STUDY OF THE SLOWING DOWN OF HIGH ENERGY PROTON SHOTS THROUGH METALS VIA A MONTE CARLO SIMULATION OF THE FOKKER-PLANCK EQUATION

by

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The aim of this work is to analyze the diffusion and the slowing down of high energy proton shots through a target. Analyzing the phenomenon rigorously, with the full transport equations, means tackling many difficulties, most of which arise from the long range nature of the Coulomb interactions, involving more than one particle simultaneously. The commonly used approach of neglecting the multi-body collisions, though correct for rarefied neutral gases, often leads to very poor approximations when charged particles moving through dense matter are considered. Here we present a Monte Carlo simulation of the Fokker-Planck equation where the multi-body collisions are taken into account. The model allows the calculation of a point-wise distribution of energy and momentum transferred to the target.

Key words: Fokker-Planck equation, Monte Carlo simulation, charged particles, multiple interactions

INTRODUCTION

When charged particles move through solid matter, energy and momentum exchanges occur through a large variety of processes in which the electromagnetic interactions predominate. Analyzing the system by the transport equation means to tackle many difficulties, most of which arise from the long range nature of the Coulomb interactions. The commonly used approximation of neglecting the multi-body collisions often leads to very poor approximation when solid matter is considered.

In this paper, a numerical simulation of the Fokker-Planck equation is presented, where the multi-body collisions are taken into account.

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THE FOKKER-PLANCK EQUATION

Let's focus our attention on a proton which moves through a target. The trajectory of the test particle in the phase space can be studied as the Brownian motion of a heavy particle within a medium composed of a large number of light particles: the heavy particle undergoes many collisions with little energy and momentum exchange. In the long run, these interactions lead the system toward the equilibrium. In this paper, protons impinging on a solid target are considered, which is the reason why the test particle mass is smaller than the field particle masses; however, most interactions are "large" impact parameter shielded collisions and the deflections are accordingly small.

It is known that the Brownian motion can be studied as a stochastic process whose mathematical formulation is the Fokker-Planck equation [1, 2, 3]. After introducing a function $\varphi(\vec{v},\Delta\vec{v})$, which represents the probability that a particle with speed $\vec{v}$ undergoes a velocity variation $\Delta\vec{v}$ within the time Δt, the distribution function f can be determined by solving the equation:

$$\frac{\partial}{\partial t} f(\vec{r},\vec{v},t) + \vec{v} \cdot \vec{\nabla} f(\vec{r},\vec{v},t) = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \vec{\nabla}_v^n (\alpha^n f) \quad (1)$$

where the coefficients α^n are obtained averaging the powers of $\Delta \vec{v}$:

$$\alpha^n = \frac{1}{\Delta t} \int (\Delta \vec{v})^n \varphi(\vec{v}, \Delta \vec{v}) d(\Delta \vec{v}) \qquad (2)$$

The first two terms of the above series are referred to as the dynamical friction factor, $\langle \Delta \vec{v} \rangle$, and the diffusion velocity tensor, $\langle \Delta \vec{v} \Delta \vec{v} \rangle$.

To determine these coefficients, knowledge of interaction processes that allows calculating explicitly the transition probability function $\varphi(\vec{v}, \Delta \vec{v})$ is needed. Usually, a Boltzmann type assumption is made and only binary collisions are considered.

Presented here is a numerical simulation where the effects of large impact parameter multi-body collisions are considered.

NUMERICAL SIMULATION

One of the main difficulties in simulating the trajectory of a charged particle through solid matter consists in the fact that one cannot speak of a mean free path. Due to the long range nature of the Coulomb force, the particles interact continuously.

