Stopping power of M-shell electrons for heavy charged particles

Hans Bichsel
1211 22nd Avenue East, Seattle, Washington 98112
(Received 18 October 1982; revised manuscript received 7 March 1983)

The stopping-power data given by Khandelwal and Merzbacher have been reevaluated because, according to Choi, their expressions for the M-shell form factors were in error. Present results are (20–45)% smaller. In addition, the coefficients for the asymptotic expression were calculated.

I. INTRODUCTION

The stopping number $B(l,\theta,\eta)$ for M-shell electrons with angular momentum quantum number l has been calculated with the method given by Khandelwal and Merzbacher[1] for $0.01<\eta<100$ (the index M is omitted here and θ as well as η depend on l). The form factors $|F_{W,l}(Q)|^2$ were taken from Choi.[2]

The asymptotic expression,[3] valid for $\eta >> 1$, is given by

$$B(l,\theta,\eta)=S(l,\theta)\ln\eta+T(l,\theta)-U(l,\theta)/\eta \ . \tag{1}$$

The coefficients S, T, and U have been determined with the method outlined by Inokuti.[4] The "shell corrections" are defined by

$$C(l,\theta,\eta)=S(l,\theta)\ln\eta+T(l,\theta)-B(l,\theta,\eta) \ . \tag{2}$$

These functions depend much less on the atomic number Z than B does. For large η, $C(l,\theta,\eta)$ is given approximately by $U(l,\theta)/\eta$.

II. NUMERICAL CALCULATIONS

The numerical integrations needed to obtain $B(l,\theta,\eta)$ and the coefficients of Eq. (1) were performed with the rectangular approximation $\int_{x_1}^{x_u} g(x)\,dx = g(x_m)(x_u-x_1)$. A geometrical progression was used for successive values of x: $x_u=x_1 10^{\delta}$ and $x_m=(x_1x_u)^{1/2}$. The integrals were calculated with several values of δ (typically 0.01, 0.005, 0.002, and 0.001), until the differences between successive calculations were small. The relative error of the calculations is estimated to be less than 10^{-3}. For $50<\eta<100$, the difference between the exact calculation of $B(l,\theta,\eta)$ and the asymptotic expression of Eq. (1) was less than 3×10^{-4} for all values of l, η, and θ. The results given here are (20–45)% less than those in Ref. 1. Calculations of collision cross sections agreed with the results of Choi[2] and Johnson, Basbas, and McDaniel[5] very well for $\eta<1$, but were bigger by approximately 1% at $\eta=10$.

III. RESULTS

In order to reduce the amount of numerical data presented, results are given for the shell corrections of Eq. (2) and the coefficients of Eq. (1), rather than for the stopping numbers.

The difference between the exact value for the stopping number B and the asymptotic expression given by Eq. (1) can be further reduced if a term V/η^2 is subtracted. While in principle the value of V could be determined with the methods[6] used to obtain U, I have found that the accuracy of the present numerical calculations was not adequate to give V. Therefore, V has been obtained empirically. The stopping number B can then be calculated with

$$B(l,\theta,\eta)=S(l,\theta)\ln\eta+T(l,\theta) - U(l,\theta)/\eta - V(l)/\eta^2 \tag{1a}$$

with the values for S, T, U, and V given in Table I. Now, the fractional difference between the exact calculation and the asymptotic expression of Eq. (1a) amounts to less than 3×10^{-4} for η greater than 2.5, 2, or 1 for $3s$, $3p$, or $3d$ electrons, respectively.

TABLE I. Coefficients for the calculation of the stopping number with the asymptotic expression of Eq. (1a). V is equal to 0.01, 0.188, and 0.138 for $3s$, $3p$, and $3d$ electrons, respectively. For accuracy of interpolations, more digits are given than warranted by the accuracy of the theory. For $\eta<2.5$ ($\eta<1$ for $3d$ electrons), Tables II–IV should be used.

