

## Quantum Mechanical Calculation of Neutron Stopping Power\*

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The stopping power of matter is calculated quantum mechanically for high-energy neutrons. The contribution from low- $Q$  collisions (in which the binding of atomic electrons is important) is shown to be insignificant at neutron energies of the order of  $4Z^{0.35}$  GeV or greater, where  $Z$  is the atomic number of the medium traversed. The quantum mechanical result shows a weaker dependence on neutron energy than an earlier semiclassical computation, applicable up to 10 GeV, although the two calculations give comparable numerical values in the range 5–10 GeV. A simple stopping-power formula is given for neutrons with energies between  $4Z^{0.35}$  and 500 GeV, where the neutron magnetic form factor becomes important. A more complicated formula is given and evaluated numerically to 7000 GeV. The density effect and radiative corrections are not treated.

### I. INTRODUCTION

Using the formalism developed in the preceding paper,<sup>1</sup> we calculate quantum mechanically the stopping power of matter for high-energy neutrons. Results are compared with those of an earlier semiclassical calculation.<sup>2</sup> The energy loss to atomic electrons occurs through the interaction of the neutron's spin and spatial distribution of magnetic moment with the charge and spin (magnetic moment) of the electron.

We proceed as in the theory of stopping power for charged particles.<sup>3</sup> As the neutron's energy increases, the relative probability increases for transferring an amount of energy which is large compared with the binding energies of the atomic electrons in the medium traversed. At very high neutron energies, to be specified more precisely below, we assume that collisions of this type are primarily responsible for the neutron stopping power. We calculate the stopping power in this "high- $Q$ " approximation, integrating over energy losses  $Q$  greater than some value  $\eta$ , of the order of the average binding energy of an atomic electron in the medium. At sufficiently high energies the dependence on  $\eta$  itself becomes negligible.

"Low- $Q$ " collisions, in which the binding of the electrons must be taken into account, are treated separately. Relevant parts of the cross-section formula are expanded in powers of  $Q$  and only the lowest-order nonvanishing term retained. We assume that this "low- $Q$ " approximation is valid for energy losses up to  $\eta$ , over which range we integrate to estimate the low- $Q$  contribution to the stopping power. In principle, higher-order terms in  $Q$  could be included to improve the low- $Q$  computation, but we do not do so here.<sup>4</sup>

We adopt the same notation as that used in Ref.

1, which also coincides with Ref. 3 (when  $\hbar=c=1$ ). Equation numbers  $N$  from Ref. 1 will be preceded here by the letter I, e.g., Eq. (I- $N$ ).

### II. FORM FACTOR FOR NEUTRON MAGNETIC MOMENT

The high- $Q$  approximation governs collisions in which  $Q$  falls between  $\eta$  and its maximum value,<sup>5</sup>

$$Q_{\max} = 2\gamma^2 M m \beta^2 / (M + 2\gamma m). \quad (1)$$

To treat these collisions when  $\gamma m/M$  is not small, we introduce the spatial distribution of the neutron's magnetic moment. As in a similar study for protons,<sup>6</sup> this is conveniently done by using the empirically fit form factor  $G_M(Q)$  suggested by Hand, Miller, and Wilson.<sup>7</sup> Using their numerical values, we write (for  $Q$  in cgs units and  $\mu = -1.91$  in units of  $e\hbar/2M_p c$ , where  $M_p$  is the mass of proton)

$$\begin{aligned} G_M(Q) &= \mu \sum_{i=1}^3 \frac{\lambda_i}{1 + \nu_i Q} \\ &= \mu \left( \frac{-0.839}{1 + 0.545Q} + \frac{2.461}{1 + 1.127Q} \right. \\ &\quad \left. + \frac{-0.622}{1 + 1.034Q} \right). \quad (2) \end{aligned}$$

It is instructive to see how large the neutron's energy must be in order for the  $Q$  dependence of the form factor to be significant. Expanding Eq. (3) to first order in  $Q$  and squaring,<sup>8</sup> we find that

$$G_M^2 = \mu^2 (1 - 3.345Q). \quad (3)$$

Setting the second term equal to 10% of the first at  $Q_{\max}$ , viz.,  $33Q_{\max} \sim 1$ , implies that  $\gamma \sim 500$ . Therefore, the error introduced by assuming the constant form factor is about 10% at 500 GeV.