By using the molecular dynamics technique, the trajectory of each particle is built calculating the positions, $\vec{r}_1$, $\vec{r}_2$, ..., $\vec{r}_N$, and the velocities, $\vec{v}_1$, $\vec{v}_2$, ..., $\vec{v}_N$ at the end of the time intervals Δt_1, Δt_2, ..., Δt_N into which the story is divided. After choosing the number and the length of the intervals opportunely, the electric field acting on the test particle is assumed constant within each interval and calculated starting from a given probability distribution which depends on target composition and density. In this way, the transition probability from point $(\vec{r}_k, \vec{v}_k)$ to point $(\vec{r}_{k-1}, \vec{v}_{k-1})$ is governed by the force

$$\vec{F} = -\nabla U(\vec{r}) \qquad (3)$$

generated by the multi-body potential

$$U(\vec{r}) = \sum_{i=1}^{N} \frac{1}{4\pi\varepsilon_0} \frac{eq_i}{\|\vec{r}_i - \vec{r}\|} \qquad (4)$$

here expressed as sum of pair potentials which are simpler to implement into a program. In equation [4], e is the electron charge, q_i is the i-th field particle charge, and ε_0 is the vacuum dielectric constant. The computation of $U(\vec{r})$, which demands the knowledge of the target particle distribution function, is the central problem. If treated without any approximation, the effect of all the particles in the system must be taken into account and the equation of motion must be solved for each particle. This increases dramatically the run time of the code.

The equation of motion is solved only for the test particle. The distribution of field particles, both in physical and momentum space, is determined from the knowledge of their distribution function. A test particle is assumed to interact only with the field particles contained in a spherical volume S_F whose radius is of the order of the Fermi length

$$\lambda_F = \sqrt{\frac{2\varepsilon_0 E_f}{3ne^2}} \qquad (5)$$

where E_f is the Fermi energy and n is the electron gas mean density. A further hypothesis is that the probability of finding N particles within the Fermi sphere follows Poisson distribution

$$p_N = \frac{n_F^N}{N!} e^{-n_F} \qquad (6)$$

where n_F is the mean number of particles containe in S_F, which depends on the target density. In this way, the potential is given by the sum of the terms

$$U(\vec{r}) = \sum_{i=1}^{N} \frac{1}{4\pi\varepsilon_o} \frac{eq_i}{\|\vec{r}_i - \vec{r}\|} + U_2(\vec{r}) \qquad (7)$$

where $U_2(r)$ is the potential due to the particles outside of the Fermi sphere. At each step, after determining the number and position of the target particles in S_F, it is possible to evaluate the force accelerating the test particle:

$$\vec{F} = e \sum_{s=1}^{S} \sum_{i=1}^{N_s} \frac{1}{4\pi\varepsilon_0} \frac{q_s}{\|\vec{r}_{s,i} - \vec{r}\|^3} (\vec{r} - \vec{r}_{s,i}) - \nabla U_2(\vec{r}) \qquad (8)$$

where the subscript s refers to the s-th field particle species. When a proton interacts with an atom at very short distance, $i.\,e.$, when the impact parameter is shorter than the atomic radius, instead of eq. 8 the following equation is used

$$\vec{F} = \frac{1}{4\pi\varepsilon_0} \frac{Ze^2 e^{-\lambda_F \|\vec{r} - \vec{r}_0\|}}{\|\vec{r}_0 - \vec{r}\|^3} (\vec{r} - \vec{r}_0) - \nabla U_2(\vec{r}) \qquad (9)$$

being $\vec{r}_0$ the position of the atom. In this case the proton interacts with the screened field of the nucleus. Applying the model to a metal target, in order to evaluate $U_2(\vec{r})$, the nearly free electron gas approximation was used, considering the metal (aluminum) as a dense plasma composed by free electrons and once-ionized atoms. The proton is viewed as a travelling charge that induces a displacement field in the electron gas of the target. Hence, ∇U_2 is a frictional term which dissipates the energy of the proton. Poisson's equation was used to determine the electrostatic potential whose gradient in the di-

rection of motion is the stopping power. By using the Fourier transform, one finds [4]

$$\frac{dE}{ds} = \frac{2\hbar^2}{\pi a_o m v^2} \int \frac{p \, \omega}{\left(p^2 + \frac{\omega^2}{v^2}\right)} \Im\left(\frac{1}{\varepsilon(p,\omega)}\right) dp \, d\omega \quad (10)$$

where a_0 is the Bohr radius, $\omega = E/\hbar$, p is the $\vec{p}$ component perpendicular to the direction of the motion and $\Im$ denotes the imaginary part of the argument. The following hypothesis is made

