electron being removed. A graph of ξ^* would show breaks in its curves between the $d^6 \rightarrow d^5$ and $d^5 \rightarrow d^4$ transitions. The graph would also show that most of the ξ^*'s are negative (i.e., $\Delta E_{\text{obs}} < \Delta E_{\text{one electron}}$). The exceptions occur for the high-lying point cases of Fig. 5. Inspection of Table IX shows that the one case of an apparently small average of configuration $\Delta E_{\text{one electron}}$ is for a high-lying point transition (V IV $\rightarrow$ V). The fact that the ξ's and ξ^*'s are generally out of line for the same transitions suggests that experimental rather than computational errors are the cause. The writer reran the pertinent H-F calculations as a check. No errors were uncovered.

VII. CONCLUSION

We have seen that the Hartree-Fock results are generally in poor agreement with experiment. While the total energies are accurate to better than one percent, the observables we are trying to predict by taking total energy differences are even smaller and thus poorly predicted. The calculated F^k $(3d,3d)$ integrals poorly predict the multiplet spectra. This is in large part due to the inadequacies of the Hartree-Fock formalism and to a lesser part due to the assumption of common radial functions for all the multiplet states of a configuration. The lower state one-electron energies are found to be in very good agreement with ionization energies. This is due to a remarkable cancellation of errors. Finally we have the unsurprising behavior of the 3d electron "correlation" energy with its sudden increase for more than half filled shells.

ACKNOWLEDGMENTS

The author wishes to express his gratitude to Professor J. C. Slater for his support and assistance with this research. The writer is also indebted to Professor R. K. Nesbet of Boston University who introduced the writer to his version of the Roothaan procedure and supplied the important computer programs. Finally, the author wishes to acknowledge the aid of the members of the Solid-State and Molecular Theory Group and of the staff of the Whirlwind Computer.

PHYSICAL REVIEW VOLUME 118, NUMBER 4 MAY 15, 1960

Range-Energy Relations for Protons in Various Substances*

R. M. STERNHEIMER
Brookhaven National Laboratory, Upton, New York
(Received December 30, 1959)

An expression is obtained for the range-energy relation $R(T_p)$ for protons (T_p=proton kinetic energy) as a function of the mean excitation potential I which enters into the Bethe-Bloch formula for the ionization loss dE/dx. The expression for $R(T_p)$ is obtained by an interpolation of the previously calculated range-energy relations for Be, Al, Cu, and Pb. The resulting expression for $R(T_p)$ can be used for any substance, provided an appropriate value of I is assumed. Values are also obtained for the quantity $q=(I/R)(dR/dI)$ which gives the fractional change of R for a small variation of the excitation potential I.

I. INTRODUCTION

RANGE-ENERGY relations for protons[1] have been recently calculated for six substances (Be, C, Al, Cu, Pb, and air). These range-energy relations are based on values of the ionization loss dE/dx which include the shell corrections at low proton energies and the density effect correction which becomes important in the high-energy region. The values of dE/dx depend mainly on the value of the mean excitation potential I of the atoms of the substance considered. The following values of I were used in the previous calculations: $I_{\text{Be}}=64$ ev, $I_{\text{C}}=78$ ev, $I_{\text{Al}}=166$ ev, $I_{\text{Cu}}=371$ ev, $I_{\text{Pb}}=1070$ ev, and $I_{\text{air}}=94$ ev.

In the present paper, we will obtain an expression which gives the range $R(T_p)$ for an arbitrary value of I, as a function of the proton kinetic energy T_p, and which can therefore be used to obtain the range-energy relation for any substance, if an appropriate value of I is assumed. The general expression for $R(T_p)$ is obtained by an interpolation of the previous results[1] for Be, Al, Cu, and Pb. It is estimated that the resulting range-energy relation is accurate to $\lesssim 1\%$ for values of I lying in the range from $I_{\text{Be}}=64$ ev to $I_{\text{Pb}}=1070$ ev.

