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Proton-induced fine-structure transitions in O IV

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Proton-impact excitation of fine-structure transitions in $O^{3+}\,{}^2P^0$ ions is studied in a quasimolecular representation. The ${}^2\Pi$ and ${}^2\Sigma^+$ states of the OH^{4+} molecule formed by the approach of H^+ and $O^{3+}\,{}^2P^0$ are represented with self-consistent-field wave functions which include the effects of polarization. Accurate, close-coupled solutions of the nuclear scattering equations are obtained and used to assess the accuracy of some approximate scattering descriptions. The elastic approximation is found to overestimate the cross sections at all energies. The Coulomb-Born approximation is accurate at both high and low energies but greatly overestimates the cross sections at intermediate energies. A simple unitarity correction to the Coulomb-Born approximation reduces the errors substantially. For high partial waves, the Coulomb-Born approximation is satisfactory at all energies and cross sections for fine-structure excitation by proton impact can be calculated accurately and efficiently with the use of a combination of close-coupled and Coulomb-Born results. Cross sections accurate to within 25% can be obtained with very little computational effort by a combination of the elastic and Coulomb-Born approximations.

I. INTRODUCTION

Parameters characterizing the internal structure of plasmas can be inferred from observations of emission lines. Seaton[1] pointed out that forbidden ${}^2P_{3/2}$-${}^2P_{1/2}$ emission lines in the solar corona are excited directly by proton and electron impacts and indirectly by collisional excitation to higher levels followed by cascading. Rate coefficients for the processes are required to interpret the observed line intensities and to derive the characteristics of the physical environment. Essential features of a reliable theoretical description of the collision processes include a proper representation of the interaction and an accurate solution of the scattering equations.

Following Seaton's analysis, most studies of fine-structure excitation by proton impact have utilized semiclassical Coulomb excitation theory.[2] Landman[3] and Landman and Brown[4] used it to calculate cross sections for a number of cases of astrophysical interest. Bahcall and Wolf[5] used direct integration of the semiclassical impact-parameter equations for low-energy collisions. Bely and Faucher[6] adopted a simplified version to calculate reaction rates for the $O^{3+}\,{}^2P_{1/2}$-${}^2P_{3/2}$ transition considered here and Faucher[7] extended the calculations to include transitions in Ca^{14+}, Fe^{20+}, and Ni^{14+}.

In all these studies, transitions were assumed to be induced by the Coulomb interaction of the proton with the permanent quadrupole moment of the target ion. This approximation is inadequate for high-energy penetrating collisions where it leads to cross sections that decrease with energy E as $E^{-1/2}$ instead of the correct E^{-1}. Reid and Schwarz,[8] Masnou-Seeuws and McCarroll,[9] Faucher and Landman,[10] and Doyle, Kingston, and Reid[11] cut off the quadrupole interaction at small internuclear separations to avoid its divergence at the origin. The impact-parameter studies indicated that, because of the Coulomb repulsion, the cross sections are insensitive to the cutoff procedure except at high energies. At high energies coupling to higher states is likely to be important also.

More approximate treatments of proton-induced fine-structure transitions have been carried out by Sahal-Bréchot[12] using semiclassical perturbation theory with a cutoff quadrupole interaction and by Kastner[13] and Kastner and Bhatia[14] who developed semiempirical formulas for cross sections as functions of energy.

Fine-structure excitation through proton impact has also been treated quantum mechanically. Faucher[15] compared quantal close-coupled results with those of the Born approximation at high energies and semiclassical Coulomb excitation theory at low energies. Faucher and Landman[10] found that semiclassical impact-parameter and quantal results agreed for quadrupole-induced transitions. Mies[16] compared accurate quantal calculations with Born-approximation results for proton impacts with neutral fluorine at low energy and concluded that the Born approximation was accurate only for high-order partial waves and was inadequate for total excitation cross sections. Mies[17] represented the collisions using continuum molecular wave functions. We use a similar formulation adapted for Coulomb scattering.

Although transitions are coupled at long range by the quadrupole interaction, the Coulomb repulsion makes transition amplitudes vanishingly small at low energies. At higher energies where the transition amplitudes are not negligible, the wavelength $\lambda = 2\pi(2\mu E)^{-1/2}$ is very small and a semiclassical description of the scattering can be used. We find that a quantal scattering description can also be employed efficiently despite the difficulties of evaluating matrix elements between rapidly oscillating wave functions over extended interaction regions.

