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Shell correction in Bohr stopping theory

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Abstract. The shell correction is a term $\propto \langle v_e^2 \rangle$ in the electronic-stopping force on a charged particle, where v_e denotes the speed of a target electron. This term has been evaluated as a function of impact parameter within the scheme underlying Bohr's classical stopping theory, applying free-Coulomb scattering to close and a multipole expansion to distant interactions. Unlike the leading term in the stopping force, the shell correction is dominated by contributions from close collisions, and its magnitude differs from that found from the Bethe theory. Findings are also compared with the predictions of kinetic theory. Implications are mentioned on the stopping of swift heavy ions.

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1 Introduction

Shell corrections account for the effect of the internal motion of target electrons on the electronic stopping of a swift charged particle [1]. Their relative significance on the stopping force is governed by the ratio $\langle v_e^2 \rangle / v^2$, where v and v_e are the speeds of the moving particle and a target electron, respectively. Consequently, these corrections become significant at low projectile speed [2]. While neglected in the original versions of classical and quantal stopping theory [3,4], shell corrections are an essential ingredient in quantitative estimates, in particular for inner shells. Theoretical treatments are based on the Born approximation applied to model targets such as hydrogenic atoms [5], Fermi gas [6], or harmonic oscillator [7]. Moreover, shell corrections have been evaluated by adopting transformation laws from binary-collision kinematics [8].

Bohr's classical theory serves as a useful reference standard in particle stopping because of transparency, calculational ease and physical insight provided. For example, the Z_1^3 or Barkas effect was first treated within this scheme [9], well ahead of elaborate quantal calculations. Somewhat surprisingly, an estimate of shell corrections within this scheme does not seem available. With an increasing use of Bohr's concepts in heavy-ion stopping [10–13] there has arisen a need also for shell corrections. The present paper is intended to provide a theoretical basis for such estimates.

2 Fundamentals

With the stopping force in standard notation,

$$-\frac{\mathrm{d}E}{\mathrm{d}x} = \frac{4\pi Z_1^2 e^4}{mv^2} N Z_2 \, L, \tag{1}$$

where N is the number density of the target and Z_1 and Z_2 are atomic numbers of projectile and target, respectively, the pertinent physics is contained in the stopping number L. The prediction for L of the Bohr theory reads[1]

$$L = \log \frac{Cmv^3}{Z_1 e^2 \omega} + \Delta L, \qquad C = 1.1229, \tag{2}$$

where ω is the resonance frequency of a target electron modelled as a classical oscillator[2]. In principle, ΔL stands for a multitude of corrections [12], but only shell corrections will be considered here.

Theoretical treatments based on quantal perturbation theory [1,6,7] all yield

$$\Delta L = -\frac{\langle v_e^2 \rangle}{v^2} + \mathcal{O}\left(\frac{\langle v_e^4 \rangle}{v^4}\right). \tag{3}$$

It is by no means evident that equation (3) should be valid also within the classical scheme: after all, the zero-order term in equation (2) differs from the Bethe logarithm $\log(2mv^2/\hbar\omega)$, and so do the force fields governing target motion.

Bohr's stopping theory separates projectile-target interactions into distant and close collisions according to the impact parameter p. The boundary between the two regimes is chosen such as to minimize its influence on the resulting stopping force. Distant interactions are treated as in classical dispersion theory, as the effect on a target electron of the time-dependent electric field set up

[1] For a discussion of the behavior of equation (2) near and below the zero of the logarithm the reader is referred to reference [10].

[2] With the aim of a transparent notation, only a single resonance is considered. Extension to multiple resonances is straightforward.

by the penetrating particle, that field being assumed slowly-varying in space. This picture breaks down for close interactions which instead are treated as binary free-Coulomb interactions, neglecting electron binding.

The present treatment follows Bohr's scheme except for the inclusion of the initial motion of target electrons up to second order. Within the Born approximation, shell corrections to that order appear model-independent, *cf.* equation (3). While the restriction to quadratic terms sets a limit on the numerical accuracy toward low projectile speeds, useful insight is provided not the least on the impact-parameter dependence which turns out to differ substantially from that of the leading contribution to the energy loss.

