Z_1^3 contribution to the energy loss of heavy charged particles

S. H. Morgan, Jr.
Program Development, George C. Marshall Space Flight Center, Huntsville, Alabama 35812

C. C. Sung*
Health and Safety Research Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830
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The Z_1^3 contribution of distant collisions to the average energy loss of heavy charged particles is obtained by extending Bethe's quantum-mechanical calculation to the next highest order in Z_1. The second-order Born approximation for the inelastic-collision cross section is simplified by using two major approximations. The infinite summation over terms arising from the coupling to intermediate states of the target atom is approximated with the aid of a parameter and the closure relation. This parameter is proportional to the average excitation energy of the intermediate states as described in the literature. The atomic form factors are simplified through a dipole expansion. Results are obtained in terms of an average excitation energy of the medium. Exemplary results for stopping in Al are presented for estimated values of the average excitation energy of the intermediate states. These results approach the classical and experimental values as the velocity of the penetrating particle increases, agreeing within 20% at $\beta = 0.3$.

I. INTRODUCTION

Calculations of the ionization and excitation energy loss of charged particles traversing matter were made prior to the development of quantum mechanics. The first classical calculation by Bohr[1] has been followed by the quantum-mechanical treatment by Bethe[2] and by the method of impact parameters by Williams.[3] In Bloch's subsequent quantum-mechanical treatment, the connection between the method of Bohr and Bethe was established.[4] Mott[5] demonstrated the equivalence of Bethe's method and the method of impact parameters. The classical approach is expected to be valid when $Z_1/137\beta \gg 1$, where the charge of the incident particle is $Z_1 e$ and βc is the velocity. The validity of the quantum-mechanical approach, in the first-order Born approximation, requires that $Z_1/137\beta \ll 1$.

All of the above theories find the energy loss in terms of Z_1^2 or, as Bloch found even powers of Z_1. However, different ranges for positive and negative Σ hyperons having the same initial energy have been reported[6] from nuclear emulsion experiments. Similar results have been found for pions.[7] In addition, claims of finding super-heavy ($Z_1 \sim 92$) nuclei in cosmic ray experiments have been published.[8] These results have supplied the motive for recent attempts to extend the theory of stopping power to include higher orders in Z_1.

Using a classical formulation of the interaction between a heavy charge with given impact parameter and a harmonically bound electron, Ashley, Ritchie, and Brandt[9] found a Z_1^3 contribution to the portion of energy loss due to distant collisions, i.e., collisions in which atomic electron binding effects are included. Jackson and McCarthy[10] repeated the calculation of Ashley *et al.* without limiting the incident particle to nonrelativistic motion and made a different choice of the minimum impact parameter. The Z_1^3 contribution is given in terms of tabulated functions.[11]

Hill and Merzbacher[12] also considered the harmonic oscillator model of the atom, but treated the problem quantum mechanically. The Z_1^3 contribution is obtained through an exact evaluation of the dipole contribution with the quadrupole contribution treated as a perturbation. Their results are identical with those obtained by Ashley *et al.*

Higher-order Z_1 contributions to energy loss for close collisions (collisions where atomic electron binding effects are ignored and arise from relativistic effects) have been made by Eby and Morgan,[13] by Jackson and McCarthy,[10] and recently by Ahlen.[14] Eby and Morgan found the higher-order contributions to all orders in Z_1 by using the exact Mott cross section, while Jackson and McCarthy obtained the Z_1^3 contribution for close collisions by using the second-Born-Mott cross section. Ahlen's calculation uses a Z_1^7 expansion of the cross section. For a recent review see Ref. 15.

The calculation described in this paper extends Bethe's nonrelativistic quantum-mechanical calculation for stopping power to the next highest order in Z_1. We obtained the Z_1^3 contribution for distant collisions by using the second-order Born approximation and repeating Bethe's calculation. The evaluation of the infinite sum over intermediate states required by the cross section is approxi-

mated by introducing, as a parameter, the mean excitation energy of the intermediate states and by using closure. This method has been used by Birman and Rosendorff[16] in calculating the collision cross section for elastic scattering of electrons by helium in the second-order Born approximation. The parameter was adjusted by these authors to fit the experimental results. In our calculation we follow the same procedure, but estimate the parameter by comparing our results with a different calculation using the techniques of Holt and Moiseiwitsch.[17]

The Holt-Moiseiwitsch approach is to truncate the sum over intermediate states at a low level, set all remaining energy levels equal to the next highest excitation level, and use closure to sum the remaining terms.

