$$\tau_{n-1} = (\Psi_{n-1}, \Psi_{n-1}) = -\tau_{n-2}^{-1}(\Psi_{n-2}, \rho_1)^2$$
$$= -\tau_{n-2}^{-1}(\Psi_{n-2}', \rho_1)^2 . \quad (95)$$

We may introduce a second spurious constant if $\tau_{n-2}$ is small. But at most a finite number of interchanges will eliminate the spurious constants as there is only one wave function.

ACKNOWLEDGMENT

I would like to thank Dr. F. Coester for several stimulating conversations on portions of this paper.

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# Ionization of Positive Ions*

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The classical binary-encounter model for ionization by charged-particle impact is modified to permit evaluation of the cross section for ionization of positive ions by electron impact. General scalable expressions are obtained and compared with available experimental data and quantum-theoretical approximations. The dependence on ionic charge is discussed, and a simple physical interpretation emerges. Our results indicate that this model is nearly as reliable as the Born approximation for this process; i.e., they agree well with existing experimental data for energies much larger than threshold and are everywhere within a factor of two.

## I. INTRODUCTION

The lack of solutions to the three-body problem presents a distinctly larger handicap in considering the ionization of ions by charged-particle impact than in ionization of neutrals because of the effects of the residual ionic field. For the neutrals, the binary-encounter approximation has been found to provide a reasonable description of the phenomena. Furthermore, recent work[1-3] has indicated the utility of even a classical binary-encounter approximation for charged-particle ionization of neutrals.

For ionization, the primary motivation for the

use of a classical binary-encounter model is that it provides a simple framework for estimates, which turn out to be quite reliable at high energy and within a factor of about 2 everywhere.[1-4] In addition, the model has been shown[5] to be related to a quantum treatment. Its practical significance is greatest for multi-electron atoms (and diatomic molecules), where even the Born approximation becomes difficult because of the numerical integrations involved. We have thus deemed it appropriate to provide a modification of the model to make it applicable to the reactions

$$e + A^{(n)+} \rightarrow A^{(n+1)+} + e + e\,, \tag{1}$$

$$p + A^{(n)+} \rightarrow A^{(n+1)+} + p + e\,. \tag{2}$$

In Sec. II we evaluate the effects of the residual ion field on the cross section within the binary-encounter framework. Section III contains a comparison of our results with the available experimental data and with quantum treatments extant. We discuss only reaction (1); the changes required for reaction (2) are straight forward. Our results agree well with experiment for energies much larger than threshold, and are everywhere within a factor of 2. They are nearly as reliable as the Coulomb-Born approximation. Our formulation also provides some interpretational advantages. For very large energies, our model yields a $1/E$ dependence, while the Born and Born-Coulomb approximations both yield an $(\ln E)/E$ dependence for low-lying states. This matter has been discussed in Ref. 5; in practice the differences are small.

## II. MODEL FOR ION IONIZATION

The binary-encounter approximation consists of the assumption that the significant interaction is the energy exchange between the incident charged particle, of velocity $\vec{v}_1$, and an atomic electron of velocity $\vec{v}_2$. Thus the cross section for ionization of a neutral atom is

$$\sigma_{\text{ion}} = \sum_i n_i \int_{U_i}^{E_1} \sigma_{\Delta E}^{\text{eff}}(v_1, v_{2i})\, d(\Delta E)\,, \tag{3}$$

where $\sigma_{\Delta E}^{\text{eff}}$ is the cross section for exchange of energy $\Delta E$, in the laboratory frame, averaged over all orientations of $\vec{v}_{2i}$, and $n_i$ is the number of equivalent electrons whose energy is $U_i$. The result (3) is to be averaged over the speed distributions of the bound electrons.

In this section we present a model for calculating the cross sections for reaction (1), taking into account the effects of the residual field of the ion. Atomic units are used throughout.

