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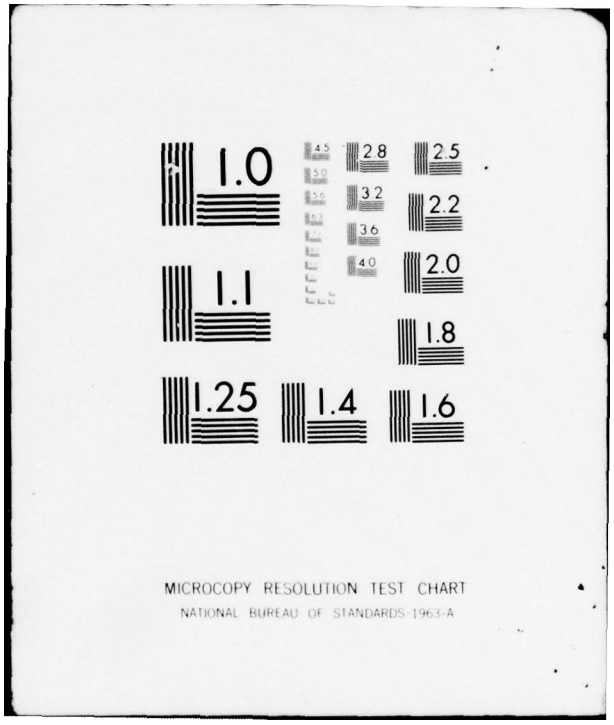
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NRL Memorandum Report 3733

Report of Progress in the Development of an Electron Impact Ionization Model

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LEVEL II

March 1978

NAVAL RESEARCH LABORATORY
Washington, D.C.

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SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE

READ INSTRUCTIONS BEFORE COMPLETING FORM

1. REPORT NUMBER: NRL Memorandum Report 3733 (14 NRL-MR-)
2. GOVT ACCESSION NO.
3. RECIPIENT'S CATALOG NUMBER

4. TITLE (and Subtitle): REPORT OF PROGRESS IN THE DEVELOPMENT OF AN ELECTRON IMPACT IONIZATION MODEL. (6)
5. TYPE OF REPORT & PERIOD COVERED: Interim report on a continuing NRL problem. (9)
6. PERFORMING ORG. REPORT NUMBER

7. AUTHOR(s): M. Blaha* and J. Davis (10) JACK / DAVIS
8. CONTRACT OR GRANT NUMBER(s): 16 RR0130 1 — 17 RR0130143

9. PERFORMING ORGANIZATION NAME AND ADDRESS: Naval Research Laboratory, Washington, D.C. 20375
10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS: NRL Problem H02-46, ONR Task RR0130143

11. CONTROLLING OFFICE NAME AND ADDRESS: Office of Naval Research, Arlington, Virginia 22217
12. REPORT DATE: March 1978
13. NUMBER OF PAGES: 27 (12 29p.)

14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)
15. SECURITY CLASS. (of this report): UNCLASSIFIED
15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

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19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Ionization
Electron
Distorted wave

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Electron impact ionization cross sections are calculated in the distorted wave approximation. Preliminary results are given for the ground state ionization cross section for H, He^+, and Mg^+ as well as for the 2s excited level for H and are compared with the corresponding calculations using the Born approximation. In the case of H, individual and total angular momenta contributions to the partial collision strength are presented.

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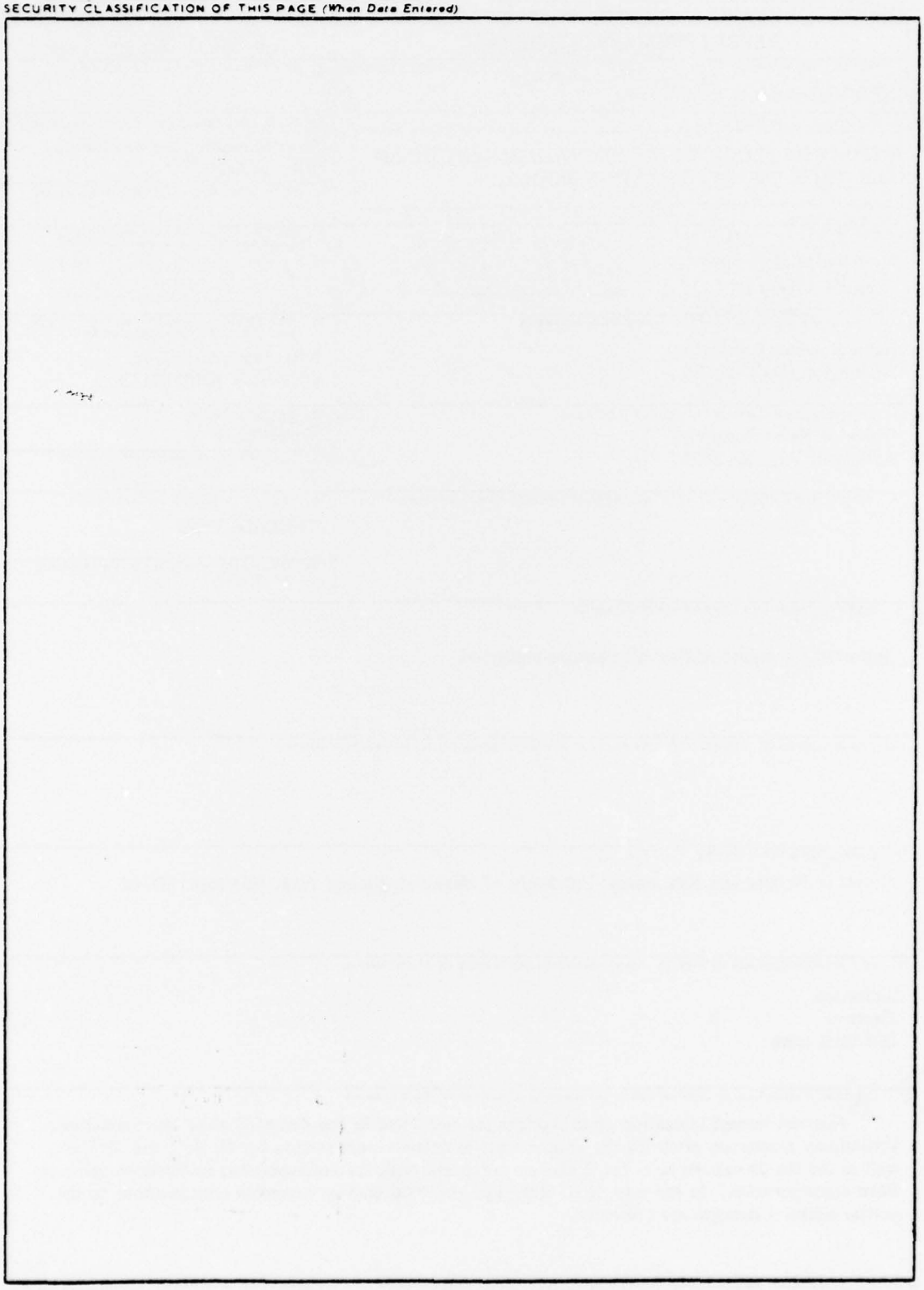

CONTENTS

REPORT OF PROGRESS IN THE DEVELOPMENT OF AN ELECTRON IMPACT IONIZATION MODEL

I. Introduction

The radiative emissions from high temperature laboratory and solar plasmas contain a potential wealth of information about its chemical composition, temperature and density structure, and radiative cooling rate. However, before any reliable quantitative information can be deduced from the plasmas' spectral emission features, some knowledge must be available on the fundamental processes leading to the spectrum formation. In principle this involves the construction of a plasma model that includes all the relevant and competing physical processes necessary to describe the dynamic evolution of the spectral emission features. Prominent among these processes is electron impact ionization and its inverse process, three-body recombination.