A dipole expansion of the atomic form factors is employed in our calculation leading to results in the form of moments of dipole oscillator-strength distributions.

In Sec. II the formalism leading to the second-order Born approximation for distant collisions is described. Results and a comparison of the present calculation with the classical theoretical results and with experiment is discussed in Sec. III.

II. THEORY

A. General

The average energy loss per unit path length of a charged particle as it traverses a material is given by

$$-\frac{dE}{dx}=N\sum_n (E_n-E_0)\sigma_{0n}=N\sum_n (E_n-E_0)\int \frac{d\sigma_{0n}}{d\Omega}\times d\Omega .$$

The summation extends over all excited states, and σ_{0n} is the total inelastic cross section that leads to final atomic state n. The energy loss in the collision is (E_n-E_0), the difference between the energy level of the excited state E_n and ground state E_0, and N is the density of atoms. In momentum coordinates

$$-\frac{dE}{dx}=2\pi N k_0^{-2}\sum_n (E_n-E_0)\int_{q_{\min}}^{q_{\max}} q\,dq|f_{n0}(\vec{q})|^2 . \quad (1)$$

The scattering amplitude is $f_{n0}(\vec{q})$, $\hbar\vec{k}_n$ and $\hbar\vec{k}_0$ are the final and initial momenta of the incident particle, respectively, and $\hbar\vec{q}=\hbar\vec{k}_0-\hbar\vec{k}_n$ is the momentum transferred in the collision. The minimum and maximum momentum is approximately $(E_n-E_0)/\hbar v_1$ and $2mv_1^2/\hbar$, respectively.

Since the lower limit of Eq. (1) depends upon n, the integration and summation cannot be interchanged. The interchange however can be accomplished by introducing $\bar{q}_{\min}=W/\hbar v_1$, where $W=(E_n-E_0)_{\rm av}$ is the average excitation energy of the medium. W is defined by writing Eq. (1) as[2]

$$-\frac{dE}{dx}=2\pi N k_0^{-2}\int_{\bar{q}_{\min}}^{q_{\max}} q\,dq\sum_n (E_n-E_0)|f_{n0}(\vec{q})|^2 \quad (2)$$

with the auxiliary requirement that

$$\sum_n \int_{W/\hbar v_1}^{(E_n-E_0)/\hbar v_1} q\,dq\,(E_n-E_0)|f_{n0}(\vec{q})|^2=0 , \quad (3)$$

which serves to define W.

Notice that the average excitation energy, W in Eq. (2) will be different from that obtained by Bethe who calculated the scattering amplitude in the first order Born approximation. This will be discussed in greater detail in Sec. II C.

The general form of Eq. (2) may be conveniently put in the form of an expansion in Z_1^n

$$-\frac{dE}{dx}=\frac{4\pi(Z_1e^2)^2NZ_2}{mv_1^2}\times[L_0(v_1,Z_2)+Z_1L_1(v_1,Z_2)+\cdots], \quad (4)$$

where $L_0=\ln(2mv_1^2/I_B)$ is Bethe's nonrelativistic results from first-order perturbation theory, L_1 is the Z_1^3 contribution, etc.

B. Second-order Born approximation

The Z_1^3 contribution to the average energy loss may be obtained by using, as the scattering amplitude, the Born expansion to second order. That is,

$$f_{n0}=\lambda f_{n0}^{(1)}+\lambda^2 f_{n0}^{(2)}$$

where

$$f_{n0}^{(1)}=-\frac{1}{4\pi}\int \exp[i(\vec{k}_0-\vec{k}_n)\cdot\vec{R}]V_{n0}(\vec{R})\,d\vec{R}$$

and

$$f_{n0}^{(2)}=\left(\frac{1}{4\pi}\right)^2\sum_m\int\int e^{-i\vec{k}_n\cdot\vec{R}'}e^{i\vec{k}_0\cdot\vec{R}}V_{nm}(\vec{R}')\times V_{m0}(\vec{R})\frac{\exp(ik_m|\vec{R}-\vec{R}'|)}{|\vec{R}-\vec{R}'|}\,d\vec{R}\,d\vec{R}' .$$

