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Stopping Power Calculations for Heavy Relativistic Ions

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Abstract

Recent theoretical results have led to improvements in formulas for $\mathrm{d}E/\mathrm{d}x$, particularly in the regime of high projectile charge and moderate to highly relativistic velocities. In addition, integration of $\mathrm{d}E/\mathrm{d}x$ leads to predictions of total range given initial energy and, reciprocally, initial energy given total range. We have compiled theoretical formulas for $\mathrm{d}E/\mathrm{d}x$ from a variety of sources into a computer code which we will make publicly available over the World Wide Web. We will also discuss comparisons of our code with experiment.

1 Introduction:

The simultaneous measurement of charge and energy of a particle passing through a solid state detector, for example a track-etch detector, requires knowledge of the rate of energy loss, $\mathrm{d}E/\mathrm{d}x$ as a function of charge and energy. For a number of combinations of charge and initial energy, we predict the values of $\mathrm{d}E/\mathrm{d}x$ along a track, and use these to predict the energies along the track. With the values Z and $E(x)$ we find the detector response using an empirically determined response function, $\xi(Z, \beta)$. The predicted response is compared to the measured response, and the best value of charge and energy is found from maximum likelihood methods.

Provided beams of known charge and energy are available, it is usually straightforward to determine the response function $\xi(Z, \beta)$. The calculation of $\mathrm{d}E/\mathrm{d}x$, however is a subject fraught with difficulty. Previously, we have relied on what amounts to a polynomial fit to empirical determinations of range as a function of energy. This method is described in Benton & Henke (1969), which is itself an extension of the work of Barkas & Berger (1964). The code which results from this technique is extremely fast, since no integrals are involved. For the purposes of the analysis of the Trek experiment (Weaver et al., 1998), we demonstrated experimentally that this was adequate for the reconstruction of charge and energy. However, there is no evidence of comparison of this code with experimental ranges for ion species above $^{40}\mathrm{Ar}$. The extrapolation to higher charge is especially complicated by the increasing probability of ion shielding due to orbital electron capture. In this case, it is appropriate to seek theoretical guidance in improving $\mathrm{d}E/\mathrm{d}x$ calculations. The monumental work of Ahlen (1980) on stopping powers must stand as the starting point for any modern calculation. It is particularly interesting to note that calculations of stopping power for uranium ions were confirmed in an experiment by Ahlen & Tarlé (1983), therefore, any modern calculation should be able to reproduce this result.

2 Overall form:

The overall form of the stopping-power formula can be obtained from classical arguments (Jackson, 1975). In the convenient units A MeV $\mathrm{g}^{-1}\ \mathrm{cm}^2$, that formula is

$$-\frac{1}{\rho}\frac{\mathrm{d}E}{\mathrm{d}x} = 4\pi N_\mathrm{A} m_\mathrm{e} c^2 r_\mathrm{e}^2 \frac{Z_1^2 Z_2}{A_1 A_2}\frac{1}{\beta^2} L. \tag{1}$$

Here, we have used Z_1 and A_1 for the charge and mass (in amu) of the projectile, Z_2 and A_2 for the atomic number and molecular weight (g mol^{-1}) of the target material, N_A is Avogadro's number, $m_\mathrm{e}c^2 = 0.511$ MeV, and $r_\mathrm{e} = e^2/4\pi\epsilon_0 m_\mathrm{e} c^2$ is the classical electron radius.

The devil, they say, is in the details. In this case, the detail is the correction factor L, also known as the stopping logarithm. Following Lindhard & Sørensen (1996), we set

$$L_0 = \ln\left(\frac{2m_\mathrm{e}c^2\beta^2\gamma^2}{I}\right) - \beta^2 - \frac{\delta}{2}. \tag{2}$$

This is the form derived originally from quantum perturbation theory, and the first two terms are typically called the Bethe result. The third term is the density effect originally calculated by Fermi (1940) and extended by Sternheimer & Peierls (1971). Here, I is the effective ionization potential of the target material. Although there are theoretical means to determine I, for the most part, the experimentalist should regard it as an empirical parameter. We will refer to L_0 as the "Bethe" result, inclusive of the density effect.

For an accurate calculation, further corrections of the form $L = L_0 + \Delta L$ are required. It will be useful here to define the quantity $\eta \equiv \alpha Z_1/\beta$, where $\alpha = e^2/4\pi\epsilon_0\hbar c$ is the usual fine-structure constant. It is most desirable to find formulas for ΔL which will be valid for all values of η. In particular, for uranium, $\eta > 1$ when $\beta < 0.671$! Thus, any formula which loses validity for $\eta > 1$ will be useless for describing the energy loss of uranium ions in matter.

