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JANUARY 1979

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SCATTERING OF SUPRATHERMAL IONS
BY PARTIALLY IONIZED IMPURITIES

BY

P. L. ANDREWS AND R. J. GOLDSTON

**PLASMA PHYSICS
LABORATORY**

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SCATTERING OF SUPRATHERMAL IONS BY PARTIALLY IONIZED IMPURITIES

P. L. Andrews and R. J. Goldston

Plasma Physics Laboratory, Princeton University
Princeton, New Jersey 08540

ABSTRACT

The pitch-angle scattering of suprathermal ions by partially ionized impurities in laboratory fusion-oriented plasmas is treated using the Thomas-Fermi statistical model for the charge density of the electron cloud and the impulse approximation for the angular deviation resulting from a collision. An analytic approximation to the exact Thomas-Fermi potential for an ion of arbitrary ionization is found and used to calculate the addition required to the classical $\ln \Lambda$ for 10% - 90% ionized impurities and incident energies in the range $(10^{-2} - 10^3) \text{ keV} \times Z_n^{4/3}$ where Z_n is the nuclear charge of the impurity. The correction can be comparable in magnitude to the classical result, e.g., for 40 keV protons incident on 30 times ionized tungsten ions the addition to $\ln \Lambda$ is approximately 6.

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INTRODUCTION

It has been previously recognized that in the calculation of the scattering of energetic protons by partially ionized impurities in laboratory fusion-oriented plasmas, a significant underestimate could occur, due to the contribution from incident protons with impact parameters allowing penetration of the screening electron cloud of the target ion [1]. These protons would in effect be scattered by a greater positive charge than that of the shielded nucleus. In order to treat this problem quantitatively a model is required for the distribution of electronic charge remaining with the impurity ion.

It was also suggested that a statistical model might be used for this purpose [1] and such an approach has several advantages. The Thomas-Fermi statistical model results in a potential that scales with Z_n in depth and with $Z_n^{-1/3}$ in width (Z_n is the nuclear charge), but has a form dependent only on the degree of ionization, A , where $A \equiv Z_s/Z_n$, Z_s being the net, or 'shielded' charge of the ion, $A = 1$ corresponding to a bare nucleus and $A = 0$ to a neutral atom. Hence we need only concern ourselves with the scattering as a function of A and the incident energy while the results can be scaled in the appropriate manner with Z_n to cover the whole range of impurities.

The Thomas-Fermi derived potential has been shown to be a fair approximation to the scattering potential in ion-atom encounters [2]. The theory does have some drawbacks however; as a statistical model it presumes the presence of a large number of electrons and so is unreliable for very low Z_s impurities; also it requires a distinct radial cut-off for the electron density in the case of ions rather than a more physical exponential decay. It in addition disregards exchange effects and other quantum corrections. However for present usage it appears adequately accurate.

The Thomas-Fermi Potential

If the potential at a distance r from the nucleus is $V(r)$ and the radius of the ion is R (all of the electronic charge is confined within a sphere of radius R) then we define the dimensionless variable χ by $\chi \equiv r/a$ with

$$a \equiv \left(\frac{9 \pi^2}{128 Z_n} \right)^{1/3} \frac{\hbar^2}{m_e e^2} = 0.88534 Z_n^{-1/3} \frac{\hbar^2}{m_e e^2} \quad (1)$$

where m_e is the mass of the electron.

The Thomas-Fermi function $\psi(\chi)$ is defined by

$$\psi(\chi) \equiv \frac{r}{Z_n e} (V(r) - V(R)) \quad (2)$$

If $n(r)$ is the electron number density then Poisson's equation gives

$$n(r) = \frac{Z_n}{4\pi a^3} \frac{\psi''(\chi)}{\chi} \quad (3)$$

Statistical reasoning, based on assuming that the electrons form a homogeneous sea of Fermions, in ground state, gives

$$n(r) = \frac{Z_n}{4\pi a^3} \frac{\psi^{3/2}}{\chi} \quad (4)$$

and the Thomas-Fermi equation is given by equating the two forms;

$$\psi'' = \frac{\psi^{3/2}}{\chi^{1/2}} \quad (5)$$

In order to achieve a physically acceptable solution we must also ensure ψ obeys three boundary conditions:

$$\psi(0) = 1 \quad (\text{near the nucleus the potential equals the potential of a bare nucleus}) \quad (F)$$

$$\text{if } x \equiv \frac{R}{a}, \psi(x) = 0 \quad (\text{continuity of } V \text{ at the boundary}) \quad (7)$$

$$\psi'(x) = -\frac{A}{x} \quad (\text{continuity of } dV/dr \text{ at the boundary}) \quad (8)$$