### III. NEUTRON STOPPING POWER IN HIGH- $Q$ APPROXIMATION

The neutron cross section in the high- $Q$  approximation is given by Eq. (I-39), in which  $G_E = 0$  and  $m$  is negligible in comparison with  $Q$ . Expressing  $G_M$  by means of Eq. (2) and making use of Eq. (I-40), we write

$$d\sigma = \frac{2\pi e^4 Z \mu^2}{m\beta^2} \frac{dQ}{Q} \left[ \frac{\tau}{1+\tau} \left( \frac{1}{Q} - \frac{\beta^2}{Q_{\max}} \right) + \frac{Q}{2E^2} \right] \times \left( \sum_{i=1}^3 \frac{\lambda_i}{1+\nu_i Q} \right)^2, \quad (5)$$

where  $\tau = mQ/2M^2$ , as found from Eqs. (I-7) and (I-8). Introducing the symbols

$$a = 2M^2, \quad (6)$$

$$\sigma_i = m - a\nu_i, \quad (7)$$

$$A = (a + mQ_{\max})/(a + m\eta), \quad (8)$$

and

$$B_i = (1 + \nu_i Q_{\max})/(1 + \nu_i \eta), \quad (9)$$

we find the high- $Q$  contribution to the stopping power,

$$\left( -\frac{dE}{ds} \right)_{Q>\eta} \equiv N \int_{\eta}^{Q_{\max}} Q d\sigma \quad (10)$$

$$= \frac{1}{2} \kappa \mu^2 \left\{ \sum_i \lambda_i^2 \left[ \left( \frac{\nu_i m}{\sigma_i} + \frac{m\beta^2}{\sigma_i Q_{\max}} + \frac{1}{2E^2 \nu_i} \right) \frac{\eta - Q_{\max}}{(1 + \nu_i Q_{\max})(1 + \nu_i \eta)} + \frac{m}{\sigma_i^2} \left( m + \frac{a\beta^2}{Q_{\max}} \right) \ln \frac{A}{B_i} + \frac{1}{2E^2 \nu_i^2} \ln B_i \right] \right. \\ \left. + \sum_{i \neq j} \lambda_i \lambda_j \left[ \frac{m}{\sigma_i \sigma_j} \left( m + \frac{\beta^2 a}{Q_{\max}} \right) \ln A + \frac{1}{\nu_j - \nu_i} \left( \frac{2m\nu_i}{\sigma_i} + \frac{2m\beta^2}{\sigma_i Q_{\max}} + \frac{1}{E^2 \nu_i} \right) \ln B_i \right] \right\}, \quad (11)$$

where  $\kappa = 4\pi e^4 NZ/m\beta^2$ . Expression (11) is exact within the high- $Q$  approximation. The value of  $\eta$  for any element is so small that  $\nu_i \eta \ll 1$  and  $m\eta \ll a$ , and we henceforth drop these terms compared with unity. For  $\gamma$  not too close to unity, we also have  $Q_{\max} \gg \eta$ .<sup>9</sup> Under this condition the low- $Q$  collisions make an insignificant contribution to the stopping power, as shown in Sec. V. Therefore, the neutron stopping power is then given by ( $Q_{\max} \gg \eta$ ),<sup>10</sup>

$$-\frac{dE}{ds} = \frac{1}{2} \kappa \mu^2 \left\{ \sum_i \lambda_i^2 \left[ -\left( \frac{\nu_i m}{\sigma_i} + \frac{m\beta^2}{\sigma_i Q_{\max}} + \frac{1}{2E^2 \nu_i} \right) \frac{Q_{\max}}{1 + \nu_i Q_{\max}} + \left( -\frac{m^2}{\sigma_i^2} - \frac{ma\beta^2}{\sigma_i^2 Q_{\max}} + \frac{1}{2E^2 \nu_i^2} \right) \ln(1 + \nu_i Q_{\max}) \right] \right. \\ \left. + m \left( m + \frac{a\beta^2}{Q_{\max}} \right) \ln \left( 1 + \frac{mQ_{\max}}{a} \right) \sum_{i,j} \frac{\lambda_i \lambda_j}{\sigma_i \sigma_j} + \sum_{i \neq j} \lambda_i \lambda_j \left( \frac{2m\nu_i}{\sigma_i} + \frac{2m\beta^2}{\sigma_i Q_{\max}} + \frac{1}{E^2 \nu_i} \right) \frac{\ln(1 + \nu_i Q_{\max})}{\nu_j - \nu_i} \right\}. \quad (12)$$