The expansion parameter is $\lambda=Z_1e^2\mu/\hbar^2$, where μ is the reduced mass of the system and $\hbar\vec{k}_m$ is the momentum of the intermediate states. The matrix elements from initial atomic state s to excited state t are given by

$$V_{ts}(\vec{R})=-2\left\langle t\left|\sum_{i=1}^{Z_2}\left(\frac{1}{|\vec{R}-\vec{r}_i|}-\frac{1}{R}\right)\right|s\right\rangle .$$

$\vec{R}$ is the coordinate of the incident ion relative to the nucleus, and $\vec{r}_i$ is the internal atomic coordinate. The sum over m implies a summation over the discrete states and an integration over the continuum.

Using the Fourier transform,

$$\frac{\exp(ik_m|\vec{R}-\vec{R}'|)}{|\vec{R}-\vec{R}'|} = \lim_{\epsilon\to 0}\int \frac{\exp[i\vec{K}\cdot(\vec{R}-\vec{R}')]}{(K^2-k_m^2-i\epsilon)}\,d\vec{K},$$

and an integral given by Bethe,

$$\int \frac{e^{i\vec{K}\cdot\vec{R}'}}{|\vec{R}-\vec{R}'|}\,d\vec{R}' = \frac{4\pi e^{i\vec{K}\cdot\vec{R}}}{K^2},$$

one may immediately integrate over the ion coordinate obtaining the first- and second-order contribution to the scattering amplitude

$$f_{n0}^{(1)}(\vec{q}) = 2F_{n0}(-\vec{q})/q^2$$

and (5)

$$f_{n0}^{(2)} = 2\pi^{-2}\Big(\sum_m J_n[k_m^2; F_{nm}(-\vec{K}_2)F_{m0}(\vec{K}_1)] - J_n[k_n^2; F_{n0}(\vec{K}_1)] - J_n[k_0^2; F_{n0}(\vec{K}_2)]\Big)$$

where the J_n integrals are defined as

$$J_n[k_s^2; F_{tp}(\vec{K})] = \lim_{\epsilon\to 0}\int \frac{F_{tp}(\vec{K})\,d\vec{K}}{(K^2-k_s^2-i\epsilon)K_1^2K_2^2} \quad (6)$$

with $\vec{K}_1 = \vec{K}-\vec{k}_0$ and $\vec{K}_2 = \vec{K}-\vec{k}_n$. The inelastic form factor is defined by

$$F_{tp}(\vec{K}) = \sum_{i=1}^{Z_2}\langle t|e^{-i\vec{K}\cdot\vec{r}_i}|p\rangle. \quad (7)$$

The J_n integrals are discussed in detail in Refs. 16 and 18 and are readily evaluated. One finds

$$\mathrm{Re}(J_n[k_s^2;1]) = \begin{cases} -\pi^3 M/q, & k_s^2 > k_0^2 > k_n^2 \\ -\pi^3 M/2q, & k_s^2 = k_0^2 > k_n^2 \\ 0, & k_0^2 > k_s^2 > k_n^2 \\ \pi^3 M/2q, & k_0^2 > k_s^2 = k_n^2 \\ \pi^3 M/q, & k_0^2 > k_n^2 > k_s^2 \end{cases}, \quad (8)$$

where

$$M = [k_s^2 q^2 + (k_s^2-k_0^2)(k_s^2-k_n^2)]^{-1/2}.$$

The Z_1^3 contribution to the stopping power is given by the expression

$$\delta\left(\frac{dE}{dx}\right) = 2\pi N\lambda^3 k_0^{-2} \times \int_{q_{\min}}^{q_{\max}} q\,dq\sum_n (E_n-E_0)(2\,\mathrm{Re}f_{n0}^{(1)}f_{n0}^{(2)}). \quad (9)$$

Terms to order λ^4 are omitted in Eq. (9) since we have not included terms to this order that would have appeared from the third-order Born expansion. The calculation performed consistently to order λ^3 thus requires that terms to order λ^4 be omitted.