II. EXPRESSION FOR $R(T_p)$

In order to obtain the interpolation formula for $R(T_p)$, we note that the Bethe-Bloch formula for dE/dx can be written as follows:

$$-\frac{1}{\rho}\frac{dE}{dx}=\frac{Z}{A}M(\beta)\left[\ln\frac{N(\beta)}{I^2}-2\beta^2-\delta-U\right], \qquad (1)$$

where ρ is the density of the medium (in g/cm^3), A is the atomic weight, $M(\beta)$ and $N(\beta)$ are functions of the

* This work was performed under the auspices of the U. S. Atomic Energy Commission.
[1] R. M. Sternheimer, Phys. Rev. **115**, 137 (1959). This paper will be referred to as I.

velocity $v=\beta c$ only. If $-(1/\rho)(dE/dx)$ is expressed in units Mev/g cm^{-2}, $M(\beta)$ is given by

$$M(\beta)=0.1536/\beta^2. \tag{2}$$

$N(\beta)$ is given by

$$N(\beta)=2mv^2W_{\max}/(1-\beta^2), \tag{3}$$

where m is the electron mass, and $W_{\max}$ is the maximum energy transfer from the incident proton to an atomic electron. For energies $T_p\ll(m_p^2/2m)c^2$, where m_p = proton mass, $W_{\max}$ is given by

$$W_{\max}=2mv^2/(1-\beta^2). \tag{4}$$

In Eq. (1), δ is the correction for the density effect due to the polarization of the medium, and U is the shell correction term. Aside from the terms δ and U, the square bracket of (1) is a function only of β and $\ln I$.

The range $R(T_{p,1})$ as obtained in I, is calculated from the following expression

$$R(T_{p,1})=R(2\text{ Mev})+\int_{2\text{ Mev}}^{T_{p,1}}\frac{dT_p}{-(1/\rho)(dE/dx)}, \tag{5}$$

where $R(2$ Mev$)$ must be obtained from experiment,[2] in view of the fact that the Bethe-Bloch formula becomes inapplicable for $T_p\lesssim 2$ Mev, on account of the possibility of electron capture by the incident proton.

If one assumes that the effect of the terms δ and U is a function of I only, the integral of Eq. (5) can be written as follows:

$$\int_{2\text{ Mev}}^{T_{p,1}}\frac{dT_p}{(Z/A)P(\beta,\ln I)}, \tag{6}$$

where P is a function of β and $\ln I$ only.

In view of Eqs. (5) and (6), we define the function $\Phi(T_p)$ as follows:

$$\Phi(T_p)\equiv(2Z/A)[R(T_p)-R(2\text{ Mev})]. \tag{7}$$

Except for the effect of the terms δ and U, $\Phi(T_p)$ is a function only of T_p and $\ln I$. We now define a function G as follows:

$$G(T_p)\equiv\Phi(T_p,I)/\Phi_{\text{Al}}(T_p), \tag{8}$$

where $\Phi(T_p,I)$ pertains to an arbitrary I, while $\Phi_{\text{Al}}(T_p)$ is the function Φ for Al. Φ_{Al} can be obtained from the table of $R(T_p)$ for Al, as given in I, which was calculated for $I_{\text{Al}}=166$ ev. Values of Φ_{Al} are given in Table I of the present paper.

In the approximation that the effect of the terms δ and U is a function of I only, $G(T_p)$ will be a function only of χ defined as:

$$\chi\equiv\log_{10}(I/I_{\text{Al}})=\log_{10}(I/166\text{ ev}). \tag{9}$$

G can be expressed as a power series in χ:

$$G=1+G_1\chi+G_2\chi^2+G_3\chi^3+\cdots, \tag{10}$$

where G_1, G_2, and G_3 are functions of T_p only. Of course, for $\chi=0$ ($I=I_{\text{Al}}=166$ ev), we have $G=1$.

It was found that sufficient accuracy ($\lesssim 1\%$) can be obtained by using four terms in the expansion of G, i.e., all terms up to $G_3\chi^3$. The values of G_1, G_2, and G_3 were determined by fitting the values of Φ for Be, Cu, and Pb, as obtained from the range tables of I. The corresponding values of χ for $I_{\text{Be}}=64$ ev, $I_{\text{Cu}}=371$ ev, and $I_{\text{Pb}}=1070$ ev are -0.4140, 0.3493, and 0.8093, respectively.

The resulting values of G_i are given in Table I, together with the function Φ_{Al}. As expected, the values of the G_i vary smoothly with the energy T_p. In view of Eqs. (7), (8), and (10), the range $R(T_p,I)$ for an arbitrary value of I is given by

$$R(T_p,I)=R(2\text{ Mev},I)+(A/2Z)\Phi_{\text{Al}}(T_p)\times(1+G_1\chi+G_2\chi^2+G_3\chi^3), \tag{11}$$

where $R(2$ Mev, $I)$ is the range for $T_p=2$ Mev. $R(2$ Mev$)$ must be obtained empirically, from the data of Bichsel et al.,[2] as was done in I. Its value ranges from ~ 0.01 g/cm^2 for light elements (Be, C, Al) to ~ 0.04 g/cm^2 for heavy elements (Pb).

