Approximate, analytic solutions of the Bethe equation for charged particle range

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By either performing a Taylor expansion or making a polynomial approximation, the Bethe equation for charged particle stopping power in matter can be integrated analytically to obtain the range of charged particles in the continuous deceleration approximation. Ranges match reference data to the expected accuracy of the Bethe model. In the non-relativistic limit, the energy deposition rate was also found analytically. The analytic relations can be used to complement and validate numerical solutions including more detailed physics.

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INTRODUCTION

The deceleration of ions as they pass through matter is important in a wide range of fields: medical ion irradiation therapy, such as the treatment of tumors [1]; radiography with ions [2]; radiolysis of chemical compounds [3]; ion implantation in material processing and semiconductor doping [4]; gas discharge plasmas [5]; locality of energy deposition in nuclear fusion plasmas, including ion beam heating for controlled thermonuclear fusion [6] and space craft [7]; and particle physics experiments [8]. Energy loss for different combinations of ion specie, ion energy, and decelerating material has been measured since the early 20th century [9], with a corresponding development in theoretical work. Calculations of ion energy loss, and hence range, are very frequently performed using variants of the Bethe [11] and Bethe-Bloch [12] relations. Experimental and theoretical developments have focused on making corrections to the original Bethe relation to account for details of interactions with bound electrons and crystal structures at low energies [13, 14], and quantum-mechanical limits to the transfer of energy under extreme relativistic conditions [15]. The original Bethe relation is still used widely, particularly when a reliable, approximate result is needed rapidly, or in the fairly wide range of energies where the Bethe relation is adequately accurate [16].

The Bethe relation describes the stopping power: the rate at which a moving ion loses energy to the surrounding material. It is not trivial to use this relation to obtain the range of an ion, i.e. the distance for it to lose all of its kinetic energy. In practice, ranges are calculated using numerical integration in multi-physics computer programs, or from scaling laws normalized to the range for other energies or masses. However, reliance on sophisticated computer programs for infrequent calculations, without the ability to make a compact analytic estimate, can lead to errors. Analytic solutions are also valuable for validating computer programs reproducing the same physics. Here we point out analytic solutions to accurate approximations of the Bethe relation, which can give good estimates of ion ranges in matter.

RANGE FROM STOPPING POWER

In the continuous deceleration approximation, charged particles traversing matter lose kinetic energy $E$ at a rate depending on their instantaneous energy and the local material. Expressed as the energy loss rate per distance traveled, the stopping power $dE/dx$ can be used to determine the range $l$ of the particle, by integrating the deposition until the particle is stationary:

$$\int_{E_0}^{l} \frac{dE(x)}{dx} \, dx = -E_0. \quad (1)$$

However, $dE/dx$ is expressed naturally in terms of $E$ rather than $x$. Rearranging,

$$l = \int_{E_0}^{E} \frac{dx}{dE} \, dE. \quad (2)$$

The integral can be found numerically for arbitrary stopping powers, or analytically for stopping powers of sufficiently simple form.

The Bethe equation [11] describes the deceleration of charged particles by interaction with the electrons in matter:

$$\frac{dE}{dx} = -\frac{4\pi}{m_e c^2} \frac{NZ^2}{\beta^2} \left( \frac{q^2}{4\pi\epsilon_0} \right)^2 \left[ \ln \frac{2m_e c^2 \beta^2}{\tilde{I} (1 - \beta^2)} - \beta^2 \right] \quad (3)$$

where $\beta = v/c$, $v$ is the ion speed, $\tilde{I}$ is the effective ionization of the target material, $Z$ and $z$ are the atomic numbers of the target and ion species respectively, $N$ is the number density of target nuclei, $m_e$ is the mass of an electron, $\epsilon_0$ is the permittivity of free space, and $c$ is the speed of light.

To find the range of charged particles from Eq. [3] Eq. [2] can be integrated numerically, though this is not straight-
forward because of a singularity at low energies. We have not found an analytic solution for the integral.

**TAYLOR EXPANSION**

\[-dx/dE\] can be expanded as a Taylor series to make it more tractable for integration. This can be done for Eq. 3 with a relativistic expression for \(\beta(E)\); we do it also for a non-relativistic \(\beta(E)\) because the resulting integral is more amenable to subsequent manipulation.