3 Distant collisions

3.1 Basic equations

Bohr's theory describes electron binding by a harmonic force. Hence, the initial motion of a target electron is given by

$$\mathbf{r}_0(t) = \mathbf{a}_0 \cos\omega t + \mathbf{b}_0 \sin\omega t, \tag{4}$$

where $\mathbf{a}_0$ and $\mathbf{b}_0$ are 3-dimensional vectors, distributed at random in accordance with

$$\langle \mathbf{a}_0 \rangle = \langle \mathbf{b}_0 \rangle = \langle \mathbf{a}_0 \cdot \mathbf{b}_0 \rangle = 0; \quad \left\langle \mathbf{a}_0^2 \right\rangle = \left\langle \mathbf{b}_0^2 \right\rangle = \frac{\langle v_e^2 \rangle}{\omega^2} \cdot \tag{5}$$

With the interaction force

$$\mathbf{F}(t) = \int \mathrm{d}^3\mathbf{k}\, V(k)(-\mathrm{i}\mathbf{k})\mathrm{e}^{\mathrm{i}\mathbf{k}[\mathbf{r}(t)-\mathbf{R}(t)]} \tag{6}$$

due to a uniformly-moving projectile,

$$\mathbf{R}(t) = \mathbf{p} + \mathbf{v}t; \qquad \mathbf{p} \perp \mathbf{v} \tag{7}$$

the electron trajectory is given by

$$\mathbf{r}(t) = \mathbf{r}_0(t) + \frac{1}{m\omega}\int_{-\infty}^{t} \mathrm{d}t' \sin\omega(t-t')\mathbf{F}(t'). \tag{8}$$

At large t, equations (4, 6, 8) lead to

$$\mathbf{r}(t) = (\mathbf{a}_0 - \mathbf{S})\cos\omega t + (\mathbf{b}_0 + \mathbf{C})\sin\omega t \tag{9}$$

with

$$\mathbf{C} = \frac{1}{m\omega}\int_{-\infty}^{\infty} \mathrm{d}t\, \cos\omega t\, \mathbf{F}(t);$$
$$\mathbf{S} = \frac{1}{m\omega}\int_{-\infty}^{\infty} \mathrm{d}t\, \sin\omega t\, \mathbf{F}(t). \tag{10}$$

The energy transfer Q for a given set $\mathbf{a}_0, \mathbf{b}_0$ is then found from the relation

$$Q = \frac{1}{2}m(\dot{\mathbf{r}}^2 - \dot{\mathbf{r}_0}^2) + \frac{1}{2}m\omega^2(\mathbf{r}^2 - \mathbf{r}_0{}^2)$$
$$= \frac{1}{2}m\omega^2\left(C^2 + S^2 + 2\mathbf{b}_0\cdot\mathbf{C} - 2\mathbf{a}_0\cdot\mathbf{S}\right), \tag{11}$$

which is exact within the assumption of uniform projectile motion.

3.2 Series expansion

In conventional Bohr theory the term $\mathbf{r}(t)$ in the exponential in equation (6) is ignored because it leads to terms of higher than second order in Z_1. In the presence of $\mathbf{r}_0$ in (8) an expansion

$$\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}(t)} = 1 + \mathrm{i}\mathbf{k}\cdot\mathbf{r}(t) - \frac{1}{2}\left[\mathbf{k}\cdot\mathbf{r}(t)\right]^2 \ldots \tag{12}$$

needs to be made, much like in the theory of the Barkas effect [9], of $\mathbf{C}$ and $\mathbf{S}$ up to second order in the perturbance Z_1 and in the initial motion $\mathbf{r}_0(t)$. Insertion into equation (11), dropping higher-order terms and consideration of equation (5) leads to

$$\left\langle C^2 + S^2 \right\rangle = -\frac{1}{m^2\omega^2}\int_{-\infty}^{\infty}\mathrm{d}t\int_{-\infty}^{\infty}\mathrm{d}t'\cos\omega(t-t')$$
$$\times\int \mathrm{d}^3\mathbf{k}\int \mathrm{d}^3\mathbf{k}'\, V(k)V(k')(\mathbf{k}\cdot\mathbf{k}')\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{R}(t)-\mathrm{i}\mathbf{k}'\cdot\mathbf{R}(t')}$$
$$\times\left\{1 - \frac{1}{6}\left\langle a_0^2\right\rangle\left[k^2 + k'^2 + 2\mathbf{k}\cdot\mathbf{k}'\cos\omega(t-t')\right]\right\}, \tag{13}$$

where the term independent of $\langle a_0^2\rangle$ in equation (13) represents Bohr's result.