[This is done correctly by Fluegge [3], but the original paper by Baker [4] is in error.]

The Thomas-Fermi potential is not an exact solution for electronic distribution and little accuracy is lost, (and much convenience gained) in the use of an analytic approximation to the exact solution of (5). It is convenient to let the approximation be of the form $\phi(u)$ where $u \equiv \frac{X}{x} = \frac{r}{R}$.

In order to achieve a good approximation we endeavor to satisfy five criteria: (6), (7) and (8) are the first three:

$$\phi(0) = 1 \quad (9)$$

$$\phi(1) = 0 \quad (10)$$

$$\phi'(1) = -A \quad (11)$$

The fourth follows from the requirement of having the correct number of electrons inside the screening cloud,

$$\text{i.e.,} \quad (1-A)Z_n = 4\pi \int_0^R n(r)r^2 dr, \quad (12)$$

using the expression for $n(r)$ from (3), (12) is immediately satisfied. However, this is not necessarily true for the statistically derived form in (4), so we demand

$$1-A = x^{3/2} \int_0^1 \phi^{3/2}(u) u^{1/2} du \quad (13)$$

Finally Firsov has shown [5] that $\psi(x)$ is the function which minimizes the integral

$$L = \int_0^x \left(\frac{1}{2} (\psi'(x))^2 + \frac{2}{5} \frac{\psi^{5/2}(x)}{x^{1/2}} \right) dx$$

for the neutral case, $A = 0$, $x \rightarrow \infty$, and that the minimization of L is equivalent to the minimizing of the energy of the atom. This procedure was used by Csavinsky [6] to optimize his approximation for the neutral Thomas-Fermi potential.

We carry this result over to the ionic case, without proof, and require

$$\int_0^1 \left[\frac{1}{2} \frac{(\phi'(u))^2}{x} + \frac{2}{5} x^{1/2} \frac{\phi^{5/2}}{u^{1/2}} \right] du \quad (14)$$

be a minimum .

The form chosen for ϕ is:

$$\phi(u) = (1 - u) \left(\frac{1 + B u}{1 + C u} \right)^2$$

with B & C parameters to be determined. (9) and (10) are satisfied by construction; (11) implies $B = (1+C)\sqrt{A} - 1$; (13) gives x in terms of C for any value of C , and C is varied so as to minimize (14). The integrations in (13) and (14) are performed numerically. The resulting values of C are plotted against A in Fig. 1. In Fig. 2, x , found in this manner, is plotted against A . In the same graph, x , found by numerical integration of (5), is also plotted against A for comparison. This approximation is only weakly dependent on deviations of C away from the values found by satisfying (14) and as A nears zero, ϕ becomes the Tietz approximation to the neutral Thomas-Fermi solution [3], [7].

$$C = 4.5 + 15 (A - 0.54)^2$$

is a useful approximation.

In Table 1, the values of C , x found from (13), and x found by numerical integrating (5) directly are given for values of A between 0.1 and 0.9. In Fig. 3 the potential ψ , found by direct numerical integration of (5), is compared to the approximation ϕ for three values of A . The good agreement with the numerical solution suggests that this approximate form of ψ could be used for a number of problems in addition to the one at hand; for example, the scattering of neutral hydrogen atoms off of partially stripped impurities [8].

The Scattering Calculation

We must first decide which, if any, of the standard approximations will be valid in the regime of interest. The ranges of validity of the Born and classical approximations for scattering are discussed by Messiah [9], Mott and Massey [10] and Sivukhin [11].