The values of Table I extend up to $T_p=100$ Bev. As was pointed out in reference 1, the proton range $R(T_p)$ is a purely mathematical quantity above ~ 1 Bev, since nuclear interactions will attenuate a proton beam to a negligible intensity for distances greater than $\sim R(1$ Bev$)$, which corresponds to ~ 4 mean free paths. The part of the table for $T_p=1$–100 Bev was calculated mainly because of its applicability to μ mesons (of energies ~ 0.1–10 Bev) [see Eq. (14) of I].

The accuracy of Eq. (10) for G was checked by calculating G for carbon ($I=78$ ev, $\chi=-0.3280$), and comparing it with the value of G as obtained directly from the range table for C given in I. The agreement was to within 0.5% throughout the energy range from $T_p=10$ Mev to 100 Bev. The expression for $R(T_p)$ has also been checked by comparing it with the previously calculated range-energy relation for air[1] ($I=94$ ev, $\chi=-0.2470$), and with the range-energy relation of Barkas[3] for nuclear emulsion ($I=331$ ev, $\chi=0.2997$). For air, the agreement for R is to within 1% for T_p between 10 Mev and 1 Bev. For $T_p\gtrsim 1$ Bev, the density effect correction for dE/dx increases $R(T_p)$ for solid materials (Be, Al, Cu, Pb) by several percent, so that the interpolation formula [Eq. (11)] cannot be used for gases. For emulsion, the present expression for R agrees with the results of Barkas[3] to within 1% for T_p between 10 Mev and 10 Bev.

In order to obtain an additional check on the accuracy of Eq. (11), we have calculated a range-energy relation for a value of $I=659$ ev, giving $\chi=0.5988$. This value

[2] H. Bichsel, R. F. Mozley, and W. A. Aron, Phys. Rev. **105**, 1788 (1957). See also S. K. Allison and S. D. Warshaw, Revs. Modern Phys. **25**, 779 (1953).

[3] W. H. Barkas, Nuovo cimento **8**, 201 (1958).

TABLE I. Values of the functions G_1, G_2, G_3, and Φ_{Al} which enter into the expression for the proton range-energy relation [Eq. (11)].

T_p (Mev)	G_1	G_2	G_3	Φ_{Al} (g/cm²)	T_p (Mev)	G_1	G_2	G_3	Φ_{Al} (g/cm²)
3	0.634	0.450	0.495	0.01016	375	0.295	0.085	0.055	91.16
4	0.595	0.379	0.468	0.02313	400	0.293	0.083	0.054	101.09
5	0.570	0.336	0.436	0.03871	450	0.288	0.081	0.053	121.80
6	0.551	0.307	0.404	0.05681	500	0.285	0.080	0.051	143.54
7	0.537	0.285	0.378	0.07734	550	0.282	0.079	0.049	166.19
8	0.525	0.269	0.353	0.1002	600	0.279	0.078	0.047	189.65
9	0.515	0.257	0.330	0.1254	700	0.273	0.077	0.045	238.6
10	0.507	0.247	0.309	0.1528	800	0.268	0.075	0.044	289.8
12	0.493	0.229	0.278	0.2142	900	0.264	0.074	0.042	342.8
14	0.481	0.218	0.250	0.2841	1000	0.259	0.073	0.041	397.2
16	0.472	0.211	0.225	0.3622	1250	0.251	0.071	0.040	537.6
18	0.464	0.204	0.205	0.4484	1500	0.243	0.068	0.039	682.2
20	0.457	0.198	0.189	0.5424	1750	0.236	0.066	0.038	829.4
22.5	0.449	0.193	0.172	0.6708	2000	0.231	0.064	0.037	977.9
25	0.442	0.188	0.158	0.8108	2250	0.226	0.063	0.035	1127.1
27.5	0.436	0.183	0.146	0.9625	2500	0.222	0.062	0.033	1276.6
30	0.430	0.180	0.136	1.1253	2750	0.218	0.061	0.030	1426.1
35	0.420	0.173	0.120	1.4839	3000	0.215	0.060	0.029	1575.5
40	0.412	0.166	0.109	1.8855	3500	0.209	0.058	0.024	1873.1
45	0.404	0.161	0.100	2.328	4000	0.205	0.057	0.020	2169
50	0.397	0.157	0.093	2.811	4500	0.200	0.056	0.017	2463
55	0.391	0.152	0.088	3.333	5000	0.197	0.056	0.013	2754
60	0.385	0.148	0.084	3.894	6000	0.190	0.055	0.007	3331
65	0.380	0.144	0.081	4.491	7000	0.185	0.054	0.002	3900
70	0.376	0.141	0.078	5.124	8000	0.181	0.054	−0.002	4463
75	0.372	0.138	0.076	5.793	9000	0.177	0.053	−0.007	5019
80	0.368	0.136	0.074	6.496	10 000	0.174	0.053	−0.011	5569
90	0.361	0.131	0.071	8.003	12 500	0.168	0.054	−0.019	6924
100	0.356	0.127	0.068	9.639	15 000	0.163	0.054	−0.026	8255
110	0.350	0.123	0.066	11.400	17 500	0.158	0.054	−0.032	9564
120	0.345	0.120	0.065	13.280	20 000	0.155	0.055	−0.037	10 857
130	0.341	0.117	0.064	15.276	22 500	0.152	0.056	−0.042	12 135
140	0.338	0.114	0.063	17.381	25 000	0.149	0.056	−0.046	13 400
150	0.334	0.112	0.061	19.593	27 500	0.147	0.057	−0.050	14 655
160	0.331	0.110	0.060	21.91	30 000	0.145	0.057	−0.054	15 900
180	0.326	0.106	0.058	26.83	40 000	0.139	0.060	−0.065	20 797
200	0.321	0.102	0.057	32.13	50 000	0.134	0.062	−0.074	25 594
225	0.316	0.098	0.057	39.24	60 000	0.131	0.064	−0.082	30 316
250	0.311	0.095	0.057	46.85	70 000	0.128	0.065	−0.088	34 978
275	0.307	0.092	0.057	54.92	80 000	0.126	0.066	−0.093	39 589
300	0.303	0.090	0.057	63.41	90 000	0.124	0.067	−0.097	44 158
325	0.300	0.088	0.056	72.30	100 000	0.122	0.069	−0.101	48 691
350	0.297	0.086	0.055	81.56					

