the diffusion constant, $1/\lambda$ is the expected interarrival time between hard collisions, and $p(\Omega)=\frac{1}{\sigma}\frac{d\sigma}{d\Omega}$ is the scattering probability density of the projectile with the scattering centers in the target medium. The notation $\Omega-\tilde{\Omega}$ is symbolic for vector addition on the unit sphere. See [2] for vector addition formulas. Because $p(\Omega)$ is a probability density, eqn (1) may be rewritten:

$$\left[\frac{\partial}{\partial t} \;+\; \Omega\cdot\nabla_r \;-\; \frac{D}{2}\Delta_\Omega \;+\; \lambda\right] f(t,\Omega,r) \;\;=\;\; \lambda \int_S d\tilde{\Omega}\; p(\tilde{\Omega})\; f(t,\Omega-\tilde{\Omega},r) \tag{2}$$

which is a diffusional equation with a right-hand side referred to as the interaction term.

The derivation of eqn (1) in [1] is similar to the derivation of the conventional diffusion equation in Einstein's 1905 Brownian motion paper discussed in [3]. A solution algorithm for eqn (1) is developed in §5 of [1], but for which the computational complexity is not readily apparent nor for which existing numerical recipes would apply. On the other hand, viewing the equivalent eqn (2) from a Green function perspective leads to a conventional solution algorithm, and provides additional insight into the model.

2. GREEN FUNCTION SOLUTION

As in [1] we incorporate initial conditions for density f by writing $f(t,\Omega,r)=f(t,\Omega,r|0,\Omega_0,O)$ where $f(t,\Omega,r|t,\Omega_1,r_1)=\delta(\Omega-\Omega_1)\delta(r-r_1)$. Consider the case when the interaction in eqn (2) vanishes. The homogeneous solution is given by:

$$\left[\frac{\partial}{\partial t} \;+\; \Omega\cdot\nabla_r \;-\; \frac{D}{2}\Delta_\Omega \;+\; \lambda\right] e^{-\lambda t}\; f_{\mathrm{diff}}(t,\Omega,r|0,\Omega_0,O) \;\;=\;\; 0 \tag{3}$$

where f_{diff} is the solution of eqn (4.13) in [1]:

$$\left[\frac{\partial}{\partial t} \;+\; \Omega\cdot\nabla_r \;-\; \frac{D}{2}\Delta_\Omega\right] f_{\mathrm{diff}}(t,\Omega,r|0,\Omega_0,O) \;\;=\;\; 0 \tag{4}$$

The density f_{diff} describes the process in which hard collisions have been eliminated; i.e., $\lambda=0$. It characterizes collisions only as a diffusion or a continuous Brownian motion on the unit sphere in momentum space; i.e., as soft collisions. The homogeneous solution to eqn (2), $e^{-\lambda t} f_{\mathrm{diff}}$, is this diffusional density multiplied by the probability that no hard collisions occur during the interval $[0,t]$; it is the probability density of transitioning from $(0,\Omega_0,O)$ to (t,Ω,r) with no hard collisions. The Green function associated with eqn (3) is:

$$G(t,\Omega,r|t_1,\Omega_1,r_1) \;\;=\;\; e^{-\lambda(t-t_1)}\; f_{\mathrm{diff}}(t,\Omega,r|t_1,\Omega_1,r_1)\; \Theta(t-t_1) \tag{5}$$

where $\Theta(\tau)$ is the Heaviside or step function:

$$\Theta(\tau) \;\;:=\;\; \begin{cases} 1 & \tau>0 \\ 0 & \tau\le 0 \end{cases} \tag{6}$$