The theoretical study of electron impact ionization of atoms and ions has been under intensive investigation for a period of years. However, only in recent years has substantial progress been achieved with the aid of large computers. Nevertheless, the majority of calculations employ either the Born approximation or some variation thereof and a variety of semi-classical and empirical methods. It is well known that outside the threshold region the accuracy and validity of the Born approximation becomes better the higher the incident energy. Unfortunately, the magnitude of the ionization rate is often dominated by the threshold region. Hence, the development of semi-classical and empirical methods to attempt to characterize the threshold region. Of the many methods available the Exchange Classical Impact Parameter (ECIP) method

Note: Manuscript submitted February 10, 1978.

has met with some success, but it is not yet fully understood why. For charge states greater than about 25 Lotz's empirical results are often applied.

The purpose of this report is to summarize our progress to date on the development of an electron impact ionization formalism and computer code. The collision process is treated quantum mechanically using the method of distorted waves. The results of some benchmark calculations with hydrogen will be presented.

II. Outline of the General Theory of Electron Impact Ionization of Atoms

We shall consider the ionization of an atom or ion with n equivalent electrons and we shall assume that the conditions of the LS coupling are satisfied for all atomic electrons. Atomic units ($e = m = \hbar$) will be used throughout this report.

The total cross section $Q(\ell^n SL; k_o)$ for ionization of an atom in the initial state $\ell^n SL$ by collisions with electrons having incident energy $\frac{1}{2} k_o^2$ and random spin orientation is given by

$$Q(\ell^n SL; k_o) = \sum_{S'L'} q\,(\ell^n SL; k_o \rightarrow \ell^{n-1} S'L') \text{ (in atomic units } a_o^2) , \qquad (1)$$

where q is the cross section for the ionization processes in which the final state of the ion is specified by quantum numbers S'L'. After an ionizing collision, the two free electrons have momenta $\vec{k}_1$ and $\vec{k}_2$ and because they cannot be distinguished, it is not possible to say which one is the scattered and which one is the ejected electron. Without the loss of generality we therefore adopt the convention $k_2 \leq k_1$. In analogy to the classical description of ionization, the electron having momentum k_2 will be called henceforth the "ejected" electron.

The cross section q can be written as an integral over the energy of the ejected electrons[1],

$$q(\ell^n SL; k_o \to \ell^{n-1} S'L') = k_o^{-1} \int_o^{E/2} k_1 k_2 \sigma(\ell^n SL; k_o \to \ell^{n-1} S'L'; k_1 k_2)\, d\,(\tfrac{1}{2} k_2^2), \quad (2)$$

where $E = \frac{1}{2} k_o^2 - E_i$, E_i being the ionization energy, and σ is given by the scattering amplitudes f describing the individual ionization processes,

$$\sigma(\ell^n SL; k_o \to \ell^{n-1} S'L'; k_1 k_2) = [8\pi(2S+1)\,(2L+1)]^{-1} \sum_{\substack{M_S M_L \mu_o \\ M_S' M_L' \mu_1 \mu_2}}$$

$$\int \left| f(\ell^n SL M_S M_L \mu_o; \vec{k}_o \to \ell^{n-1} S'L' M_S' M_L' \mu_1 \mu_2; \vec{k}_1 \vec{k}_2) \right|^2 d\hat{k}_o\, d\hat{k}_1\, d\hat{k}_2. \quad (3)$$

In (3), $\hat{k}_o$, $\hat{k}_1$ and $\hat{k}_2$ are unit vectors in the direction of $\vec{k}_o$, $\vec{k}_1$, $\vec{k}_2$ and μ_o, μ_1, μ_2 specify the spin orientations of the free electrons before and after the collision. $|f|^2$ is integrated over all orientations of $\vec{k}_1$, $\vec{k}_2$, summed over all final states characterized by M_S' M_L' $\mu_1\mu_2$ and averaged over all directions of incident electrons and all initial states $M_S M_L \mu_o$.

The scattering amplitudes f are defined by the asymptotic form of the total wave function $\underline{\Psi}$ describing the scattering of electrons with incident energy $\frac{1}{2} k_o^2$. The asymptotic form of $\underline{\Psi}$ for the case of two electrons in the field of an ion was derived by Peterkop[2,3] and by Rudge and Seaton[4]. The knowledge of the correct form of $\underline{\Psi}$ in the

asymptotic region permits us to write an explicit expression for the scattering amplitude as an integral[1]

$$f(\ell^n SLM_S M_L \mu_o;\ \vec{k}_o \to \ell^{n-1} S'L'M_S'M_L'\mu_1\mu_2;\ \vec{k}_1\vec{k}_2)$$

$$= -(2\pi)^{-\frac{5}{2}}\, e^{i\Delta(\vec{k}_1\vec{k}_2)}\, n^{\frac{1}{2}} \int \underline{\Psi}\,(\vec{x}_2 \text{----} \vec{x}_{n+1};\ \vec{x}_1)[H(1,2) + E' - E]$$

$$X[\Psi^*(\ell^{n-1} S'L'M_S'M_L';\ \vec{x}_3 \text{----} \vec{x}_{n+1})\{\gamma(\mu_1;\ \sigma_1)\ \chi_1\ (Z_1\vec{-k}_1;\ \vec{r}_1) \qquad (4)$$

$$X\gamma(\mu_2;\ \sigma_2)\ \chi_2\ (Z_2\vec{-k}_2;\ \vec{r}_2) - \gamma(\mu_1;\ \sigma_2)\ \chi_1\ (Z_1\vec{-k}_1;\ \vec{r}_2)\ \gamma\ (\mu_2;\ \sigma_1)$$

$$X\ \chi_2(Z_2\vec{-k}_2;\ \vec{r}_1)\}]\ d\vec{x}_1 \text{----}\ d\vec{x}_{n+1}\ .$$

H(1,2) is the hamiltonian of electrons labeled 1,2, E' the energy of the final state of the ion, E the total (positive) energy of the system and $\vec{x}_i$ represents spatial and spin coordinates of the i-th electron. $\underline{\Psi}\,(\vec{x}_2 \ldots\ldots \vec{x}_{n+1};\ \vec{x}_1)$ is the exact solution of the Schrödinger equation

$$H\underline{\Psi} = E\underline{\Psi} \qquad (5)$$

and it is normalized so that for $r_1 \to \infty$ it has the form

$$\underline{\Psi} \sim \Psi\,(\ell^n SLM_S M_L;\ \vec{x}_2 \text{----} \vec{x}_{n+1})\ \gamma\ (\mu_1;\sigma_1)\ [1+Z^2\{ik_o^2(k_o r_1 - \vec{k}_o\vec{r}_1)\}^{-1}] \qquad (6)$$

$$x\ \exp\ [i\vec{k}_o\vec{r}_1 - i\ (Z/k_o)\ \log\ (k_o r_1 - \vec{k}_o\vec{r}_1)]$$

$$+ \text{scattered waves}$$

for collisions with atoms or ions with asymptotic charge Z(Z=0 for neutral atoms). $\underline{\Psi}$ is antisymmetric with respect to $\vec{x}_2$ .... $\vec{x}_{n+1}$ only. $\gamma(\mu_i;\sigma_k)$ in (4), (5) and (6) is a spin function representing spin orientation μ_i and σ_k is the spin coordinate of the k-th electron. Ψ is the antisymmetric function of the atom before or after the ionizing collision.

