The Importance of Elastic Scattering to Particle Direction Determination in Monte Carlo Calculations of DT Reactions in Flight

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THE IMPORTANCE OF ELASTIC SCATTERING TO PARTICLE DIRECTION DETERMINATION IN MONTE CARLO CALCULATIONS OF DT REACTIONS IN FLIGHT

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ABSTRACT

The importance of single, large-angle, nuclear-coulombic, nuclear-hadronic, hadronic-coulombic interference, and multiple nuclear-coulombic scattering is investigated for tritons incident on deuterium, iron, and plutonium for very high temperatures and densities and for ordinary liquid and solid densities at low temperature. Depending on the accuracy desired, we conclude that for 10-keV-temperature DT plasmas it is not necessary to include elastic scattering deflection in reaction-in-flight calculations. For higher temperatures or where angular accuracies greater than 10° are significant or for higher Z targets or for other special circumstances, one must include elastic scattering from coulomb forces.

I. INTRODUCTION

In the passage of a deuteron or triton through a DT plasma it is of interest to know the deflection of the incident particle caused by elastic scattering because such deflection will, of course, add to the angular distribution of any subsequent interactions, i.e., to the final extra thermal neutrons. We will show that at low projectile energies the elastic scattering of projectiles by target nuclei is important (indeed dominant) in the slowing down in high-temperature plasmas and that large angular scattering is possible. However, we believe that the numbers do not justify the inclusion of elastic scattering in reaction-in-flight (RIF) calculations unless the temperature exceeds 10 keV or so, although we offer a formalism for the inclusion of the effect if desired. It turns out that multiple electronic nuclear scattering is the major source of the deflections; nuclear forces or hadronic scattering is also important. Ten to fifty times larger deflections occur in heavier media. We give a representative calculation of the various relevant quantities.

II. THE SCATTERING ANGLE AND CROSS SECTION OF THE COULOMB FIELD DEFLECTION OF A CHARGED PARTICLE: RUTHERFORD SCATTERING

As a heavy charged particle passes through matter, it loses energy through being deflected by: (a) electrons, (b) nuclei from both coulomb and hadronic elastic scattering plus their interference, (c) nuclear reactions which can change the particle or its parameters, and (d) nuclear bremsstrahlung (a small effect). In the RIF patch, the coulomb interactions with electrons and nuclei are explicitly accounted for in slowing down of the charged particles, but not the resulting angular deviations. The angular deviation of a heavy ion caused by electrons is negligible; that by ions may not be. The possible change in angle in a single collision can be large, although usually with low probability. In this section we give the probability and angles of coulomb deflections, i.e., deflections by the electrostatic repulsions of ions from the target nuclei. For like particles, particular quantum effects come into play because of the indistinguishability of the particles that must be represented in the theory.¹ For unlike particles, the famous Rutherford scattering cross section for charged interactions only is

$$d\sigma_R/d\Omega = \frac{z_1^2 z_2^2 e^4 (m_1 + m_2)^2}{4E_0^2 m_2^2 (2 \sin^2 \frac{\theta}{2})^2} \quad (1)$$

giving the center-of-mass (CM) differential scattering cross section where 1 refers to the incident particle and 2 to the target. Ze is charge, m is mass, E_0 is the initial kinetic energy (laboratory system), and θ is the CM angle of deflection. Equation (1) cannot be used for like particles because particular quantum effects of their distinguishability come into play (see Ref. 1). Note that Eq. (1) blows up at $\theta = 0$, that is, $d\sigma_R/d\Omega = \infty$. Indeed, the total scattering cross section of a "bare" charge is infinite. But bare charges are impossible; they are always neutralized if one goes out far enough, and anyway, the deflections for large cross sections are negligibly small. The Rutherford cross section is indeed strongly peaked forward. The effect is increased in transformation to the laboratory system by the increase of the forward velocity of the center of mass itself. The governing equations² are

$$\tan \theta_L = \sin \theta \left[\left(\frac{m_1}{m_2} \right) + \cos \theta \right]^{-1} \quad (2)$$

and

$$\sigma'_{RL}(\theta_L) = \left[1 + 2 \left(\frac{m_1}{m_2} \right) \cos \theta + \left(\frac{m_1}{m_2} \right)^2 \right]^{3/2} \cdot \left| 1 + \left(\frac{m_1}{m_2} \right) \cos \theta \right|^{-1} \sigma'_R(\theta), \quad (3)$$

where the unlabeled variables refer to the CM system and the variables labeled "L" to the laboratory system.