**Relativistic**

The relativistic relation between \(\beta\) and kinetic energy \(E\) is

\[
\beta(E) = \sqrt{E(E + 2m_i c^2)} / E + m_i c^2
\]

where \(m_i\) is the rest-mass of the moving ion. For later convenience, we scale key quantities to be dimensionless. Substituting into Eq. 3 and expanding about zero,

\[
-\frac{dx}{dE} = \frac{4\pi e_0 m_e c^2}{q^4 z^2 N Z} \left[ \frac{2E}{L} - \frac{3E^2 (L - 1)}{L^2} \right] + O(E^3)
\]

where

\[
\dot{E} = \frac{E}{m_i c^2}, \quad \dot{i} = \frac{i}{2m_e c^2}
\]

are the scaled kinetic energy and mean ionization, and

\[
L \equiv \ln \frac{2E}{\dot{i}}.
\]

Integrating Eq. 2 the range is

\[
l = \frac{4\pi e_0^2 m_e c^2 m_i c^2}{q^4 z^2 N Z} \frac{1}{2} \dot{E} i Ei(2L) + \frac{3}{4} \dot{E}^3 i Ei(3L) - \frac{3\dot{E}^3}{L}
\]

where \(Ei(z)\) is the exponential integral function,

\[
Ei(z) \equiv - \int_{-\infty}^{\infty} \frac{e^{-t}}{t} dt.
\]

**Non-relativistic**

In the non-relativistic limit, \(\beta(E) = \sqrt{2E/m_i}\). Following the same procedure as above, we find that the non-relativistic form of each of \(-dx/dE\) and \(l\) is simply the first term of the corresponding relativistic relation.

**MIXED-SPECIES TARGETS**

For a target comprising multiple elements, the stopping power can be estimated from the combination of stopping powers from each element \(s\)

\[
\frac{dE}{dx} \simeq \sum_s \frac{dE}{dx}(Z_s, N_s)
\]

– the Bragg addition rule. This relation is approximate because of chemical bond formation, which alters the effective ionization. For ion energies much greater than the bond energies, the approximation should be accurate.

Expanding as before and gathering terms, the range can be expressed very similarly to that for single-element targets. In the relativistic case,

\[
l = \frac{4\pi e_0^2 m_e c^2 m_i c^2}{q^4 z^2 Z} \left[ \frac{1}{2} \dot{E} i Ei(2\dot{L}) + \frac{3}{4} \dot{E}^3 i Ei(3\dot{L}) - \frac{3\dot{E}^3}{\dot{L}} \right]
\]

where

\[
\dot{I} \equiv \exp \sum \frac{N_s Z_s}{Z} \ln \dot{i}_s, \quad \dot{L} \equiv \ln \frac{2\dot{E}}{\dot{i}}
\]

and

\[
\dot{Z} \equiv \sum \frac{N_s Z_s}{Z}
\]

is the total electron density in the target.

In the non-relativistic case,

\[
l = \frac{2\pi e_0^2 m_e c^2 m_i c^2}{q^4 z^2 Z} \dot{E} i (2\dot{L}),
\]

which is again simply the first term of the relativistic relation.

**POLYNOMIAL FIT TO THE STOPPING DISTANCE SCALE**

Although well-characterized numerical approximations to the exponential integral exist [17], they are not available as standard functions in mainstream computer languages, and require significant effort to implement from scratch. However, the logarithmic terms in the stopping power and range vary slowly compared with the powers of \(E\); over wide ranges of energy, the stopping power can be approximated accurately by low-order polynomials. The use of polynomial approximations avoids the need to evaluate the exponential integral function. We define a stopping distance scale

\[
D \equiv \frac{\dot{E} i dx}{dE},
\]

which is particularly well-behaved above the low-energy singularity as it tends to zero with \(E\), and increases
monotonically (Fig. 1). This quantity can be used as a crude, $O(1)$, (over)estimate of particle range, without requiring any series expansion or integration. Approximating $D$ by a polynomial

$$D_p(E) = \sum_j a_j E^j,$$

the range (Eq. 2) is simply

$$l_p \simeq a_0 \ln E + \sum_{j>0} \frac{a_j E^j}{j}.$$  \hspace{1cm} (17)

$a_0$ must be zero, since $E^n/\ln(E) \rightarrow 0$ as $E \rightarrow 0$.

To find the charged particle range in a specific substance, it is straightforward to tabulate $D(E)$ using Eq. 3 (and Eq. 10 for a multi-species target), fit a polynomial $D_p(E)$, and evaluate Eq. 17. However, it is also possible to find a universal polynomial fit. Defining for convenience a different scaled energy

$$F \equiv \frac{4m_e E}{Im_i} = \frac{2\hat{E}}{I},$$

the stopping distance scale is (using Eq. 5)

$$D(F) = \frac{\pi\epsilon_0^2}{2m_e q^2} \frac{m_i \hat{F}^2}{z^2 N Z} \left[ \frac{F^2}{\ln F} + \frac{3}{8 \overline{m}_c^2} \frac{\hat{F}}{(\ln F)^2} F^3 \right],$$

where the first term is the non-relativistic approximation. The prefactor comprises universal constants and a simple problem-specific factor $m_i \hat{F}^2/z^2 N Z$. The relative magnitude of the relativistic term to the non-relativistic term depends only on $\overline{I}$. Thus, by finding polynomial approximations

$$-\frac{F^2}{\ln F} \simeq P_{NR}(F) = \sum_j n_j F^j,$$  \hspace{1cm} (20)

it is straightforward to find the polynomial coefficients for any problem:

$$a_j = \frac{\pi\epsilon_0^2}{2m_e q^2} \frac{m_i \hat{F}^2}{z^2 N Z} \left( \frac{4m_e}{Im_i} \right)^j \left( n_j + \frac{3}{8 \overline{m}_c^2} \hat{I} r_j \right)$$

and hence the range through Eq. 17.