If, in addition,  $\gamma \lesssim 500$ , Eq. (12) reduces to a simpler form. From Eq. (4) we see that we can represent the form factor (2) by writing  $\lambda_1 = 1$ ,  $\lambda_i = 0$  for  $i > 1$ , and  $\nu_1 = \nu = 1.7 \text{ erg}^{-1}$ . Expansion of Eq. (12) to first order in  $\nu$  then gives ( $Q_{\max} \gg \eta$ ,  $\gamma \lesssim 500$ )<sup>11</sup>

$$-\frac{dE}{ds} = \frac{1}{2} \kappa \mu^2 \left\{ \left( 1 + \frac{M(M+2\gamma m)}{\gamma^2 m^2} \right) \left( 1 + \frac{4M^2 \nu}{m} \right) \ln \left( 1 + \frac{\gamma^2 m^2 \beta^2}{M(M+2\gamma m)} \right) - \beta^2 \right. \\ \left. + \left( \frac{\gamma m \beta^2}{M+2\gamma m} \right)^2 + 2\nu M \beta^2 \left[ \left( \frac{\gamma^2 m (\beta^2 - 2)}{M+2\gamma m} \right) - \frac{2M}{m} - \frac{4\gamma^4 m^3 \beta^4}{3(M+2\gamma m)^3} \right] \right\}. \quad (13)$$

Finally, at high  $Q$ , we treat the condition  $\gamma m/M \ll 1$ . We can ignore the  $Q$  dependence of the form factor, but cannot assume that  $Q_{\max} \gg \eta$ . With  $\lambda_1 = 1$  and  $\lambda_i = 0$  for  $i > 1$ , Eq. (11) gives in the limit  $\nu_1 \rightarrow 0$ ,

$$\left( -\frac{dE}{ds} \right)_{Q>\eta} = \frac{1}{2} \kappa \mu^2 \left[ \frac{\beta^2}{Q_{\max}} (\eta - Q_{\max}) + \frac{Q_{\max}^2}{4E^2} + \left( 1 + \frac{a\beta^2}{mQ_{\max}} \right) \ln \left( \frac{a + mQ_{\max}}{a} \right) \right]. \quad (14)$$

From Eq. (1) we now have  $Q_{\max} = 2\gamma^2 m \beta^2$ . Furthermore, since  $mQ_{\max}/a = \beta^2 \gamma^2 m^2/M^2 \ll 1$ , the logarithm can be accurately represented by expanding it to first order in this parameter. With these substitutions Eq. (14) gives

$$\left( -\frac{dE}{ds} \right)_{Q>\eta} = \frac{1}{2} \kappa \mu^2 \left( \frac{m}{M} \right)^2$$

$$\times \left( \gamma^2 \beta^2 (1 + \beta^2) + \frac{\eta M^2}{2\gamma^2 m^3} \right). \quad (15)$$

This formula will be considered further after calculation of the low- $Q$  contribution to  $-dE/ds$ .

### IV. LOW- $Q$ CONTRIBUTION TO STOPPING POWER

At low  $Q$ , the inelastic-scattering cross section for the neutron is given by Eq. (I-32) with  $G_E^2 = 0$ ,

$G_M^2 = \mu^2$ , and  $\tau \ll 1$ . In addition, we make the approximation that  $Q/m \ll 1$ . The matrix elements are expanded into powers of  $|\vec{q}|$  and only the first nonvanishing terms retained. In terms of the optical-dipole-oscillator strengths  $f_n$ ,

$$|F_n|^2 = Q f_n / E_n, \quad (16)$$

$$|\vec{\beta}_t \cdot \vec{G}_n|^2 = \beta_t^2 E_n f_n / 2m, \quad (17)$$

and

$$|\vec{G}_n|^2 = 3E_n f_n / 2m. \quad (18)$$

With  $Q$  small, the scattering angle is also small, and so

$$\beta_t^2 = \beta^2(1 - Q_{\min}/Q), \quad (19)$$

where

$$Q_{\min} = E_n^2 / 2m\beta^2 \quad (20)$$

is the minimum value of  $Q$ .<sup>3</sup> Under these conditions Eq. (I-32) yields the simple result

$$d\sigma_n = \frac{\pi e^4 Z \mu^2 f_n}{M^2 \beta^2 E_n} \times \left( \beta^2 - \frac{E_n^2}{\gamma^2(E_n^2 - 2mQ)} \right) dQ. \quad (21)$$