Our model can be simply stated as follows: we consider an electron with kinetic energy $E_1$ incident on a fixed positive ion with net charge $Z'$. At a distance $\xi$ from the nucleus, the incident electron undergoes an essentially binary collision with a bound electron, of binding energy $U$, resulting in an energy transfer $\Delta E \geq U$. At the distance $\xi$, the incoming electron has a kinetic energy

$$E_1' = E_1 + Z'/\xi \geq E_1\,, \tag{4}$$

so that the total cross section for the energy exchange collision is given by

$$\sigma'(E_1', E_1, U) = \left\langle \int_U^{E_1} \sigma_{\Delta E}^{\text{eff}}(v_1', v_2)\, d(\Delta E) \right\rangle_{\text{av}}\,, \tag{5}$$

where $\langle\ \rangle_{\text{av}}$ denotes an averaging over the speed distribution $f(v_2)$ of the bound electron. In Eq. (5), the upper limit of the integral must be $E_1$, not $E_1'$, since for ionization, both electrons are to be in positive energy states after collision. The total cross section for ionization will be related to $\sigma'$ as indicated in Fig. 1. We assume that $\sigma'$ determines an average off-axis distance $\rho$ from the relation $\sigma' = \pi\rho^2$. The parameters $\xi$ and $\rho$ then determine a trajectory for the incident electron in the presence of the asymptotic charge $Z'$ prior to the binary encounter. This trajectory in turn specifies the initial impact parameter $b$

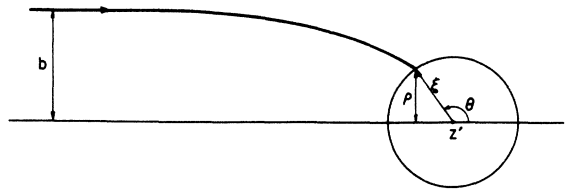


FIG. 1. Geometry for electron-ion collision.

for the incident electron. The total cross section for ionization is then $\sigma = \pi b^2$. Our final result is presented in the form of a correction factor to an appropriate result for neutrals.

The collision radius $\xi$ depends on both the distance of the bound electron from the nucleus $\vec{r}_A$ and an electron-electron separation $\vec{\delta}$ such that an energy exchange $\Delta E \geq U$ can occur. We use an average over relative orientations,

$$\xi \equiv |\vec{r}_A + \vec{\delta}|_{\text{av}} = (1/3r_A)(3r_A^2 + \delta^2), \quad \text{if } r_A > \delta ;$$

$$= (1/3\delta)(3\delta^2 + r_A^2), \quad \text{if } r_A < \delta . \tag{6}$$

Classically, an average $r_A$ can be determined from the virial theorem result $(Z'+1)/2r_A = U$, where $U$ is the binding energy, at least for hydrogenic ions. We adopt this result for all cases.

$\delta$ is related only to an energy exchange collision between the two electrons. Consider the simpler case of an isolated two-electron system in which one electron is initially at rest and the other is incident with energy $E_{1d}$. For this situation, the minimum laboratory scattering angle $\theta_m$, such that a minimum energy transfer $\Delta E = U$ may occur is given by[6]

$$\sin^2\theta_m = U/E_{1d} , \tag{7}$$

corresponding to a maximum (center of mass) impact parameter,

$$s_m = E_{1d}^{-1}\cot(\Theta_m/2), \tag{8}$$

where $\Theta_m = 2\theta_m$ is the center of mass scattering angle. Using the center of mass orbit equation,[6] together with (7) and (8), we find that the largest distance of closest approach $d$, such that an energy transfer of at least $U$ can occur, is

$$d = E_{1d}^{-1}[(E_{1d}/U)^{1/2} + 1] . \tag{9}$$

This result was derived for one electron initially at rest; if both electrons have nonzero laboratory frame velocities, $E_{1d}$ is the relative kinetic energy. But if we average over a spherically symmetric distribution of velocities for one electron, the resultant relative energy is the total laboratory frame energy. Thus we set $E_{1d} = E_1 - U$ in (9) and adopt this as the value of $\delta$:

$$\delta \equiv (E_1 - U)^{-1}[(E_1/U - 1)^{1/2} + 1] . \tag{10}$$

Equations (10), (6), and (4) complete our specification of $E_1'$:

$$E_1' = E_1 + 3Z'r_A/(3r_A^2 + \delta^2), \quad r_A > \delta ; \qquad E_1' = E_1 + 3Z'\delta/(r_A^2 + 3\delta^2), \quad r_A < \delta ;$$

with $r_A = (Z'+1)/2U$ and $\delta$ as defined in (10).