$$\overline{U}_2 = \frac{dE}{ds} \frac{\vec{v}}{v} \quad (11)$$

In determining the dielectric function $\varepsilon(p,\omega)$, one can use the relationship [5]

$$\frac{\partial}{\partial E} f(p, E) = \frac{2E}{\pi E_p^2} \Im\left(\frac{1}{\varepsilon(p,\omega)}\right) \quad (12)$$

where

$$E_p = \sqrt{\frac{\hbar^2 e^2}{m_e \varepsilon_0} n} \quad (13)$$

is the plasmon energy, describing the collective oscillation of the electron gas, with one electron from each atom. The function f is the generalized oscillator strength (GOS) given by [6]:

$$f(p, E) = \frac{2mE}{\hbar^2 p^2} \left| M_{if} \right|^2 \quad (14)$$

where M_{if} is the matrix element for optical dipole transition. Under the action of the force $\vec{F}$ the proton acquires the acceleration $\vec{a}_k$ and undergoes the transitions:

$$\vec{v}_{k+1} = \vec{v}_k + \vec{a}_k \Delta t \quad (15)$$

and

$$\vec{r}_{k+1} = \vec{r}_k + \vec{v}_k \Delta t + \frac{1}{2} \vec{a}_k (\Delta t)^2 \quad (16)$$

from state $(\vec{r}_k, \vec{v}_k)$ to state $(\vec{r}_{k+1}, \vec{v}_{k+1})$.

APPLICATION OF THE MODEL

The model has been used to study the slowing down of 1.5 MeV protons through an aluminum target.

The space distribution of free electrons and once-ionized atoms within the target has been considered uniform. The probability of finding one of these particles in a shell of thickness dr, at a distance r from the test particle, is given by

$$p(r)dr = \frac{4\pi r^2 \, dr}{\frac{4}{3}\pi \lambda_F^3} = \frac{3r^2}{\lambda_F^3} dr \quad (17)$$

and the cumulative probability of finding a particle at a shorter distance than r will be

$$\int_0^r p(t)dt = \frac{r^3}{\lambda_F^3} \quad (18)$$

Concerning the momentum space, a Fermi distribution was assumed for free electrons and a Maxwellian distribution for the atoms. Figure 1 shows the proton range obtained for different proton initial energies. In fig. 2, one can see the proton distribution as a function of depth, at time 10^{-9} s.
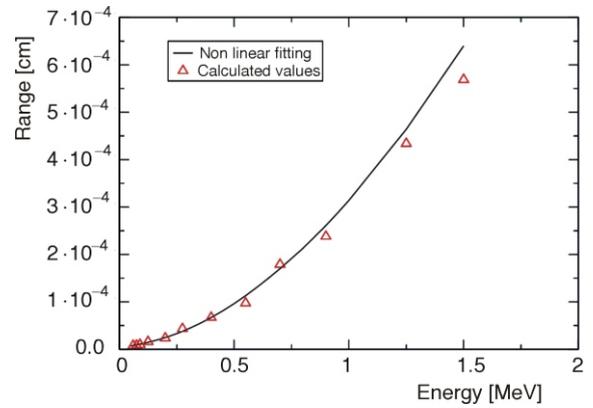
Figure 1. Proton range
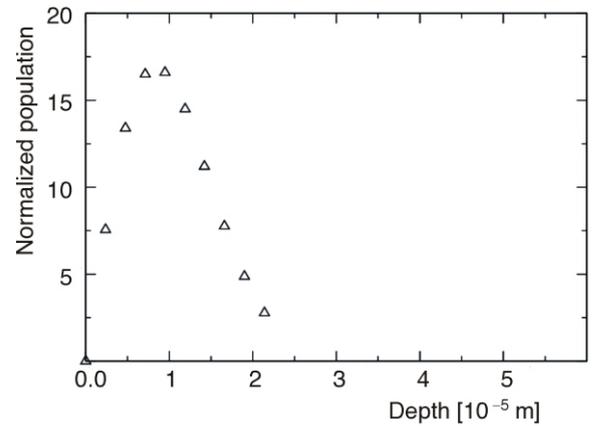
Figure 2. Proton space distribution at time 10^{-9} s

Figure 3 shows the proton energy distribution for a proton shot of 1.5 MeV, at depth 10^{-7} m. One can see that the spectrum is almost monochromatic. Figure 4 depicts the proton spectrum at depth 10^{-6} m, where the momentum straggling of the proton beam is sensibly increased.