The infinite summation over intermediate states has been approximated using several approaches. The earliest and simpliest is that of Massey and Mohr[19] (MM), who set the energy of all intermediate levels equal to the ground-state energy and used the closure relation

$$\sum_s \Psi_s^*(\vec{r}')\Psi_s(\vec{r}) = \delta(\vec{r}-\vec{r}')$$

to obtain

$$\sum_m \langle n|F(-\vec{K}_2)|m\rangle\langle m|F(\vec{K}_1)|0\rangle = \langle n|F(\vec{q})|0\rangle.$$

This approach is reasonable for high-energy penetrating particles. However, when one sets $k_m^2 = k_0^2$ in the first integral of Eq. (5), the resulting integral vanishes (cf. Ref. 16). Further inadequacies of the MM approximation are shown by the calculations of Holt and Moiseiwitsch,[17] which indicate that for the $1S \to 2S$ excitation of hydrogen by electron impact this approach is not reliable except at large angles and high energies. Holt and Moiseiwitsch point out, however, that the MM approach may be rendered more reliable by setting the intermediate energy levels equal to an excited state level instead of the ground state.

Other approaches have been to truncate the sum after using the exact value of k_m^2 for the first p terms and dropping the remaining terms[20] or, alternatively, setting $k_m^2 = k_{p+1}^2$ for the remaining terms, and use the closure relation.[17] However, these methods are difficult, in general, because of the great amount of computational effort required even for small values of p. In addition, one must use the explicit excited-state form factors. These approaches have thus only been attempted in a limited way for scattering of electrons and protons by hydrogen and helium.[17,20]

The approach used in this paper is similar to that used by Birman and Rosendorff,[16] who modified the MM approximation. We set $k_m^2 = k_0^2 - \Delta$ in Eq. (9) and use the closure relation. The free parameter Δ is interpreted as being proportional to the mean excitation energy of the intermediate states. One notes from the behavior of the J_n integrals as expressed by Eq. (8) that the $m=0$ terms may be conveniently separated from the $m>0$ terms. After making this separation and using closure, one finds that the cross terms of the squared modulus of the scattering amplitude that are responsible for the Z_1^3 contribution may be expressed as

$$\lambda^3 f_{n0}^{(1)}f_{n0}^{(2)} \approx 4\lambda^3(\pi q)^{-2}\{J_n[k_0^2; F_{0n}(\vec{q})F_{n0}(-\vec{K}_2)F_{00}(\vec{K}_1) - F_{0n}(\vec{q})F_{n0}(-\vec{K}_2)] + J_n[k_0^2-\Delta; |F_{0n}(\vec{q})|^2 - F_{0n}(\vec{q})F_{n0}(-\vec{K}_2)F_{00}(\vec{K}_1)] - J_n[k_n^2; F_{0n}(\vec{q})F_{n0}(\vec{K}_1)]\}. \quad (10)$$

C. Distant collisions

The excited-state form factors are not known in general. In order to obtain a reasonably tractable solution we make a dipole expansion through the quadrupole terms with the definitions

$$\vec{D}_{n0} = \left\langle n \left| \sum_{i=1}^{Z_2} \vec{r}_i \right| 0 \right\rangle \quad \text{and} \quad Q_{n0} = \left\langle n \left| \sum_{i=1}^{Z_2} |\vec{r}_i|^2 \right| 0 \right\rangle .$$

Including, in Eq. (9), only those real terms that survive the change in parity selection rules, we find

$$\delta\left(\frac{dE}{dx}\right)_{\text{dist}} = 8\pi^2 N\lambda^3 k_0^{-2} \sum_n (E_n - E_0) \times \int_{q_{\min}}^{q_{\max}} (g+h)\, dq , \tag{11}$$

where

$$g = [S - (k_n q)^{-1}]\, |D_{0n}|^2 ,$$
$$h = [q^2 S + 4(k_n - k_0)/k_0 k_n]|\, Q_{0n}|^2 ,$$
$$S = \{(k_0^2 - \Delta)\, q^2 + \Delta[\Delta - (k_0^2 - k_n^2)]\}^{-1/2} .$$

Since a dipole expansion has been made in arriving at Eq. (11) one would not expect the integration to be valid for $qa_0 \gg 1$. We therefore divide the integration into two regions $[\bar{q}_{\min}, q_0]$ and $[q_0, q_{\max}]$. The first region corresponds to "distant" collisions which are associated with small momentum transfers. For the second or "close" collision region one assumes, in most calculations, that the momentum transfer is high enough so that the binding energies of the atomic electrons may be neglected. The intermediate momentum transfer, q_0, is analogous to the minimum impact parameter of the classical treatment. Jackson and McCarthy[10] used the quantal radius of the harmonic oscillator, i.e., $b_{\min} = (\hbar/2m\omega_0)^{1/2}$, where ω_0 is the effective harmonic-oscillator frequency. Ashley *et al.*[9] set $b_{\min} = \eta r$, where η is a parameter nearly equal to 1, and r is the shell radius of the "atom." We used $q_0 = (2m\omega_0/\hbar)^{1/2}$ in order to make a comparison with the classical results.

