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S. M. Sepke

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Notes on Light Ion Continuous Slowing Down in HYDRA

Scott M. Sepke

Lawrence Livermore National Laboratory
7000 East Avenue, Livermore, California, 94550
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Introduction

Charged particle stopping power in HYDRA is composed of three terms arising from (i) free electrons, (ii) bound electrons, and (iii) ions. Each of these terms has a corresponding Coulomb logarithm denoted by \mathcal{L}_e , \mathcal{L}_b , and \mathcal{L}_i , respectively, and these are given formally by the equations

$$\begin{aligned}\mathcal{L}_e &= \frac{1}{2} \log \left(1 + \left[\frac{2m_e v_e^2}{\hbar \omega_p} \left(\frac{0.321 + 0.259f^2 + 0.0707f^4 + 0.05f^6}{1 + 0.130f^2 + 0.0500f^4} \right) \right]^2 \right) \\ \mathcal{L}_b &= \frac{1}{2} \log \left(1 + \left[\frac{2m_e v_p^2}{T [\text{erg}]} \right]^2 \right) \\ \mathcal{L}_i &= \frac{1}{2} \log \left(\frac{\lambda_{De}^2}{\lambda_{CA}^2 + \lambda_{Qi}^2} \right).\end{aligned}$$

The resulting total stopping power is then

$$\begin{aligned}-\frac{1}{m_p} \frac{dE}{ds} &= \left[\frac{2\pi e^4 Z_p^2}{E_p} \right] \left(\left\{ \frac{n_b \mathcal{L}_b + n_e \mathcal{L}_e}{m_e} \right\} \left[\text{erf} \left(\frac{v_p}{v_e} \right) - \left(\frac{2v_p}{\sqrt{\pi} v_e} \right) e^{-v_p^2/v_e^2} \right] + \left[\frac{n_b \mathcal{L}_b + n_e \mathcal{L}_e}{n_e \mathcal{L}_{e0}} \right] \sum_i \frac{Z_i^2 n_i}{m_i} \mathcal{L}_i \right) \\ &\approx \left[\frac{2\pi e^4 Z_p^2}{E_p} \right] \left(\left\{ \frac{n_b \mathcal{L}_b + n_e \mathcal{L}_e}{m_e} \right\} \left[\text{erf} \left(\frac{v_p}{v_e} \right) - \left(\frac{2v_p}{\sqrt{\pi} v_e} \right) e^{-v_p^2/v_e^2} \right] + \sum_i \frac{Z_i^2 n_i}{m_i} \mathcal{L}_i \right),\end{aligned}$$

where

$$\mathcal{L}_{e0} = \ln \left(\frac{2m_e v_e^2}{\hbar \omega_p} [0.321] \right)$$

is the free electron Coulomb logarithm in the limit that the projectile speed v_p is much less than the characteristic electron speed v_e : *i.e.* $f \equiv (v_p/v_e) \ll 1$.

The free electron stopping power has been derived using the random phase approximation (RPA) with an empirical fit used to bridge the gap between the Fermi and Boltzmann limits[2], bound electron stopping is simply the Bethe-Bloch form, and the ion Coulomb stopping power is the form used by many including Li and Petrasso[1] in the limit that the projectile speed far surpasses the background ion thermal speed.

Heretofore, most of parameters have been left undefined, and the remainder of this section will strive to develop practical definitions for each with engineering (numerical) formulae whenever possible. Before diving into that, however, a brief comment on notation is in order. Throughout this document — unless otherwise noted — subscript “p” will denote a variable associated with the projectile that is slowing down, “e” refers to free electrons, “b” to bound electrons, and “i” to background ions. In practice, background ions are typically amalgamated using an appropriate average so that only a single ion species is considered. This “average species” is denoted by subscript “ α .”

In addition, m denotes mass, m_{klr} denotes reduced mass for species k and l , n number density, Z charge state, E energy, v speed, ω angular frequency, T electron temperature in keV, $e = 4.8032 \times 10^{-10}$ statC is the charge of an electron, $k_B = 1.602176487 \times 10^{-9} \frac{\text{erg}}{\text{keV}}$ is Boltzmann’s constant, $u = 1.66054 \times 10^{-24} \frac{\text{g}}{\text{AMU}}$, $h = 2\pi\hbar = 6.6260692851436918 \times 10^{-27}$ erg · s is Planck’s constant, and all units are CGS unless noted.