Computing the momentum given to the incident particle following the collision by matching momenta and energy before and after the collision, and then the postcollision energy of that particle, we can compute the loss of energy from the elastic scattering through an angle θ_L .

$$\Delta E = E_0 \left\{ 1 - \left(\frac{m_1}{m_1 + m_2} \right)^2 \left[\cos \theta_L \pm \sqrt{\cos^2 \theta_L - \left(\frac{m_1^2 - m_2^2}{m_1^2} \right)^2} \right]^2 \right\} \quad (4)$$

where the "+" goes with $\theta_L \leq 90^\circ$ and the "-" with $\theta_L \geq 90^\circ$. Table I gives a numerical sample of these expressions for a 2-MeV triton incident on a deuteron. Unlabeled variables are in CM; those labeled "L" are in the laboratory system. Thus with the exception of the singular point at $\theta_L = 41.81^\circ$, we see that larger angles have much lower cross sections. The singular point at $\theta_L = 41.81^\circ$ is a point of zero measure so it does not invalidate the remark. The singular point is caused by slowdown and the reversal of laboratory angular deflection rate of increase as the CM velocity exceeds the triton velocity in the CM and occurs for $\cos \theta = m_2/m_1$ [see Eq. (3)]. For $m_2 > m_1$ these singular points do not occur.

Table I indeed shows that small-angle scattering is overwhelmingly more likely but does not show the net effect nor compare nuclear scattering with electron scattering. We will compute the mean coulomb scattering angle in Section V, but first we calculate the net effect of the various processes by giving the mean rate of energy loss for each.

TABLE I
RUTHERFORD SCATTERING OF A 2-MeV t ON d

θ	0	10°	20°	30°	60°	90°	120°	131.81°	150°	180°
θ_L	0	2.85°	5.68°	8.45°	16.1°	21.8°	23.4°	41.81°	17.0°	0
$\sigma_R'(b/\text{sr})$	=	35.1	2.23	0.45	0.032	0.006	0.0036	0.0029	0.0023	0.0020
$\sigma_{RL}'(b/\text{sr})$	=	218.9	13.8	2.8	0.192	0.047	0.033	=	0.0041	0.00051
$\Delta E(\text{MeV})$	0	0.0074	0.029	0.065	0.232	0.418	0.48	1.46	1.74	1.92

III. RATE OF ENERGY LOSS FROM COULOMB ELASTIC SCATTERING OF A HEAVY ION FROM ELECTRONS AND NUCLEI

To compare the net importance in slowing down by the electrons and the nuclei of a target, we calculate the rates of energy loss and compare. The mean or standard deviation of the net angular deflection is to be found in Section V. Following Longmire,³ for electrons labeled 2,

$$\frac{dE}{dx} = - N_2 \cdot 4\sqrt{\pi} Z_1^2 Z_2^2 e^4 \cdot (EkT)^{-1/2} \cdot \ln(2/\theta_m) \cdot \sqrt{m_2/m_1} \cdot \left[\frac{E}{(3/2) kT} - 1 \right] , \quad (5)$$

where N_2 is the electron density, $Z_2 e$ is the electron charge, E is the incident ion energy, $Z_1 e$ the incident ion charge, x is the distance, and kT is the temperature of the plasma target. θ_m , the minimum CM angle, is the larger of

$$\text{Classical: } \theta_m = Z_1 Z_2 e^2 / E \lambda_D \quad (6)$$

or

$$\text{Quantum Mechanical: } \theta_m = \hbar / [\lambda_D \cdot \sqrt{2mE}] , \quad (7)$$

where the Debye length, λ_D , is

$$\lambda_D = \sqrt{kT / 4\pi N_e e^2} . \quad (8)$$

m is the reduced mass:

$$m = m_1 m_2 / (m_1 + m_2) . \quad (9)$$

N_e is the electron density.

For nuclei,³ when $(m_2/m_1)(E/kT) \gg 1$, we have

$$\frac{dE}{dx} = - (N_2/E) \cdot 2\pi Z_1^2 Z_2^2 e^4 \cdot \ln(2/\theta_m) \cdot (m_1/m_2) , \quad (10)$$

where now N_2 is the atom density of target nuclei and $Z_2 e$ their charge.