Expansion of the remainder of equation (11) needs terms in $\mathbf{C}$ and $\mathbf{S}$ of first order in $\mathbf{a}_0$ or $\mathbf{b}_0$ and up to second order in $V(k)$. Therefore, all three terms listed in the expansion (12) are in fact needed. However, systematic use of equation (5) and mutual cancellation of equivalent terms between $\mathbf{b}_0\cdot\mathbf{C}$ and $\mathbf{a}_0\cdot\mathbf{S}$ leave only one nonvanishing term,

$$\left\langle 2\mathbf{b}_0\cdot\mathbf{C} - 2\mathbf{a}_0\cdot\mathbf{S}\right\rangle = -\frac{\langle a_0^2\rangle}{3m^2\omega^2}\int_{-\infty}^{\infty}\mathrm{d}t\int_{-\infty}^{\infty}\mathrm{d}t'$$
$$\times\sin^2\omega(t-t')\int\mathrm{d}^3\mathbf{k}\int\mathrm{d}^3\mathbf{k}'\, V(k)V(k')$$
$$\times(\mathbf{k}\cdot\mathbf{k}')^2\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{R}(t)-\mathrm{i}\mathbf{k}'\cdot\mathbf{R}(t')}. \tag{14}$$

3.3 Integration

Collection of equations (13, 14) in equation (11), leaving out the zero-order term, leads to the shell correction

$$\Delta T = \langle\Delta Q\rangle = \frac{\langle a_0^2\rangle}{6m}\int_{-\infty}^{\infty}\mathrm{d}t\int_{-\infty}^{\infty}\mathrm{d}t'\int\mathrm{d}^3\mathbf{k}\int\mathrm{d}^3\mathbf{k}'$$
$$\times V(k)V(k')\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{R}(t)-\mathrm{i}\mathbf{k}'\cdot\mathbf{R}(t')}(\mathbf{k}\cdot\mathbf{k}')^2\cos 2\omega(t-t'). \tag{15}$$

After insertion of equation (7) and integration over the time variables, $\mathbf{k}$-dependent factors in the integrand may be replaced by differentiations with respect to $\mathbf{p}$. For Coulomb interaction[3], $V(k) = -Z_1e^2/2\pi^2k^2$,

[3] Only point charges will be considered here. The effect of screening can be incorporated when necessary [11].

the integrations over $\mathbf{k}$ and $\mathbf{k}'$ can be carried out, leading to

$$\Delta T = \frac{2Z_1^2 e^4 \langle a_0^2 \rangle}{3mv^2} \left[\nabla_p \cdot \nabla_{p'} + \left(\frac{2\omega}{v}\right)^2 \right]^2 \times K_0\left(2\frac{\omega p}{v}\right) K_0\left(2\frac{\omega p'}{v}\right) \Big|_{\mathbf{p}'=\mathbf{p}} \quad (16)$$

or

$$\Delta T = \frac{8Z_1^2 e^4 \langle v_e^2 \rangle}{3mv^4} \left(\frac{2\omega}{v}\right)^2 \left\{ \frac{3}{2}\left[K_0\left(2\frac{\omega p}{v}\right)\right]^2 + 2\left[K_1\left(2\frac{\omega p}{v}\right)\right]^2 + \frac{1}{2}\left[K_2\left(2\frac{\omega p}{v}\right)\right]^2 \right\}, \quad (17)$$

where K_n is a modified Bessel function in standard notation. In comparison with Bohr's expression for the leading term,

$$T = \frac{2Z_1^2 e^4}{mv^2} \left(\frac{\omega}{v}\right)^2 \left\{ \left[K_0\left(\frac{\omega p}{v}\right)\right]^2 + \left[K_1\left(\frac{\omega p}{v}\right)\right]^2 \right\}, \quad (18)$$

two differences appear most significant,

- the dependence on $2\omega p/v$ instead of $\omega p/v$ causes a more rapid decrease at large impact parameters,
- the occurrence of the Bessel function $K_2(2\omega p/v)$ in addition to K_0 and K_1 causes a more pronounced divergence at small impact parameters.