Integration over the range of the low- $Q$  collisions gives

$$E_n \int_{Q_{\min}}^{\eta} d\sigma_n = \frac{\pi e^4 Z \mu^2 f_n}{M^2 \beta^2} \left( \beta^2(\eta - Q_{\min}) + \frac{E_n^2}{2m\gamma^2} \ln \frac{E_n^2 - 2m\eta}{E_n^2 - 2mQ_{\min}} \right). \quad (22)$$

Substituting (20) and summing over all excited states, we obtain ( $\sum_n f_n = 1$ )

$$\sum_n E_n \int_{Q_{\min}}^{\eta} d\sigma_n = \frac{\pi e^4 Z \mu^2}{m M^2 \beta^2} \left[ \beta^2 m \eta - \frac{1}{2} \sum_n E_n^2 f_n + \frac{1}{2\gamma^2} \sum_n E_n^2 f_n \ln \gamma^2 \beta^2 \left( \frac{2m\eta}{E_n^2} - 1 \right) \right]. \quad (23)$$

For most collisions at low- $Q$  we expect that  $2m\eta/E_n^2 \gg 1$ . Therefore, we shall neglect the unit term in the argument of the logarithm in the last term in Eq. (23). Any overestimate of this term thus introduced is of little significance, because this term is small, as shown below.

The low- $Q$  contribution to the stopping power is obtained from Eq. (23) by multiplying by  $N$ , the number of atoms per unit volume. It follows that

$$\left( -\frac{dE}{ds} \right)_{Q < \eta} = \frac{\kappa \mu^2}{4M^2} \left( \beta^2 m \eta - \frac{1}{2} \sum_n E_n^2 f_n - \frac{1}{\gamma^2} \sum_n E_n^2 f_n \ln \frac{E_n}{\gamma \beta (2m\eta)^{1/2}} \right). \quad (24)$$

The sums are evaluated in the Appendix. Substituting Eqs. (A15) and (A16), we obtain

$$\left( -\frac{dE}{ds} \right)_{Q < \eta} = \frac{1}{2} \kappa \mu^2 \left( \frac{m}{M} \right)^2 \left( \frac{\eta \beta^2}{2m} - \frac{8(Z-0.3)^3}{3m^2} \mathfrak{R}^2 - \frac{16(Z-0.3)^3 \mathfrak{R}^2}{3\gamma^2 m^2} \ln \frac{8(Z-0.3)^3 \mathfrak{R}}{\gamma \beta (2m\eta)^{1/2} Z^{2.4}} \right), \quad (25)$$

where  $\mathfrak{R}$  denotes the rydberg energy.

#### V. NEUTRON STOPPING POWER WHEN $\gamma m/M \ll 1$

The total stopping power at low  $\gamma$  is represented by the sum of (15) and (25). Omitting the first term from (25) in comparison with the last term from (15), we write

$$-\frac{dE}{ds} = \frac{1}{2} \kappa \mu^2 \left( \frac{m}{M} \right)^2 \left( \gamma^2 \beta^2 (1 + \beta^2) + \frac{\eta M^2}{2\gamma^2 m^3} - \frac{8(Z-0.3)^3 \mathfrak{R}^2}{3m^2} - \frac{16(Z-0.3)^3 \mathfrak{R}^2}{3\gamma^2 m^2} \ln \frac{8(Z-0.3)^3 \mathfrak{R}}{\gamma \beta (2m\eta)^{1/2} Z^{2.4}} \right) \quad (26)$$

$$\equiv \frac{1}{2} \kappa \mu^2 \left( \frac{m}{M} \right)^2 \sum_{i=1}^4 T_i. \quad (27)$$

The terms  $T_i$  in Eq. (27) are defined in the order of their appearance in (26). In contrast to the corresponding formula for charged particles, the intermediate energy  $\eta$  does not drop out. The main dependence on  $\eta$  comes from the second high- $Q$  term, which decreases as  $\gamma^2$ .

