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Transfer Cross Section Matrix for Elastic Nuclear Scattering
of Low Z Ions in Deuterium

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Transfer Cross Section Matrix for Elastic Nuclear Scattering of Low Z Ions in Deuterium

Some discussion and work has been devoted^{1,2} to the extraction of cross sections for the elastic scattering of charged particles by the nuclear force field. This utilization of such cross sections was incorporated into some Monte Carlo codes along with the effects of the long range Coulomb force field, which dominate at very small scattering angles.

Attempts are now being made to include the large angle nuclear scattering into codes that use multigroup diffusion of energetic ions slowing down in a plasma, which is considered predominantly deuterium. If the nuclear scattering cross section matrix σ_{if} is known, where "i" and "f" denote the initial and final energy groups of an energetic ion, the ion density in group i has the following time rate of change due to nuclear scattering:

$$\frac{\partial n_{P_i}}{\partial t} = -n_D n_{P_i} v_{P_i} \sum_{f>i} \sigma_{if} + n_D \sum_{j<i} n_{P_j} \sigma_{ji} v_{P_j} \quad , \quad (1)$$

where n_{P_i} and v_{P_i} are the density and the speed of ions of species P in group i, n_D is the density of thermal deuterons, and the group structure is considered with the highest energy designated as group 1, with the lower energies in higher numbered groups. Thus the summation f is over lower energy groups into which group i ions can be scattered, and the summation j is over higher energy groups which can be scattered into group i.

The structure of the equation (1) is such that it is very amenable to the same method of solution as is the multigroup diffusion of ions by Coulomb collisions.⁷ The equation for the latter process, which includes the space rate of diffusion, is of the following form:

$$\frac{\partial n_{P_i}}{\partial t} = \nabla \cdot D_{P_i} \nabla n_{P_i} - n_{P_i} / \tau_{P_i} + S_{P_i} \quad (1a)$$

where D_{P_i} is the flux limited diffusion operator, S_{P_i} is the particle source rate, and τ_{P_i} is the time of transition of the ion due to Coulomb collisions from group i to the next lower group $i+1$. Hence, equation (1a) can simply be slightly modified to include the two terms (summations) on the R.H.S. of equation (1), which contain the effects of the nuclear scattering. It can then be solved by the method described in reference 7.

The need to include such treatment can easily be observed by considering the case of an energetic triton in a deuterium plasma. Suppose for example that a 5 Mev triton were released (from knock-on neutrons or other ions) in such a plasma at an electron temperature of 50 kev. The triton at 5 Mev has about a 37% probability of reacting in flight with a thermal deuterium before thermalization, if it is assumed to thermalize only via Coulomb collisions.³ At this high energy its reaction cross section is about 100 millibarns, whereas such a cross section rises rapidly to about 5000 millibarns when its energy drops to 180 Kev. Also, the nuclear scattering cross section of the 5 Mev triton is about 1000 m.b., which gives it an appreciable probability of instantaneous scattering down to near the resonance at 180 Kev. It is also possible that it could be scattered to below the resonance (if the ion temperature is fairly low) which would render an in-flight reaction very unlikely. Thus the time history of any one triton will be greatly affected by the nuclear scattering competing with the Coulomb scattering. Also, τ_{P_i} was found to be 0.122 shakes for a 6 Mev deuterium slowing down to 3.5 Mev in a unit density deuterium plasma at an electron temperature of

50 Kev. The corresponding mean scattering time $(n_D \sigma_{if} v_{P_i})^{-1}$ for nuclear scattering (over the same energy interval) was found to be 0.151 shakes.

Thus the cross sections for these two competing processes appear quite comparable over much of the range of the ion energies. At any rate, irrespective of the existence of any possible reaction cross section, the presence of the nuclear scattering will in general effect a more rapid thermalization of the energetic ion in a plasma.