We now need to find the impact parameter $b$, such that the incident electron intercepts the "collision sphere" at an angle defined by $\sin\theta = \rho/\xi$, where $\rho = (\sigma'/\pi)^{1/2}$, as shown in Fig. 1.[7] Considering the ion as fixed, the trajectory of the electron is given by[6]

$$1/r = (Z'/2E_1b^2)\{1 + [1 + 4E_1^2b^2/(Z')^2]\cos(\theta - \theta')\} , \tag{11}$$

where $\cos\theta' = [1 + 4E_1^2b^2/(Z')^2]^{-1/2}$ .

Using $r = \xi$ and $\theta = \sin^{-1}\rho/\xi$, together with the requirement that if $Z' = 0$, $b = \rho$ (i.e., no correction for the neutral case), we can solve (11) for $b$:

$$b = \tfrac{1}{2}\left(\rho + \{\rho^2 + (2Z'/E_1)[\xi - (\xi^2 - \rho^2)^{1/2}]\}^{1/2}\right) .$$

The total ionization cross section, remembering the definition of $\rho$, is then

$$\sigma_{\text{ion}}(E_1) \equiv \pi b^2 = \tfrac{1}{4}\sigma' \left(1 + \{1 + (2Z'\pi/E_1\sigma')[\xi - (\xi^2 - \sigma'/\pi)^{1/2}]\}^{1/2}\right)^2 ,$$

or finally, using (4) to eliminate $\xi$ and taking advantage of the fact[2] that $\sigma'$ (hence $\sigma$) is a scalable function of $E_1/U$,

$$\Sigma = \tfrac{1}{4}\Sigma' \left(1+\left[1+(2Z'\pi/\beta_1\Sigma')\left\{Z'/(\beta_1'-\beta_1)-\left[(Z')^2/(\beta_1'-\beta_1)^2-\Sigma'/\pi\right]^{1/2}\right\}\right]^{1/2}\right)^2 , \tag{12}$$

where $\Sigma = U^2\sigma$, $\Sigma' = U^2\sigma'$, $\beta_1 = E_1/U$, and

$$\begin{aligned}\beta_1' = E_1'/U &= \beta_1 + \tfrac{3}{2}Z'(Z'+1)/\left[\tfrac{3}{4}(Z'+1)^2+\Delta^2\right], \quad (Z'+1)/2 > \Delta ; \\ &= \beta_1 + 3Z'\Delta/\left[3\Delta^2+\tfrac{1}{4}(Z'+1)^2\right], \quad (Z'+1)/2 < \Delta ;\end{aligned} \tag{13}$$

with $\Delta = U\delta = (\beta_1-1)^{-1}\left[(\beta_1-1)^{1/2}+1\right]$.

Equation (12) is the desired result for the cross section for removal of an electron of binding energy $U$ from the ion whose residual charge is $Z'$. The total cross section for ionization of an ion is obtained by summing over all electrons in the ion. We need still specify the function defined by Eq. (5).

A few remarks about the nature of our result are in order. The factor in curly brackets in (12) represents the effect of magnification of the cross section due to the curvature of the electron's path in the residual field. The magnification is 1 when $Z' = 0$, as appropriate. The other difference from the model for ionization of neutrals is in requiring an increase in the incident particle energy at which the energy exchange takes place, reflected in $E_1'$. Thus, the result incorporates the major features of the effect of the ion field. Both of these effects are expected to be very small for reaction (2) because of the large mass differences.

We now return to the evaluation of $\Sigma'$ or $\sigma'$ from Eq. (5). The required expressions for $\sigma_{\Delta E}{}^{\text{eff}}(v_1', v_2)$ have been given by Gerjuoy,[4] among others. It already involves a spherical averaging over all orientations of $\vec{v}_2$ with respect to $\vec{v}_1'$. We evaluate the integral over $(\Delta E)$ by imposing the condition $U \le E_1 \le E_1'$ and taking $E_2$ fixed but arbitrary. We have, then, the following three possibilities[4] (when $E_1 \ne E_1'$):

$$\sigma'(E_1', E_2, U) = \int_U^{E_1} \sigma_{\text{iii}}(v_1', v_2)\,d(\Delta E), \qquad \text{if } U \le E_1 \le E_1' - E_2 \le E_1' ; \tag{14a}$$