TABLE II
COULOMBIC ENERGY LOSSES OF A TRITON INCIDENT ON 16-keV TEMPERATURE
DEUTERIUM, IRON, AND PLUTONIUM

Triton Energy (MeV)	Energy Loss to Deuterium at 16 keV, 4 g/cc (MeV/cm)		Energy Loss to Iron at 16 keV, 39.3 g/cc (MeV/cm)		Energy Loss to Plutonium at 16 keV, 200 g/cc (MeV/cm)	
	$\frac{dE}{dx} _{\text{nuclei}}$	$\frac{dE}{dx} _{\text{electrons}}$	$\frac{dE}{dx} _{\text{nuclei}}$	$\frac{dE}{dx} _{\text{electrons}}$	$\frac{dE}{dx} _{\text{nuclei}}$	$\frac{dE}{dx} _{\text{electrons}}$
0.1	25.2	0.58	146.5	3.4	391.8	8.3
1	2.9	3.6	19.3	25.8	56.0	76.8
2	1.5	5.6	10.3	40.4	30.5	122.5
5	0.62	9.7	4.5	71.6	13.5	221.5
10	0.32	14.6	2.4	109.4	7.3	342.5

Choosing rather extreme temperatures and densities of $kT = 16$ keV, $\rho_D = 4$ g/cm³, $\rho_{Fe} = 39.3$ g/cm³, and $\rho_{Pu} = 200$ g/cm³, we get the values of Table II.

Note from Eqs. (5) and (1) that the energy loss to free electrons varies as $(kT)^{-3/2}$, while the energy loss to nuclei is temperature independent so long as $(m_2/m_1)(E/kT) \gg 1$. Therefore, for $E \gg kT$, the dominant loss is to electrons and there is consequently little angular deflection. At high temperatures and incident energies not sufficiently greater than the temperature, nuclear scattering with its possibility of large angles becomes important. Indeed, hadronic and hadronic-coulombic interference scattering can be important, as we discuss in the next section.

IV. RATE OF ENERGY LOSS FROM HADRONIC AND HADRONIC-COULOMBIC INTERFERENCE

This section discusses the energy losses from nuclear scattering interactions and their interference with normal electric (coulombic) elastic scattering. As noted above, because coulombic losses decrease with increasing temperature, nuclear processes automatically become relatively more important. Nuclear processes are already important at $kT = 16$ keV for tritons on deuterium as a comparison of Table III with Table II shows.

V. MULTIPLE COULOMB (OR OTHER) SCATTERING

Table II shows that at low incident energy and high temperature nuclear-coulomb scattering is an important energy loss. Yet Table I implies that the angle of scattering is small but does not say how small

the net effect of many scatterings can be. This section gives that result, namely, the angular distribution from multiple coulomb (or any) scattering. Multiple scattering, being a stochastic process, leads to a normal distribution^{4,5} in the net or final angle of an incident particle in any plane relative to the original directions. If one chooses orthogonal planes, the two Cartesian normal distributions can then be replaced by polar coordinates and the integration over azimuth performed (the distributions are azimuthally symmetric) to give the radial angle, θ , distribution for finding a particle deflected by θ if the variance is $\langle \theta^2 \rangle$:

$$p(\theta) d\theta = (2\theta/\langle \theta^2 \rangle) e^{-\theta^2/\langle \theta^2 \rangle} \cdot d\theta \quad (11)$$

TABLE III

HADRONIC AND HADRONIC-COULOMBIC INTERFERENCE ENERGY LOSS
OF A TRITON INCIDENT ON 4 g/cm³ DEUTERIUM (REF. 1)

E Triton (MeV)	1	2	5	10
dE /dx (MeV/cm) T	≈1.6	2.19	4.76	9.21

If the thickness of the target medium is t or s ($t = \rho s$, ρ is density), then define θ_1 to be that angle for which there is only one collision with $\theta > \theta_1$ in the thickness t or s . Then,^{4,6}

$$\theta_1^2 = 4\pi N_2 Z_1^2 Z_2^2 e^4 \cdot (p_v^2)^{-1} \quad \text{CM system} \quad (12)$$

where s is in centimeters, p is the relative momentum, v the incident velocity, 1 refers to CM system incident, and 2 to target;

$$\theta_1^2 = 0.039228 \cdot t \cdot Z_1^2 Z_2^2 \left(\frac{m_1 + m_2}{m_2} \right)^2 / E_t^2 \quad \text{CM system} \quad (13)$$

for E_t in MeV and t in g/cm²; and

$$\theta_1^2 = 0.039228 \cdot \frac{\rho_2 s}{A_2} \cdot Z_1^2 Z_2^2 \left(\frac{m_1 + m_2}{m_2} \right)^2 / E_t^2 \quad \text{CM system} \quad (14)$$

where thickness s is in centimeters, density ρ_2 in g/cm^3 , triton energy E_t in MeV, and A_2 is the atomic weight of the target.