$\theta/9$	S	T	U
	$3s$ electrons		
0.090	1.3720	5.0310	0.2548
0.080	1.4256	5.2982	0.2552
0.070	1.4941	5.6239	0.2553
0.060	1.5845	6.0342	0.2551
0.050	1.7087	6.5745	0.2547
0.040	1.8891	7.3328	0.2541
0.035	2.0136	7.8469	0.2539
0.030	2.1737	8.5062	0.2539
	$3p$ electrons		
0.090	3.9058	15.9256	0.6484
0.080	4.0897	16.8309	0.6531
0.070	4.3349	17.9452	0.6546
0.060	4.6727	19.3686	0.6520
0.050	5.1587	21.2825	0.6457
0.040	5.8995	24.0564	0.6431
0.035	6.4289	26.0020	0.6524
	$3d$ electrons		
0.090	5.8209	28.0388	0.9791
0.080	6.0999	29.8843	1.0310
0.070	6.5217	32.2033	1.0848
0.060	7.1929	35.2355	1.1312
0.050	8.3353	39.4198	1.1432
0.040	10.4696	45.6579	1.0397

TABLE II. Shell corrections $C(l,\theta,\eta)$ for $3s$ electrons, used in the calculation of the stopping number for small velocities of the incident particle: $B(l,\theta,\eta)=S(l,\theta)\ln\eta+T(l,\theta)-C(l,\theta,\eta)$. The exact values of η are given by $\eta=10^{(p-21)/10}$, where p is the line number in the table. For $\eta>2.5$, see Table I.

η \ $\theta/9$	0.090	0.080	0.070	0.060	0.050	0.040	0.035	0.030
0.0100	−1.291	−1.272	−1.267	−1.284	−1.337	−1.448	−1.535	−1.651
0.0126	−0.980	−0.953	−0.940	−0.946	−0.984	−1.072	−1.142	−1.235
0.0158	−0.678	−0.647	−0.629	−0.629	−0.656	−0.724	−0.780	−0.853
0.0200	−0.394	−0.363	−0.343	−0.340	−0.359	−0.413	−0.456	−0.511
0.0251	−0.138	−0.110	−0.092	−0.087	−0.102	−0.143	−0.175	−0.215
0.0316	0.081	0.104	0.199	0.123	0.112	0.082	0.058	0.030
0.0398	0.256	0.275	0.287	0.290	0.281	0.258	0.241	0.223
0.0501	0.387	0.401	0.410	0.412	0.405	0.388	0.377	0.366
0.0631	0.477	0.487	0.494	0.495	0.489	0.476	0.469	0.464
0.0794	0.530	0.538	0.543	0.543	0.538	0.529	0.524	0.523
0.1000	0.554	0.560	0.563	0.563	0.559	0.552	0.549	0.550
0.1259	0.554	0.559	0.561	0.561	0.558	0.552	0.550	0.552
0.1585	0.537	0.540	0.542	0.542	0.539	0.535	0.534	0.536
0.1995	0.507	0.509	0.511	0.510	0.508	0.505	0.504	0.507
0.2512	0.468	0.470	0.471	0.471	0.469	0.467	0.466	0.468
0.3162	0.425	0.427	0.427	0.427	0.426	0.424	0.423	0.425
0.3981	0.380	0.382	0.382	0.382	0.381	0.379	0.379	0.380
0.5012	0.336	0.337	0.337	0.337	0.336	0.335	0.335	0.336
0.6310	0.294	0.294	0.294	0.294	0.294	0.293	0.292	0.293
0.7943	0.253	0.254	0.254	0.254	0.253	0.253	0.252	0.253
1.0000	0.216	0.216	0.217	0.216	0.216	0.215	0.215	0.216
1.2589	0.182	0.182	0.182	0.182	0.182	0.181	0.181	0.182
1.5849	0.151	0.152	0.152	0.152	0.151	0.151	0.151	0.151
1.9953	0.124	0.125	0.125	0.125	0.124	0.124	0.124	0.124
2.5119	0.101	0.101	0.101	0.101	0.101	0.101	0.101	0.101

TABLE III. Shell corrections for $3p$ electrons (see Table II).