The functions $\chi_j(Z_j\text{-}\vec{k}_j;\vec{r})$ satisfy equations of the form

$$[\nabla^2 + k_j^2 + 2Z_j\, r^{-1} + 2\, V_j(r)]\, \chi_j(Z_j\text{-}\vec{k}_j;\, \vec{r}) = 0, \tag{7}$$

where $V_j(r)$ may be any short-range potentials. At large r,

$$\chi_j(Z_j\text{-}\vec{k}_j;\vec{r}) \sim [1+Z_j^2\{ik_j^2(k_jr+\vec{k}_j\vec{r})\}^{-1}]\, \exp\, [-i\vec{k}_j\vec{r}\text{-}i(Z_j/k_j)\, \log\, (k_jr+\vec{k}_j\vec{r})] \tag{8}$$

$$+ \text{----} \ .$$

The charges Z_1 and Z_2 in (4), (7) and (8) are related to the phase factor $\exp\, [i\Delta(\vec{k}_1\vec{k}_2)]$ in (4) which is divergent unless Z_1, Z_2, $\vec{k}_1$ and $\vec{k}_2$ satisfy the equation

$$\frac{Z_1}{k_1} + \frac{Z_2}{k_2} = \frac{Z+1}{k_1} + \frac{Z+1}{k_2} - \frac{1}{|\vec{k}_1\text{-}\vec{k}_2|} \ . \tag{9}$$

In (4) we have omitted the term representing "classical exchange", i.e. a capture of the colliding electron and a subsequent ejection of two atomic electrons. This process has been described in Ref. 1.

Eq. (4) is the basis for the calculation of scattering amplitudes f. Cross sections can be obtained using relations (1), (2) and (3). However,

the exact solution of the Schrödinger equation (5) is unknown, and therefore $\underline{\Psi}$ has to be replaced by an approximate function. This procedure leads to various approximations. Furthermore, if $\underline{\Psi}$ is not the exact solution, f becomes dependent on the choice of potentials V_1 and V_2 in (7). In actual calculation it is difficult to satisfy eq. (9) for effective charges Z_1 and Z_2 which depend on relative directions of $\vec{k}_1$ and $\vec{k}_2$. If the requirement (9) is not satisfied, the phase factor $\exp\left[i\Delta(\vec{k}_1\vec{k}_2)\right]$ is essentially undefined and then there exists an arbitrariness in the relative phase assigned to the two terms in {---} in eq. (4), the first giving the direct part, the second the exchange part of the scattering amplitude.

III. Partial Wave Theory and Approximations

For numerical calculations it is convenient to expand the function $\chi_j(Z_j,-\vec{k}_j;\vec{r})$ into partial waves using the relation[5]

$$\chi_j(Z_j,-\vec{k}_j;\vec{r}) = 4\pi\,(k_j)^{-\frac{1}{2}}\,r^{-1}\sum_{\ell=0}^{\infty} i^{\ell}\exp\left[i(\eta_\ell+\delta_\ell)\right]F_{k_j\ell}(r) \tag{10}$$

$$\times\sum_{m=-\ell}^{+\ell} Y_{\ell m}(-\hat{k}_j)\;Y^{*}_{\ell m}(\hat{r})\,,$$

where $Y_{\ell m}$ are spherical harmonics defined by directions of $-\hat{k}_j$ and $\hat{r}$, respectively, η_ℓ is the Coulomb phase $\eta_\ell = \arg\Gamma(\ell+1-iZ_j/k_j)$ and $F_{k_j\ell}$ is the solution of the equation

$$\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + \frac{2Z_j}{r} + 2V_j(r) + k_j^2\right] F_{k_j\ell}(r) = 0 \qquad (11)$$

with the asymptotic form

$$F_{k_j\ell} \sim k_j^{-\frac{1}{2}} \sin\left[k_j r - \tfrac{1}{2}\pi\ell + (Z_j/k_j)\log(2k_j r) + \eta_\ell + \delta_\ell\right]. \qquad (12)$$

δ_ℓ is the phase shift depending on $V_j(r)$ and $\delta_\ell = 0$ if $V_j \equiv 0$.

We adopt the following approximations:

(a) The wave function $\underline{\Psi}$ of the total system appearing in (4) is replaced by

$$\Psi(\ell^n SLM_S M_L;\ \vec{x}_2 \text{----} \vec{x}_{n+1})\ \gamma\ (\mu_o;\sigma_1)\ \chi_o\ (Z\vec{k}_o;\vec{r}_1)\ , \qquad (13)$$

where $\chi_o(Z\vec{k}_o;\vec{r}_1)$ is defined similarly to (7) and (8), and Z is the asymptotic charge of the atom or ion before the collision. We assume that the radial functions of atomic electrons remain unchanged by the ionizing collision. The potential $V_o(r)$ in equation (7) for $\chi_o(Z\vec{k}_o;\vec{r}_1)$ represents the modification of the Coulomb potential Z/r near the nucleus and in our approximation it is given by

$$V_o(r) = nr^{-1} - n\,Q(r) \qquad (14)$$

$$\text{with } Q(r) = r^{-1}\int_o^r P_\ell^2\ dr + \int_r^\infty r^{-1}\,P_\ell^2\ dr, \qquad (15)$$

where n is the number of atomic electrons before the ionizing collision and $P_\ell(r)$ is the radial function of atomic electrons.

(b) We will assume that charges Z_2 and Z_1, which determine the asymptotic forms of the wave functions χ_2 and χ_1 of the ejected and scattered electrons, are not dependent on the direction of $\vec{k}_1$ and $\vec{k}_2$. This assumption substantially simplifies the evaluation of the cross sections, but it is in violation of requirement (9). In the majority of calculations on ionizing collisions it has often been assumed that $Z_1 = Z$ and $Z_2 = Z + 1$. We intend to study the effect of different choices of Z_1 and Z_2 including non-integer values of these charges. The short-range potentials V_1 and V_2 in (7) may be arbitrary and the result will depend on their form. One of many possibilities is to set

$$V_j = (n-\mathcal{E}_j) \left[r^{-1} - Q(r)\right] \tag{16}$$

with Q(r) defined by (15). $\mathcal{E}_j$ is such that

$$Z_j = Z + \mathcal{E}_j \tag{17}$$

and $0 \leq \mathcal{E}_j \leq 1$. This particular choice of V_1 and V_2 would make our approximation similar to the distorted-wave method in the calculation of collisional excitations. Born and Coulomb-Born approximations would be obtained if we put $V_o(r) = V_1(r) = V_2(r) = 0$, $Z_1 = Z$, $Z_2 = Z + 1$.