Following the general procedure as in reference 2, to calculate the effect of the nuclear contribution to the elastic scattering, the total (measured) elastic differential cross section was obtained from the "charged particle cross sections book"⁴, published literature⁵ and private communication. From the total differential elastic cross section the calculated Coulomb cross section was subtracted, which resulted in the nuclear cross section (plus that contribution from the nuclear-coulomb interference). Letting $z = \cos \theta$, where θ is the polar scattering angle in the C. M. system, the difference expression

$$\left. \frac{d\sigma}{dz} \right|_{\Delta} (z, E_P) = \left. \frac{d\sigma}{dz} \right|_{\text{meas.}} - \left. \frac{d\sigma}{dz} \right|_{\text{coul.}} \quad (2)$$

was obtained by means of data over the z range from -1 to +1 and for values of E_P (the ion's energy) from the approximate range of 1 to 15 Mev.

$$\left. \frac{d\sigma}{dz} \right|_{\text{coul.}} = \begin{cases} \frac{z_1^2 e^4}{E_P^2} \left[\frac{1}{(1-z)^2} + \frac{1}{(1+z)^2} + \frac{2 \cos \left(\frac{z_1^2 e^2}{\hbar v_o} \ln \frac{1-z}{1+z} \right)}{1-z^2} \right] \\ \frac{z_1^2 z_2^2 e^4 (m_1 + m_2)^2}{4 E_P^2 m_2^2 (1-z)^2} \end{cases} \quad (3)$$

where the upper expression is for like particles and the lower expression for unlike particles.¹ The subscript 1 refers to the projectile particle and 2 refers to the target particle initially "at rest" in the lab system, which in these applications is the deuteron. z_1 and z_2 are the number of charges of the ions, v_0 is the ion's velocity, and m is the mass. The ions selected were the proton, deuteron, triton and alpha. For each ion species and for each value of E_p , the differential nuclear data $\left. \frac{d\sigma}{dz} \right|_{\Delta}$ were integrated numerically over the angular range to yield the "total" cross section vs. E_p . The differential and angle integrated data were supplied to the CLYDE code, which, given the desired energy group structure of the ion, the following transfer cross sections (P→P') were obtained.

$$\sigma(\Delta E_{P_{i+\frac{1}{2}}}, \Delta E_{P'_{j+\frac{1}{2}}}) = \frac{\int_{E_{P_i}}^{E_{P_{i+1}}} \phi(E_{P_i}) dE_{P_i} \cdot 2\pi \int_{z_j}^{z_{j+1}} \left. \frac{d\sigma}{dz} \right|_{\Delta}(z, E_{P_i}) dz}{\int_{E_{P_i}}^{E_{P_{i+1}}} \phi(E_{P_i}) dE_{P_i}} \quad (4)$$

where $\Delta E_{P'_{j+\frac{1}{2}}}$ denotes an energy interval (or group) with the boundaries $E_{P'_j}$ and $E_{P'_{j+1}}$, which correspond to the scattering angle cosines z_j and z_{j+1} . Similarly $\Delta E_{P_{i+\frac{1}{2}}}$ is the initial ion group bounded by E_{P_i} and $E_{P_{i+1}}$. $\phi(E_{P_i})$ is the flux of incident particles in the group $\Delta E_{P_{i+\frac{1}{2}}}$. Such a flux was considered flat (set equal to unity) for these applications.

The CLYDE code interpolates values of $\left. \frac{d\sigma}{dz} \right|_{\Delta}$ over appropriate energy intervals in order to carry out the necessary numerical integration between group boundaries. The z_j limits of the integrals are converted to the corresponding energy values of the scattered ion by means of the formula⁴

$$\frac{E_{p'}}{E_p} = 1 - \frac{2m_1 m_2}{(m_1 + m_2)^2} (1 - \cos \theta) \quad , \quad (5)$$

where E_p and $E_{p'}$ are the projectile ion energies before and after scattering. Hence the integration is effected with the differential cross section over energy space instead of angular space.⁶

For the following ions, the first table is the angle integrated nuclear scattering cross section (numerically integrated by either parabolic fits to the data or by the trapezoidal rule, whichever appeared more appropriate) plotted vs. the ion energy in a deuterium plasma.