3 The Bloch-Mott-Ahlen corrections:

The Bloch correction (Bloch, 1933) arose from an investigation of the limiting behavior of classical and quantum-mechanical calculations of stopping power. Further details may be found in Ahlen (1980). It is most important at moderate energies 10 A MeV $< E <$ 1000 A MeV. The Mott correction (Ahlen, 1978) was first investigated when corrections to the stopping power of order higher than Z^2 became apparent. Ahlen's form of the Mott correction relied on parameterizations of the Mott cross section (Curr, 1955; Doggett & Spencer, 1956). Interested readers should note that the best derivation of the Mott correction may be found in Ahlen (1982). The Mott correction has a serious defect: it becomes large and negative at low energies, leading to unphysical behavior of the stopping power if the Mott correction is not cut off below some arbitrary energy. It has been experimentally demonstrated that the Bloch and Bloch+Mott corrections are inadequate in regimes of both high charge and high energy (Ahlen & Tarlé, 1983). A third correction is necessary. This is the "relativistic Bloch" correction of Ahlen (1982). Henceforth we will refer to this as the Ahlen correction. Altogether, these three corrections form what we will call the BMA group.

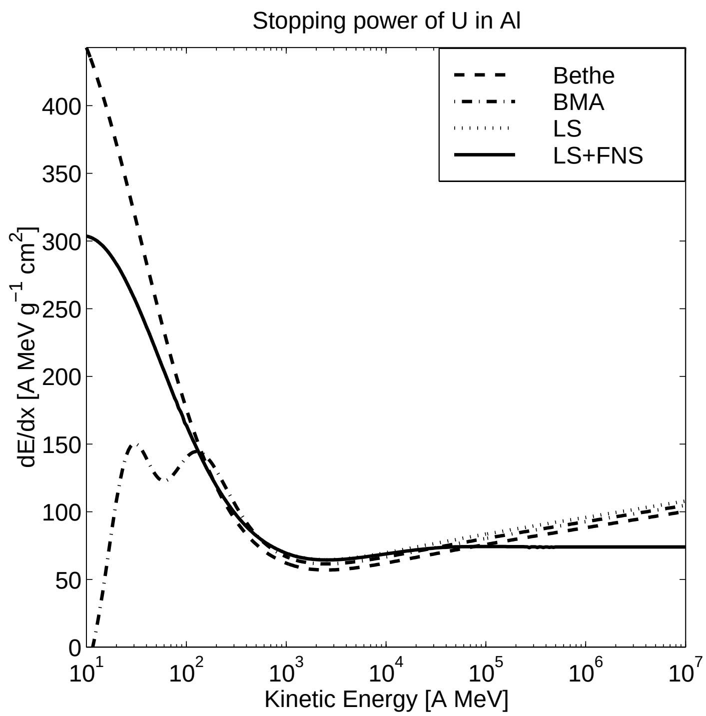

Figure 1: $\mathrm{d}E/\mathrm{d}x$ plotted versus energy for different corrections described in this paper. The projectile is uranium and the target is aluminum. Note the absence of the relativistic rise for the LS+FNS corrections.

4 The Lindhard-Sørensen correction:

It has been known for some time (Rose, 1961; Bhalla & Rose, 1962) that exact solutions of the Dirac equation exist not only for the Coulomb potential, but for any spherically symmetric potential. Only very recently (Lindhard & Sørensen, 1996) have these solutions been applied to the theory of stopping power. What we will term the Lindhard-Sørensen (LS) correction *replaces* the BMA group. (This definition of the Lindhard-Sørensen correction differs from that of Scheidenberger & Geissel (1998).) The LS correction is expressed as an infinite sum over Coulomb scattering phase shifts of increasing angular momentum quantum number. The sum converges fairly rapidly.

4.1 Finite nuclear size effects: In their paper Lindhard & Sørensen (1996) also derive a correction due to the finite size of atomic nuclei. The finite nuclear size effect arises as a modification to the Coulomb phase shifts in the basic LS correction. The numerical evaluation of these phase shifts can be tricky unless fully complex arithmetic can be implemented. In particular the convergence of the LS+FNS correction seems to be limited by the behavior of the confluent hypergeometric function. Convergence has been demonstrated out to Lorentz factors of $\gamma \simeq 10/R'$ (Sørensen, 1999), where $R' = Rm_{\rm e}c/\hbar = .003056A^{1/3}$ and $R = 1.18A^{1/3}$ fm is the nuclear radius. For ^{238}U this evaluates to $\gamma \simeq 500$ which is well into the ultrarelativistic regime.