(c) We omit exchange contributions to the scattering amplitude, i.e. we ignore the second term in {---} in eq. (4). Effects of exchange will be studied later. In a non-exchange approximation the value of the phase factor $\exp[i\Delta(\vec{k}_1\vec{k}_2)]$ is irrelevant.

With the assumptions (a), (b) and (c), the calculation of the ionization cross sections is considerably simplified and the problem is in many respects analogous to collisional excitation.

The function $\chi_o(Z\vec{k}_o;\vec{r}_1)$ may also be expanded into partial waves according to (10), where for convenience we write $Y^*_{\ell_o m_o}(\hat{k}_o)\, Y_{\ell_o m_o}(\hat{r}_1)$ instead of $Y_{\ell_o m_o}(\hat{k}_o)\, Y^*_{\ell_o m_o}(\hat{r}_1)$.

Using the notation

$$\varphi_j(\ell_j m_j \mu_j k_j;\vec{x}_i) \equiv \gamma(\mu_j;\sigma_i)\, r_i^{-1} F_{k_j \ell_j}(r_i)\, Y_{\ell_j m_j}(\hat{r}_i) \tag{18}$$

for a one-electron wave function with spin μ_j, the expression (4) for the scattering amplitude takes the form

$$f\left(\ell^n SLM_S M_L \mu_o;\ \vec{k}_o \rightarrow\ \ell^{n-1} S'L'M_S'M_L'\ \ \mu_1\mu_2;\ \vec{k}_1\ \vec{k}_2\right)$$

$$= -(2\pi)^{-5/2} \exp\left[i\Delta(\vec{k}_1\vec{k}_2)\right] n^{1/2}\ (4\pi)^3\ (k_o k_1 k_2)^{-1/2}$$

$$\times \sum_{\ell_o \ell_1 \ell_2} i^{\ell_o+\ell_1+\ell_2} \exp\left[i(\eta_{\ell_o}+\eta_{\ell_1}+\eta_{\ell_2}+\delta_{\ell_o}+\delta_{\ell_1}+\delta_{\ell_2})\right] \sum_{m_o m_1 m_2} Y^*_{\ell_o m_o}(\hat{k}_o) \tag{19}$$

$$\times Y_{\ell_1 m_1}(-\hat{k}_1) Y_{\ell_2 m_2}(-\hat{k}_2) \int \Psi(\ell^n SLM_S M_L;\vec{x}_2 \text{----} \vec{x}_{n+1})\ \varphi_o(\ell_o m_o \mu_o k_o;\vec{x}_1)$$

$$\times [H(1,2)+E'-E]\ \Psi^*(\ell^{n-1} S'L'M_S'M_L';\ \vec{x}_3 \text{----} \vec{x}_{n+1})\ \varphi_1^*(\ell_1 m_1 \mu_1 k_1;\ \vec{x}_1)$$

$$\times \varphi_2^*(\ell_2 m_2 \mu_2 k_2;\ \vec{x}_2)\ \ d\vec{x}_1 \text{----} d\vec{x}_{n+1}\ .$$

With the functions $F_{k\ell}$ satisfying (11) and with $E' - E = -\frac{1}{2}k_1^2 - \frac{1}{2}k_2^2$, $H(1,2) + E' - E$ in (19) may be replaced by

$$(Z_1\text{-}Z\text{-}n)\ r_1^{-1} + (Z_2\text{-}Z\text{-}n)\ r_2^{-1} + V_1(r_1) + V_2(r_2) + r_{12}^{-1} \qquad (20)$$

where r_{12} is the interelectronic distance.

If φ_o is orthogonal to φ_1 and if the wave functions of bound electrons are orthogonal to φ_2, which is always satisfied for $\ell_o \neq \ell_1$ and $\ell \neq \ell_2$, the first four terms in (20) give no contributions to the integral in (19) and can be omitted. If $\ell = \ell_2$, the orthogonality of P_ℓ and $F_{k_2\ell}$ can be achieved by various methods, e.g. by redefining the potential V_2 in (11) or by replacing $F_{k_2\ell}$ by $F_{k_2\ell} - P_\ell \int F_{k_2\ell}\, P_\ell\, dr$, or by solving eq. (11) with the right-hand side replaced by $\lambda\, P_\ell$, where λ is to be adjusted so that $\int P_\ell\, F_{k_2\ell} dr = 0$. In the case of $\ell_1 = \ell_o$ we can use similar methods, or we can put $Z_1 = Z$ and $V_1(r) = V_o(r)$ in (7) and (11). Then φ_o and φ_1 will be orthogonal because $k_o \neq k_1$. In the following we shall assume that the orthogonality properties are always satisfied and that (20) may be replaced by r_{12}^{-1}.

The one-electron functions defined by (18) represent states of definite orbital and spin angular momentum. Using vector-coupling coefficients we therefore define

$$\Psi[(\ell^n SL)\ell_o;\ S^T L^T M_S^T M_L^T;\ k_o;\ \vec{x}_2 \ldots \vec{x}_{n+1};\ \vec{x}_1] \qquad (21)$$

$$= \sum_{M_S \mu_o M_L m_o} C^{S\ \frac{1}{2}\ S^T}_{M_S \mu_o M_S^T}\, C^{L\ \ell_o\ L^T}_{M_L m_o M_L^T}\ \Psi(\ell^n SLM_S M_L; \vec{x}_2 \ldots \vec{x}_{n+1})\, \varphi(\ell_o m_o \mu_o k_o; \vec{x}_1).$$

$S^T L^T M_S^T M_L^T$ specify spin and angular momenta of the total system. It follows that

$$\Psi(\ell^n SLM_S M_L; \vec{x}_2 \cdots \vec{x}_{n+1}) \varphi(\ell_o m_o \mu_o k_o; x_1) = \sum_{M_S^T M_L^T} C^{S\ \frac{1}{2}\ S^T}_{M_S \mu_o M_S^T} C^{L\ \ell_o\ L^T}_{M_L m_o M_L^T}$$

(22)

$$\times \Psi[(\ell^n SL)\ell_o;\ S^T L^T M_S^T M_L^T;\ k_o;\ \vec{x}_1 \cdots \vec{x}_{n+1};\ \vec{x}_1].$$

Similarly to (22) we can write in (19) the product $\Psi(\ell^{n-1} S'L'M_S'M_L'; \vec{x}_3 \cdots \vec{x}_{n+1})\ \varphi_2(\ell_2 m_2 \mu_2 k_2; \vec{x}_2)$ in terms of $\Psi[(\ell^{n-1} S'L')\ \ell_2;\ S^F L^F M_S^F M_L^F;\ k_2;\ \vec{x}_3 \cdots \vec{x}_{n+1};\ \vec{x}_2]$, where $S^F L^F M_S^F M_L^F$ characterize the final state of the ion + ejected electron, and then the product $\Psi[(\ell^{n-1} S'L')\ell_2;\ S^F L^F M_S^F M_L^F;\ k_2;\ \vec{x}_3 \cdots \vec{x}_{n+1};\ \vec{x}_2]\ \varphi_1(\ell_1 m_1 \mu_1 k_1;\ \vec{x}_1)$ in terms of

$$\Psi[\{(\ell^{n-1} S'L')\ \ell_2;\ S^F L^F\}\ell_1;\ S^T L^T M_S^T M_L^T;\ k_2 k_1;\ \vec{x}_3 \cdots \vec{x}_{n+1};\ \vec{x}_2;\ \vec{x}_1]. \qquad (23)$$

The integral in (19) can be expanded in a series of terms and only those terms for which the quantum numbers $S^T L^T M_S^T M_L^T$ defined by (21) and (22) are identical to $S^T L^T M_S^T M_L^T$ specified by (23) will give non-vanishing contributions.