The critical parameter is $Z_n e^2 / h v \equiv \gamma$, where v is the proton velocity. For $\gamma > 1$ the classical approximation is indicated and for $\gamma < 1$ the Born. Hence for $E/Z_n^2 < 25$ keV, with E the proton kinetic energy, the classical approximation will hold. We are therefore justified in using the classical approximation for interaction between neutral injected ions in fusion plasmas [$E_i = 15$ -1000 keV] and moderate to high Z_n impurities.

We expect the major contribution to the scattering cross section to come from small angle scattering events and we therefore use the impulse approximation [9] where

$$\Delta\theta = - \frac{be}{E} \int_b^{\infty} \frac{V'(r) dr}{(r^2 - b^2)^{1/2}} \quad (15)$$

with $\Delta\theta$ the scattering angle due to an encounter with impact parameter b .

We are concerned only with impact parameters less than the ionic radius R . Using our approximation to the Thomas-Fermi potential and splitting up the integral range, (15) becomes:

$$\Delta\theta = \frac{Z_n e^2 b}{E} \left[\int_R^\infty \frac{A dr}{r^2 (r^2 - b^2)^{1/2}} - \frac{1}{b^2} \int_{u_0}^1 \frac{\phi'(u) u du}{(u^2 - u_0^2)^{1/2}} \right] \quad (16)$$

after one integration by parts, with $u_0 \equiv b/R$.

This can be performed analytically to give

$$\Delta\theta = \frac{Z_n e^2}{E b} \left\{ A \left[1 - \left(1 - \frac{b^2}{R^2} \right)^{1/2} \right] + I(u_0) \right\}.$$

$I(u_0)$ is the contribution to the scattering of the proton due to its passage through the electron cloud. The integration is straightforward though cumbersome.

If we write $\beta \equiv 1/C$ then with the following definitions we can give an expression for $I(u_0)$.

$$\text{If } I_n = \int_{u_0 + \beta}^{1 + \beta} \frac{x^n dx}{[(x - \beta)^2 - u_0^2]^{1/2}}.$$

$$l = 2\beta^2(1 - \beta\beta)^2 (1 + \beta),$$

$$m = \beta^2(1 - \beta\beta) (3\beta\beta + 2\beta - 1),$$

$$n = \beta^2 \cdot \beta^2,$$

$$\text{then } I(u_0) = -\beta l I_{-3} + (l - \beta m) I_{-2} + m I_{-1} - \beta n I_0 + n I_1.$$

The various I_n are given by

$$I_0 = \ln \left[\frac{1 + (1 - u_0^2)^{1/2}}{u_0} \right]$$

$$I_1 = (1 - u_0^2)^{1/2} + \beta I_0$$

$$I_{-1} = \begin{cases} \frac{1}{(u_0^2 - \beta^2)^{1/2}} \arccos \left(\frac{u_0^2 + \beta}{u_0(1 + \beta)} \right), & \beta^2 \leq u_0^2 \\ \frac{1}{(\beta^2 - u_0^2)^{1/2}} \ln \left(\frac{u_0(1 + \beta)}{u_0^2 + \beta - (\beta^2 - u_0^2)^{1/2}(1 - u_0^2)^{1/2}} \right), & u_0^2 \leq \beta^2 \end{cases}$$

$$I_{-2} = \frac{\beta}{(\beta^2 - u_0^2)} I_{-1} - \frac{(1 - u_0^2)^{1/2}}{(\beta^2 - u_0^2)(1 + \beta)}$$

$$I_{-3} = \left(\frac{3\beta^2}{\beta^2 - u_0^2} - 1 \right) \frac{I_{-1}}{2(\beta^2 - u_0^2)} - \left(\frac{1}{1 + \beta} + \frac{3\beta}{(\beta^2 - u_0^2)} \right) \times \frac{(1 - u_0^2)^{1/2}}{2(\beta^2 - u_0^2)(1 + \beta)}$$

We now have $\Delta\phi$ but the quantity of interest is the diffusion cross section.

