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Letter to the Editor

Shell correction in stopping theory

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Abstract

The shell correction in the stopping force on a point charge is shown to consist of two distinct contributions, a kinematic correction for the neglect of orbital motion and a mathematical correction for an asymptotic expansion limited to high projectile speed. The latter can be identified by separating Bloch's expression for the stopping number into the classical Bohr contribution and an inverse-Bloch correction.

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There are three obvious problems with the shell correction in stopping theory:

- the name is not particularly descriptive,
- the definition is ambiguous, and
- there is no agreement about its physical origin.

These problems are mutually related. Leaving aside the name for a moment and considering the definition, we write the electronic stopping force on a point charge Z_1e with a velocity v in a medium with NZ_2 electrons per volume in standard form

$$-\frac{\mathrm{d}E}{\mathrm{d}x}=\frac{4\pi Z_1^2Z_2e^4}{mv^2}NL. \tag{1}$$

Bethe evaluated the stopping number L within the first Born approximation in both a nonrelativistic [1] and a relativistic [2] version. Although the shell correction has a relativistic aspect, discussion of the above three points does not require to include it in the present discussion. Therefore, relativity will be ignored here.

Within this limitation, the stopping number L_{Born} may be written in the form

$$L_{\mathrm{Born}}=\frac{1}{2}\sum_n\int\frac{\mathrm{d}Q}{Q}f_{n0}(Q), \tag{2}$$

where the $f_{n0}(Q)$ are generalized oscillator strengths, the limits of the Q-integral are specified by $(\hbar\omega_{n0})^2\leqslant 2mv^2Q$, and ω_{n0} is a transition frequency in the target atom from its ground state to state n.

The famous Bethe formula approximates the stopping number by

$$L_{\mathrm{Bethe}}=\ln\frac{2mv^2}{I}, \tag{3}$$

where the logarithmic mean excitation energy I is uniquely defined over dipole oscillator strengths.

Eq. (3) is an asymptotic formula valid at high speed. It breaks down at low speed and becomes unphysical for $2mv^2<I$, whereas the exact expression (2) cannot give a negative stopping number if the target atom is in its ground state. Hence, at low velocities, explicit evaluation is required either of Eq. (2) or of the difference

$$\Delta L=L_{\mathrm{Born}}-L_{\mathrm{Bethe}}. \tag{4}$$

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Numerous estimates of this quantity may be found in the literature, starting from [3]. An extensive review may be found in [4].

Eq. (4) defines the shell correction ΔL uniquely within the range of validity of the first Born approximation. Problems arise with the inclusion of higher orders in the Born series, the Barkas–Andersen correction, as well as the Bloch correction. Both become significant in the velocity range where the shell correction is appreciable.

Early estimates of the Barkas–Andersen correction [5,6] invoke logarithmic expressions much like Eq. (3) which turn negative at some velocity. Evidently, such terms need a shell correction. Does this have to be included in ΔL? And if so, which of several logarithmic expressions proposed in the literature should be the reference standard?

A similar situation is found for the Bloch correction [7],

$$\Delta L_{\mathrm{Bloch}} = \psi(1) - \mathrm{Re}\psi\left(1 + \mathrm{i}\frac{Z_1 e^2}{\hbar v}\right), \tag{5}$$

where $\psi(\zeta) = \mathrm{d}\ln\Gamma(\zeta)/\mathrm{d}\zeta$. When this is added to L_{Bethe}, one arrives at the Bohr stopping formula [8] at the low-velocity end. Bohr stopping is likewise governed by a logarithmic stopping number that turns negative at some value of the argument and hence needs to be corrected. That correction differs from ΔL. Hence, there must be a shell correction to the Bloch term. Is this to be included in ΔL, or is it something else?

Clearly, there is an ambiguity about the basic definition of the shell correction. One way to resolve this is by keeping to the original definition (4), as was done in a recent study of aluminium [9]. However, evaluation of a shell correction so defined warrants attention to the corresponding corrections in higher-order Born terms and the Bloch correction. Failure to do so may severely limit the usefulness of an improved scheme.