The second table is that of the transfer cross section in barns. The group boundaries used here are the following:

Group Number	
1	14.1 MEV
2	14.0
3	10.0
4	7.24
5	4.80
6	2.20
7	0.50
8	0.15
	0.03

The larger table is the result of the transfer cross section calculations repeated for different boundaries, this time with the boundaries at integral MEV values starting at 16 MEV; i.e. group 1 is between 16 and 15 MEV, group 2 is between 15 and 14 MEV, etc. . . . down to group 16 between 1 and 0 MEV.

A. Proton

E_p (Mev)	$\int \frac{d\sigma}{d\Omega} d\Omega$ (Barns)
1.00	2.82
1.50	2.34
2.00	2.13
3.00	1.87
4.00	1.61
5.00	1.50
7.90	1.06
9.70	0.92
20.60	0.37

Incident Group

Emission Group	1	2	3	4	5	6
1	.007	0	0	0	0	0
2	.388	.257	0	0	0	0
3	.124	.254	.278	0	0	0
4	.051	.107	.360	.413	0	0
5	.064	.076	.158	.523	.683	0
6	.067	.109	.215	.409	.880	1.024
7	0	0	0	0	.196	.611
8	0	0	0	0	0	.029

Incident Group

Emission
Group

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	.054	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	.100	.060	0	0	0	0	0	0	0	0	0	0	0	0	0
3	.085	.111	.067	0	0	0	0	0	0	0	0	0	0	0	0
4	.070	.093	.123	.075	0	0	0	0	0	0	0	0	0	0	0
5	.057	.076	.103	.137	.083	0	0	0	0	0	0	0	0	0	0
6	.045	.061	.083	.113	.152	.093	0	0	0	0	0	0	0	0	0
7	.036	.049	.066	.090	.124	.168	.104	0	0	0	0	0	0	0	0
8	.028	.038	.051	.071	.097	.136	.188	.115	0	0	0	0	0	0	0
9	.021	.029	.039	.054	.075	.105	.151	.215	.134	0	0	0	0	0	0
10	.015	.021	.029	.040	.055	.078	.114	.172	.259	.174	0	0	0	0	0
11	.011	.015	.021	.028	.040	.056	.080	.120	.195	.314	.226	0	0	0	0
12	.010	.012	.015	.020	.027	.038	.055	.078	.122	.215	.373	.282	0	0	0
13	.019	.019	.020	.020	.023	.028	.038	.056	.084	.136	.236	.427	.335	0	0
14	.047	.048	.049	.048	.047	.047	.048	.055	.071	.101	.154	.257	.522	.428	0
15	.030	.045	.062	.083	.106	.131	.158	.168	.172	.180	.197	.241	.360	.717	.648
16	0	0	0	0	0	0	.003	.035	.085	.154	.238	.348	.524	.855	1.760

B. Deuteron

E_D (Mev)	$\int \frac{d\sigma}{d\Omega} d\Omega$ (Barns)
0.96	4.52
1.49	4.27
2.01	4.04
2.51	3.84
3.02	3.65
3.50	3.49
4.46	3.19
6.00	2.80
8.20	2.41
10.50	2.13
12.10	2.00
13.80	1.88
16.00	1.79

Incident Group

Emission Group	1	2	3	4	5	6
1	.001	0	0	0	0	0
2	.687	.455	0	0	0	0
3	.201	.383	.482	0	0	0
4	.171	.228	.564	.673	0	0
5	.257	.301	.470	.920	1.235	0
6	.388	.432	.553	.766	1.347	3.845
7	.093	.116	.183	.302	.508	.538
8	.009	.012	.026	.068	.243	.511
9	4×10^{-4}	5×10^{-4}	.001	.003	.013	.096
10	3×10^{-6}	4×10^{-6}	1×10^{-5}	3×10^{-5}	1×10^{-4}	.001