We also make use of the expansion for the inverse interelectronic distance,

$$r_{12}^{-1} = 4\pi \sum_{\lambda\mu} (2\lambda + 1)^{-1}\ \frac{r_<^{\lambda}}{r_>^{\lambda+1}}\ Y_{\lambda\mu}(\hat{r}_1)\ Y^*_{\lambda\mu}(\hat{r}_2) \qquad (24)$$

and substitute f from (19) with all changes into (3). The integration over $\hat{k}_o$, $\hat{k}_1$, and $\hat{k}_2$ can be easily performed using orthogonal properties of spherical harmonics and the summation over angular momenta and their

components as well as spin orientations can be carried out using properties of vector-coupling and Racah coefficients. Together with the summation over S'L' we obtain

$$\sum_{S'L'} \sigma\,(\ell^n SL;\ k_o \rightarrow \ell^{n-1} S'L';\ k_1 k_2) \;=\; \frac{16\,\pi\,n}{k_o\ k_1\ k_2} \tag{25}$$

$$\times \sum_{\ell_o \ell_1 \ell_2 \lambda} (2\lambda+1)^{-1}(2\ell_o+1)(2\ell_1+1)(2\ell_2+1)\begin{pmatrix} \ell_o & \ell_1 & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{pmatrix} \ell & \ell_2 & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2 R_\lambda^2(\ell\ell_o;\ell_2\ell_1)\ .$$

The radial integrals are defined by

$$R_\lambda(\ell\ell_o;\ell_2\ell_1) = \int P_\ell(r_2)\ F_{k_o\ell_o}(r_1)\ \frac{r_<^\lambda}{r_>^{\lambda+1}}\ F_{k_2\ell_2}(r_2) F_{k_1\ell_1}(r_1)\ dr_1 dr_2. \tag{26}$$

The total ionization cross sections can be calculated from (1), (2) and (25). In (25), the 3-j symbols have non-vanishing values only if triangular conditions for vectors $\ell_o\ell_1\lambda$ and $\ell\ell_2\lambda$ are satisfied. In particular that means that $\ell_2 \leqq \ell + \lambda$. The value of R_λ usually rapidly decreases with increasing λ and therefore only few low values of the angular momenta ℓ_2 of the ejected electron need to be taken into account. The situation is illustrated in the next section for the ionization of hydrogen.

The ionization of a complex atom with n equivalent electrons in the outer shell can be treated similarly, if we redefine the potentials $V_j(r)$ in (7), (11), (14) and (16) by adding contributions arising from additional nuclear charge and screening of inner electrons.

IV. Results of Preliminary Calculations

In our preliminary calculations we have computed ionization cross sections for H, He, He^+ and Mg^+ in a distorted-wave approximation in order to compare the results with other methods.

We have put $Z_1 = Z$, i.e. the asymptotic charge Z_1 for the scattered electron equal to the charge seen by the incoming electron, and also $V_o(r) = V_1(r)$ and V_o defined by (14), so that the orthogonality of φ_o and φ_1 in (19) is satisfied. The asymptotic charge Z_2 acting on the ejected electron was taken to be equal to $Z + 1$ and $V_2(r)$ given by (16) with $\mathcal{E}_2 = 1$. The orthogonality of P_ℓ and $F_{k_2\ell}$ was achieved by solving eq. (11) with the right-hand side replaced by λP_ℓ and with λ appropriately adjusted.

The results of the present calculations are compared with other methods and with experimental values on Fig. 1 - 5. (Crosses represent results of the present DW calculations. E_0 = energy of the incident electrons, E_i = ionization energy). Our distorted-wave method is very close to the Born (b) approximation[1]. In fact, the two methods differ for ionization of neutral atoms just by the form of functions $F_{k\ell}$ which are solutions of eq. (11). In the Born (b) and the DW approximations the upper limit of integration according to (2) is E/2, while in the Born (a) method the limit is E and therefore this approximation always gives higher results for cross sections. Near threshold, however, the DW results are higher than the Born (b) values (Figs. 1 and 4), probably because of the focusing effect of the short-range nuclear potential.

It is not clear why there is a discrepancy between the DW approximation and the Coulomb-Born method for Mg^+ (Fig. 5). The CB calculation[10]

is based on atomic wave functions generated in a scaled Thomas-Fermi potential. Moreover, contributions from excitations to autoionizing levels were also taken into account. In our DW calculations, Hartree-Fock orbitals of all atomic electrons were employed.

In almost all cases where a comparison with experimental results is possible, theoretical ionization cross sections are larger than the measured values.[1] With respect to many simplifying assumptions made during the calculations, it is not obvious what is the main cause of the discrepancy. One possible reason may be the incorrect choice of asymptotic charges Z_1 and Z_2 (see below).

For the ionization of hydrogen, the total cross section Q may be written as

$$Q(1s,k_o) = \frac{\pi}{k_o^2} \int_o^{E/2} \sum_{\ell_o \ell_2} \Omega_{\ell_o} (1sk_o \rightarrow \ell_2 k_2)\, d\,(\tfrac{1}{2} k_2^2), \qquad (27)$$

where $\Omega_{\ell_o} (1sk_o \rightarrow \ell_2 k_2)$ is the partial collision strength corresponding to incoming electrons with angular momentum ℓ_o and to ejected electrons with ℓ_2 and momentum k_2.

In Table 1, the importance of individual partial contributions is shown for $E_o/E_i = 4$ and $k_2 = 0$. The largest contribution comes from $\ell_2 = 1$, i.e. from the dipole transition s → p, and contributions from higher ℓ_2 rapidly decrease.

Table 2 presents the dependence of $\Omega (1sk_o \rightarrow \ell_2 k_2) = \sum_{\ell_o} \Omega_{\ell_o} (1sk_o \rightarrow \ell_2 k_2)$ on the energy of the ejected electron $\frac{1}{2} k_2^2$. For low values of ℓ_2, this quantity decreases with k_2 indicating that the most important region for the calculation of cross sections corresponds to low energies of the ejected electrons.

The effect of the choice of the asymptotic charge Z_2 acting on the ejected electron is demonstrated in Table 3 for ionization of hydrogen. The calculation has been made for $E_o/E_i = 4$ and with $Z = Z_1 = 0$. The Table shows that a slight increase of Z_2 leads to a substantial improvement of the result in comparison with experiment. However, at the present time it is not clear why a specific choice of Z_2 should be preferable from the theoretical point of view.

V. Summary

A distorted wave treatment has been developed to describe the electron impact ionization on atoms and ions. Preliminary calculations were carried out for the ground state ionization cross sections of H, He^+, He, and Mg^+ as well as the 2s excited level of H and are found to be in a good agreement with the Born (b) approximation[1] except at the threshold region where the DW method yields higher values. In the case of H, individual and total angular momenta contributions to the partial collision strength are presented. In terms of the individual angular momentum contributions, at threshold for the ejected electron, the dipole contribution to the partial collision strength is generally the largest, but not always as evidenced by the combination of (ℓ_o, ℓ_2), (0,1) and (1,0). As the ejected electron energy is increased the dipole partial collision strength remains the dominant term but steadily decreases in value.