The angular standard deviation, σ , squared of the distribution is given by:^{4,6}

$$\sigma^2 \equiv \langle \theta^2 \rangle = 2\theta_1^2 \ln(\theta_1/\theta_m) \quad \text{CM system} \quad (15)$$

θ_m is the minimum angle of scattering, given for plasmas in Eqs. (6) and (7).

A more physically meaningful measure of a distribution is the median (the 50th percentile) or for errors, the probable error, which we label τ and define

$$0.5 = \int_0^\tau p(\theta) d\theta \quad (16)$$

Substituting Eq. (11) and performing the integration give

$$\tau = \sqrt{\ln 2} \cdot \sqrt{\langle \theta^2 \rangle} = 0.83255\sigma \quad (17)$$

The transformation [Eq. (2)] from the CM to the laboratory system is, for CM angles not too large, i.e., $\cos \theta < (m_{\text{incident}}/m_{\text{target}})$, an isomorphism and the median transforms into the median.

Choosing a high temperature, $kT = 16$ keV, and very dense materials we give in Table IV the median, τ_L , of the multiple coulomb scattering angular distributions for tritons incident on deuterium, iron, and plutonium calculated from Eqs. (14), (15), (17), and (2) for a distance $s = 0.01$ cm and a fixed incident energy. Note that at lower incident energies and at higher charges of the target atoms, the energy loss is appreciable in passing through the foil so that the assumption of a fixed energy of the projectile is inaccurate and the numbers should be used for comparison only. Such comparative numbers are marked with an asterisk (*).

It is evident from Table IV, with an eye to the range of the triton from $dE/dx/\text{nuclei} + dE/dx/\text{electrons}$ in Table II, that the coulombic multiple scattering leads to median net scatterings of 6 to 10° over the range of the triton to just below about 1 MeV. In heavier material the multiple small-angle electronic scattering is much larger. At lower temperatures the median scattering decreases weakly as

TABLE IV

MULTIPLE COULOMB SCATTERING THROUGH 0.01 cm THICKNESS**
TEMPERATURE, $kT = 16$ keV

Target Isotope and mass density	Incident Triton Energy E_t (MeV)	Minimum Angle of Scatter θ_m (radians)	Laboratory Scattering Angle Median τ_L (degrees)
D (4 g/cm ³)	0.1	4.18(-5)	39.7°
	1.0	7.65(-6)	5.7°
	2	5.41(-6)	2.8°
	5	3.42(-6)	1.1°
	10	2.42(-6)	0.53°
Fe (39.3 g/cm ³)	0.1	1.39(-3)	>180°*
	1.0	1.39(-4)	84.3°*
	2	6.96(-5)	41.6°*
	5	2.79(-5)	16.6°*
	10	1.39(-5)	8.3°*
Pu (200 g/cm ³)	0.1	9.2 (-3)	>180°*
	1.0	9.2 (-4)	>180°*
	2	4.6 (-4)	159.4°*
	5	1.84(-4)	63.2°*
	10	9.2 (-5)	31.6°*

*Indicates significant ($\geq 10\%$) E_t slowing down in the sample distance of 0.01 cm, so that the resulting numbers apply as comparisons or at E_t only.

**Computed on the basis that the $kT = 16$ keV motion of the target is negligible, which is certainly not a good approximation for $E_t = 100$ keV.

$(1/2)\ln kT$ [Eqs. (8), (6), (7), and (15)]. Indeed, for comparison we include the laboratory median, τ_L , for the scattering of tritons by 0.01 cm of deuterium, iron, and plutonium at solid or liquid densities and at nonplasma temperatures. See Table V.