Integrating Eq. (11), assuming that Δ is independent of q, one obtains for dipole transitions

$$\delta\left(\frac{dE}{dx}\right)_{\text{dist}} = 8\pi^2 N\lambda^3 k_0^{-2} \sum_n |D_{0n}|^2 (E_n - E_0) \times [(k_0^2 - \Delta)^{-1/2} A - (4k_n)^{-1} \ln(2mv_1^2\hbar\omega_0/I'^2)] , \tag{12}$$

where

$$A = \sinh^{-1}\left[\left(\frac{2m\hbar\omega_0(k_0^2 - \Delta)}{\hbar^2\Delta[\Delta - (k_0^2 - k_n^2)]}\right)^{1/2}\right] - \sinh^{-1}\left[\left(\frac{(k_0^2 - \Delta)I'^2}{\Delta[\Delta - (k_0^2 - k_n^2)]\hbar^2 v_1^2}\right)^{1/2}\right] .$$

We make the substitution $\Delta = 2\mu\bar{\epsilon}/\hbar^2$ in Eq. (12), where $\bar{\epsilon}$ is the average excitation energy of the intermediate states. Expanding the $\sinh^{-1}$ functions, dropping terms to order $(\Delta/k_0^2)^2$ and smaller, one obtains in the high-velocity limit

$$L_1 = \frac{\pi e^2}{v_1^3\hbar^3 Z_2} \sum_n (E_n - E_0)|D_{0n}|^2[\bar{\epsilon} - (E_n - E_0)] \times \ln(2mv_1^2\hbar\omega_0/I'^2) . \tag{13}$$

$\bar{\epsilon}$ will be considered later in more detail. However, if we compare the trends predicted by Birman and Rosendorff[16] with the results of Holt and Moiseiwitsch,[17] it is clear that $\bar{\epsilon}$ lies between the ground-state energy level and one of the lower excited-state energy levels. Thus a value of $\bar{\epsilon}$ larger than the ground-state energy, but not arbitrarily large, is required to fit the experimental results.

I' is the average excitation energy obtained from the second-order Born approximation. This is obtained by noting that the auxiliary requirement given by Eq. (3) may be written in terms of two auxiliary equations when the second-order Born approximation is used. That is,

$$\sum_n \int_{I_B/\hbar v_1}^{(E_n - E_0)/\hbar v_1} q\, dq\, (E_n - E_0)\, |f_{n0}^{(1)}(\vec{q})|^2 = 0 \tag{14}$$

and

$$\sum_n \int_{I'/\hbar v_1}^{(E_n - E_0)/\hbar v_1} q\, dq\, (E_n - E_0) \times [2\,\text{Re} f_{n0}^{(1)}(\vec{q}) f_{n0}^{(2)}(\vec{q})] = 0 . \tag{15}$$

Equation (14) defines Bethe's average excitation energy from the first-order perturbation calculation, while Eq. (15) serves as the definition of the average excitation energy that must be used for the Z_1^3 contribution. Thus Eq. (15) becomes

$$\sum_n (E_n - E_0)|D_{0n}|^2[\bar{\epsilon}/\mathcal{R} - (E_n - E_0)] \times \ln[(E_n - E_0)/I'] = 0 \tag{16}$$

where $\mathcal{R}$ is the Rydberg energy.

The parameter $\bar{\epsilon}$ in Eq. (13) was estimated by using a modification of the MM approximation. The intermediate-state energy levels were set equal to an excited-state level instead of the ground state as was the case with the MM approximation. This approach is expected to be more reliable than the MM approximation.[17] The results using this improved, yet manageable, approach were then compared with Eq. (13) to obtain a rough estimate of $\bar{\epsilon}$.