$\sigma = \int_{b_0}^{b_m} (\Delta\phi)^2 2\pi b db$ where b_0 and b_m are the minimum and maximum impact parameters considered. The usual cutoff arguments identify b_m as the Debye length, and b_0 as the distance from the scattering center at which the potential energy is twice the initial kinetic energy of the scattered particle.

This integral can only be partially completed analytically; if we write

$$w = \left(1 - \left(\frac{b_0}{R} \right)^2 \right)^{1/2} \quad \text{and} \quad u_m = b_0/R$$

we then have

$$\sigma = 2\pi \left(\frac{Z_s e^2}{E} \right)^2 \left[\ln \Lambda + \frac{1}{A^2} \int_{u_m}^1 \left[1^2 - 2IA(1 - (1-u_0^2)^{1/2}) \right] \frac{du_0}{u_0} \right. \\ \left. - \ln u_m + \frac{w}{2} (4w - 1) - \ln \left(\frac{1+w}{1-w} \right) \right], \quad (17)$$

where $\Lambda = b_0/b_m$.

There are two departures from the usual result, $\sigma = 2\pi \left(\frac{Z_s e^2}{E} \right)^2 \ln \Lambda$. First, b_0 must be found in a different manner due to the non-coulombic form of the potential. In Fig. 4 the effective degree of ionization seen by the proton at the minimum impact parameter, which must be used in finding b_0 , is plotted against energy. We define A_{eff} to be $b_0 2E/e^2 Z_n^{4/3}$. This contributes a correction of order $\ln(1/A)$ or less to the usual $\ln \Lambda$.

For most energies, however, the dominant contribution is from the extra terms in (17). This correction is plotted in Fig. 5 for A from 0.1 to 0.9, and on a different scale for A from 0.5 to 0.9 in Fig. 6.

It can be seen that this correction is of comparable magnitude to the original $\ln \Lambda$ term of impurities which are not highly ionized, e.g. tungsten in multi-keV electron temperature plasmas, or iron in plasmas with T_e equal to several hundred electron volts. As we would expect, the slope of the corrections in Fig. 6 is approximately $1/A^2 - 1$ at high energies, since this corresponds to scattering from the nuclear charge Z_n , the influence of the screening cloud declining as the incident energy increases.

ACKNOWLEDGMENT

This work was supported by the Department of Energy contract number EY-76-C-02-3073.

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Table 1.

<u>A</u>	<u>C</u>	<u>X (Approx.)</u>	<u>X (Numerical)</u>
0.1	7.33	10.7	11.0
0.2	5.84	6.73	6.98
0.3	5.06	4.90	5.05
0.4	4.68	3.75	3.83
0.5	4.52	2.91	2.95
0.6	4.56	2.25	2.26
0.7	4.82	1.69	1.69
0.8	5.50	1.19	1.18
0.9	7.47	0.691	0.687

FIGURE CAPTIONS

- Fig. 1. The value of C which minimizes the energy of the ion, plotted against ionization ratio. (PPL-786163)
- Fig. 2. Comparison of the ionic radius as a function of ionization ratio, found by direct integration of the Thomas-Fermi equation (solid line) and by the approximate method described in the text (dotted line). (PPL-786164)
- Fig. 3. Comparison of ψ , found by numerical integration of the Thomas-Fermi equation (solid line), and ϕ , our approximate solution (dotted line), for three values of the ionization ratio. (PPL-786217)
- Fig. 4. The effective ionization ratio seen by a scattered ion in a minimum impact parameter encounter as a function of incident energy, nuclear charge and ionization ratio. (PPL-786165)
- Fig. 5. The additive correction to the conventional $\ln \Lambda$ term as a function of incident energy, nuclear charge, and ionization ratio. (PPL-786168)
- Fig. 6. The additive correction to the conventional $\ln \Lambda$ as a function of incident energy, nuclear charge, and ionization ratio, for ionization ratios greater than 0.5. (PPL-786167)

Fig. 1. 786163

Fig. 2. 786164

Fig. 3. 786217

Fig. 4. 786165

Fig. 5. 786168

Fig. 6. 786167

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