For the minimum scattering angle in un-ionized media we used the larger of:⁶

$$\text{Classical: } \theta_m = 3.8 Z_2^{4/3} e^2 (m_1 + m_2) / (2 m_2 E_t a_0) \quad (18)$$

or

$$\text{Quantum Mechanical: } \theta_m = 2.10 Z_2^{1/3} \sqrt{m_1 + m_2} / \left(m_2 \sqrt{2 m_1 E_t} a_0 \right), \quad (19)$$

where $a_0 \equiv \hbar^2 / m_e e^2$ is the Bohr radius, 1 refers to the incident triton, and 2 to the target nucleus. The values used are found in Table V.

TABLE V
MULTIPLE COULOMB SCATTERING
LIQUID AND SOLID DENSITIES (UN-IONIZED), 0.01-cm THICKNESS

Target Isotope and Mass Density	Incident Triton Energy (MeV)	Minimum Scattering Angle θ_m (radians)	Rate of Energy Loss with Distance dE_t/dx (MeV/cm)	Median Laboratory Scattering Angle τ_L (degrees)*
D (0.14 g/cm ³)	0.1	1.29(-3)	2.5(2)	4.82°
	1.0	2.61(-4)	1.2(2)	0.44°
	2	1.84(-4)	67	0.21°
	5	1.17(-4)	33	0.077°
	10	8.25(-5)	17	0.036°
Fe (7.96 g/cm ³)	0.1	0.042	1.6(3)	$\sigma > 180^\circ$
	1.0	0.0042	1.8(3)	25.7°
	2	0.0021	1.3(3)	12.8°
	5	0.00084	8.0(2)	5.1°
	10	0.00042	4.9(2)	2.6°
Pu (19.84 g/cm ³)	0.1	0.224	1.9(3)	$\sigma > 180^\circ$
	1.0	0.0224	2.2(3)	64.8°
	2	0.0119	1.5(3)	32.3°
	5	0.00448	9.3(2)	12.9°
	10	0.00224	6.4(2)	6.5°

*The median values in this column are computed on the basis that the energy remains as given in column two throughout the thickness of 0.01 cm, which column four shows cannot be true. Hence, these values are so to speak initial values per 0.01-cm thickness and are meant to be comparative only.

dE_t/dx is taken from the encyclopedic work of Anderson and Ziegler.⁷ For the rest of Table V we used Eqs. (14), (15), (17), and (2).

VI. DISCUSSION AND CONCLUSIONS

At very high temperatures, because the energy loss of a charged particle to electrons varies roughly as $(kT)^{-3/2}$ [Eq. (5)], the usual dominant electron losses (Table V) begin to be dominated by nuclear losses at 16-keV temperature (Table II), especially at lower incident energy. Nuclear interactions imply much greater angular deflections, although the greatest probability still is for slight deflections (Table I). However, two questions remain: (1) can the multiple nuclear coulomb scatterings add up to a significant net deflection, and (2) what is the effect of hadronic (i.e., nuclear forces) scattering? If 10° (or 20°) or so is a negligible deflection, one can ignore multiple coulomb elastic scattering (Table IV) of triton on deuterons or deuterons on tritons at $kT \leq 16$ keV, but not on higher Z targets. For higher Z or higher temperatures or for better than 10 - 20° angular accuracy over the full range of a deuteron or triton, one is going to have to sample a normal distribution [Eq. (11), two dimensional] over the deflection angle with variance given by Eq. (15). In practice, one suspects that each case might have to be examined individually to see if this complication is really necessary.

Comparing Tables III and II for tritons on deuterium we see that already at 16-keV temperature the hadronic energy loss is significant. And, as a rule of thumb, such scatterings at low incident energies always involve large CM angular deflections. The large motion of the CM in deuterium on triton or triton on deuterium ameliorates the large deflections to a degree.

At lower temperatures (the extremes of low temperatures where the targets are not ionized are given in Table V), the rate of energy loss to the electrons is so great that the chance of large-angle scattering by the nuclei is reduced to negligible. Note that the large angles shown in Table V are often not realizable because energy degradation is so swift that the triton range is less than the thickness, 0.01 cm, for which the net deflections were calculated.

We conclude (depending on the accuracy desired) that for, say, ≤ 10 keV DT plasma temperatures it is not necessary to include elastic scattering deflections in the RIF patch. For higher DT temperatures or where 10° is an important random deflection or for special circumstances, i.e., where rare large scattering could be important, elastic scattering from nuclear forces and multiple elastic scattering from coulomb force must be included.

The angular deflections from multiple scattering of heavy ions from electrons are taken to be negligible.

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