Incident Group

Emission
Group

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	.093	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	.244	.104	0	0	0	0	0	0	0	0	0	0	0	0	0
3	.162	.260	.117	0	0	0	0	0	0	0	0	0	0	0	0
4	.110	.167	.277	.130	0	0	0	0	0	0	0	0	0	0	0
5	.083	.113	.174	.294	.142	0	0	0	0	0	0	0	0	0	0
6	.070	.086	.117	.185	.311	.152	0	0	0	0	0	0	0	0	0
7	.066	.074	.090	.123	.198	.332	.176	0	0	0	0	0	0	0	0
8	.063	.070	.081	.097	.134	.215	.361	.209	0	0	0	0	0	0	0
9	.062	.068	.077	.091	.112	.153	.232	.393	.250	0	0	0	0	0	0
10	.064	.069	.075	.086	.102	.128	.174	.256	.445	.306	0	0	0	0	0
11	.067	.072	.079	.088	.100	.117	.146	.197	.291	.514	.390	0	0	0	0
12	.075	.078	.083	.093	.106	.119	.142	.176	.226	.331	.603	.517	0	0	0
13	.094	.096	.099	.105	.119	.139	.157	.181	.216	.270	.382	.713	.687	0	0
14	.130	.133	.138	.148	.159	.175	.194	.219	.248	.285	.346	.471	.885	.977	0
15	.200	.208	.218	.231	.245	.262	.281	.304	.341	.390	.448	.527	.686	1.183	1.593
16	.230	.253	.277	.301	.321	.344	.388	.442	.517	.617	.758	.959	1.235	1.688	2.676

C. Triton

$E_T(\text{Mev})$	$\int \frac{d\sigma}{d\Omega} d\Omega$ (Barns)
1.80	1.63
2.96	1.12
3.86	1.15
4.46	1.07
5.06	1.08
5.96	1.21
6.87	1.42
7.77	1.63
8.67	1.81
9.57	1.90
10.47	1.88
11.97	1.81
13.49	1.71
14.99	1.59
16.49	1.49

Incident Group

Emission Group	1	2	3	4	5	6
1	.0317	0	0	0	0	0
2	.869	.689	0	0	0	0
3	.147	.254	.479	0	0	0
4	.190	.230	.257	.201	0	0
5	.116	.177	.247	.194	.164	0
6	.311	.438	.644	.582	.591	.213
7	0	.011	.136	.273	.386	.119
8	0	0	0	0	.024	.031

Incident Group

Emission Group	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	.254	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	.374	.269	0	0	0	0	0	0	0	0	0	0	0	0	0
3	.176	.388	.287	0	0	0	0	0	0	0	0	0	0	0	0
4	.060	.168	.399	.301	0	0	0	0	0	0	0	0	0	0	0
5	.025	.053	.157	.402	.311	0	0	0	0	0	0	0	0	0	0
6	.028	.028	.047	.143	.394	.314	0	0	0	0	0	0	0	0	0
7	.042	.036	.033	.044	.126	.373	.301	0	0	0	0	0	0	0	0
8	.061	.057	.050	.043	.046	.109	.332	.260	0	0	0	0	0	0	0
9	.068	.076	.077	.069	.059	.056	.094	.264	.218	0	0	0	0	0	0
10	.067	.077	.088	.096	.094	.083	.072	.084	.192	.130	0	0	0	0	0
11	.057	.070	.083	.096	.109	.118	.108	.085	.079	.138	.081	0	0	0	0
12	.039	.050	.063	.080	.098	.114	.122	.114	.089	.077	.112	.058	0	0	0
13	.029	.033	.040	.051	.066	.084	.097	.099	.090	.071	.071	.121	.060	0	0
14	.038	.045	.054	.062	.068	.074	.081	.081	.076	.060	.053	.080	.169	.077	0
15	.149	.159	.171	.184	.199	.218	.248	.264	.263	.242	.192	.168	.217	.401	.090
16	.090	.120	.157	.203	.260	.332	.428	.520	.582	.616	.635	.659	.690	.845	.228