The derivation presented above is valid for any choice of units. The Bethe relation breaks down when the logarithm changes sign, i.e. when $\hat{E}$ approaches $Im_i/4m_e$. Physically meaningful distances are obtained for greater energies. Using the Bloch estimate \[12\] for the effective ionization of the material,

$$\overline{I} \simeq 10Zq,$$  \hspace{1cm} (23)

the relations are valid for $E \geq 4600Zq$. Polynomial fits were calculated over a range suitable for hadrons of energy $\sim$MeV to GeV (Table I). The relativistic term diverges rapidly outside the fitting region.

### ENERGY DEPOSITION PROFILE

Given $E(x)$, the profile of energy deposition $-dE(x)/dx$ (Bragg curve) can be calculated. $E(x)$ is the inverse of the range, $l(E)$.

For the non-relativistic range relation, $E(x)$ can be expressed in terms of the inverse of the exponential integral function,

$$-\frac{dE(x)}{dx} \simeq \frac{q^4 z^2 N Z}{4\pi\epsilon_0 \overline{I}} \exp \left( \frac{1}{2} \text{Ei}^{-1}(ax) \right) \text{Ei}^{-1}(ax)$$

where

$$\alpha = \frac{2m_e q^4 z^2 N Z}{\pi\epsilon_0^2 \overline{I}^2 m_i}.$$  \hspace{1cm} (25)

If the stopping distance scale is represented locally in energy by a sufficiently simple polynomial, then it too

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**TABLE I: Polynomial fits to stopping distance scale functions.**

| Parameter | $5 \leq F \leq 100$ | $100 \leq F \leq 10000$ |
|-----------|---------------------|-------------------------|
| $r_1$     | 2.17423             | 1.64377 $\times 10^{-1}$ |
| $r_2$     | 2.29035 $\times 10^{-1}$ | 1.31696 $\times 10^{-1}$ |
| $r_3$     | -3.36317 $\times 10^{-4}$ | -4.55336 $\times 10^{-6}$ |
| $r_4$     | 2.07676 $\times 10^{-10}$ | 2.07676 $\times 10^{-10}$ |

$\ln F - 1 \overline{F}^{-2} \overline{F}^3 \simeq P_R(F) = \sum_j r_j F^j$  \hspace{1cm} (21)
deposited energy (MeV/mm) vs. distance from rest (mm)

**FIG. 2:** Example calculation of Bragg curve via a polynomial (quadratic) fit to \( D(E) \): protons in water. The curve is presented backward from its usual form: as if the particles are accelerating from rest. Conceptually, the curve can be continued to arbitrarily high energies, i.e. long ranges.

may be used to calculate \(-dE/dx\). For example, taking a local quadratic fit

\[
D_p = a_1 E + a_2 E^2 \quad \Rightarrow \quad l_p = a_1 E + \frac{a_2}{2} E^2, \quad (26)
\]

one obtains

\[
-\frac{dE}{dx} \simeq \frac{1}{\sqrt{a_1^2 + 2a_2x}} \quad (27)
\]

(Fig. 2).

**EXAMPLE CALCULATIONS**

Reference calculations are used to validate radiation protection simulations using different computer programs. Here we compare the analytic solutions of the Bethe relation with results from widely-used programs SRIM [18], which uses numerical solutions of more detailed stopping powers developed from the Bethe relation, and MCNP [19], which collects Monte-Carlo statistics for the simulated interaction of individual particles. Trial calculations were made for protons and \( \alpha \)-particles stopping in Al and water.

We use the Bloch estimate, Eq. 23, for the effective ionization of the target material. More accurate calculations have been developed more recently, but the original Bloch estimate serves to demonstrate the correctness of our analysis.

The results are consistent with the accuracy of the Bethe relation itself (Table I), and are consistent with direct numerical integration of the Bethe equation without being affected by the low energy singularity. The greatest difference was for relativistic protons in Al. In this regime, radiative losses and nuclear reactions become significant [17], and the Bethe relation requires additional corrections.

**CONCLUSIONS**

Analytic solutions were found to power series expansions and polynomial fits to the Bethe relation. These solutions provide a convenient way to calculate ion ranges and energy deposition in regimes where the Bethe relation is valid, i.e. kinetic energies of roughly 1-100 MeV/u, without depending on numerical integration. The use of a Taylor series restricts the accuracy at high energy; the relativistic expansion thus incorporates relativistic contributions to the range but is not valid to arbitrarily high energies. However, the analytic solutions can readily be used with more accurate formulations of the effective ionization. The accuracy was demonstrated by comparison with simulations from widely-used computer programs of ion ranges in Al and water.

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