$$= \int_U^{E_1'-E_2} \sigma_{\text{iii}}\,d(\Delta E) + \int_{E_1'-E_2}^{E_1} \sigma_{\text{i}}(v_1', v_2)\,d(\Delta E), \quad \text{if } U \le E_1' - E_2 \le E_1 \le E_1' ; \tag{14b}$$

$$= \int_U^{E_1} \sigma_{\text{i}}(v_1', v_2)\,d(\Delta E), \qquad \text{if } E_1' - E_2 \le U \le E_1 \le E_1' ; \tag{14c}$$

where $\int^{\Delta E} \sigma_{\text{i}}(v_1', v_2)\,d(\Delta E) = -\tfrac{2}{3}\pi(v_1'/v_2)(1/E_1')^2(1-\Delta E/E_1')^{3/2}(\Delta E/E_1')^{-2}$,

and $\int^{\Delta E} \sigma_{\text{iii}}(v_1', v_2)\,d(\Delta E) = -(\pi/E_1')\left[\tfrac{1}{3}v_2{}^2(\Delta E)^{-2}+(\Delta E)^{-1}\right]$,

with $E_2 = \tfrac{1}{2}v_2{}^2$, etc. Equation (14a) does not appear if $E_1 = E_1'$. In that case, Eqs. (14) reduce to Stabler's[8] result (with the appropriate changes in notation), as expected. Inserting the results of the integrations into Eqs. (14) and introducing the scaled quantities of Eqs. (12) and (13), we have

$$\Sigma_{\text{ion}}'(\beta_1', \beta_2; \beta_1) = (\pi/\beta_1')\left[\tfrac{2}{3}\beta_2(1-1/\beta_1{}^2)+(1-1/\beta_1)\right], \qquad \text{if } 0 \le \beta_2 \le \beta_1' - \beta_1 ; \tag{15a}$$

$$= \frac{\pi}{3\beta_1'}\left(2\beta_2+3-\frac{3}{(\beta_1'-\beta_2)}-\frac{2}{\beta_2{}^{1/2}}\,\frac{(\beta_1'-\beta_1)^{3/2}}{\beta_1{}^2}\right), \quad \text{if } \beta_1'-\beta_1 \le \beta_2 \le \beta_1'-1; \tag{15b}$$

$$= \frac{2\pi}{3}\,\frac{1}{\beta_1'}\,\frac{1}{\beta_2{}^{1/2}}\left((\beta_1'-1)^{3/2}-\frac{(\beta_1'-\beta_1)^{3/2}}{\beta_1{}^2}\right), \qquad \text{if } \beta_1'-1 \le \beta_2 ; \tag{15c}$$

where we have expressed the inequalities in (14) as inequalities on $\beta_2 = E_2/U$. For ionization $\beta_1 \ge 1$.

Equation (15) is required to calculate $\Sigma'(\beta_1'; \beta_1)$. If we adopt hydrogenic speed distributions for the bound electrons

$$f(k) = (32/\pi)k^2/(1+k^2)^4, \quad k^2 \equiv \beta_2 , \tag{16}$$

we have $\Sigma_{\text{av}}'(\beta_1'; \beta_1) = \int_0^\infty \Sigma_{\text{ion}}'(\beta_1', k; \beta_1) f(k)\,dk$. (17)

The integral (17), using (15) and (16), results in the following expression:

$$\Sigma'(\beta_1';\beta_1) = (32/3\beta_1')\Big( [(\beta_1'-1)^{1/2}/2\beta_1'][\tfrac{5}{8} - 1/4\beta_1' - 1/(\beta_1')^2]$$
$$+[(\beta_1'-\beta_1)^{1/2}/2\beta_1(c-\beta_1)][(c-\beta_1)^{-2} + (2-\beta_1)/4\beta_1(c-\beta_1) - (2+3\beta_1)/8\beta_1]$$
$$+\tfrac{5}{16}\tan^{-1}(\beta_1'-1)^{1/2} - [(3\beta_1+2)/16\beta_1^2]\tan^{-1}(\beta_1'-\beta_1)^{1/2}$$
$$-[3(\beta_1')^{1/2}/c^4]\ln\{\beta_1^{1/2}[(\beta_1')^{1/2} + (\beta_1'-1)^{1/2}]/[(\beta_1')^{1/2} + (\beta_1'-\beta_1)^{1/2}]\}$$
$$+3\beta_1'\{[(\beta_1'-c)/6\beta_1'c][(\beta_1'-\beta_1)^{1/2}/(c-\beta_1)^3 - (\beta_1'-1)^{1/2}/(\beta_1')^3]$$
$$+[\tfrac{5}{24}(\beta_1'-c)/\beta_1'c + 1/4c^2][(\beta_1'-\beta_1)^{1/2}/(c-\beta_1)^2 - (\beta_1-1)^{1/2}/(\beta_1')^2]$$
$$+[\tfrac{5}{16}(\beta_1'-c)/\beta_1'c + 3/8c^2 + 1/2c^3][(\beta_1'-\beta_1)^{1/2}/(c-\beta_1) - (\beta_1'-1)^{1/2}/\beta_1']$$
$$-[\tfrac{5}{16}(\beta_1'-c)/\beta_1'c + 3/8c^2 + 1/2c^3 + 1/c^4][\tan^{-1}(\beta_1'-1)^{1/2} - \tan^{-1}(\beta_1'-\beta_1)^{1/2}]\}\Big) , \quad (18)$$

where $c = \beta_1' = 1$.

We note that by setting $\beta_1' = \beta_1$, we can obtain the averaged ionization cross section for neutral hydrogen in the binary-encounter model from (18):

$$\sigma_{\text{ion};H}(E_1) = \Sigma'(\beta_1' = \beta_1)/U_H^2, \quad \text{where } E_1 \equiv U_H\beta_1 .$$

The numerical calculations of Kingston[9] are in agreement with the results obtained from the exact expression (18) with $\beta_1' = \beta_1$. It should be noted that this exact result is proportional to $1/\beta_1$ as $E_1 \to \infty$; this is not in agreement with the Coulomb-Born $(\ln E)/E$ behavior.[5]

## III. RESULTS AND COMPARISONS

Since both (12) and (18) are already in scaled form, the application of these results to the ionization of any ion merely requires a sum of expressions (12) for each bound electron:

$$\sigma_{\text{ion}} = \sum_i [n_i U_i^{-2}\Sigma(\beta_{1i}'\beta_{1i})] , \quad (19)$$

where $n_i$ is the number of equivalent electrons having binding energy $U_i$, $\beta_{1i} = E_1/U_i$ and $\beta_{1i}'$ is given by (13). Since we are using atomic units, $\sigma$ will be given in units of Bohr radii squared $(r_0^2)$; note that the $U_i$ are in a.u. (27.2 eV), and $\Sigma$ has dimensions (a.u.)$^2(r_0^2)$.

One test of our model is provided by a comparison with existing quantum treatments for $He^+$. Figure 2 shows such a comparison with two first-Born calculations: the Coulomb-Born [CB(i)] approximation of Burgess and Rudge,[10] and the Coulomb-Born [CB(ii)] calculations of Rudge and Schwartz.[11] The figure shows only the values explicitly calculated, not including their extrapolation to higher energies. Also shown are the experimental values of Dolder *et al.*[12] The Coulomb-Born-exchange (CBE) calculations of Rudge and Schwartz[11] lie very close to the experimental values, while the close coupling approximation values of Burke and Taylor[13] lie close to the CB(ii) curve, neither of these is shown. It can be seen that our model gives results consistent with the CB(i) approximation, but not as close to the experimental values as the CB(ii) or CBE approximations. We point out that all of these CB approximations require extensive numerical integration, expecially at higher energies.