Note that although a correction to a correction may be small, Barkas–Andersen and Bloch terms may become comparable in magnitude to L_{Bethe} around and below the stopping maximum, dependent on the ion–target combination.

At this point, let us look at the origin of the shell correction. According to Fano [10], ΔL may, for a one-electron atom, be written as

$$\Delta L \simeq -\frac{\langle v_e^2\rangle}{v^2} - \frac{\langle v_e^4\rangle}{2v^4} - \frac{5\pi}{3}\left(\frac{v_0}{v}\right)^4 a_0^3\rho(0), \tag{6}$$

where v_e is the orbital velocity and $\rho(r)$ the electron density at a distance r from the nucleus. Here, the two first terms indicate that the orbital motion of the target electrons has not been fully taken into account in Eq. (3). However, the third term has a different form and, more importantly, the expansion Eq. (6) cannot be carried further since $\langle v_e^6\rangle$ diverges.

Similar indications emerge from the work of Lindhard and Winther [11] who found

$$\Delta L = -\frac{3}{5}\frac{v_F^2}{v^2} - \frac{3}{14}\frac{v_F^4}{v^4}\cdots \tag{7}$$

for stopping in a Fermi gas with the Fermi speed v_F. It is easily verified that this is equivalent to the first two terms in Eq. (6).

Eqs. (6) and (7) indicate a strong connection between the shell correction and the orbital motion of the target electrons. In case of the Fermi gas, one might be inclined to assume the shell correction to be purely kinematic. Otherwise one would expect terms proportional to $\hbar\omega_P/mv^2$ and/or $(\hbar\omega_P/mv^2)^2$, where ω_P, the plasma frequency, is known to replace $I/\hbar$ in the Bethe formula [12]. One may object that Eq. (7) only describes the high-speed behavior of L. However, the only material parameter determining the behavior at low projectile speed, according to [11], is the Fermi speed v_F.

Based on this background, one of us [13] developed a kinetic theory of stopping that treats the shell correction as a purely kinematical effect. The heart of this theory – which is exact for free binary collisions – is a transformation of the stopping number L_0, evaluated in a reference frame where the target electron is initially at rest, to the laboratory system where it moves with an orbital speed v_e (a similar transformation was also provided for straggling). An expansion of the type of Eqs. (6) and (7) was derived in general terms and tested on a number of cases such as the Fermi gas and the quantal harmonic oscillator [14].

Extensive tests on the full transformation, going beyond asymptotic expansion, were performed by Sabin and Oddershede in [15] and numerous subsequent studies. A weak point in those calculations is the question of how to treat the velocity range where the Bethe logarithm becomes negative. Here, the best available solution in 1982 was to set $L = 0$ for $2mv^2/I < 1$.

A fundamental problem with this scheme is the fact that the assumption of a bound electron at rest violates the uncertainty principle, and that, consequently, a rigorous evaluation of Eq. (2) is strictly impossible for an electron at rest because of the lack of a valid description of the target atom in such a state. Although this problem is less accentuated in case of the Fermi gas, were the assumption of all electrons initially being at rest 'only' violates the Pauli principle and not the uncertainty principle, it would be desirable to have a 'legitimate' system for a direct evaluation of whether the shell correction is purely kinematic or, if not, for separating the kinematic contribution from whatever else might be significant.

Here we make reference to the wellknown fact that the function

$$L_{\mathrm{Bloch}} = L_{\mathrm{Bethe}} + \Delta L_{\mathrm{Bloch}}, \tag{8}$$

with $\Delta L_{\mathrm{Bloch}}$ defined in Eq. (5), reduces to the Bohr logarithm

$$L_{\mathrm{Bohr}} = \ln\left(\frac{Cmv^3}{Z_1 e^2\omega}\right) \tag{9}$$

at low projectile speed, where $C = 1.1229$ and $\omega = I/\hbar$. At high projectile speed, $\Delta L_{\mathrm{Bloch}}$ goes to zero, cf. Eq. (5).