Defining the Details

Stopping By Free Electrons

The free electron Coulomb logarithm is modeled after that derived by Maynard and Deutsch using the random phase approximation with a Padé approximant fit in f used to account for the temperature effects

described in the reference. The fit bridges the gap between the calculated low and high temperature limits and is defined such that

$$\mathcal{F}(f) = \frac{0.321 + 0.259f^2 + 0.0707f^4 + 0.05f^6}{1 + 0.130f^2 + 0.0500f^4}$$

where $f \equiv (v_p/v_e)$ as stated above.

In addition to this fit, electron time and speed scales appear within this formulation. The time scale is simply the electron plasma response time here expressed in terms of the Langmuir frequency

$$\omega_p = \sqrt{\frac{4\pi e^2 n_e}{m_e}} = (5.64172 \times 10^4) \sqrt{n_e [\text{cm}^{-3}]} \text{sec}^{-1}.$$

The speed scale is the thermal electron speed, but since plasma conditions within an ICF capsule may be Fermi degenerate, a Boltzmann description is not sufficient.

Characteristic Electron Speed: v_e

The desired Fermi thermal speed can be simply expressed by the compact expression

$$v_e = \frac{\hbar\pi^{1/2}}{m_e} (4n_e [1 + \exp(-\eta)])^{1/3}, \quad (1)$$

where η is the chemical potential of the system normalized to the electron temperature. With the electron number density and temperature specified, this speed is, in principle, known since the chemical potential depends only on these properties. Practically speaking, however, the chemical potential is not easily expressed in closed form and must be either approximated or computed numerically. In this case, a functional fit is chosen to make this calculation practical for the enormous number of stopping power computations required in modeling a full scale ICF target.

Begin with the standard distribution for a non-relativistic Fermi (electron) gas

$$dN = \frac{g d\tau}{1 + e^{\epsilon-\eta}} = \frac{g dp_x dp_y dp_z dV}{h^3 (1 + e^{\epsilon-\eta})} = \frac{2V m_e^{3/2} T^{3/2}}{2^{1/2} \pi^2 \hbar^3} \frac{\epsilon^{1/2} d\epsilon}{e^{\epsilon-\eta} + 1},$$

where N is the number of particles, g is the spin degeneracy parameter — 2 for an electron — V is the system volume, and p_j is the j^{th} -direction momentum component associated with a normalized energy $\epsilon = E/T$. Thus, the overall number density is

$$n_e = \frac{1}{V} \int_0^\infty dN = \left(\frac{4\pi [2m_e T]^{3/2}}{h^3} \right) \int_0^\infty \frac{\epsilon^{1/2} d\epsilon}{e^{\epsilon-\eta} + 1} = \left(\frac{4\pi [2m_e T]^{3/2}}{h^3} \right) F_{1/2}(\eta),$$

where $F_{1/2}(\eta)$ has been implicitly defined as the Fermi integral of order 1/2.

By rearranging this expression, the parameter ξ can be defined such that

$$F_{1/2}(\eta) = \frac{n_e h^3}{4\pi [2m_e T]^{3/2}} = \frac{2}{3} \left[\frac{(\frac{3n_e}{8\pi})^{2/3} \frac{h^2}{2m_e}}{T} \right]^{3/2} = \frac{2}{3} \left(\frac{E_F}{T} \right)^{3/2} \equiv \frac{2}{3} \xi^3,$$

where the numerator of the third term has been noted to be equal to the Fermi energy, E_F , which is the highest energy occupied state for this density at a temperature of absolute zero. The newly defined parameter ξ can be expressed using the simple engineering formula

$$\xi = \sqrt{\frac{E_F}{T}} = (1.9096 \times 10^{-9}) \left[\frac{(n_e [\text{cm}^{-3}])^{1/3}}{(T_e [\text{keV}])^{1/2}} \right],$$

and with this parameter defined, the normalized chemical potential can now be fit to facilitate computing the thermal speed such that:

$$\frac{1}{1 + \exp(-\eta)} \approx 1 - e^{-\zeta_0} \quad (2)$$

$$\zeta_0 = \frac{(.7531 + \xi(.1679 + .3108\xi)) * \xi^3}{1. + \xi(.2676 + \xi(.2280 + .3099\xi))}.$$

The Fermi degeneracy corrected electron thermal speed is then given by the engineering formula

$$v_e = 3.2572 \left[\frac{n_e [\text{cm}^{-3}]}{1 - \exp(-\zeta_0)} \right]^{1/3} \frac{\text{cm}}{\text{s}}. \quad (3)$$

for arbitrary values of the normalized chemical potential, η .

