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Ionization of atomic hydrogen by bare ions with charges 1 to 6 in the Glauber approximation

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Total cross sections for the ionization of atomic hydrogen by the impact of bare ions with charge $Z_1 = 1-6$ evaluated in the Glauber approximation are presented and compared to recent data for $Z_1 = 1-3$ and to other theoretical predictions. At projectile velocities $v < Z_1$ (in atomic units) the Glauber results lie below data observed. For $v > Z_1$ the Glauber results converge to observed results better than other theoretical calculations now available.

I. INTRODUCTION

Recently there has been interest, both experimentally and theoretically, in the ionization of atomic hydrogen by fully stripped ions of charge Z_1 from 1 through 6 at projectile velocities near and above the peak of the ionization cross section. Experimentally[1–3] there are recent[2] data (for $Z_1 = 1$, 2, and 3) and expected[3] data ($Z_1 = 4$, 5, and 6) from about 15 keV/amu to about 1 MeV/amu bare projectiles on atomic hydrogen. The accuracy of this data is typically better than 10%. This improved accuracy enables a more detailed test of theory in a region where perturbation theory (which is quite useful at sufficiently high projectile velocities) is no longer applicable.

Concurrently there has been a recent development of theoretical models[4–10] which possibly may be applied to situations where perturbation theory is inapplicable. Classical calculations[4] have been successful in predicting total vacancy production (electron capture plus ionization) cross sections in atomic hydrogen near the peak of the cross section. Continuum distorted-wave (CDW) calculations,[5] based on solving the Schrödinger equation with an approximation satisfying Coulombic asymptotic boundary conditions, have been reported for ionization of hydrogen by proton and α-particle impact. Quite recently the unitarized distorted-wave Born approximation[6] (UDWBA) has been applied to a variety of reactions with atomic hydrogen. For protons and α particles on hydrogen a dipole close-coupling approximation,[7] coupling the $1s$ wave function to continuum pseudostates via dipole coupling has been reported. In addition to these approximate solutions, recent progress has been made toward exact numerical solutions using close-coupling techniques[8,9] with large basis sets and by integration of the Schrödinger equation with the use of the finite element method.[10]

The Glauber approximation[11–13] is a comparatively simple method for solving the Schrödinger equation by retaining, in an eikonal approximation, all terms in the Born expansion. This approximation introduced[11] over 20 years ago was (and is being) used in nuclear and high-energy physics, as well as atomic physics where it was introduced[14] in 1969. The first applications to atomic ionization[15] were reported for electron impact about 1974, where the total cross sections for $e + \mathrm{H}$ and $e + \mathrm{He}$ were in reasonable agreement with observed data near and above the peak of the cross section. Such agreement is typical of many Glauber applications and is somewhat better than what is expected theoretically. However, Glauber results[16] for $p + \mathrm{H}$ and $p + \mathrm{He}$ tended to lie below observed results near the peak of the cross sections. This discrepancy was attributed[17] to the effects of charge transfer to the continuum,[18] omitted in the theoretical calculations. A calculation[19] for atomic ionization of hydrogen by α-particle impact was briefly reported in 1976, but with a lack of data or alternative nonperturbative calculations to test the theory, no further calculations for ionization were performed.

With both experiment and theory now available for comparison, calculations in the Glauber approximation for ionization of atomic hydrogen by ions of charges 1 to 6 are presented in this paper.

II. CALCULATIONS

In order for the reader to understand the nature of the results presented here, it is useful to briefly and simply review the Glauber approximation itself. Although there exist various derivations, each giving some insight, the conventional derivation[11] is illustrative. Consider

$$\left[\frac{-\nabla^2}{2M}+V\right]\Psi=E\Psi\ , \tag{1}$$

and choosing $\Psi=e^{i\vec{k}\cdot\vec{R}}\,\phi(R)$, the above Schrödinger equation becomes

$$\left[\frac{k^2}{2M}+\frac{-\nabla^2}{2M}+\frac{-i\vec{k}\cdot\vec{\nabla}}{M}+V\right]\phi=E\phi\ , \tag{2}$$

then setting $k^2/_{2M}=E$, choosing $\hat{Z}=\hat{k}$, and assuming that ϕ does not vary rapidly with R so that $\nabla^2\phi \ll 2\vec{k}\cdot\vec{\nabla}\phi$, one has

$$\left[-iv\frac{d}{dZ}+V\right]\phi=0 \tag{3}$$

corresponding to the eikonal approximation, namely,

$$\Psi=e^{i\vec{k}\cdot\vec{R}}\phi=e^{i\vec{k}\cdot\vec{R}}e^{i/v\int^{Z}V\,dZ'}\ , \tag{4}$$

so that Ψ corresponds to a plane wave (as in the first Born approximation) times an eikonal phase proportional to the average of the perturbing potential over the trajectory of the particle. The corresponding scattering amplitude f may be expressed

$$f=\frac{-M}{2\pi}\int d\vec{k}\,e^{-i\vec{k}_f\cdot\vec{R}}\,V\Psi$$
$$=\frac{-M}{2\pi}\int d\vec{R}\,e^{i(\vec{k}_f-\vec{k}_i)\cdot\vec{R}}\,Ve^{i/v\int^{Z}V\,dZ'}\ . \tag{5}$$