It should be apparent that while the magnification factor in Eq. (12) was obtained in a rather direct fashion and is relatively insensitive to the parameters used in the model, the interaction energy $E_1'$ is considerably more model dependent. Since the model only attempts plausible approximations to the exact three-body effects, we have

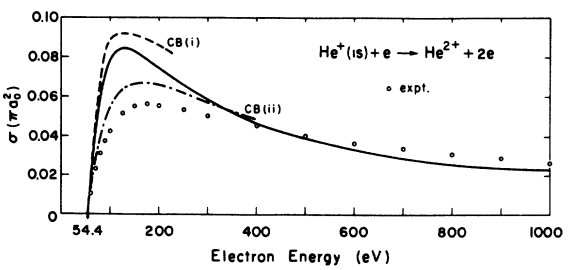


FIG. 2. Ionization of helium ions by electron impact. Solid curve, present results; broken curves, Coulomb-Born approximations (Ref. 10 and 11); circles, experimental results (Ref. 12).

examined various schemes for varying $\beta_1'$. The solid curve in Fig. 3 is our "best" result for $He^+$, obtained by using $\beta_1' = \beta_1 + 2$ in (18) and using this value of $\Sigma'$ in (12). The explicit $\beta_1'$ dependence of (12) is still determined by (13). (The dashed curve in this figure is a semi-empirical cross-section discussed below.) We note that this result lies everywhere below the CB(ii) curve of Fig. 2, except in the region from threshold to 100 eV.

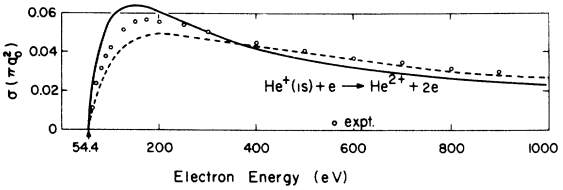


FIG. 3. Comparison of modified binary-encounter results. Solid curve, result using $\Sigma'_N$; dashed curve, result using $\Sigma'_{H,\,exp}$; circles, experiment (Ref. 12).

We denote the result obtained by using $\beta_1' = \beta_1 + 2$ in (18) by $\Sigma'_N$. Table I gives the value of $\Sigma'_N$ for the range of values of $\beta_1$ of any practical significance.

It is apparent that this choice of the energy dependence of $\Sigma'$ improves agreement with experiment near threshold, and goes smoothly to the

TABLE I. Scaled Cross Sections $\Sigma'_N$.

| $\beta_1 = E_1/U$ | $\pi^{-1}\Sigma'_N(\beta_1' = \beta_1 + 2)$ (a.u.) |
|---|---|
| 1.25 | 0.1137 |
| 1.50 | 0.1720 |
| 1.75 | 0.2033 |
| 2.00 | 0.2202 |
| 2.50 | 0.2320 |
| 3.00 | 0.2304 |
| 5.0 | 0.1955 |
| 7.0 | 0.1623 |
| 10.0 | 0.1274 |
| 20.0 | 0.0729 |
| 30.0 | 0.0508 |

unmodified result at higher energies. (As the incident energy is increased, the effects of the residual field become less important.) The effect of using $\Sigma'_N$ simulates in some fashion exchange effects. On this basis, we suggest that the total cross section for ionization of ions can be well approximated by (19), with the use of $\Sigma'_N$ in (12).

The dependence on residual charge $Z'$ is illustrated in Fig. 4. There the reduced cross-section $Q_R = (U_H)^{-2}\Sigma$, where $U_H$ is the ionization energy of hydrogen, is plotted for various values of $Z'$.

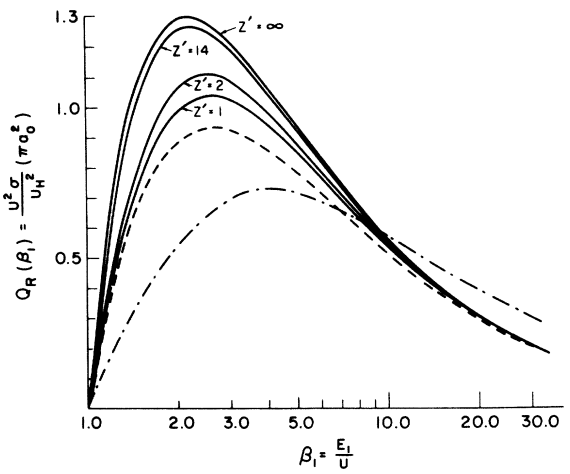


FIG. 4. $Z'$ dependence of reduced cross sections. Solid curves, reduced cross sections for various $Z'$; dashed curve, "unmagnified" reduced cross section, $\Sigma'_N/U_H^2$; broken curve; reduced semi-empirical cross section, $\Sigma_{H,\,exp}/U_H^2$.