η \ $\theta/9$	0.090	0.080	0.070	0.060	0.050	0.040	0.035
0.0100	−2.077	−2.029	−2.061	−2.225	−2.605	−3.341	−3.908
0.0126	−1.198	−1.118	−1.110	−1.221	−1.524	−2.139	−2.617
0.0158	−0.342	−0.239	−0.201	−0.269	−0.507	−1.016	−1.412
0.0200	0.471	0.587	0.644	0.606	0.420	0.005	−0.318
0.0251	1.214	1.333	1.397	1.379	1.233	0.898	0.640
0.0316	1.857	1.968	2.032	2.025	1.910	1.643	1.442
0.0398	2.372	2.470	2.527	2.525	2.434	2.222	2.070
0.0501	2.740	2.823	2.871	2.870	2.797	2.632	2.521
0.0631	2.959	3.027	3.066	3.064	3.004	2.877	2.799
0.0794	3.040	3.095	3.125	3.122	3.072	2.975	2.924
0.1000	3.006	3.050	3.073	3.069	3.028	2.954	2.924
0.1259	2.884	2.919	2.937	2.932	2.897	2.842	2.827
0.1585	2.701	2.728	2.742	2.736	2.707	2.667	2.662
0.1995	2.475	2.497	2.508	2.502	2.478	2.448	2.450
0.2512	2.223	2.240	2.248	2.243	2.223	2.200	2.207
0.3162	1.955	1.969	1.975	1.970	1.954	1.937	1.946
0.3981	1.683	1.695	1.699	1.695	1.681	1.669	1.679
0.5012	1.419	1.428	1.432	1.428	1.417	1.408	1.417
0.6310	1.173	1.180	1.183	1.180	1.171	1.164	1.173
0.7943	0.952	0.958	0.960	0.957	0.950	0.945	0.953
1.0000	0.762	0.766	0.768	0.766	0.760	0.756	0.763
1.2589	0.603	0.606	0.608	0.606	0.601	0.598	0.604
1.5849	0.473	0.476	0.477	0.476	0.472	0.470	0.474
1.9953	0.370	0.372	0.373	0.372	0.369	0.367	0.371
2.5119	0.289	0.291	0.291	0.290	0.288	0.286	0.290

TABLE IV. Shell corrections for $3d$ electrons (see Table II).

η \ $\theta/9$	0.090	0.080	0.070	0.060	0.050	0.040
0.0100	1.187	1.727	2.074	1.971	0.824	−2.889
0.0126	2.485	3.077	3.504	3.530	2.604	−0.683
0.0158	3.755	4.391	4.887	5.025	4.301	1.414
0.0200	4.976	5.644	6.192	6.423	5.876	3.361
0.0251	6.117	6.800	7.379	7.678	7.281	5.105
0.0316	7.131	7.806	8.394	8.736	8.460	6.590
0.0398	7.958	8.603	9.175	9.536	9.355	7.760
0.0501	8.532	9.129	9.667	10.026	9.916	8.563
0.0631	8.799	9.335	9.825	10.168	10.109	8.969
0.0794	8.730	9.199	9.635	9.950	9.927	8.971
0.1000	8.334	8.736	9.115	9.397	9.396	8.600
0.1259	7.659	7.997	8.321	8.568	8.580	7.921
0.1585	6.785	7.066	7.338	7.550	7.570	7.027
0.1995	5.808	6.039	6.265	6.445	6.468	6.022
0.2512	4.822	5.011	5.197	5.347	5.370	5.007
0.3162	3.902	4.055	4.208	4.332	4.354	4.058
0.3981	3.095	3.218	3.342	3.444	3.464	3.224
0.5012	2.420	2.519	2.620	2.703	2.720	2.526
0.6310	1.877	1.956	2.037	2.104	2.119	1.963
0.7943	1.450	1.513	1.578	1.633	1.645	1.520
1.0000	1.120	1.171	1.222	1.266	1.276	1.176

It is seen that S and T change considerably with θ. On the other hand, U is almost constant for $3s$ and $3p$ electrons and changes only little for $3d$ electrons. For S and T, linear interpolation for the product $S\sqrt{\theta}$ or $T\sqrt{\theta}$ will give an accuracy of about 0.1% for intermediate values.