ACKNOWLEDGMENT

This work was supported by the Office of Naval Research. One of us (M.B.) would like to acknowledge a partial support from NASA.

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Table 1

PARTIAL COLLISION STRENGTH $\Omega_{\ell_o}(1sk_o \rightarrow \ell_2 k_2)$

FOR IONIZATION OF HYDROGEN. $\frac{1}{2}k_o^2 = 4$ ryd, $k_2 = 0$.

(Numbers in parentheses are decadic exponents)

	ℓ_2				
ℓ_o	0	1	2	3	4
0	3.75(-1)	2.03(-1)	5.68(-3)	3.47(-4)	1.21(-6)
1	7.74(-1)	2.13(-1)	3.54(-2)	8.43(-4)	7.89(-6)
2	4.36(-1)	1.33	5.76(-2)	2.12(-3)	9.86(-6)
3	1.62(-1)	2.01	5.46(-2)	3.94(-3)	1.30(-5)
4	4.47(-2)	2.09	1.12(-1)	4.44(-3)	2.60(-5)
5	8.71(-3)	1.82	1.73(-1)	4.00(-3)	7.83(-5)
6	8.99(-4)	1.44	2.09(-1)	4.16(-3)	1.10(-4)
7	7.49(-7)	1.08	2.14(-1)	4.93(-3)	1.16(-4)
8		7.89(-1)	1.96(-1)	5.83(-3)	1.10(-4)
9		5.68(-1)	1.65(-1)	6.39(-3)	1.02(-4)
10		4.09(-1)	1.32(-1)	6.92(-3)	9.88(-5)

Table 2

PARTIAL COLLISION STRENGTHS $\Omega(1sk_o \rightarrow \ell_2 k_2)$ FOR IONIZATION OF HYDROGEN AS FUNCTION OF $\frac{1}{2} k_2^2$

(ENERGY OF THE EJECTED ELECTRON($\frac{1}{2} k_o^2 = 4$ ryd)

			ℓ_2		
$\frac{1}{2} k_2^2$ (ryd.)	0	1	2	3	4
0.0	1.80	13.01	1.88	0.055	0.0007
0.5	0.69	3.57	1.22	0.26	0.026
1.0	0.35	1.44	0.69	0.24	0.055
1.5	0.20	0.70	0.40	0.18	0.063

Table 3

DEPENDENCE OF THE IONIZATION CROSS SECTION FOR HYDROGEN ON THE ASYMPTOTIC CHARGE Z_2 (FOR THE EJECTED ELECTRON). $E_o/E_i = 4$.

Z_2	$Q\ (\pi a_o^2)$
0.4	1.34
0.6	1.36
0.8	1.21
1.0	1.01
1.2	0.80
1.4	0.62
1.6	0.48
Experiment[7]	0.69

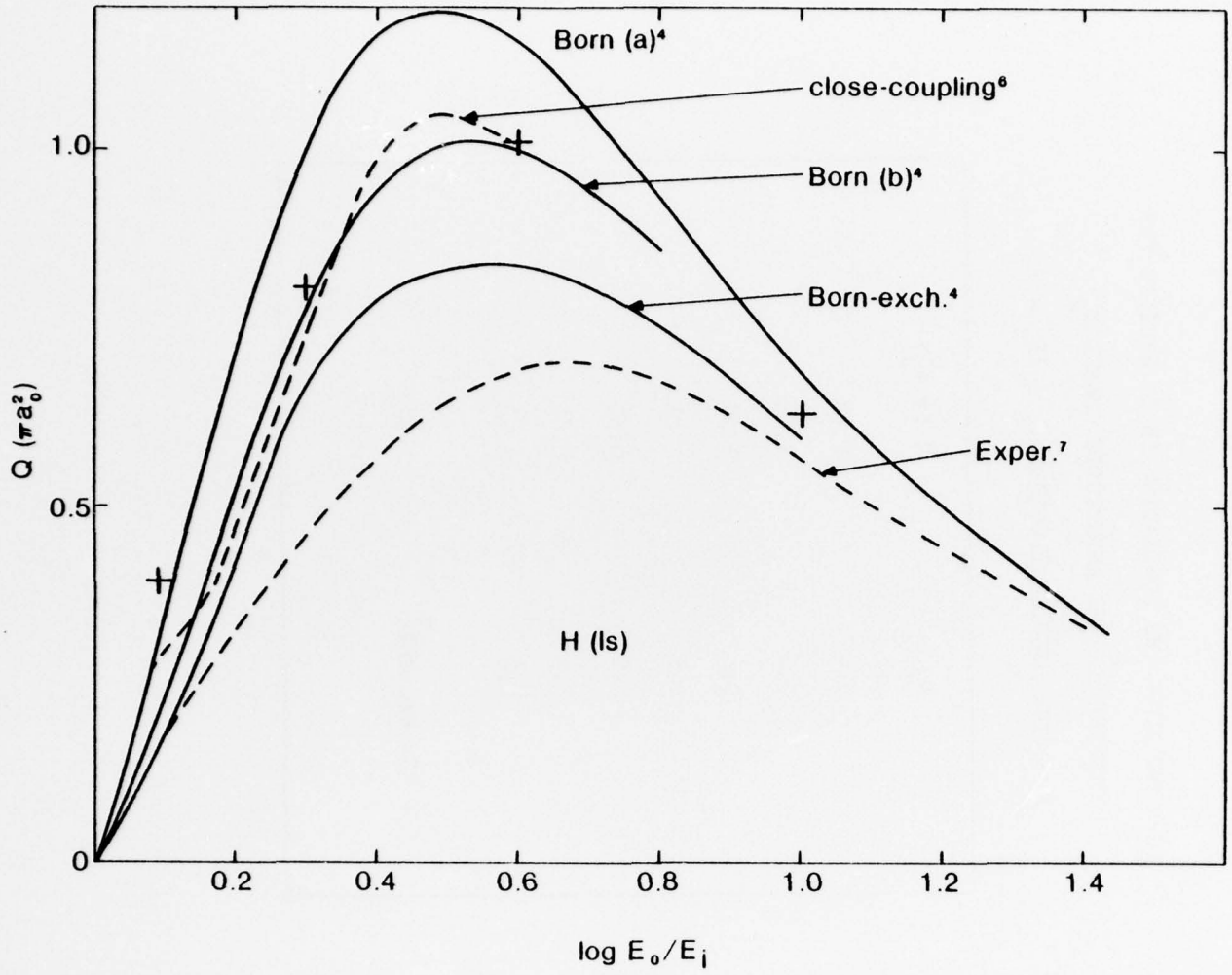
Born (a)[4]
close-coupling[6]
Born (b)[4]
Born-exch.[4]
Exper.[7]
H (ls)
Q (πa₀²)
1.0
0.5
0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
log E₀/Eᵢ