If one applies the same procedure as was used to obtain Eq. (12) and Eq. (13) to the modified MM approximation one finds after expanding the $\sinh^{-1}$ functions

$$\delta\left(\frac{dE}{dx}\right)_{\text{dist}} = 8\pi^2 N\lambda^3 k_0^{-2} \sum_n (E_n - E_0)|D_{n0}|^2 \times [(2k')^{-1} - (4k_n)^{-1}] \times \ln(2mv_1^2\hbar\omega_0/I'^2), \quad (17)$$

where k' corresponds to an excited-state excitation level.

We restrict k' in Eq. (17) to correspond to optically allowed excitations only. For example, for $1S \rightarrow 2P$ excitations we select k' to correspond to the next highest optically allowed state, the $3P$ state. Specifically

$$k_0^2 - k'^2 = 2\mu(E_{3P} - E_{1S})/\hbar^2 .$$

The next highest level is chosen because of the restrictions of Eq. (8). One notes from Eq. (8) that the J_n integrals vanish unless

$$\Delta > k_0^2 - k_n^2 \text{ or } \bar{\epsilon} > (E_n - E_0) .$$

We consider only one excitation level, namely the $1S \rightarrow 2P$ excitation. Thus

$$\bar{\epsilon} > (E_{2P} - E_{1S})$$

and k'^2 must correspond to at least the E_{3P} energy level.

Comparing Eq. (17) with Eq. (13), one obtains the approximate relation

$$k_2 \approx (k_0^2 - \Delta)^{1/2}$$

or

$$\Delta \approx k_0^2 - k_2^2 ,$$

then

$$\bar{\epsilon} \approx E_{3P} - E_{1S} . \quad (18)$$

The estimated value of $\bar{\epsilon}$ given by Eq. (18) was obtained from the first optically allowed state only. If more intermediate states were included, Eq. (17) would be much more complicated as would Eq. (18).

We next introduce the dipole oscillator-strength distributions:

$$S(a) = \sum_n f_n (E_n - E_0)^a ; \quad (19)$$

$$L(a) = \sum_n f_n (E_n - E_0)^a \ln(E_n - E_0) ; \quad (20)$$

where f_n is the oscillator strength given by

$$a_0^2 \mathcal{R} f_n = (E_n - E_0)|D_{n0}|^2 .$$

Returning to Eq. (14) and Eq. (15), Bethe found upon solving Eq. (14)

$$\ln(I_B/\mathcal{R}) = L(0)/S(0) . \quad (21)$$

In our case we have an additional relationship for I', according to Eq. (15). Thus,

$$\left[\frac{\bar{\epsilon}}{\mathcal{R}}\frac{S(0)}{S(1)} - 1\right]\ln(I'/\mathcal{R}) = \frac{\bar{\epsilon}}{\mathcal{R}}\frac{L(0)}{S(1)} - \frac{L(1)}{S(1)} . \quad (22)$$

It should be pointed out that I' must not be interpreted as a correction to I_B.

Substituting Eq. (22) into Eq. (13), one finds the expression

$$L_1 = \frac{\pi}{4(137\beta)^3}\frac{S(1)}{S(0)}\left[\left(\frac{\bar{\epsilon}}{\mathcal{R}}\frac{S(0)}{S(1)} - 1\right)\ln(2mv_1^2/\mathcal{R}) - \frac{\bar{\epsilon}}{\mathcal{R}}\frac{L(0)}{S(1)} + \frac{L(1)}{S(1)}\right] . \quad (23)$$

In the high-velocity limit Jackson and McCarthy found

$$L_1 = \frac{3\pi}{8(137\beta)^3}\frac{S(1)}{S(0)}\left(\ln(2mv_1^2/\mathcal{R}) - \frac{L(1)}{S(1)} - 1.04\right) . \quad (24)$$

In comparing Eq. (23) and Eq. (24), one finds certain similarities. Both have the same v_1^{-3} velocity dependence and both are proportional to $S(1)$. $S(1)$ is approximately equal to the absolute value of the total binding energy and $S(0) = Z_2$ from the oscillator strength sum rule.[21] If one multiplies Eq. (23) by the $S(1)/S(0)$ factor the results are in the form

$$L_1 \sim \left[\frac{\bar{\epsilon}}{\mathcal{R}} - \frac{S(1)}{S(0)}\right]\ln(2mv_1^2/\mathcal{R}) - \frac{\bar{\epsilon}}{\mathcal{R}}\frac{L(0)}{S(0)} - \frac{L(1)}{S(0)} .$$

Thus the logarithmic term, which will be the dominate term for high energies, is proportional to the difference between the average excitation energy of the intermediate states and the absolute value of the binding energy per atomic electron.