D. Alpha

E_{α} (Mev)	$\int \frac{d\sigma}{d\Omega} d\Omega$ (Barns)
1.76	1.23
2.86	1.56
3.92	1.19
4.96	1.01
7.02	0.96
16.00	1.64

Incident Group

Emission Group	1	2	3	4	5	6
1	.016	0	0	0	0	0
2	.572	.325	0	0	0	0
3	.186	.228	.157	0	0	0
4	.206	.219	.258	.124	0	0
5	.384	.372	.361	.460	.471	0
6	.129	.192	.305	.402	.780	.288
7	0	0	0	0	.057	.047

Incident Group

Emission Group	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	.195	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	.268	.174	0	0	0	0	0	0	0	0	0	0	0	0	0
3	.124	.235	.153	0	0	0	0	0	0	0	0	0	0	0	0
4	.059	.116	.205	.131	0	0	0	0	0	0	0	0	0	0	0
5	.041	.059	.110	.179	.110	0	0	0	0	0	0	0	0	0	0
6	.048	.049	.061	.105	.158	.088	0	0	0	0	0	0	0	0	0
7	.062	.058	.058	.067	.103	.142	.066	0	0	0	0	0	0	0	0
8	.074	.071	.068	.066	.074	.103	.131	.046	0	0	0	0	0	0	0
9	.080	.081	.079	.077	.076	.082	.106	.125	.026	0	0	0	0	0	0
10	.075	.083	.087	.087	.086	.085	.090	.112	.125	.019	0	0	0	0	0
11	.071	.080	.088	.094	.097	.096	.095	.099	.120	.142	.027	0	0	0	0
12	.104	.098	.096	.100	.106	.110	.110	.107	.109	.143	.180	.052	0	0	0
13	.155	.150	.145	.139	.134	.132	.133	.134	.130	.144	.199	.271	.163	0	0
14	.202	.202	.200	.197	.193	.190	.186	.182	.180	.185	.216	.292	.479	.354	0
15	.043	.071	.101	.132	.164	.197	.231	.257	.259	.257	.260	.310	.422	.663	.167
16	0	0	0	0	0	0	0	.010	.047	.083	.114	.166	.274	.429	.136

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Upon request, these tables can easily be recalculated for any desired group structure or flux spectrum.

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3. The 37% probability can be calculated by using the expression for the space rate of slowing down of a charged particle⁷,

$$\frac{dE_i}{ds} = -Z_i^2 \left[\frac{1.56 \times 10^{-18} \mu_i}{E_i} \sum_x \frac{n_x Z_x^2}{\mu_x} + \frac{1.83 \times 10^{-20} E_i^{1/2}}{\mu_i^{3/2} T_e} \sum_x n_x Z_x \right] \text{ Kev/cm},$$

where E_i , Z_i and μ_i are the energy, charge and mass (in proton mass units) of the charged particle, T_e is the electron temperature of the plasma, and n_x is the number of ions of species x per cm^3 , where the subscript x refers to the field ions through which the charged particle (labelled i) is traveling. E_i and T_e are in kilovolts. Also needed is $\sigma_{\text{react.}}(E_i)$, which is the reaction cross section of the charged particle at energy E_i with a plasma thermal deuteron and can be obtained from Reference 4.

Thus the probability of the charged particle reacting in flight can be written to a good approximation for pure deuterium:

$$P(E_i, T_e) = 1 - \exp \left\{ - \int_0^{E_i} \frac{\sigma_{\text{react.}}(E_i) dE_i}{3/2 k T_e Z_i^2 \left[\frac{7.80 \times 10^{-19} \mu_i}{E_i} + \frac{1.83 \times 10^{-20} E_i^{1/2}}{\mu_i^{1/2} T_e^{3/2}} \right]} \right\}.$$

The foregoing integral can be solved numerically on a computer.

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