($\Sigma'_N$ has been used.) It can be seen that at high energies $\Sigma$ becomes independent of $Z'$, a result which can also be obtained directly from (12) and (13). The dashed curve in Fig. 4 is the "unmagnified" result; that is, it is just the reduced cross-section $\Sigma'_N/U_H^2$. The broken curve is the semi-empirical reduced cross-section discussed below.

The usefulness of a classical formulation is made evident here. Quantum treatments[10,11] obtain the same general features displayed in Fig. 4, but their interpretation is not evident. From (12) we see that the $Z'$ dependence of the reduced cross-section is primarily due to the curvature of the electron in the residual field of the ion. As $Z'$ increases, the actual curvature produced by the residual field increases, but the mean distance of the bound electron from the nucleus decreases. These two effects eventually compensate each other, so that the reduced cross-section approaches a limiting curve as $Z' \to \infty$. The cross-section itself, of course, has additional $Z'$ dependence in that it is proportional to $U^{-2}$.

Further comparisons with experiment are presented in Figs. 5 and 6. The experimental results are from Refs. 14 through 17. In each case, the upper solid curve is the direct evaluation of (19) with $\beta_1'$ as given by (13), and the lower curve the result of using $\Sigma'_N$ in (12), then using (13) in (12) to determine (19). The required inner-shell ionization energies were taken to be Clementi's Hartree-Fock values.[18] Agreement with experiment is gratifying, considering the simplicity of the model, especially for the calculations involving $\Sigma'_N$. Even the direct model results, however, are seen to be everywhere within a factor of about 2, and much better at high energies.

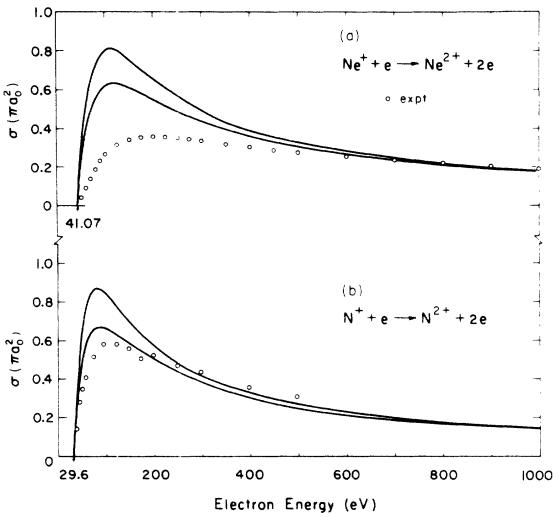


FIG. 5. Electron impact ionization cross sections. In each case, the upper solid curve is the direct model result, the lower curve is the values using $\Sigma'_N$. (a) Neon ions; circles, experimental results (Ref. 14). (b) Nitrogen ions; circles, experimental results (Ref. 15).

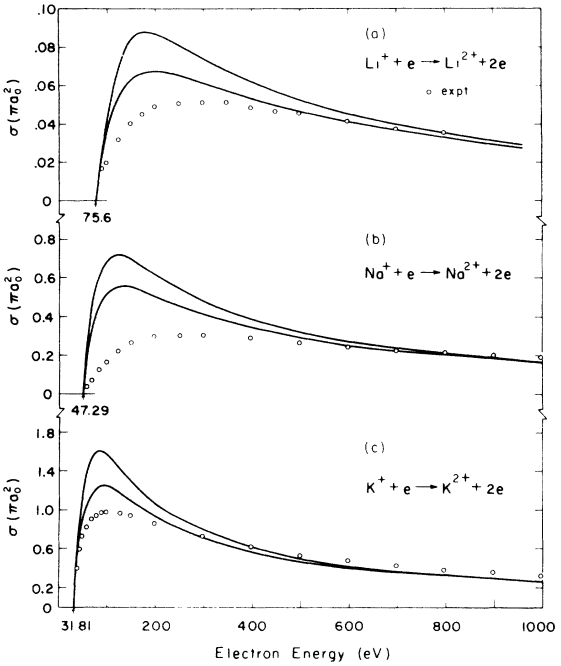


FIG. 6. Electron impact ionization of alkali ions. In each case the upper solid curve is the direct model result, the lower curve is the values using $\Sigma'_N$. (a) Lithium ions; circles, experiment (Ref. 16). (b) Sodium ions; circles, experiment (Ref. 16). (c) Potassium ions; circles, experiment (Ref. 17).