III. RESULTS

The distributions in Eq. (24) may be obtained from the normalized moment integrals

$$S(a) = \int_0^\infty g(\omega)\omega^a d\omega$$

$$L(a) = \int_0^\infty g(\omega)\omega^a \ln(\omega)\, d\omega ,$$

where $g(\omega)$ is the oscillator strength distribution, normalized such that $S(0) = 1$. This was done in the earlier classical calculations by using the Thomas-Fermi statistical model as suggested by Lindhard and Scharff[22] with the Lenz-Jensen approximation for the statistical-model number density.[23] That is,

$$g_{LJ}(\omega) = \int \rho_{LJ}(\vec{r})\delta(\omega - \omega(\vec{r}))\, d\vec{r} .$$

Subsequent to the first classical calculations,[9-11] Dehmer *et al.*[21] and Inokuti *et al.*[24] published the moments $S(a)$ and $L(a)$ for $-6 \leq a \leq 1$, obtained from the Hartree-Slater oscillator-strength distributions

for He through Ar. Recently Ritchie and Brandt[25] applied the Hartree-Slater distributions to their classical approach reported earlier.[9] The Lenz-Jensen approach is not expected to yield reliable results for $Z_2 \leq 54$.[25] We therefore used the published results of the Hartree-Slater distributions in our calculations.

Ashley *et al.* published their results in the form of a tabulated function $\mathcal{K}(b, x)$, where

$$L_1 = L_0(x)\mathcal{K}(b, x)Z_2^{-1/2}x^{-1}$$

with $L_0 = \ln(2mv_1^2/K_B Z_2)$. K_B is Bloch's constant ≈ 9.76 eV, $x = (137\beta)^2 Z_2^{-1}$, and b is a parameter related to the minimum impact parameter cutoff.

Figure 1 is a plot of L_1 vs β [Eq. (23)] for charged particles incident on Al with the parameter $\bar{\epsilon}/\mathcal{R} = 125$ and 100. The curve representing the experimental data was obtained from the best fit equation given by Andersen *et al.*[26] The classical results of Ashley *et al.* with $b = 1.6$ are included for comparison along with the results of Jackson and McCarthy (high-velocity limit). One notes from the figure that the quantum results for $\bar{\epsilon}/\mathcal{R} = 100$ and the experimental results are about a factor of 2 larger than the classical results with $b = 1.6$. However, if one reduces the minimum impact parameter cutoff by setting $b = 1.4$ in $\mathcal{K}(b, x)$, L_1 is increased by a factor of 2 over the $b = 1.6$ values[25] and the classical, quantum, and experimental results are in closer agreement. One also notes from the figure that the quantum results fit the experimental curve fairly well for $\bar{\epsilon}/\mathcal{R} = 100$. The value of $(E_{3P} - E_{1S})$ is approximately $11\mathcal{R}$ for Al.

The cross section for excitation depends upon the energy of the penetrating particle, which is partially contained in the velocity dependence of Δ. One can treat Δ as a parameter and fit the experimental data as did Birman and Rosendorff in their calculation of the differential cross section. They examined the scattering of 200 and 700 eV electrons by helium. For low-momentum transfers they found that $\Delta \approx 5a_0^2$ at 200 eV and $\Delta \approx 7a_0^2$ at an initial kinetic energy of 700 eV gave relatively good agreement with experiment. This trend is also evident in the results of Fig. 1, where the proper $\bar{\epsilon}/\mathcal{R}$ depends on β. In view of the experimental uncertainity, we found the best fit for $\Delta(v_1)$. If $\Delta(v_1)$ varies from $E_{2P} - E_{1S}$ from high v_1 to $a(E_{3P} - E_{1S})$, where $a < 1$, we probably can fit the velocity dependence of dE/dx very well throughout the range of available experimental data.