Numerical evaluations of the four terms from Eqs. (26) and (27) are given in Table I, for which we have assumed  $\eta$  to be of the order of the average binding energy of an atomic electron,  $\eta \sim Z^{1.4}$ . The last two terms in (26) are negligible ex-

cept when  $\gamma$  is very close to unity. The second term becomes small compared with the first for somewhat larger values of  $\gamma$ , depending on the atomic number. A separate computation shows that the value of the second term is one-tenth that of the first when  $\gamma \sim 4Z^{0.35}$ . Thus when  $4Z^{0.35} < \gamma \ll M/m$  the neutron stopping power is given by

$$-\frac{dE}{ds} = \frac{1}{2} \kappa \mu^2 \left( \frac{m}{M} \right)^2 \gamma^2 \beta^2 (1 + \beta^2). \quad (28)$$

TABLE I. Values of terms in Eqs. (26) and (27) at different  $\gamma$  for  $Z=13$  and  $Z=82$ .

$\gamma$	$Z=13$				$Z=82$			
	$T_1$	$T_2$	$T_3$	$T_4$	$T_1$	$T_2$	$T_3$	$T_4$
2	5.25	408	$-3.87 \times 10^{-6}$	$8.52 \times 10^{-6}$	5.25	5380	$-1.03 \times 10^{-3}$	$2.33 \times 10^{-3}$
5	47.0	65.3	$-3.87 \times 10^{-6}$	$1.69 \times 10^{-6}$	47.0	860	$-1.03 \times 10^{-3}$	$4.59 \times 10^{-4}$
10	197	16.3	$-3.87 \times 10^{-6}$	$4.76 \times 10^{-7}$	197	215	$-1.03 \times 10^{-3}$	$1.30 \times 10^{-4}$
50	5000	0.65	$-3.87 \times 10^{-6}$	$2.40 \times 10^{-8}$	5000	8.60	$-1.03 \times 10^{-3}$	$6.51 \times 10^{-6}$

Equation (28) can be compared with the corresponding semiclassical formula, Eq. (23) of Ref. 2, which is valid for  $1 < \gamma \lesssim 10$ .<sup>12</sup> The ratio of the quantum mechanical and semiclassical stopping powers is found to be

$$\frac{(-dE/ds)_{\text{QM}}}{(-dE/ds)_{\text{SC}}} = \frac{18(2\gamma^2 - 1)}{(\gamma^2 - 1)(\gamma^2 + 3)}. \quad (29)$$

When  $\gamma=5$ , the ratio is 1.3; when  $\gamma=10$ , it is 0.35. The two computations give comparable values for the stopping power in the range of  $\gamma$  where they overlap. The semiclassical formula shows a stronger dependence on  $\gamma$ , due possibly to the abrupt falloff ( $r^{-3}$ ,  $r^{-5}$ , and  $r^{-7}$ ) of the classical force components with neutron-electron separation.

## VI. NUMERICAL RESULTS

Table II gives the neutron stopping power calculated from Eq. (12) and multiplied by  $A/Z\rho$ , where  $A$  is the atomic mass number and  $\rho$  the density of the medium traversed. The quantity  $(-dE/\rho ds) \times A/Z$  is the same for all elements. From the foregoing discussion, these values are accurate at high  $\gamma$ . Calculations were carried out through  $\gamma=7000$ , where the magnetic form factor is very small and where the charge form factor may be comparable in magnitude. The error at low  $\gamma$  is

TABLE II. Neutron stopping power as a function of  $\gamma$  and neutron energy  $E$ .

$\gamma$	$E$ (GeV)	$-\frac{dE}{\rho ds} \left( \frac{A}{Z} \right)$ (MeV g <sup>-1</sup> cm <sup>2</sup> )
10	9.38	$1.89 \times 10^{-5}$
50	47.0	$5.62 \times 10^{-4}$
100	94.0	$2.03 \times 10^{-3}$
150	141	$4.10 \times 10^{-3}$
250	235	$9.07 \times 10^{-3}$
500	470	$2.04 \times 10^{-2}$
750	705	$2.72 \times 10^{-2}$
1000	940	$3.07 \times 10^{-2}$
2000	1880	$3.45 \times 10^{-2}$
4000	3760	$3.58 \times 10^{-2}$
5000	4700	$3.62 \times 10^{-2}$
7000	6580	$3.66 \times 10^{-2}$

$\sim 10\%$  when  $\gamma \sim 4Z^{0.35}$ . The total energy  $E$  of the neutron at each value of  $\gamma$  is also shown in the table.