4 Close collisions

Close collisions are treated by classical binary scattering theory, taking into account the initial velocity $\mathbf{v}_e$ of the target electron. The kinematics are well-known [8,14], but inclusion of the impact-parameter dependence is a noticeable complication that requires care.

For a target particle in motion, in the absence of a binding force, the definition of the impact parameter is not unique. In order to ensure compatibility with the distant-collision regime, the initial (uniform) motion of the electron will be characterized by

$$\mathbf{r}_0(t) = \mathbf{a}_0 + \mathbf{v}_e t, \quad (19)$$

with

$$\langle \mathbf{a}_0 \rangle = \langle \mathbf{v}_e \rangle = \langle \mathbf{a}_0 \cdot \mathbf{v}_e \rangle = 0; \qquad \langle \mathbf{a}_0^2 \rangle = \frac{\langle v_e^2 \rangle}{\omega^2}, \quad (20)$$

the projectile trajectory (7) remaining unaffected. Equation (19) represents a feasible match of a uniform to a periodic trajectory: both the average behavior and that around $t = 0$ agree with equation (4)[4].

For a heavy projectile the c.m.s. velocity is identical in practice with the projectile velocity. In a system moving along with the projectile the unperturbed electron trajectory reads

$$\mathbf{r}_e(t) = \mathbf{s} + \mathbf{w}t; \qquad \mathbf{s} = \mathbf{a}_0 - \mathbf{p}; \qquad \mathbf{w} = \mathbf{v}_e - \mathbf{v}. \quad (21)$$

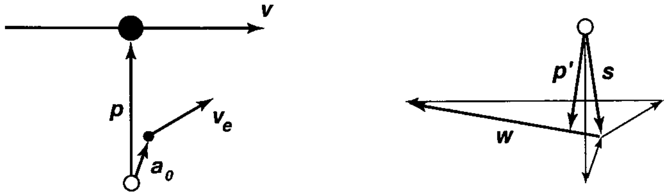

Fig. 1. Projectile interaction with moving target electron in lab (left) and projectile frame (right).

Figure 1 defines the vectorial impact parameter $\mathbf{p}'$ to the electron,

$$\mathbf{p}' = \mathbf{s} - \frac{\mathbf{s} \cdot \mathbf{w}}{w^2}\mathbf{w}. \quad (22)$$

With a scattering angle $\theta = \theta(w, p')$, the velocity after a collision reads

$$\mathbf{w}' = \mathbf{w}\cos\theta + \frac{\mathbf{p}'}{p'} w \sin\theta. \quad (23)$$

This defines the energy transfer Q in the laboratory system

$$Q = \frac{m}{2}\left[(\mathbf{v} + \mathbf{w}')^2 - v_e^2)\right] = m(v^2 - \mathbf{v}\cdot\mathbf{v}_e)(1-\cos\theta) + mw\mathbf{v}_e \cdot \frac{\mathbf{p}'}{p'}\sin\theta. \quad (24)$$

The energy transfer per unit time at the impact-parameter interval $\mathrm{d}^2\mathbf{p}'$ is given by $NwQ\,\mathrm{d}^2\mathbf{p}'$. Projection of that area on $\mathrm{d}^2\mathbf{p}$ in the lab system provides a factor $|\mathbf{v}\cdot\mathbf{w}|/vw$. With this one arrives at the stopping cross-section

$$S = \int \mathrm{d}^2\mathbf{p}\, T(\mathbf{p}) \quad (25)$$

with

$$T(\mathbf{p}) = \left\langle \frac{\mathbf{v}\cdot\mathbf{w}}{v^2} Q \right\rangle. \quad (26)$$

The same result can be obtained by considering the momentum transfer per unit time to the projectile in the moving system[5].