For $0.01 < \eta < 2.5$, the expression

$$B(l,\theta,\eta) = S(l,\theta,\eta)\ln\eta + T(l,\theta) - C(l,\theta,\eta) \qquad (2a)$$

is used to obtain the stopping number. For $\eta < 0.01$, $B = 0$ can be assumed. Values of $C(l,\theta,\eta)$ are given in Tables II–IV. For values of θ in between the tabulated ones, linear interpolation in general should be adequate, but for η, a Lagrange interpolation scheme is suggested.[7]

It may be noted that the dependence on θ of $C(l,\theta,\eta)$ is mostly quite small for $3s$ and $3p$ electrons, and only moderate for $3d$ electrons. The dependence is large only for small η, where

$$C(l,\theta,\eta) \approx S(l,\theta)\ln\eta + T(l,\theta) \ .$$

IV. CALCULATION OF STOPPING POWER

The values of the stopping number B for a given subshell in a specific atom with Z electrons are obtained from Eqs. (1a) or (2a). The variable η is given by

$$\eta = mc^2\beta^2/2\epsilon_a = 18\,787\beta^2/(Z-d)^2 \ ,$$

where $\epsilon_a = (Z-d)^2$ Ry. It is suggested that the "orbital exponent" ζ given by Clementi, Raimondi, and Reinhardt[8] be used for $(Z-d) = 3\zeta$, and for θ, the observed ionization potential,[9] divided by $\epsilon_a/9$. If the spin-orbit splitting of the energy levels is substantial, ϵ_a should be determined for each level, and the contribution from the $3p$ electrons is assigned a weight of $\frac{1}{3}$ for the M_{II} energy, $\frac{2}{3}$ for M_{III}, for that from the $3d$ electrons a weight of $\frac{2}{5}$ for M_{IV} and $\frac{3}{5}$ for M_{V} is used. With

$$k = 4\pi z^2 e^4/mv^2 = 5.099\times10^{-19} z^2/\beta^2 \ \mathrm{eV\,cm^2} \ ,$$

the stopping cross section is then obtained as $\tau = kB$, and the stopping power is $dE/dx = kNB$.

V. CONCLUSIONS

The present results can be used in the calculation of theoretical stopping-power values for the comparison with experimental data. I assume that the shell corrections given will be more appropriate than the values obtained to date with the scaling procedure proposed by Bethe to Hirschfelder and Magee,[10] later used by Bichsel[11] and Janni.[12]

No reliable guidance can be given for the range of validity of the present results. Substantial corrections should be expected for $\eta < 0.03$. An estimate can be obtained from the experimental data[13] on M-shell excitation by protons in gold. The deviations between theory and experiment are quite small for $n > 0.01$. For bismuth,[13] on the other hand, experimental values amount to only 60% of the calculated ones.

ACKNOWLEDGMENTS

This study was partially funded by the U.S. Air Force under ILIR 82-15 research. Dr. B.-H. Choi was kind enough to send me copies of his program and some numerical results.

[1]G. S. Khandelwal and E. Merzbacher, Phys. Rev. 144, 349 (1966).
[2]B.-H. Choi, Phys. Rev. A 7, 2056 (1973).
[3]L. M. Brown, Phys. Rev. 79, 297 (1950).
[4]M. Inokuti, Rev. Mod. Phys. 43, 297 (1971).
[5]D. E. Johnson, G. Basbas, and F. D. McDaniel, At. Data Nucl. Data Tables 24, 1 (1979).
[6]M. C. Walske, Phys. Rev. 88, 1283 (1952); 101, 940 (1956).
[7]A FORTRAN subroutine implementing this scheme is available, e.g., in IBM System/360 Scientific Subroutine Package or the CERN CDC subroutines.
[8]E. Clementi, D. L. Raimondi, and W. P. Reinhardt, J. Chem. Phys. 47, 1300 (1967); 38, 2686 (1963).
[9]D. A. Shirley, R. L. Martin, S. P. Kowalczyk, F. R. McFeely, and L. Ley, Phys. Rev. B 15, 544 (1977); J. A. Bearden and A. F. Burr, Rev. Mod. Phys. 39, 125 (1967).
[10]J. O. Hirschfelder and J. L. Magee, Phys. Rev. 73, 207 (1948).
[11]H. Bichsel, in *American Institute of Physics Handbook*, 2nd ed., edited by D. Gray (McGraw-Hill, New York, 1963); see also *ibid.*, 3rd ed. (McGraw-Hill, New York, 1972).
[12]J. F. Janni, At. Data Nucl. Data Tables 27, 150 (1982).
[13]K. Sera, K. Ishii, A. Yamadera, A. Kuwako, K. Kamiya, M. Sebata, S. Morita, and T. C. Chu, Phys. Rev. A 22, 2536 (1980).