Using $\frac{d}{dt}\,\Theta(t-t_1)=\delta(t-t_1)$ we have:

$$\left[\frac{\partial}{\partial t} \;+\; \Omega \cdot \nabla_r \;-\; \frac{D}{2}\Delta_\Omega \;+\; \lambda\right] G(t,\Omega,r|t_1,\Omega_1,r_1) \;\;=\;\; \delta(t-t_1)\;\delta(\Omega-\Omega_1)\;\delta(r-r_1) \tag{7}$$

as required of a Green function. Now consider adding an interaction in the form of a multiplication by a function $U(t,\Omega,r)$ of the state $f(t,\Omega,r|0,\Omega_0,O)$:

$$\left[\frac{\partial}{\partial t} \;+\; \Omega \cdot \nabla_r \;-\; \frac{D}{2}\Delta_\Omega \;+\; \lambda\right] f(t,\Omega,r|0,\Omega_0,O) \;\;=\;\; U(t,\Omega,r)\; f(t,\Omega,r|0,\Omega_0,O) \tag{8}$$

This is reminiscent of the diffusional imaginary-time Schrödinger equation of motion:

$$\left[\frac{\partial}{\partial \tau} \;+\; H\right] \Psi(r,\tau) \;\;=\;\; -\frac{2m}{\hbar^2}\; U(r,\tau)\; \Psi(r,\tau) \tag{9}$$

where $\tau = i\hbar t/2m$, H is the "free" or "unperturbed" Hamiltonian, and U the interaction potential. The distinction is that in eqn (8) f is a classical probability density, while in the Schrödinger equation Ψ is a quantum mechanical probability amplitude. However, in either case U has the effect of modifying the solution so that it is distinct from the free solution $e^{-\lambda t} f_{\text{diff}}$ or Ψ_{free} , reflecting the influence of the interaction. Following the standard procedure of quantum mechanics, eqn (8) may be rewritten in the form of an integral equation:

$$\begin{aligned} f(t,\Omega,r|0,\Omega_0,O) \;=\; & e^{-\lambda t}\; f_{\text{diff}}(t,\Omega,r|0,\Omega_0,O) \\ +\; & \int_S d\Omega_1 \int_{\mathbb{R}^3} dr_1 \int_{-\infty}^{\infty} dt_1\; G(t,\Omega,r|t_1,\Omega_1,r_1)\; U(t_1,\Omega_1,r_1)\; f(t_1,\Omega_1,r_1|0,\Omega_0,O) \end{aligned} \tag{10}$$

where S is the unit sphere in momentum space. Now consider a potential operator $\hat{U}$ which is defined for an integrable function f as follows:

$$\hat{U}\; f(t,\Omega,r|t_1,\Omega_1,r_1) \;\;:=\;\; \lambda \int_S d\tilde{\Omega}\; p(\tilde{\Omega})\; f(t,\Omega-\tilde{\Omega},r|t_1,\Omega_1,r_1) \tag{11}$$

The interaction $\hat{U}$ is a coupling of a weighted sum of probability densities for all trajectory directions at point r. The coupling constant λ is the inverse of the expected interarrival time between hard collisions. The weight $p(\tilde{\Omega}) = \frac{1}{\sigma}\frac{d\sigma}{d\tilde{\Omega}}$ is the scattering probability density. A density $f(t,\Omega-\tilde{\Omega},r|t_1,\Omega_1,r_1)$ is most heavily weighed for highly probable scattering angles, and the entire interaction more significantly influences the density as λ increases, or as the interarrival time between hard collisions decreases. With $\hat{U}$ the equation of motion becomes:

$$\left[\frac{\partial}{\partial t} \;+\; \Omega \cdot \nabla_r \;-\; \frac{D}{2}\Delta_\Omega \;+\; \lambda\right] f(t,\Omega,r|0,\Omega_0,O) \;\;=\;\; \lambda \int_S d\tilde{\Omega}\; p(\tilde{\Omega})\; f(t,\Omega-\tilde{\Omega},r|0,\Omega_0,O) \tag{12}$$

which has the integral-equation representation:

$$\begin{aligned} f(t,\Omega,r|0,\Omega_0,O) \;=\; & e^{-\lambda t}\; f_{\text{diff}}(t,\Omega,r|0,\Omega_0,O) \\ +\; & \lambda \int_S d\Omega_1 \int_{\mathbb{R}^3} dr_1 \int_{-\infty}^{\infty} dt_1 \int_S d\tilde{\Omega}\; p(\tilde{\Omega})\; G(t,\Omega-\tilde{\Omega},r|t_1,\Omega_1,r_1)\; f(t_1,\Omega_1,r_1|0,\Omega_0,O) \end{aligned} \tag{13}$$