Figure 1

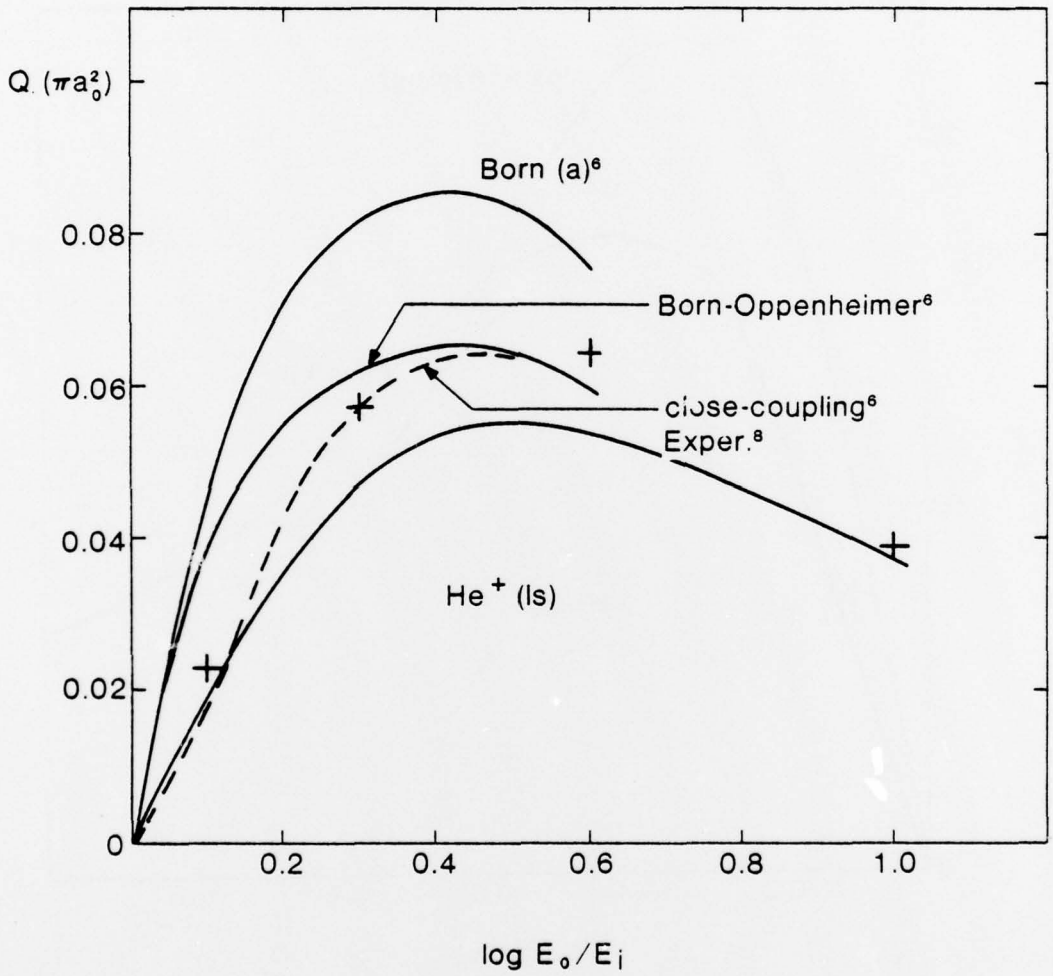
Q (πa_0^2)
Born (a)[6]
0.08
Born-Oppenheimer[6]
0.06
close-coupling[6]
Exper.[8]
0.04
He$^+$ (1s)
0.02
0
0.2
0.4
0.6
0.8
1.0
log E_o/E_i

Figure 2

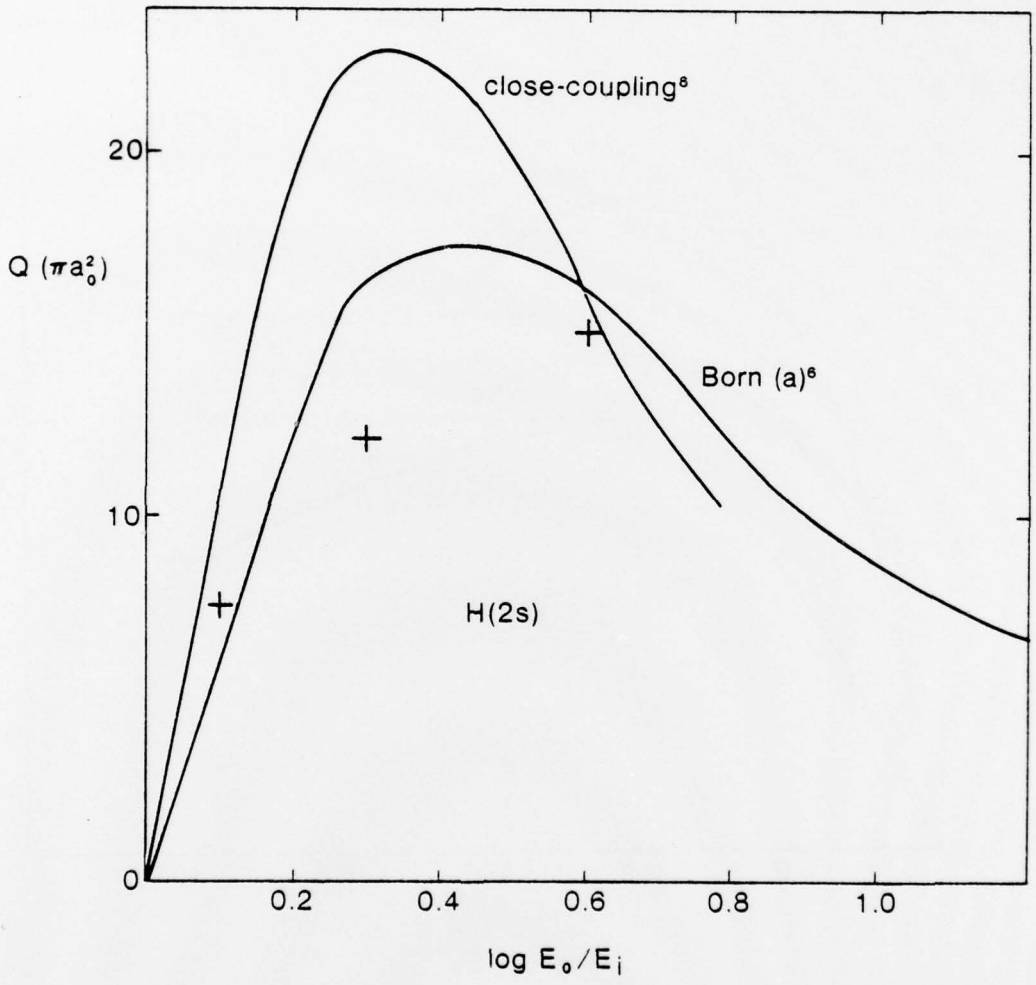
close-coupling[6]
Born (a)[6]
H(2s)
Q (πa_0^2)
20
10
0
0.2
0.4
0.6
0.8
1.0
log E_0/E_i