of I was chosen partly because the corresponding χ lies approximately in the middle of the range from $\chi_{Cu}=0.3493$ to $\chi_{Pb}=0.8093$, and therefore the deviations of Eq. (11) from the actual calculated R are expected to be largest there. For all values of T_p, the ratio ξ of the value of G obtained from Eq. (10) to the actual G as determined from the calculated range was between 0.996 and 1.009. Typical values of ξ and the corresponding values of G are as follows: at 5 Mev: $\xi=0.9963$, $G=1.5611$; at 10 Mev: $\xi=0.9979$, $G=1.4615$; at 1 Bev: $\xi=0.9982$, $G=1.1922$; at 10 Bev: $\xi=1.0025$, $G=1.1180$; at 100 Bev: $\xi=1.0090$, $G=1.0665$.

As an example of the use of Eq. (11), one can calculate a range-energy relation for silver, using a value of $I=586$ ev, which is the average of the I values determined in the experiments of Bichsel et al.[2] and Burkig and MacKenzie.[4] The corresponding value of χ is 0.5478. For $R(2$ Mev), we use the value 0.0263 g/cm² obtained by Bichsel et al.[2] For example, for $T_p=50$ Mev, with $G_1=0.397$, $G_2=0.157$, $G_3=0.093$, one thus obtains $G=1.2799$. With $\Phi_{Al}=2.811$ g/cm² and $2Z/A=0.8713$, the second term on the right-hand side of Eq. (11) has the value 4.129 g/cm². Upon adding $R(2$ Mev), one obtains $R(50$ Mev$)=4.155$ g/cm². Similarly, for $T_p=100$ Mev, one finds $G=1.2443$, and $R=13.79$ g/cm².

Conversely, one can use Eq. (11) to determine the value of I from a measurement of the range R at a particular energy $T_{p,1}$. From the value of $R(T_{p,1})$, one obtains $G(T_{p,1})$:

$$G(T_{p,1})=(2Z/A)[R(T_{p,1})-R(2\text{ Mev})]/\Phi_{Al}(T_{p,1}). \quad (12)$$

Then one solves Eq. (10) for χ, which in turn gives the value of I. In this connection, a plot of G vs χ for $T_p=T_{p,1}$ may be helpful.

We note that the approximation that δ depends on I only, which underlies the use of the interpolation formula (10) for $T_p \gtrsim 2$ Bev, probably does not introduce any significant inaccuracies, for the following

[4] V. C. Burkig and K. R. MacKenzie, Phys. Rev. **106**, 848 (1957).

TABLE II. Values of $q=(I/R)(dR/dI)$ for Be, C, Al, Cu, and Pb.