II. THEORY

Assuming *l*-*s* coupling is valid, we consider the process described by

$$A(nlsj) + \mathrm{H}^+ \rightarrow A(nlsj') + \mathrm{H}^+ , \tag{1}$$

where A is an ion or neutral atom initially in the quantum state $(nlsj)$, specified by its principal, orbital, spin, and total angular quantum numbers. If μ is the reduced mass of the nuclei, the full Hamiltonian in center-of-mass coordinates can be written

$$H = T_R + V_{\vec{s}\cdot\vec{l}} + H_{\mathrm{el}} , \tag{2}$$

where $T_R = -(\hbar^2/2\mu)\nabla_R^2$ is the nuclear kinetic energy operator, $V_{\vec{s}\cdot\vec{l}}$ is the spin-orbit interaction operator, and H_{el} is the electronic Hamiltonian. If Z_A is the nuclear charge of the N-electron ion A with electrostatic Hamiltonian H_A, transitions are induced between states of the Hamiltonian

$$H_0 = T_R + \frac{(Z_A - N)}{R} + V_{\vec{s}\cdot\vec{l}} + H_A \tag{3}$$

by proton-electron interactions given asymptotically by

$$H' \sim -\sum_{L=1}^{\infty} \frac{1}{R^{L+1}} \sum_{i=1}^{N} r_i^L P_L(\cos\theta_i) , \tag{4}$$

where the electron coordinates are $\underline{r}_i$, denoted collectively by $\underline{r}$, and θ_i is the angle between $\vec{r}_i$ and the proton-ion direction $\vec{R}$. The leading nonzero term in Eq. (4) is the proton-ionic quadrupole interaction.

For an initial quantum state α with total energy E, the scattering states describing process (1) are solutions of the Lippmann-Schwinger equation

$$\Psi^{(+)}(E,\alpha) = \Psi^{(0)}(E,\alpha) + G^{(+)}(E) H' \Psi^{(+)}(E,\alpha), \tag{5}$$

where $\Psi^{(0)}$ is a product of the target eigenfunction and a free Coulomb-state eigenfunction, satisfying

$$H_0 \Psi^{(0)} = E \Psi^{(0)}$$

and $G^{(+)}(E)$ is the Coulomb Green's function. In the close-coupled approximation, the state vectors are expanded in a truncated set of eigenstates giving rise to a coupled set of radial equations from which the transition amplitudes may be obtained. A close-coupled formulation for similar processes involving neutral particle collisions has been given in terms of laboratory-fixed coordinates by Reid and Dalgarno.[18]

If the total angular momentum quantum number is J with projection M along a space-fixed axis and if L is the proton-ion orbital angular momentum, the cross section for process (1) is given by

$$\sigma(j' \leftarrow j) = \frac{\pi}{(2j+1)k_\alpha^2} \times \sum_{JLL'} (2J+1) \left| S_{\alpha'\alpha} - \delta_{\alpha'\alpha} \right|^2 , \tag{7}$$

where $S_{\alpha'\alpha}$ is the scattering matrix element between initial state $\alpha \equiv (JnlsjL)$ and final state $\alpha' \equiv (Jnlsj'L')$, and the threshold energy and wave number for state α are E_α and $k_\alpha = \hbar^{-1}[2\mu(E - E_\alpha)]^{1/2}$, respectively. In terms of energy-normalized wave functions, the transition amplitude is

$$T_{\alpha'\alpha} = (\Psi_{\alpha'}^{(0)}, H' \Psi_\alpha^{(+)}) . \tag{8}$$

The scattering matrix is given in terms of the transition matrix by

$$S_{\alpha'\alpha} = S^{L'}(\alpha')(\delta_{\alpha'\alpha} - 2\pi i^{L'-L+1} T_{\alpha'\alpha}), \tag{9}$$

where $S^{L'}(\alpha')$ is the Coulomb S matrix

$$S^{L'}(\alpha') = \frac{\Gamma(L'+1+i\gamma_{\alpha'})}{\Gamma(L'+1-i\gamma_{\alpha'})} \tag{10}$$

and

$$\gamma_{\alpha'}=\frac{(Z_A-N)e^2\mu}{k_{\alpha'}} . \qquad (11)$$

The Coulomb-Born approximation is the zero-order approximation to Eq. (8) and may be written

$$T^{\text{CB}}_{\alpha'\alpha}=(\Psi^{(0)}_{\alpha'},H'\Psi^{(0)}_{\alpha}) . \qquad (12)$$

To characterize better the interaction potential, given asymptotically in Eq. (4), we consider process (1) in the adiabatic molecular representation as an inelastic transition between electronic eigenstates,

$$A\text{H}^+(nl\Lambda s)\rightarrow A\text{H}^+(nl\Lambda's) ,$$

where Λ is the absolute magnitude of the projection m_l of the electronic orbital angular momentum $\vec{l}$ along the internuclear axis. The angular momentum $\vec{l}$ is well defined in the asymptotic limit, but not elsewhere.

