PHYSICAL REVIEW A VOLUME 43, NUMBER 7 1 APRIL 1991

Stopping power of hydrogen atoms

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(Received 12 November 1990)

The stopping number of hydrogen atoms calculated with Bethe's theory in the first Born approximation is tabulated. A comparison is made with the asymptotic approximation and with a model based on the harmonic oscillator.

In their study of the Bethe theory of stopping power for a harmonic oscillator, Sigmund and Haagerup[1] compared their results for the stopping number with that for the hydrogen atom given in Fig. 4 of Fano.[2] They found differences which exceeded their expectations and therefore suggested that a more accurate function be published.

The stopping power for a heavy particle with charge ze and speed v is given by[3]

$$S=\frac{2\pi e^4 z^2}{mv^2}NB \; , \tag{1}$$

where e is the electron charge, m its mass, N the number of atoms per unit volume, and B the stopping number (in some papers L is used), defined by

$$B(\eta)=\sum_n^{\infty}\int_{Q_n}^{\infty} f_n(Q)d\ln Q + \int_1^{\infty} d(E/R)\int_{Q_m}^{\infty} f(E/R,Q)d\ln Q \; , \tag{2}$$

where $\eta=v^2/v_0^2$, $v_0=c/137$ the Bohr speed, and $R=13.606$ eV the Rydberg energy. $f_n(Q)$ is the generalized oscillator strength (GOS) for an excitation from the ground state of the hydrogen atom to a discrete energy level (where the particle loses an energy E_n and suffers a momentum change q, $Q=q^2/2m$), while $f(E,Q)$ is the GOS leading to a continuum state, with energy loss E.[4,5] The minimum momentum change corresponds to $Q_n=E_n^2/2mv^2$ and $Q_m=E^2/2mv^2$. The expressions for $f_n(Q)$ and $f(E,Q)$ were given in Refs. 3–6, and the func-

TABLE I. Stopping number B of hydrogen atoms, as a function of $\eta=v^2/v_0^2$. $B_d(\eta)$ is the sum over energy losses to all discrete levels, $B_c(\eta)$ is the sum over energy losses to all continuum levels, and $B(\eta)$ the sum of the two. δ_W is the relative difference to Eq. (3), and δ_S is the relative difference to the function in Ref. 1.

η	$B_d(\eta)$	$B_c(\eta)$	$B(\eta)$	δ_W (%)	δ_S (%)
0.1000	0.020 02	0.005 05	0.025 07		31
0.1334	0.038 99	0.013 21	0.052 2		33
0.1778	0.069 84	0.031 75	0.101 59		30
0.2371	0.115 69	0.07	0.185 69		23
0.3162	0.178 52	0.141 61	0.320 13		15
0.4217	0.258 76	0.263 58	0.522 34		8
0.5623	0.355 38	0.453 26	0.808 64		3.2
0.7499	0.466 38	0.723 85	1.190 23		2.5
1.0000	0.589 32	1.079 78	1.6691		−0.3
1.3335	0.721 81	1.514 18	2.235 99		−0.9
1.7783	0.861 72	2.009 93	2.871 65		−1.4
2.3714	1.007 30	2.544 12	3.551 42		−1.36
3.1623	1.157 16	3.093 85	4.251 01	17	−1.01
4.2170	1.310 23	3.640 86	4.951 09	4.4	−0.74
5.6234	1.465 71	4.173 56	5.639 27	0.9	−0.39
7.4989	1.622 98	4.686 71	6.309 69	0	−0.17
10.0000	1.781 61	5.179 67	6.961 28	−0.17	−0.1
13.3352	1.941 23	5.654 44	7.595 67	−0.16	−0.1
17.7828	2.101 61	6.114 11	8.215 72	−0.13	−0.085
23.7137	2.262 55	6.561 86	8.824 41	−0.11	−0.077
31.6228	2.423 92	7.000 55	9.4244	−0.09	−0.076
42.1697	2.585 59	7.432 46	10.018	−0.08	−0.07
56.2341	2.747 51	7.859 37	10.6069	−0.07	−0.061
74.9894	2.909 60	8.282 62	11.1922	−0.06	−0.055

tions are shown in Ref. 5. The stopping number was calculated numerically, with double-precision arithmetic, with $d\ln Q = 0.009$ for the discrete excitations, $d\ln Q = 0.0115$ for the continuum ones. The error of the calculations (less than 0.02%) was estimated by performing them also with $d\ln Q$ twice as large. The sum was calculated for $n < 300$, the residual to ∞ estimated from an approximation replacing the sum by an integral. Results are given in Table I. The relative deviation between the function calculated with[6]

$$B_W = 2\ln\eta + 2.578\,61 - \frac{2}{\eta} - \frac{25}{3\eta^2} + \frac{49}{\eta^3} \approx 2\ln\frac{2mv^2}{I} \quad \text{where } I = 1.102R \;, \tag{3}$$

and $B(\eta)$, $\delta_W = B_W/B(\eta) - 1$, is also given. For $\eta > 6$ this is well within the error quoted in Ref. 6. Tables of the stopping number $B_K(\Theta_K, \eta_K)$ calculated incidentally to the above calculations agree to better than 0.5% with Table II in Ref. 6.

The function $\frac{1}{2}B(\eta)$ exceeds the values of L shown in Fig. 4 of Ref. 2 by as much as 20% for $\eta < 1$, apparently due[7] to the use of a coarse grid in the integration over Q.

The relative deviation of the Sigmund-Haagerup[1] function is given as δ_S. The table given here should only be used for comparison with other calculations at the same level of approximation. For practical applications, various corrections should be included.[8]

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