The neutron stopping power increases by about a factor of 100 between  $\gamma=10$  and 100 and by another order of magnitude between  $\gamma=100$  and 1000. Thereafter, it rises only slightly when  $\gamma$  is increased to 7000.

The possibility of detecting neutron energy losses to atomic electrons was discussed in Ref. 2 on the basis of the semiclassical calculation. The quantum mechanical results do not appear to alter the suggestion made there for their possible detection.

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## APPENDIX: EVALUATION OF LOW- $Q$ SUMS

The first sum in Eq. (24) is immediately available.<sup>13-15</sup> In terms of the quantities  $S_r$ , defined in Ref. 13, we have

$$\sum_n E_n^2 f_n = \lim_{Q \rightarrow 0} \frac{1}{Q} \sum_n E_n^3 |F_n|^2 = \left( \frac{S_3}{Q} \right)_{Q=0}. \quad (A1)$$

The second sum in (24) is more difficult to evaluate. Treating the exponent  $r$  as a continuous variable, one may write<sup>14</sup>

$$\sum_n E_n^r f_n \ln E_n = \frac{\partial}{\partial r} \sum_n E_n^r f_n. \quad (A2)$$

In terms of the  $S_r$ , the sum needed in Eq. (24) is related to

$$\sum_n E_n^2 f_n \ln E_n = \left[ \frac{\partial}{\partial r} \left( \frac{S_r}{Q} \right)_{Q=0} \right]_{r=3}. \quad (A3)$$

This quantity can be estimated from a plot of  $(S_r/Q)_{Q=0}$  vs  $r$  at  $r=3$ .

To make such a plot, the relevant quantities were obtained as follows. For  $r=1, 2$  we have<sup>13,15</sup>  $S_1/Q \equiv 1$  and  $(S_2/Q)_{Q=0} = \frac{4}{3} \langle T \rangle$ , where  $\langle T \rangle$  is the total kinetic energy of the atomic electrons. By the virial theorem,  $\langle T \rangle$  is also equal to the total elec-