Before leaving this topic, consider the non-degenerate limit: *i.e.* as $\eta \rightarrow -\infty$. In that case, the Fermi integral can be carried out analytically

$$F_{1/2}(\eta \rightarrow -\infty) \rightarrow e^\eta \int_0^\infty \varepsilon^{1/2} e^{-\varepsilon} d\varepsilon = \frac{\sqrt{\pi} e^\eta}{2} = \frac{n_e h^3 \sqrt{2}}{16\pi T^{3/2} m_e^{3/2}}$$

yielding a closed form relationship between the chemical potential and the electron density and temperature:

$$e^{-\eta} = \left(\frac{2\sqrt{\pi T m_e}}{h} \right)^3 \frac{1}{n_e \sqrt{2}} \approx 1 + e^{-\eta}.$$

Using this form in the original expression for the electron thermal speed given in Eq. 1 results in

$$v_e \rightarrow \frac{\hbar\sqrt{\pi}}{m_e} (4n_e e^{-\eta})^{1/3} = \frac{\hbar\sqrt{\pi}}{2\pi m_e} \left(\frac{4n_e}{\sqrt{2}n_e} \right)^{1/3} \frac{2\sqrt{\pi T m_e}}{h} = \sqrt{\frac{2T}{m_e}}, \quad (4)$$

which is, of course, the classical Boltzmann thermal speed.

Alternatively, if the high temperature, low density non-degenerate limit is taken in Eq. 1 by employing the Padé approximant of Eqs. 2 and letting ξ tend to zero,

$$v_e \rightarrow \left(\frac{4}{3\pi^{1/2} (0.7531)} \right)^{1/3} \sqrt{\frac{2T}{m_e}} \approx 0.9996 \sqrt{\frac{2T}{m_e}} \quad (5)$$

which is, of course, essentially the value obtained in Eq. 4 since $0.7531 \approx 4/(3\pi^{1/2})$ thereby demonstrating that the Padé approximant for the chemical potential does, indeed, reduce to the Maxwell Boltzmann limit.

Casting the Coulomb Logarithm Argument in Terms of Characteristic Lengths

The argument to the free electron Coulomb logarithm may be cast in terms of the more traditional ratio of maximum to minimum distances of interaction squared by noting that

$$\frac{2m_e v_e^2}{\hbar\omega_e} = \frac{\sqrt{2}\lambda_{De,\eta}}{\lambda_{Qe}} \quad (6)$$

where

$$\lambda_{De,\eta} = \frac{v_e}{\sqrt{2}\omega_e} = (4.8024 \times 10^{-5} \text{cm}) \left\{ \sqrt{n_e [\text{cm}^{-3}]} [1 - \exp(-\zeta_0)] \right\}^{-1/3}$$

is the electron Debye length — here cast in terms of the Fermi-Dirac electron speed rather than the temperature — and that

$$\lambda_{Qe} = \frac{\hbar}{2m_e v_e} = (0.1777 \text{cm}) \left[\frac{1 - \exp(-\zeta_0)}{n_e [\text{cm}^{-3}]} \right]^{1/3}$$

is the quantum distance of closest approach to an electron: that is, the electron thermal deBroglie wavelength under the approximation that the electron reduced mass is equal to the true electron mass.

The factor of $\sqrt{2}$ in Eq. 6 is included to ensure that the electron speed and temperature are correctly related by $m_e v_e^2 = 2k_B T_e$ in the Maxwell-Boltzmann limit as shown in Eqs. 4 and 5.

Stopping By Bound Electrons

The bound electron Coulomb logarithm is simply the Bethe-Bloch equation with \bar{I} equal to the average ionization potential of the material, which can be approximated as

$$\bar{I} [\text{erg}] = k_B Z_i \left[\frac{0.011 + 0.013 \frac{Z^*}{Z_i}}{\sqrt{1 - \frac{Z^*}{Z_i}}} \right],$$

where Z^* is the number of free electrons per nucleus in the background material, and as above, Z_i is the number of protons per nucleus.