This eikonal amplitude may be reduced to a Glauber amplitude by choosing the $\hat{Z}$ axis of integration so that $(\vec{k}_f-\vec{k}_i)\cdot\vec{R}=\vec{q}\cdot\vec{R}\rightarrow\vec{q}\cdot\vec{B}$, i.e., $\vec{q}\cdot\vec{Z}=0$. Then, the Z integration is easily done so that

$$f=\frac{-iM}{2\pi v}\int d^2B\,e^{i\vec{q}\cdot\vec{B}}\left(1-e^{i/v\int_{\infty}^{\infty}V\,dZ}\right)\ . \tag{6}$$

Expanding the exponent, one obtains the first Born amplitude exactly and higher Born amplitudes approximately.

For ionization in atomic hydrogen, the above expression for the scattering amplitude becomes[11–15]

$$f=\frac{-2\pi i}{mv}\langle u_f\,|\int d^2B\,e^{i\vec{q}\cdot\vec{B}}\left(1-e^{i/v\int_{\infty}^{\infty}V(\vec{R},\vec{r})dZ}\right)|\,u_i\rangle\ , \tag{7}$$

where $\langle u_f\,|\cdots|\,u_i\rangle$ denotes an integration over the electronic initial and final states $u_i(r)$ and $u_f(r)$, where $\vec{r}$ is the electron coordinate and $\vec{R}$ the internuclear coordinate. Algebraic reduction of this amplitude has been done two ways.[15,20] Both ways have given the same numerical results. Total cross sections for ionization correspond to

$$\sigma=\int |f(\vec{q},\vec{k}_e)|^2 d\vec{q}\,d\vec{k}_e\ , \tag{8}$$

where $f(\vec{q},\vec{k}_e)$ is the Glauber amplitude of Eq. (7) and $\vec{k}_e$ is the momentum of the ejected electron. Following previous techniques[15,21] this may be reduced to

$$\sigma=\Sigma_{l,m}\int dq\,dk\,e\,|f_{l,m}(q,ke)|^2\ ,$$

where the f_{lm}, corresponding to the terms in Eq. (15) of Ref. 16, are represented by a one-dimensional numerical integral of hypergeometric functions.

III. RESULTS

The results of these calculations are presented in Table I and in Figs. 1–3. The numerical error in the Glauber calculations is about 1%, caused mostly by truncation of the sun over partial waves l, in Eq. (9) past $l=4$. Also listed are Born calculations for $p+\mathrm{H}$. Since the Born calculation varies as the square of the projectile charge (i.e., as Z_1^2), values of Born cross sections for particles of charge Z_1 may be easily evaluated from Table I and compared to Glauber calculations. It is noted that for $C^{6+}+\mathrm{H}$ the difference between Glauber and Born predictions is more than 2 orders of magnitude near 20 keV/amu. Also, while the Born cross section peaks at 25 keV/amu for all values of Z_1, the peak of the Glauber cross section moves to higher projectile speeds as the charge Z_1, of the projectile increases. At the higher velocities listed, the Glauber approximation converges slowly to the Born approximation. For example, at 1 MeV for $p+\mathrm{H}$ (where charge transfer to the continuum is quite small), the Born cross sections are still 3% larger than Glauber cross sections. Thus, while the Born cross section is correct at very high velocities, inaccuracies of a few percent remain, according to our calculations, at projectile speeds in the MeV/amu region even for $p+\mathrm{H}$.