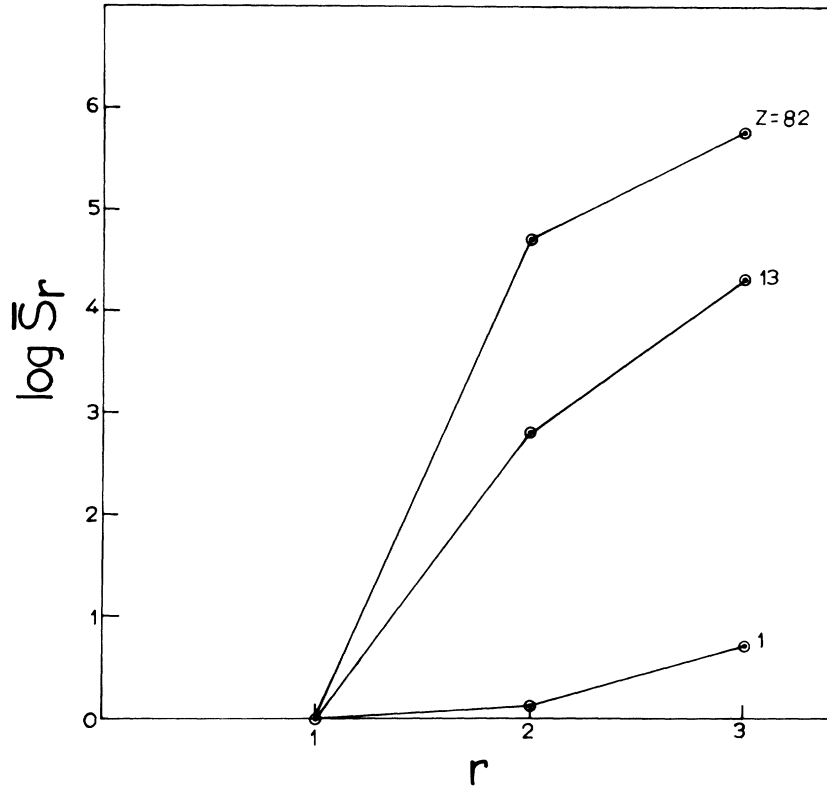


FIG. 1. Circled points show values of  $\ln \bar{S}_r$  [Eq. (A8)] for  $r=1, 2,$  and  $3$  and for  $Z=1, 13,$  and  $82$ . Points belonging to the same  $Z$  are connected by straight lines for ease in reading.

tronic binding energy, which is given approximately by  $Z^{2.4}\mathcal{R}$ ,<sup>13</sup> where  $\mathcal{R}$  is the rydberg energy. Therefore,

$$(S_2/Q)_{Q=0} \sim \frac{1}{3} Z^{2.4}\mathcal{R}. \quad (\text{A4})$$

For  $r=3$  we follow Ref. 13, taking

$$\begin{aligned} \left(\frac{S_4}{Q}\right)_{Q=0} &= \frac{4\pi\hbar^2 e^2}{3m} \sum_j \langle \delta(\vec{r}_j) \rangle \\ &= \frac{16}{3} \pi \rho \mathcal{R}^2, \end{aligned} \quad (\text{A5})$$

where  $\sum_j \langle \delta(\vec{r}_j) \rangle$  is the density of electrons at the nucleus of the atom, averaged over the ground state, and  $\rho$  is the density per cubic Bohr radius at the nucleus. Most of the contribution to  $\rho$  comes from the two  $K$ -shell electrons, for which the screened hydrogenic approximation gives  $\rho \sim 2 \times (Z - 0.3)^3/\pi$ . Therefore,

$$(S_3/Q)_{Q=0} \sim \frac{32}{3} (Z - 0.3)^3 \mathcal{R}^2. \quad (\text{A6})$$

For  $r=4$ ,

$$\left(\frac{S_4}{Q}\right)_{Q=0} = \frac{2\hbar^2}{3m} \left\langle \left( \sum_j \nabla_j V \right)^2 \right\rangle, \quad (\text{A7})$$

$\nabla_j V$  being the gradient of the potential energy taken with respect to the position coordinates of the  $j$ th electron.<sup>15</sup> The mean value in (A7) is large. In fact, this quantity diverges if the electron density at the nucleus is different from zero,<sup>14</sup> and so it

cannot be calculated by means of a hydrogenic approximation or the Thomas-Fermi model. We make no attempt to calculate (A7), this quantity not being critical for our purposes. The dimensionless quantities

$$\bar{S}_r = (S_r / QR^{r-1})_{Q=0} \quad (\text{A8})$$

are shown in a semilogarithmic plot in Fig. 1 for  $r=1, 2,$  and  $3$  and  $Z=1, 13,$  and  $82$ .<sup>16</sup> In view of the approximately linear trend shown and in view of the smallness of the contribution made by the sums in Eq. (24) when the high- $Q$  contribution is added, we assume that the value of the derivative in (A3) is approximately the same as the slope of the line drawn between the points at  $r=2$  and  $r=3$  in Fig. 1.

Specifically, introducing the dimensionless quantities

$$\mathcal{E}_n = E_n / \gamma \beta (2m\eta)^{1/2} = E_n / \zeta \quad (\text{A9})$$

and

$$P_\mu = \sum_n \mathcal{E}_n^\mu f_n = \left( \frac{S_{\mu+1}}{\zeta^\mu Q} \right)_{Q=0}, \quad (\text{A10})$$

we write for the second sum in Eq. (24),

$$\zeta^2 \sum_n \mathcal{E}_n^2 f_n \ln \mathcal{E}_n = \zeta^2 \left( \frac{\partial P_\mu}{\partial \mu} \right)_{\mu=2}. \quad (\text{A11})$$

Since  $\ln \bar{S}_r$  is assumed to vary linearly with  $r$ , the

logarithm of  $P_\mu$  in (A10) is linear in  $\mu$ . Under this condition it follows that

$$\frac{\partial P_\mu}{\partial \mu} \equiv P_\mu \frac{\partial(\ln P_\mu)}{\partial \mu} \sim P_\mu (\ln P_\mu - \ln P_{\mu-1}). \quad (\text{A12})$$