Figure 3

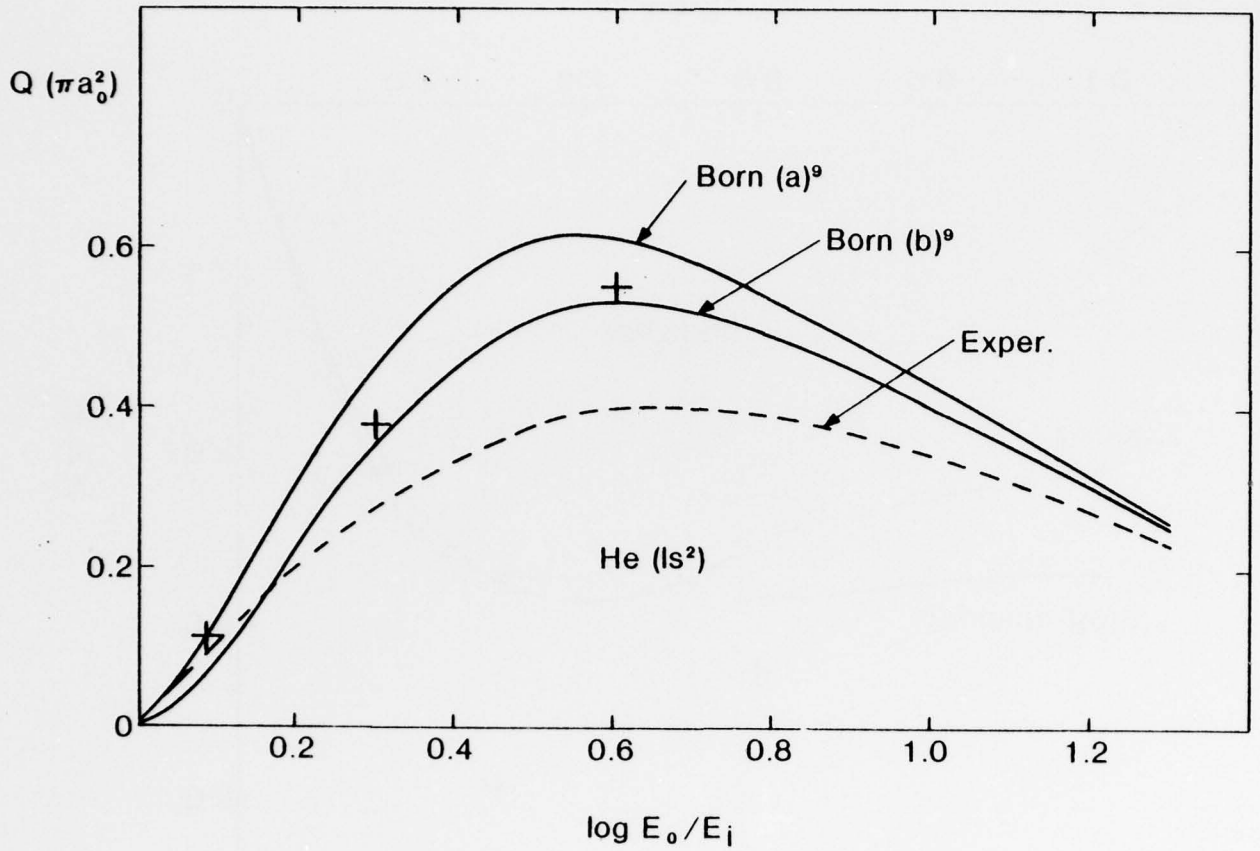
Q (πa_0^2)
Born (a)[9]
Born (b)[9]
Exper.
He ($1s^2$)
0
0.2
0.4
0.6
0.2
0.4
0.6
0.8
1.0
1.2
log E_o/E_i

Figure 4

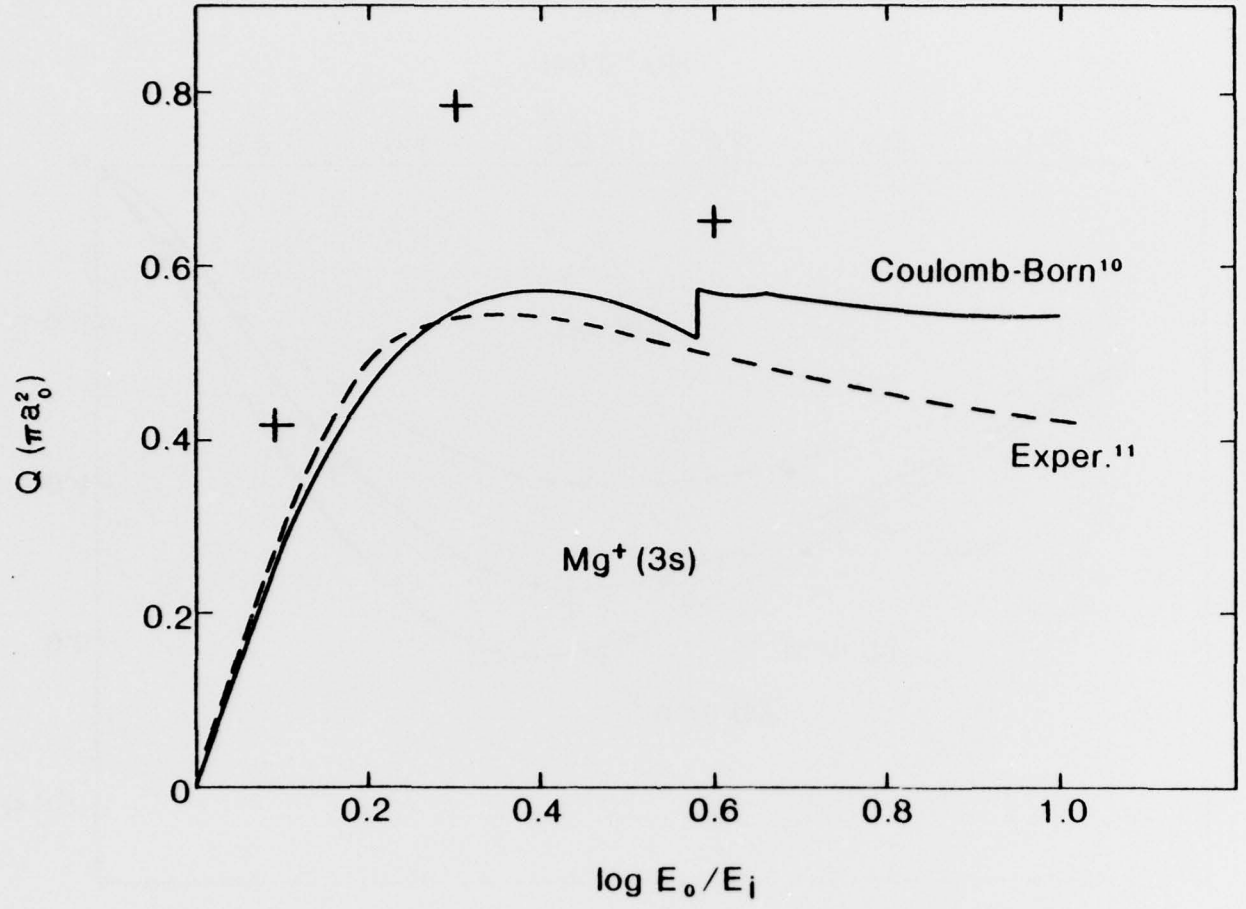
0.8
0.6
0.4
0.2
0
0.2
0.4
0.6
0.8
1.0
Q (πa_0^2)
log E_0/E_i
Coulomb-Born[10]
Exper.[11]
Mg^+ (3s)

Figure 5