[4] The resonance frequency ω occurs in equation (20) only to ensure proper specification of the displacement $\mathbf{a}_0$.

[5] The momentum transfer in a collision is

$$\Delta\mathbf{P} = m\mathbf{w}(1-\cos\theta) - mw\frac{\mathbf{p}'}{p'}\sin\theta.$$

Only the component $-(\mathbf{v}/v)\cdot\Delta\mathbf{P}$ in the direction $-\mathbf{v}$ is of interest for the stopping force. With the current density $N\mathbf{w}$, the number of electrons per unit time passing an areal element $\mathrm{d}^2\mathbf{p}$ is given by

$$-N\mathbf{w}\cdot\frac{\mathbf{v}}{v}\mathrm{d}^2\mathbf{p}.$$

The product of the two quantities yields the contribution from the areal element $\mathrm{d}^2\mathbf{p}$ to the stopping force $N\int \mathrm{d}^2\mathbf{p}\, T(\mathbf{p})$, from which $T(\mathbf{p})$, equation (26), emerges again.

Specifically, for free-Coulomb scattering[6] with $\tan\theta/2 = b'/2p'$ and $b' = -2Z_1e^2/mw^2$,

$$T(\mathbf{p}) = T^{(1)}(\mathbf{p}) + T^{(2)}(\mathbf{p}) \tag{27}$$

with

$$T^{(1)}(\mathbf{p}) = 2mv^2 \left\langle \frac{(1 - \mathbf{v}\cdot\mathbf{v}_\mathrm{e}/v^2)^2}{1 + (2p'/b')^2} \right\rangle \tag{28}$$

and

$$T^{(2)}(\mathbf{p}) = 2mv^2 \left\langle \frac{2w(\mathbf{v}_\mathrm{e}\cdot\mathbf{p}')}{v^2b'} \frac{1 - \mathbf{v}\cdot\mathbf{v}_\mathrm{e}/v^2}{1 + (2p'/b')^2} \right\rangle. \tag{29}$$

Series expansion in $\mathbf{a}_0$ and $\mathbf{v}_\mathrm{e}$, taking due account of equation (20), leads to

$$T^{(1)}(\mathbf{p}) = \frac{2mv^2}{1 + (2p/b)^2} \left\{ 1 + \frac{\langle v_\mathrm{e}^2 \rangle}{3v^2} \frac{1 - 15(2p/b)^2}{[1 + (2p/b)^2]^2} - \frac{8\langle \mathbf{a}_0^2 \rangle}{3b^2} \frac{1 - (2p/b)^2}{[1 + (2p/b)^2]^2} \right\} \tag{30}$$

and

$$T^{(2)}(\mathbf{p}) = 0 \tag{31}$$

up to second order, with $b = -2Z_1e^2/mv^2$ and

$$\frac{8\langle \mathbf{a}_0^2 \rangle}{3b^2} = \frac{2}{3} \frac{\langle v_\mathrm{e}^2 \rangle}{v^2} \xi^2; \qquad \xi = mv^3/Z_1e^2\omega. \tag{32}$$

5 Results

Figures 2 and 3 show shell corrections evaluated from equations (17, 30) as functions of the scaled impact parameter $\omega p/v$ for several values of the scaled velocity parameter $\xi = mv^3/Z_1e^2\omega$. Plotted is the quantity $p\Delta T(p)$ in proper dimensionless variables. This implies that the area under a curve reflects the contribution to the total shell correction.

Consider first the cases of $\xi = 8$ and 4 indicating the high-speed behavior (Fig. 2). The shell correction is negative at small impact parameters, turns positive after having gone through a minimum and slowly approaches zero. This appears dictated mostly by the free-Coulomb behavior. A smooth transition to the multipole limit is found, which is positive everywhere, and there is a crossover at an impact parameter p_c (Tab. 1).

A qualitatively similar behavior is still observed for $\xi = 2$ (Fig. 3), although there is no crossover since the free-Coulomb limit now is negative everywhere. While the true behavior of the shell correction is not obvious for $1 \lesssim \omega p/v \lesssim 2$, the contribution to the total shell correction from this region is moderate.