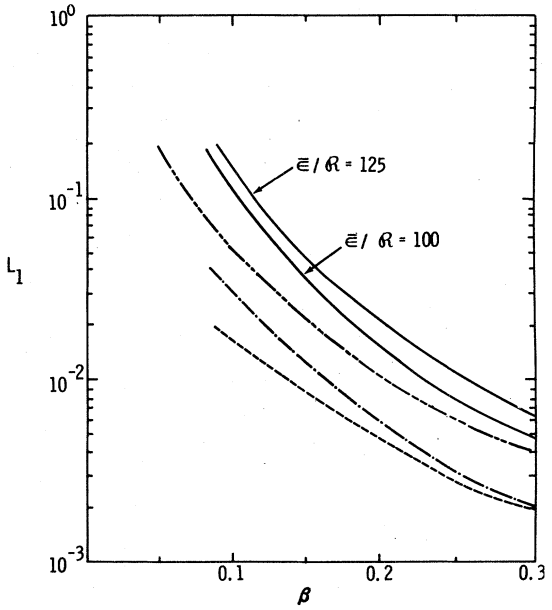

FIG. 1. Z_1^3 contributions for stopping power of Al as a function of initial velocity of the penetrating particle. The solid curves are the second-order Born results. The dash-dot-dot curve is from the experiments by Andersen *et al.* (Ref. 26). The dash-dot curve is from the classical results of Ashley *et al.* (Ref. 9) with $b = 1.6$. The dashed curve is Jackson and McCarthy's (Ref. 10) high-velocity limit.

IV. CONCLUSIONS

The calculation discussed in this paper extends Bethe's stopping-power calculation to the next highest order in Z_1. However, as was the case in the classical formulation, this is accomplished at the expense of introducing a parameter which may be estimated through the techniques used in calculating inelastic collision cross sections. We have thus presented a quantum-mechanical version of the earlier calssical calculations of the Z_1^3 contribution to energy loss.

The calculation also requires a minimum momentum-transfer cutoff separating close and distant collisions analogous to the maximum impact parameter cutoff required in the classical approach. The consequences of this cutoff are now under investigation.

The quantum results approach the classical and experimental results as the velocity of the colliding particle increases if the lower minimum impact parameter cutoffs are used in the classical results. The second-order Born results are about a factor of 2 larger than both the high-velocity limit results of Jackson and McCarthy and the results of Ashley *et al.* with $b = 1.6$. Andersen *et al.* also found their measured values of L_1 to be nearly a factor of 2 larger than the Jackson and McCarthy results. This is discussed by Lindhard,[27] who attributes this to contributions from small impact parameters that should be included in the classical

calculations. The better agreement with experiment and with the results presented in this paper if a smaller impact parameter cutoff is used would seem to support this.

The velocity dependence found in our calculation is $L_1/L_0 \sim v_1^{-3}$ as was also found in the classical high-velocity limit results. Andersen *et al.* found that the most favorable fit to their experimental data was $L_1/L_0 \sim v_1^{-2}$. Jackson and McCarthy find a velocity dependence which varies from $L_1/L_0 \sim v_1^{-2}$ to $L_1/L_0 \sim v_1^{-2.5}$ for low velocities, i.e., for $\beta \leq 0.07$. The velocity dependence of L_1/L_0, however, depends upon the minimum impact parameter cutoff chosen or alternatively the maximum momentum transfer for distant collisions. This and the varying results found thus far would lead one to conclude as stated by Hill and Merzbacher and by Inokuti *et al.*[15] that the question of Z_1^3 contributions for small impact parameters remains to be completely resolved.

Although the calculation discussed in this paper is treated as a quantum-mechanical scattering problem, a minimum momentum-transfer cutoff q_0 was required because of the dipole expansion used for the target atom from factors. This cutoff was assumed to be related to the classical minimum impact parameter and our solution should be termed, in a strict sense, semiclassical. For the quantum-mechanical first-order perturbation treatment, this cutoff is arbitrary since it cancels when the close and distant contributions are added. The relative contribution to stopping power of those collisions with momentum transfer greater than q_0 will be reported in a subsequent paper with the form factors for atomic hydrogen and other available target atoms used explicitly instead of a dipole expansion.

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*Present address: Dept. of Physics, Univ. of Alabama in Huntsville, Huntsville, Ala. 35807.

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