With  $\mu = 2$ , then,

$$\begin{aligned} \left(\frac{\partial P_\mu}{\partial \mu}\right)_{\mu=2} &\sim \left(\frac{S_3}{\xi^2 Q}\right)_{Q=0} \\ &\times \left[ \ln\left(\frac{S_3}{\xi^2 Q}\right)_{Q=0} - \ln\left(\frac{S_2}{\xi Q}\right)_{Q=0} \right] \\ &= \left(\frac{S_3}{\xi^2 Q}\right)_{Q=0} \ln \frac{(S_3/Q)_{Q=0}}{\xi(S_2/Q)_{Q=0}}. \end{aligned} \quad (\text{A13})$$

From Eqs. (A11) and (A13) it follows that the second sum is given by

$$\sum_n E_n^2 f_n \ln \mathcal{E}_n \sim \left(\frac{S_3}{Q}\right)_{Q=0} \ln \frac{(S_3/Q)_{Q=0}}{\xi(S_2/Q)_{Q=0}}. \quad (\text{A14})$$

Finally, combining Eqs. (A1) and (A6), we have

$$\sum_n E_n^2 f_n \sim \frac{32}{3} (Z - 0.3)^3 R^2. \quad (\text{A15})$$

Combining (A4), (A6), (A9), and (A14) gives

$$\sum_n E_n^2 f_n \ln \mathcal{E}_n \sim \frac{32}{3} (Z - 0.3)^3 R^2 \ln \frac{8(Z - 0.3)^3 R}{\gamma \beta (2m\eta)^{1/2} Z^{2.4}}. \quad (\text{A16})$$

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<sup>1</sup>J. E. Turner, V. N. Neelavathi, R. B. Vora, J. S. Bisht, R. K. Kher, and D. Arora, preceding paper, *Phys. Rev. B* **8**, XXX (1973).

<sup>2</sup>R. B. Vora, V. N. Neelavathi, J. E. Turner, T. S. Subramanian, and M. A. Prasad, *Phys. Rev. B* **3**, 2929 (1971).

<sup>3</sup>U. Fano, *Annu. Rev. Nucl. Sci.* **13**, 1 (1963).

<sup>4</sup>Such low- $Q$  shell corrections of the type encountered with charged particles could be carried out. Because of the extremely small rate of energy loss by the neutron at low velocity, however, they are probably unwarranted.

<sup>5</sup>A small additional term  $m^2/M$  is omitted in the denominator of (1).

<sup>6</sup>J. E. Turner, V. N. Neelavathi, R. B. Vora, T. S.

Subramanian, and M. A. Prasad, *Phys. Rev.* **183**, 453 (1969).

<sup>7</sup>L. N. Hand, D. G. Miller, and R. Wilson, *Rev. Mod. Phys.* **35**, 335 (1963).

<sup>8</sup> $G_M^2$  enters Eq. (I-32) for the scattering cross section.

<sup>9</sup>When  $\gamma = 2$ , for example,  $Q_{\max} = 6m c^2$ ;  $\eta$  is in the range  $\sim 10^2 - 10^5$  eV.

<sup>10</sup>Equation (12) can also be inferred directly from Eq. (19) of Ref. 6.

<sup>11</sup>Equation (13) can be inferred from Eq. (20) of Ref. 6.

<sup>12</sup>The term  $\gamma^2 \bar{\mu}^2$  in the parentheses of the equation should read  $\gamma^2 \bar{\mu}^2$ .

<sup>13</sup>U. Fano and J. E. Turner, in *Studies in Penetration of Charged Particles in Matter*, edited by U. Fano, National Academy of Sciences-National Research Council Publication No. 1133 (U. S. GPO, Washington, D. C., 1964), p. 47.

<sup>14</sup>Mitio Inokuti, *Rev. Mod. Phys.* **43**, 297 (1971).

<sup>15</sup>G. Placzek, *Phys. Rev.* **86**, 377 (1952).

<sup>16</sup>The right-hand side of Eq. (A6) was divided by 2 for  $Z = 1$ .