[6] The chosen notation implies negative scattering angles for attractive interaction.

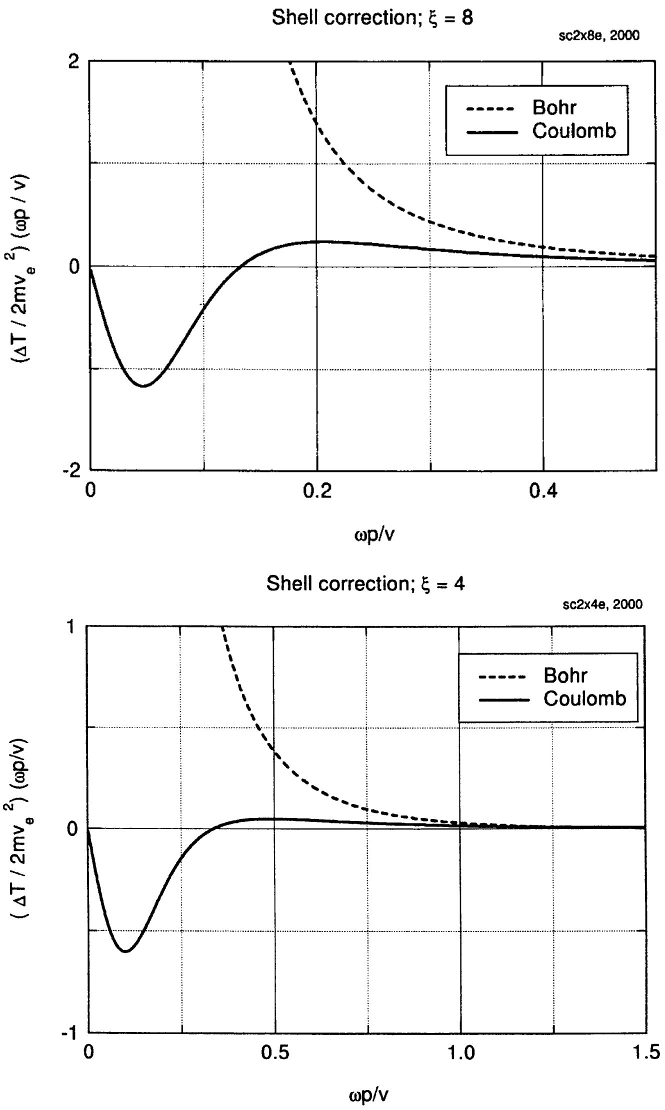

Fig. 2. Impact-parameter-dependent shell corrections in Bohr model; plotted is the quantity $(\Delta T/2m\langle v_\mathrm{e}^2\rangle)(\omega p/v)$ for $\xi = mv^3/Z_1e^2\omega = 8$ (upper graph) and 4 (lower graph).

This behavior gets accentuated for $\xi = 1$ (Fig. 3) where a feasible interpolation between the two curves can hardly be found without additional information. Clearly, the limitations of a description based solely on the first shell correction have been reached here.

Table 1 shows integrated shell corrections. It is seen that the free-Coulomb portion dominates, and that the total shell correction is close to what would be found from integration over the free-Coulomb expression over all impact parameters,

$$\Delta L_\mathrm{free} = -\frac{7}{6} \frac{\langle v_\mathrm{e}^2 \rangle}{v^2} \cdot \tag{33}$$

Note that the term $\propto \langle \mathbf{a}_0^2 \rangle$ does not contribute to equation (33). This has to be so since $\mathbf{a}_0$ merely specifies an origin in the impact plane before integration.