Substituting the Green function of eqn (5) yields:

$$\begin{aligned} f(t,\Omega,r|0,\Omega_0,O) \;=\; & e^{-\lambda t}\; f_{\text{diff}}(t,\Omega,r|0,\Omega_0,O) \\ +\; & \lambda \int_S d\Omega_1 \int_{\mathbb{R}^3} dr_1 \int_{-\infty}^{t} dt_1\; e^{-\lambda(t-t_1)} \int_S d\tilde{\Omega}\; p(\tilde{\Omega})\; f_{\text{diff}}(t,\Omega-\tilde{\Omega},r|t_1,\Omega_1,r_1) \\ & \times\; f(t_1,\Omega_1,r_1|0,\Omega_0,O) \end{aligned} \tag{14}$$

where the upper limit if the time integration is changed to t and the Heaviside function omitted. The interpretation of eqn (14) is perhaps most clear via iteration, analogous to the Born series interpretation in quantum scattering. The source term or free solution $e^{-\lambda t} f_{\rm diff}(t, \Omega, r|0, \Omega_0, O)$ represents the density of particles arriving at r, heading in direction Ω, at time t, which departed from the origin at time 0, initially heading in direction Ω_0, and which have experienced no (hard) collisions, no jumps, during their journeys. However, on their respective journeys the particles' directions changed continuously according to a Brownian motion on S in momentum space, as represented by $f_{\rm diff}$. Added to this is the first-order term:

$$\lambda \int_S d\Omega_1 \int_{\mathbb{R}^3} dr_1 \int_{-\infty}^{t} dt_1\, e^{-\lambda(t-t_1)} \int_S d\tilde{\Omega}\, p(\tilde{\Omega})\, f_{\rm diff}(t, \Omega, r|t_1, \Omega_1 + \tilde{\Omega}, r_1) \times e^{-\lambda t_1} f_{\rm diff}(t_1, \Omega_1, r_1|0, \Omega_0, O) \tag{15}$$

representing the density of particles with these same initial and final states, but which experienced one hard collision at an intermediate location r_1, at an intermediate time $0 < t_1 < t$, while heading in direction Ω_1, which abruptly changed the direction of travel by the scattering vector $\tilde{\Omega}$. However, before and after this hard collision the particles' directions changed continuously according to a Brownian motion on S in momentum space. Note the equality $f_{\rm diff}(t, \Omega - \tilde{\Omega}, r|t_1, \Omega_1, r_1) = f_{\rm diff}(t, \Omega, r|t_1, \Omega_1 + \tilde{\Omega}, r_1)$, valid for a homogeneous target medium, is used to facilitate the interpretation. Added to this is the second-order term representing particles that experienced two hard collisions during their journeys, and so forth.

Because eqn (12) is precisely eqn (2) with δ-function initial conditions, the Fredholm type 2 integral eqn (14) is the integral-equation representation with δ-function initial conditions of eqn (1), which is eqn (4.10) in [1]. Given $f_{\rm diff}$, eqn (14) may be solved using off-the-shelf Monte Carlo and variance reduction techniques. The computational complexity of Fredholm type 2 integral equations is well understood, and the convergence properties of the Neumann series solution have been thoroughly analyzed.

3. DIRECT DERIVATION

Further understanding of eqn (14) is possible via a direct derivation of the integral equation. We apply the standard thought-process of particle transport modeling. The probability of an outgoing particle from a collision occurring at time t in volume element dr at r and exiting in a direction within the solid angle $d\Omega$ about Ω is denoted $f_{\rm out}(t, \Omega, r|0, \Omega_0, O)\, d\Omega\, dr$. where the initial condition $0, \Omega_0, O$ is included in the notation. On the other hand, the probability of an incoming particle into a collision to occur in volume element dr at r and entering from a direction within the solid angle $d\Omega$ about Ω is denoted $f_{\rm in}(t, \Omega, r|0, \Omega_0, O)\, d\Omega\, dr$. Assume a new-particle density or source density $s(t, \Omega, r|0, \Omega_0, O)$. As in §2 the interarrival time between hard collisions is assumed to be distributed exponentially. The probability that the interarrival time between successive hard collisions lies between $t - t_1$ and $t - t_1 + d(t - t_1)$ is:

$$\lambda\, e^{-\lambda(t-t_1)}\, d(t - t_1) \tag{16}$$

where λ is a positive constant. Thus:

$$\int_0^{\infty} \lambda\, e^{-\lambda(t-t_1)}\, d(t - t_1) \;=\; 1 \;=\; \int_{-\infty}^{t} \lambda\, e^{-\lambda(t-t_1)}\, dt_1 \tag{17}$$

where the second integration is valid for fixed t. Therefore, the probability of an incoming particle at (t, Ω, r) is the sum of the probabilities of all outgoing particles multiplied by the probability of their reaching (t, Ω, r) and experiencing a hard collision at time t:

$$f_{\rm in}(t,\Omega,r|0,\Omega_0,O) \quad (18)$$
$$= \lambda \int_S d\Omega_1 \int_{\mathbb{R}^3} dr_1 \int_{-\infty}^{t} dt_1\, e^{-\lambda(t-t_1)}\, f_{\rm diff}(t,\Omega,r|t_1,\Omega_1,r_1)\, f_{\rm out}(t_1,\Omega_1,r_1|0,\Omega_0,O)$$

Meanwhile the probability of an outgoing particle at (t,Ω,r) equals the source at (t,Ω,r) plus probabilities of all incoming particles multiplied by the probability of their being scattered into $d\Omega$ about Ω:

$$f_{\rm out}(t,\Omega,r|0,\Omega_0,O) = s(t,\Omega,r|0,\Omega_0,O) + \int_S d\tilde{\Omega}\, p(\tilde{\Omega})\, f_{\rm in}(t,\Omega-\tilde{\Omega},r|0,\Omega_0,O) \quad (19)$$

where $p(\tilde{\Omega})$ is the probability density of the scattering angle and previously defined for eqn (11). The source term consists of particles that are outgoing from the volume element dr at r and in a direction within the solid angle $d\Omega$ about Ω, but which do not arise from a collision in dr. These then must be particles that have journeyed to (t,Ω,r) from $(0,\Omega_0,O)$ multiplied by the probability that the arrival time of their first collision exceeds t: $s(t,\Omega,r|0,\Omega_0,O) = e^{-\lambda t}\, f_{\rm diff}(t,\Omega,r|0,\Omega_0,O)$. Substituting this source term and eqn (18) into eqn (19) yields an integral equation for $f_{\rm out}$ which is precisely eqn (14). In similar fashion an integral equation for $f_{\rm in}$ may be obtained.

4. CONCLUSIONS

The model of elastic scattering as a mixed diffusion-jump stochastic process, developed in [1], may be reformulated as a standard Fredholm type 2 integral equation. The reformulation facilitates physical interpretation of the model, allows for off-the-shelf Monte Carlo solution recipes, and provides access to a considerable variety of well-known variance-reduction techniques. Future work includes incorporating the small-angle approximation of $f_{\rm diff}$.

ACKNOWLEDGEMENTS

This research has been funded in part by the Shared University Research Grants [SUR] from International Business Machines Inc., and the Indiana Genomics Initiative [INGEN]. The Indiana Genomics Initiative of Indiana University is supported in part by Lilly Endowment Inc.

REFERENCES

[1] L. Papiez and V. Tulovsky, "A stochastic model of the evolution derived from elastic velocity process with mixed diffusion-jump characteristics," *Mathematical Models and Methods in Applied Science*, **Vol. 12, No. 7**, pp. 921–941 (2002).

[2] X. Ning, L. Papiez, and G. Sandison, "Compound-Poisson-process method for multiple scattering of charged particles," *Physical Review E*, **Vol. 32, No. 5**, pp. 5621–5633 (1995).

[3] C. W. Gardiner, *Handbook of Stochastic Methods: For Physics, Chemistry and the Natural Sciences*, Springer Verlag (1996).