In Fig. 1 cross sections for p^+, He^{2+}, and Li^{3+}

projectiles on atomic hydrogen are shown, together with recent data[2] of Shah and Gilbody as well as some other theoretical predictions.[8,10,22] In the region shown, the observed data lie between the Glauber and Born calculations, including the position of the peak of the cross section. Thus the Glauber approximation underestimates the cross sections at the cross-section maxima. This could perhaps be accounted for[8] by the omission of charge transfer to the continuum in the Glauber calculations. This suggestion is supported in the case of $p+H$ by observations[17] of the energy distributions of the ejected electrons. The close-coupling calculation[8] (which includes charge transfer to the continuum) shown in Fig. 1 lies 14% above (at 50 keV) and 8% below (at 200 keV) the data, which is accurate to 3%. Near the peak of the cross section for $p+H$, this close-coupling calculation is in better agreement with observation than other quantum calculations now available. The classical results[4] shown agree well with observation for $p+H$ near the peak of the cross section. However, at higher projectile energies E, the classical cross section varies as E^{-1} rather than the correct quantum-mechanical $E^{-1}\ln E$ variation. At projectile energies above the peak of the cross sections the

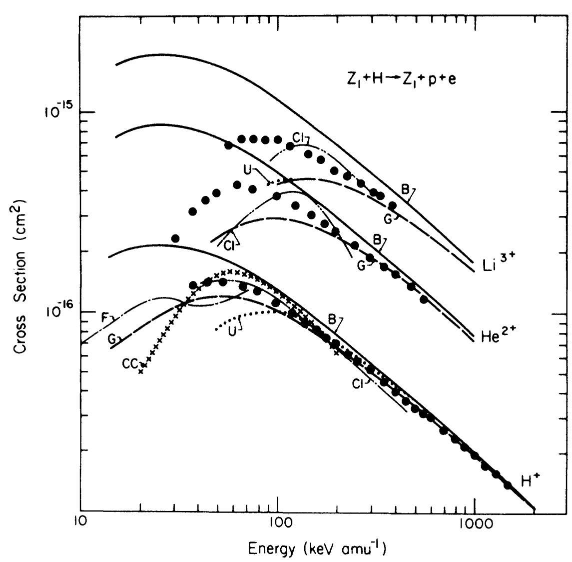

FIG. 1. Total cross section for ionization of atomic hydrogen by p^+, He^{2+}, and Li^{3+}. Data, represented by black circles, are from Shah and Gilbody (Refs. 1 and 2). The experimental uncertainty varies from 3% for p^+ to about 7% for Li^{3+}. Theoretical results include Born (B) (Ref. 21), close-coupling (CC) (Ref. 8), classical (Cl) (Ref. 4), finite element method (F) (Ref. 10), Glauber (G) (present results), and unitarized distorted-wave (U) (Ref. 6) calculations.

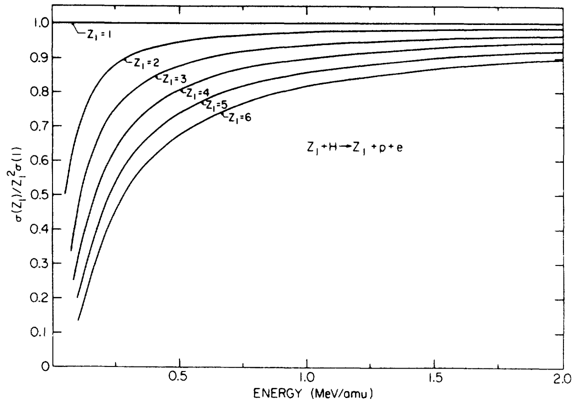

FIG. 2. Ratio of $\sigma(Z_1)/Z_1^2\sigma(1)$ in the Glauber approximation for ionization of atomic hydrogen by ions of charge $Z_1=1$, 2, 3, 4, 5, and 6. This ratio is one in the Born approximation.

Glauber approximation tends to converge to observed data in all cases shown. For example, for $p+H$ the Glauber calculations are within 3% (i.e., experimental error) of observed results at energies above 150 keV, while Born results agree within experimental accuracy only above 1 MeV. This region where the Glauber approximation fits data better than Born, was not apparent in[16] prior data. The traditional validity condition[11] for the Glauber approximation is that $Va/hv>1$, where a is the range of the potential V. For our case this condition becomes $Z_1 r/rv<1$ or $v>Z_1$ which is roughly consistent with the convergence of the Glauber results to the data in Fig. 1.

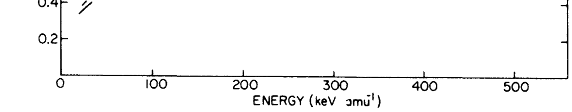

FIG. 3. Ratio of $\sigma(Z_1)/Z_1^2\sigma(1)$ for ionization of atomic hydrogen by protons and α particles. Experiment (E) is by Shah and Gilbody (Refs. 1 and 2). Theoretical results include Born (B) (Ref. 21), continuum distorted-wave (C) (Ref. 5), dipole close-coupling (D) (Ref. 7), and Glauber (G) (present results) approximations.