Finally, we observe that an alternative choice for the electron-electron interaction cross-section, $\Sigma'$, can be based upon experiment. The dashed curve in Fig. 3 is the result of using $\Sigma'_{H,\mathrm{exp}}(\beta_1)$ for $\Sigma'$ in (12), where $\Sigma'_{H,\mathrm{exp}}(\beta_1)$ has been obtained from the fit to the experimental electron-hydrogen ionization cross-sections given in Ref. 11. Similarly, the broken curve in Fig. 4 is $Q_R(\Sigma_{H,\mathrm{exp}}(\beta_1))$. Agreement with experiment is slightly improved at high energies, as expected from the results for ionization of neutrals.[9]

It appears that Eq. (19) with the reduced cross section $\Sigma$ specified by (12) includes the major physical effects involved. We have demonstrated three different ways of specifying the intermediate cross section $\Sigma'$ needed in (12): (1) using our Eq. (18); (2) using $\Sigma'_N$ from Table I; (3) a semi-empirical method using $\Sigma'_{H,\mathrm{exp}}$. All yield estimates which differ no more than a factor of 2 from experimental values, and are much better at higher energies. It is hoped that this will provide a useful guide to future experiments, especially those involving many-electron ions, where the simpler semi-empirical schemes fail and the simplest quantum estimates are difficult.

We conclude that the binary encounter model, as modified, is as reliable for predicting ionization of ions as for neutrals. Evidently, energy exchange between the incident and bound electrons is the dominant interaction occurring in this process.

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[7]The ratio $\rho/\xi$ is strictly less than unity, if $Z' \geq 1$. From Eq. (6) we see that $\xi \geq r_A$, so that $U\xi \geq Ur_A = (Z'+1)/2$. Thus

$$\rho/\xi \leq U\rho/Ur_A = [2/(Z'+1)]\,(U^2\sigma'_{\text{ion}}/\pi)^{1/2}.$$

This last factor can be shown to be less than 1 from the equations in Ref. 4.

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# Asymptotic Form of the Total Wave Function for Electron-Impact Excitation of Hydrogen Atoms

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An asymptotic form of the total wave function for electron-impact excitation of hydrogen atoms is obtained by the use of the Coulomb Green function. The result is compared with the corresponding usual form, obtained through the free-particle Green function. The validity of the Coulomb wave formulation is upheld in view of the physical quantities being finite definite.

## I. INTRODUCTION

In describing inelastic electron-atom collisions, the outgoing boundary conditions on the total wave function of a system of an electron and an atom are important. From the boundary conditions, one finds the scattering amplitudes for the processes; and from the amplitudes one can predict various physical properties, such as the probability of having a specific process, or specific energy and angular dependences. This asymptotic form of the wave function can be, in principle, derived from the Schrödinger equation with the use of either a plane wave or a Coulomb wave to represent a positive energy electron. These correspond to employing either a free-particle Green function or a Coulomb Green function.

In the literature, the former method of a free-particle Green function has been carried out[1,2] while the latter has not. However, when the method of a free-particle Green function is applied to the Coulomb potential scattering of a charged particle, the apparent asymptotic form of the wave function differs from that of the known exact Coulomb wave function by an indefinite phase factor whose argument diverges. Thus one is left with an inconsistency.

In this paper, the asymptotic form of the total wave function for the electron-atom inelastic collision process is obtained via the Coulomb Green function and compared with that of a free-particle Green function method. It is pointed out that the two forms of the same total wave functions are the same and unique, though they appear differently. It is also found that the scattering amplitudes for both electron-atom collisions and the Coulomb potential scattering in the plane wave formulation contain the undesirable indefinite phase factor, while those in the Coulomb wave formulation are finite and definite. Thus some doubts which were raised by some authors[3,4] about the validity of the Coulomb wave formulation by Kang and Foland[5] for the electron-atom collision process, are dispelled.