These simulations show that within a thickness of 10^{-5} m the protons are completely
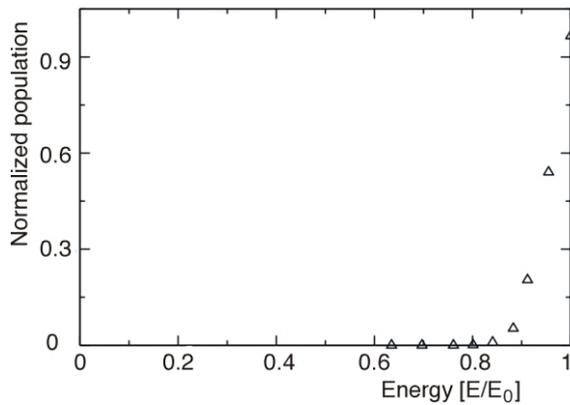
Figure 3. Proton spectrum at 10^{-7} m
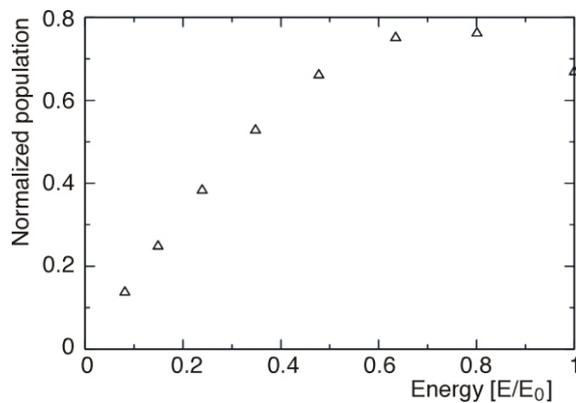
Figure 4. Proton spectrum at 10^{-6} m

thermalized. The time of the process is smaller than 10^{-7} s.

CONCLUSIONS

A numerical code that describes the diffusion of heavy ions through metallic targets has been presented. The commonly used approximation of neglecting multi-body collisions has been removed. The code was originally developed for plasmas [7] and then modified to describe heavy charged particle diffusion through solid matter [8].

The aim of this work is to obtain a Monte Carlo code that gives an exhaustive description of the slowing down process. At present, the code is still in its developmental stage. However, it has been possible to test it in order to describe the high energy proton diffusion through an aluminum sample, estimating the proton range and the proton spreading, both in the physical and the momentum space.

The knowledge of energy spectrum is important in fields such as micro-beam analysis [9] and radiation protection [10], where quantifying and identifying the reactions produced in the medium is of fundamental interest, as the phenomena induced depend on the energy of the interacting particles.

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Франческо ТЕОДОРИ, Винћенцо МОЛИНАРИ

ИСТРАЖИВАЊЕ УСПОРАВАЊА ВИСОКОЕНЕРГЕТСКОГ ПРОТОНА КОЈИ ПРОДИРЕ КРОЗ МЕТАЛЕ ПОСРЕДСТВОМ МОНТЕ КАРЛО СИМУЛАЦИЈЕ ФОКЕР-ПЛАНКОВЕ ЈЕДНАЧИНЕ

Сврха овог рада је проучавање дифузије и успоравања високоенергетског протона испаљеног у мету. Строга анализа ове појаве, помоћу потпуних транспортних једначина, представља подухват пун тешкоћа од којих многе потичу од природе Кулонових интеракција дугог домета које укључују више од једне честице истовремено. Уобичајено занемаривања вишечестичних судара, мада исправан приступ за разрђене неутралне гасове, често води врло слабим апроксимацијама када се разматра кретање наелектрисаних честица кроз густе материјале. Овде је приказана Монте Карло симулација Фокер-Планкове једначине са урачунатим вишечестичним сударима. Модел допушта израчунавање тачкасте расподеле енергије и момента пренетих на мету.

Кључне речи: *Фокер-Планкова једначина, Монте Карло симулација, наелектрисане честице, вишеструке интеракције*