TABLE I. Total cross sections for $Z_1+\mathrm{H}\rightarrow Z_1+p+e$ evaluated in the Glauber and Born approximations for $Z_1=1$, 2, 3, 4, 5, 6 in units of $\pi a_0^2=8.79\times10^{-17}$ cm^2.

v	Glauber ionization cross sections (πa_0^2)						Born
keV/amu	$Z_1=1$	$Z_1=2$	$Z_1=3$	$Z_1=4$	$Z_1=5$	$Z_1=6$	$\sigma(Z_1)/Z_1^2$
20	9.05(−1)	1.32(0)	1.19(0)	7.93(−1)	4.55(−1)	2.85(−1)	2.39(0)
25	1.04(0)	1.54(0)	1.58(0)	1.26(0)	8.48(−1)	5.33(−1)	2.46(0)
30	1.17(0)	1.76(0)	1.88(0)	1.69(0)	1.30(0)	9.05(−1)	2.44(0)
40	1.32(0)	2.23(0)	2.43(0)	2.38(0)	2.15(0)	1.77(0)	2.31(0)
50	1.38(0)	2.65(0)	3.02(0)	3.02(0)	2.86(0)	2.59(0)	2.13(0)
75	1.32(0)	3.21(0)	4.30(0)	4.67(0)	4.63(0)	4.43(0)	1.74(0)
100	1.19(0)	3.31(0)	5.00(0)	5.98(0)	6.36(0)	6.37(0)	1.45(0)
150	9.59(−1)	3.05(0)	5.27(0)	7.14(0)	8.51(0)	9.37(0)	1.09(0)
200	7.93(−1)	2.70(0)	4.98(0)	7.22(0)	9.19(0)	1.08(1)	8.74(−1)
300	5.88(−1)	2.13(0)	4.21(0)	6.52(0)	8.87(0)	1.11(1)	6.28(−1)
400	4.69(−1)	1.75(0)	3.57(0)	5.72(0)	8.04(0)	1.04(1)	4.94(−1)
500	3.91(−1)	1.48(0)	3.09(0)	5.05(0)	7.24(0)	9.56(0)	4.09(−1)
600	3.36(−1)	1.29(0)	2.72(0)	4.51(0)	6.54(0)	8.75(0)	3.50(−1)
800	2.64(−1)	1.02(0)	2.20(0)	3.71(0)	5.47(0)	7.43(0)	2.73(−1)
1000	2.19(−1)	8.54(−1)	1.85(0)	3.15(0)	4.70(0)	6.45(0)	2.25(−1)
1500	1.55(−1)	6.08(−1)	1.34(0)	2.31(0)	3.49(0)	4.85(0)	1.58(−1)
2000	1.21(−1)	4.76(−1)	1.05(0)	1.83(0)	2.79(0)	3.91(0)	1.23(−1)

In Fig. 2 the ratio $\sigma(Z_1)/Z_1^2\sigma(1)$ is plotted versus energy in the energy region where the Glauber approximation appears to be useful. The Born approximation, which varies as Z_1^2, predicts a value of one for this ratio, independent of projectile velocity. In this region, the Glauber approximation lies below the Born approximation. Furthermore, the Glauber approximation predicts no "polarization effect"[9,21] [in which the ratio $\sigma(Z_1)/Z_1^2\sigma(1)$ rises above unity]. Deviations of several percent or more from the Z_1^2 projectile charge scaling are predicted even at energies of the order of MeV/amu.

In Fig. 3 the ratio $\sigma(Z_1)/Z_1^2\sigma(1)$ is compared to experimental observation[2] and to other theoretical calculations[5,7] for protons and α particles on atomic hydrogen. The Glauber approximation tends to converge to observed results at the higher energies, i.e., energies above the peak of the cross sections. While the other theoretical results shown do not converge to the data as well as the Glauber results, the trends are reasonable with the exception of the CDW results.[5] This apparent breakdown of the CDW results is surprising, in the author's opinion, since CDW, like Glauber, represents a better solution to the Schrödinger equation at high energies than the simpler Born approximation.

Availability of precise total-cross-section data on highly perturbed systems, including, for example, C^{6+} + H in the near future,[3] provides a useful and stringent test of new approximations, such as those included in Figs. 1 and 3, as well as more extensive, exact numerical calculations[8-10] now being developed. Even greater differences are evident in differential cross sections in our calculations than in total cross sections, providing incentive for more detailed studies.

IV. SUMMARY

In summary, calculations of cross sections for ionization of atomic hydrogen by bare ions of charge $Z_1=1-6$ have been presented (Table I). At projectile velocities $v<Z_1$, the Glauber results lie below recently observed results for $Z_1=1-3$. At velocities $v>Z_1$, the Glauber results converge to the observed data, consistent with the validity criterion.

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