4.2 The ultrarelativistic limit: Sørensen (1998) has shown that for ultrarelativistic ions, a (careful) perturbation treatment of the problem of energy loss is possible. In particular, because of finite nuclear size effects the potential energy experienced by an electron has a maximum depth of order 10 MeV, while the kinetic energies involved are very much greater than this. Thus, the stopping power calculation should be amenable to perturbation methods. For a uniformly charged nucleus, the perturbation treatment leads to a correction, $\Delta L_{\rm ultra}$, with a limiting behavior given by

$$\Delta L_{\rm ultra} = -\ln\left(\beta\gamma R'\right) - 0.2 + \beta^2/2. \tag{3}$$

The LS+FNS correction tends toward this same limit. This correction cancels the density effect correction in the ultrarelativistic limit, so that the entire stopping logarithm becomes

$$L = L_0 + \Delta L = \ln\frac{2c}{R\omega} - 0.2, \tag{4}$$

where ω is the plasma frequency of the target material. Astonishingly, this implies that *there is no relativistic rise* in stopping power in the ultrarelativistic regime. Classically, the stopping logarithm is interpreted as the logarithm of the ratio of maximum to minimum impact parameters. Here we have an (obvious) minimum of R out to the maximum of c/ω, which is the natural length scale for plasma screening. The prediction of an energy-independent $\mathrm{d}E/\mathrm{d}x$ in the ultrarelativistic regime has been confirmed with > 100 A GeV Pb ions in an Al target (Scheidenberger, 1994; Datz et al., 1996; Arduini et al., 1996).

5 Comparison with experiment:

Since the goal has been to provide accurate stopping power calculations for very high charges, we have primarily followed the experimental work of Ahlen & Tarlé (1983). In that experiment, performed at LBNL's Bevalac, a beam of uranium ions with beam energy 955.7 ± 2.0 A MeV, was brought to rest in a Lexan target. Additional stopping was provided by a block of Cu upstream from the target. For an accurate calculation, the upstream air and Al beam pipe window must also be included. The mean total range of the uranium nuclei was measured, and energy was reconstructed from stopping power calculations. Since this was primarily an experiment to determine the importance of the BMA group, low energy effects were not included in the calculation. Instead, the calculation was terminated at an energy of 150 A MeV, and a measured range (Ahlen, Tarlé, & Price, 1982) was used for the remaining energy. However, electron capture effects were included by applying an empirical formula (Pierce & Blann, 1968) for the effective charge.

The reconstructed energy is sensitive to the details of the empirical cutoff (Tarlé, 1999), but it is still possible to reconstruct the beam energy to better than 1%. No matter how the empirical range is actually added, the BMA and LS values differ by less than 1 A MeV. Thus, we believe the claim that the LS correction replaces the BMA group is empirically verified. As a further check on the validity of the LS correction, we attempted to reconstruct the beam energy without using the 150 A MeV cutoff. As mentioned above, the Mott correction becomes large and negative at low energies, and probably should not be used for energies with $Z_1/\beta < 100$ (Ahlen, 1978). Peculiarly, the integration of $\mathrm{d}E/\mathrm{d}x$ with the BMA group produces a better fit to the beam energy if we ignore the Mott cutoff. Direct integration of $\mathrm{d}E/\mathrm{d}x$ with the LS correction gives a reconstructed energy of 950.1 A MeV. Thus, any low energy effects must contribute less than 1% to the reconstruction of energy given range.

6 Stopping power code:

The code which has been developed as a result of these studies is freely and publicly available. The code is written entirely in C and should compile on most systems. The code may be downloaded from the website http://underdog.berkeley.edu/dedx/dedx.html, or via anonymous FTP ftp://underdog.berkeley.edu/pub/dedx/. We encourage anyone to suggest improvements.

A future goal will be to better understand low energies, where atomic effects become important. These include the Barkas effect (Jackson & McCarthy, 1972; Lindhard, 1976) and the shell correction (Fano, 1963). It is not entirely clear at this point what the range of validity or even the overall form of these corrections should be. We hope to locate more recent work which will clarify these matters.

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