T_p (Mev)	Be	C	Al	Cu	Pb
10	0.232	0.214	0.217	0.258	0.337
20	0.200	0.192	0.205	0.236	0.300
50	0.159	0.159	0.181	0.201	0.244
100	0.143	0.143	0.163	0.178	0.214
200	0.131	0.131	0.147	0.159	0.191
500	0.119	0.118	0.131	0.140	0.171
1000	0.106	0.106	0.119	0.128	0.155
2000	0.094	0.094	0.106	0.115	0.142
5000	0.074	0.076	0.090	0.097	0.113
10 000	0.058	0.062	0.080	0.084	0.088

reason. With increasing I, i.e., with increasing Z, δ generally decreases uniformly,[5] as is shown by Fig. 5 of reference 5. The electron density n also enters into δ, but since n generally also increases with Z, the value of δ will therefore mainly depend on I (which is approximately proportional to Z). Hence, we expect that no appreciable errors ($\gtrsim 1\%$) are introduced by the use of Eq. (11) in the high-energy region, especially since this expression fits the values of R (including the effect of δ on dE/dx) for Be, Al, Cu, and Pb.

The shell correction U is given by

$$U=2(C_K/Z)+2(C_L/Z), \tag{13}$$

where C_K and C_L are the K and L shell correction terms, first introduced by Bethe,[6] which account for the reduction of the stopping power of the K and L shells at low velocities of the incident particle. This correction becomes appreciable only at rather low energies ($T_p\lesssim 70$ Mev for Cu). U varies uniformly with increasing Z, in similarity to I. Moreover, U is very small for $T_p\gtrsim 2$ Mev: $U\lesssim 0.1$, as compared to a value of the square bracket of Eq. (1) of the order of 10. Thus the error introduced in Eq. (11) by the implicit assumption that U depends on I only, will be completely negligible.

As was discussed in I, the present proton range-energy relations can be used for other heavy particles (heavier than electrons), and in particular enable one to obtain the range of μ mesons up to energies of ~ 10 Bev [see Eq. (14) of I].

[5] R. M. Sternheimer, Phys. Rev. **91**, 256 (1953).
[6] M. S. Livingston and H. A. Bethe, Revs. Modern Phys. **9**, 261 (1937).

III. VALUES OF $q=(I/R)(dR/dI)$

It may be noted that from Eq. (11) one can obtain an expression for the derivative dR/dI, which gives the change of R for a small variation of the excitation potential I. Thus dR/dI is given by

$$\frac{dR}{dI}=\left(\frac{A}{2Z}\right)\Phi_{\mathrm{Al}}(T_p)\frac{dG/d\chi}{2.303I}$$
$$=\left(\frac{A}{2Z}\right)\Phi_{\mathrm{Al}}(T_p)\frac{(G_1+2G_2\chi+3G_3\chi^2)}{2.303I}, \tag{14}$$

where we have made use of the fact that $d\chi/dI=1/(2.303I)$. In Eq. (14), the small term $dR(2\text{ Mev})/dI$ has been neglected. This term will be unimportant, except for very low proton energies ($T_p\lesssim 10$ Mev).

As an example, for Cu and $T_p=500$ Mev, we have: $G_1=0.285$, $G_2=0.080$, $G_3=0.051$, $\chi=0.3493$, so that $dG/d\chi=0.3596$. With $\Phi_{\mathrm{Al}}=143.54$ g/cm^2, one obtains $dR/dI=0.0662$ gcm^{-2}/ev.

In connection with dR/dI, we define the quantity q as follows:

$$q\equiv(I/R)(dR/dI). \tag{15}$$

We may write q as: $(dR/R)/(dI/I)$, which shows that q gives the fractional change of R for a given small variation of I. Values of q have been calculated for Be, C, Al, Cu, and Pb, for various energies in the range from $T_p=10$ Mev to 10 Bev. These values are given in Table II. It is seen that q decreases with increasing T_p, and generally increases with increasing Z (at a fixed energy T_p). For 500-Mev protons in copper, one finds $q=0.140$, which means that a 1% error in a range measurement would lead to an error of $1/q=7.1\%$ or $0.071\times 371=26.3$ ev in the calculated value of I which is inferred from the measured range.

The fact that $1/q$ is considerably larger than 1 illustrates the well-known property that a relatively small error in the experimental range leads to a proportionately much larger error in the calculated ionization potential I. This result arises from the fact that I enters only into the logarithmic term of the Bethe-Bloch formula for dE/dx.