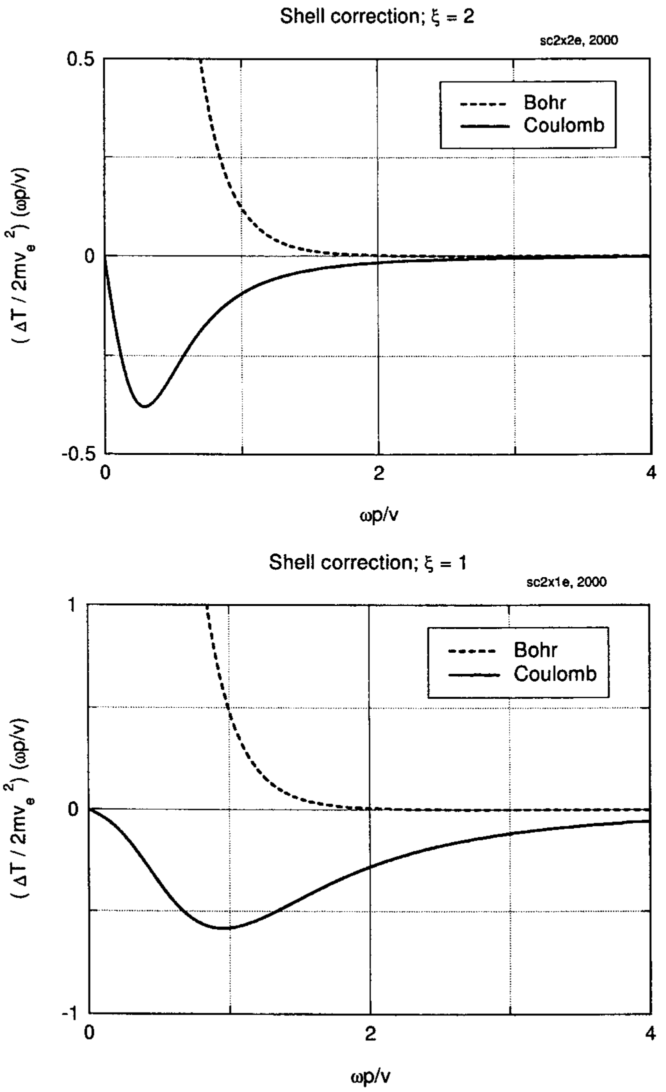

Fig. 3. Same as Figure 2 for $\xi = mv^3/Z_1e^2\omega = 2$ (upper graph) and 1 (lower graph).

The result, equation (33) is close to but not identical with the quantal result (3), and the results in Table 1 deviate even a bit more. In order to rationalize the difference in magnitude note that the minima in Figures 2 and 3 lie around or below $\omega p_{\min}/v = 1/\xi$ or, in terms of Bohr's κ-parameter $\kappa = 2Z_1v_0/v$ [15]

$$p_{\min} \lesssim \frac{\kappa}{2}\frac{\hbar}{mv}\,. \tag{34}$$

In the Bethe regime, *i.e.*, for $\kappa \lesssim 1$, this minimum lies below the de Broglie wavelength where the relation between energy loss and impact parameter is not described by classical dynamics.

6 Kinetic theory

In reference [8] a general expression was suggested for the first shell correction, based on transformation laws from

Table 1. Contributions to coefficient of first shell correction. p_c marks the crossover between free-Coulomb and multipole limit. Coulomb: contribution from impact parameters $< p_c$. Bohr: contributions from impact parameters $> p_c$.

ξ	$\omega p_c/v$	$v^2\Delta L/\langle v_e^2\rangle$		
		Coulomb	Bohr	total
10	0.866	−1.563	0.201	−1.362
8	0.917	−1.502	0.160	−1.342
6	1.018	−1.407	0.103	−1.304
4	1.283	−1.265	0.033	−1.232
3	1.846	−1.181	0.003	−1.178

binary-collision kinematics,

$$\Delta S(v) = \frac{\langle v_e^2\rangle}{v^2}\left(-\frac{1}{3}S_0(v) + \frac{v}{3}{S_0}'(v) + \frac{v^2}{6}{S_0}''(v)\right), \tag{35}$$

where $S_0(v)$ represents the stopping cross-section disregarding shell corrections, *i.e.*, the limiting expression for $v \gg v_e$, and a prime denotes the derivative with respect to v.

When (35) is applied to equation (2) one finds

$$\Delta L = -\frac{3\langle v_e^2\rangle}{2v^2}, \tag{36}$$

i.e., a result different from both (3, 33) and Table 1. It is of interest to trace the origin of this discrepancy.