Stopping By Ions

The ion Coulomb logarithm, \mathcal{L}_i , follows the typical model of depending on the ratio of the maximum to minimum impact parameters:

$$\mathcal{L} = \frac{1}{2} \log \left(1 + \left[\frac{b_{max}}{b_{min}} \right]^2 \right) \approx \frac{1}{2} \log \left(\left[\frac{b_{max}}{b_{min}} \right]^2 \right) = \frac{1}{2} \log \left(\frac{\lambda_{De}^2}{\lambda_{CA}^2 + \lambda_{Qi}^2} \right).$$

The maximum impact parameter is taken to be the electron Debye length as Coulomb effects are screened beyond this distance. Specifically, the Debye length λ_{De} can be expressed

$$\lambda_{De}^2 = \frac{T}{4\pi e^2 n_e} = (5.526441 \times 10^8) \frac{T [\text{keV}]}{n_e [\text{cm}^{-3}]}.$$

The square of the minimum approach distance is taken as the sum of the squares of the classical distance of closest approach λ_{CA} — the square bracketed term in Eq. 7 — and the deBroglie wavelength of the system λ_{Qi} — the term in parentheses below in Eq. 7:

$$\lambda_{CA}^2 + \lambda_{Qi}^2 = \left[\frac{e^2 Z_i Z_p}{m_{pir} v_{crit}^2} \right]^2 + \left(\frac{\hbar}{2m_{pir} v_{crit}} \right)^2, \quad (7)$$

where v_{crit} represents a characteristic speed described below.

The characteristic speed, v_{crit} is defined as the speed of the projectile under the condition that the electron and ion stopping powers are equal. To facilitate this calculation, the stopping power formulae are simplified somewhat and the contribution from bound electrons is neglected. The typical limit $v_i \ll v_p \ll v_e$ is taken to simplify the resulting expressions for the free electron and ion stopping powers yielding

$$\begin{aligned} -\frac{dE}{ds} \Big|_e &= \sqrt{E} \frac{8\sqrt{\pi}}{3} \left[\frac{Z_p^2 e^4 n_e}{T^{2/3}} \right] \sqrt{\frac{m_e}{m_p}} \log(\Lambda_e) \\ -\frac{dE}{ds} \Big|_i &= \sum_i \left[\frac{2\pi Z_p^2 Z_i^2 e^4 n_i}{E_p} \right] \frac{m_p}{m_i} \log(\Lambda_i), \end{aligned}$$

respectively. Taking their ratio yields

$$\frac{\frac{dE}{ds} \Big|_e}{\frac{dE}{ds} \Big|_i} = \left[\frac{4}{3\sqrt{\pi}} \frac{\frac{n_e}{m_e} \log(\Lambda_e)}{\sum_i \frac{n_i Z_i^2}{m_i} \log(\Lambda_i)} \right] \left(\frac{m_e E_p}{m_p T} \right)^{3/2}.$$

When these stopping powers are equal, this ratio is 1, and v_{crit} can be determined:

$$\frac{E_p}{A_p} = \frac{1}{2} u v_{crit}^2 = \left[\left(\frac{3\sqrt{\pi}}{4} \right) \frac{\langle \frac{Z_i^2}{A_i} \rangle \log(\Lambda_i)}{\langle Z_i \rangle \log(\Lambda_e)} \right]^{2/3} \left(\frac{u}{m_e} \right)^{1/3} k_B T,$$

where A_p is the projectile mass in AMU, and Boltzmann's constant has been introduced during this step to emphasize that T will be given in keV and E_p in ergs. Assuming a Deuterium background as typical for ICF applications and noting that

$$\frac{\log(\Lambda_i)}{\log(\Lambda_e)} \sim 1.545,$$

the proportionality constant relating E_p/A_p to T is $12.43k_B$, and thus,

$$v_{crit}^2 = \frac{2(12.43k_b)T}{u} = (2.39863 \times 10^{16}) T [\text{keV}]. \quad (8)$$

Using this characteristic speed, the square of the resulting minimum impact parameter can then be written directly as

$$\lambda_{CA}^2 + \lambda_{Qi}^2 = \frac{T [\text{keV}] + 15.961}{(2.377 \times 10^{23}) T^2 [\text{keV}]},$$

and, finally, the ion Coulomb logarithm can be written

$$\mathcal{L}_i = \frac{1}{2} \log \left(\frac{(1.31364 \times 10^{32}) \frac{T[\text{keV}]}{n_e[\text{cm}^{-3}]}}{T[\text{keV}] + 15.961} \right)$$

for a Deuterium plasma. Currently, all simulations assume that the ratio $E_p/A_p = 12.43k_B T$ regardless of the plasma conditions or constituents. In a typical ICF environment, this is generally not far from reality, and in fact, this seems to make little difference even for plasmas very dissimilar to this in test cases run to date. This restriction could be relaxed.

References

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