Note first that equation (2) (with $C = 1$) can be rationalized by assuming free-Coulomb scattering on stationary target electrons for $0 < p < p_{\max} = v/\omega$ and cutting off all interaction at larger impact parameters. The kinetic theory requires this limit to be applied in the moving system, *i.e.*, $0 \le p' \le w/\omega$ or

$$s^2 - \frac{(\mathbf{s}\cdot\mathbf{w})^2}{w^2} \le w^2/\omega^2 \tag{37}$$

according to equation (22). This affects the averaging process leading from equation (28–30). Equation (28) needs to be evaluated again, now with the boundary condition (37) also expanded up to second order in v_e. One can set $\mathbf{a}_0 = 0$ here since that term drops out after integration, as in equation (31). As a result one finds a contribution $\Delta L^{(0)} = \langle v_e^2\rangle/3v^2$ from the zero-order term in (28) and $\Delta L^{(1)} = -2\langle v_e^2\rangle/3v^2$ from the first-order term. Adding these contributions to equation (33) yields the result from kinetic theory, equation (36), as it has to for consistency.

This estimate shows that the kinetic theory overestimates the contribution from distant collisions to the shell correction. The likely reason for this is the fact that shell corrections are evaluated in that scheme by means of a transformation of the leading energy-loss term, where there is approximate equipartition between close and distant collisions.

Since the transformations discussed in reference [8] refer to integrals over the impact parameter, pertinent differential relationships are given here for completeness, although only for the case of a projectile mass $\gg m$. If the energy loss to a stationary target electron is denoted as $T_0(p,v)$, then, for binary collisions and a central force,

$$T(p,v) = \left\langle T_0(p',w)\left(\frac{\mathbf{v}\cdot\mathbf{w}}{vw}\right)^2\right\rangle. \quad (38)$$

Expansion up to second order yields

$$\begin{aligned} T(p,v) &\simeq T_0(p,v) \\ &+ \frac{\langle v_\mathrm{e}^2\rangle}{v^2}\left(-\frac{2}{3} - \frac{1}{6}p\frac{\partial}{\partial p} + \frac{1}{3}v\frac{\partial}{\partial v} + \frac{1}{6}v^2\frac{\partial^2}{\partial v^2}\right)T_0(p,v) \\ &+ \frac{\langle a_0^2\rangle}{p^2}\left(\frac{1}{6}p\frac{\partial}{\partial p} + \frac{1}{6}p^2\frac{\partial^2}{\partial p^2}\right)T_0(p,v). \quad (39)\end{aligned}$$

Integration over $2\pi p\,\mathrm{d}p$ leads back to equation (35).

7 Discussion

Figures 2 and 3 confirm the experience from Bethe theory that the shell correction results from the *motion* of a target electron, while the influence of the binding force is indirect via its effect on the zero-point motion.

The absence of some sort of equipartition in the shell correction between close and distant interactions has been established in momentum space within the Bethe theory [1]. However, equipartition was asserted in reference [1] between energy transfers below and above mv^2. In the present scheme, this corresponds to $2p/|b| = 1$ or $\omega p/v = 1/\xi$. At least for $\xi = 8$ and 4, impact parameters below that limit, *i.e.*, energy losses above mv^2, contribute with a significantly higher weight than those below mv^2.

While it is reassuring that a smooth transition between the two theoretical schemes is achieved for not too small values of ξ, the error made by applying free-Coulomb scattering at all impact parameters is limited, as shown in Table 1, and even for $\xi = 2$ and 1, where there is some uncertainty about the proper interpolation, application of the binary approximation at all impact parameters appears the most feasible approach in the lack of more detailed information.

Note that the limitations of the kinetic theory identified in the preceding section become relevant only when long-range interactions play a substantial role in the energy loss before shell correction, while the transformation equations as such are exact within the binary-collision picture. For heavy ions, shell corrections become important mainly in the velocity range where ions are more or less heavily screened [12]. With increasing screening the role of the long-range part of the interaction decreases even in zero order.

While the applicability of the binary-collision picture implies a major simplifaction in the computation of stopping forces for heavy ions, it is clear that the restriction to terms of second order in v_e cannot be adequate at velocities where shell corrections are large. However, within the binary-collision approximation, target motion can readily be allowed for to any order.

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