In this representation, the electronic Hamiltonian is diagonal with transitions occurring through off-diagonal matrix elements of T_R and $V_{\vec{s}\cdot\vec{l}}$. The adiabatic nuclear scattering equations result from an expansion

$$\Psi^{(+)}(\underline{r},\underline{R})=\sum_i \Psi_i(\underline{r},R)F_i(\underline{R}) \qquad (13)$$

in terms of electronic eigenstates

$$H_{\text{el}}\psi_{nl\Lambda s}(\underline{r},R)=\epsilon_{nl\Lambda s}(R)\psi_{nl\Lambda s}(\underline{r},R) , \qquad (14)$$

where $i\equiv nl\Lambda s$ is a composite adiabatic quantum state index.

The adiabatic nuclear wave functions remain coupled asymptotically and must be transformed into the scattering state solutions of Eq. (5). We first couple $\vec{l}$ and $\vec{s}$ according to

$$\phi_{nlsj\Omega}(\underline{r},R)=\sum_{m_l m_s}(lm_l sm_s\,|\,jm_j)\times\psi_{nl\Lambda s}(\underline{r},R)\,|\,sm_s\rangle , \qquad (15)$$

where $\vec{j}=\vec{l}+\vec{s}$, m_j is the projection of $\vec{j}$ and $\Omega=|\,m_j\,|$. Transforming from the body-fixed to the laboratory-fixed coordinate system we obtain

$$|\,JMnlsjL\,\rangle=\sum_{m_j}(-1)^{L-j+m_j}(2L+1)^{1/2}\begin{bmatrix} L & j & J \\ 0 & m_j & -m_j\end{bmatrix}|\,JMnlsjm_j\rangle , \qquad (16)$$

where $(lm_lsm_s\,|\,jm_j)$ is a Clebsch-Gordan coefficient and

$$\begin{bmatrix} L & J & J \\ 0 & m_j & -m_j\end{bmatrix}$$

is a 3-j symbol.

The operators T_R and $V_{\vec{s}\cdot\vec{l}}$ are diagonal in this representation. We ignore some additional angular coupling terms of T_R which Mies[17] has argued are small. We approximate the spin-orbit operator as $C\vec{s}\cdot\vec{l}$, where C is a constant. Then the spin-orbit matrix elements are given by

$$\langle\alpha'\,|\,V_{\vec{s}\cdot\vec{l}}\,|\,\alpha\rangle=C[j(j+1)-l(l+1)-s(s+1)]\delta_{\alpha'\alpha} . \qquad (17)$$

The constant C is chosen so that the difference in the target energies $E_\alpha=\langle\alpha\,|\,V_{\vec{s}\cdot\vec{l}}\,|\,\alpha\rangle$ and $E_{\alpha'}=\langle\alpha'\,|\,V_{\vec{s}\cdot\vec{l}}\,|\,\alpha'\rangle$ equals the measured fine-structure splitting. The spin-orbit matrix element varies with R by a factor of 2 for the case of O^{3+} from the 0.048-eV splitting of O^{3+} to the 0.092-eV splitting of F^{4+} to which the system reduces in the united atom limit. However, because the cross sections for process (1) are negligible until collision energies of at least 10 eV are attained, a constant splitting may be assumed for proton O^{3+} collisions.

In the $|\,JnlsjL\,\rangle$ representation transitions are driven by off-diagonal matrix elements of H_{el},

$$V^J_{L',j',Lj}(R)=(-1)^{L'+L-j'-j+2(l-s)}[(2L'+1)(2L+1)(2j'+1)(2j+1)]^{1/2}\times\sum_{m_jm_lm_s}\begin{bmatrix} L' & j' & J \\ O & m_j & -m_j\end{bmatrix}\begin{bmatrix} L & j & J \\ O & m_j & -m_j\end{bmatrix}\begin{bmatrix} l & s & j \\ m_l & m_s & -m_j\end{bmatrix}\begin{bmatrix} l & s & j \\ m_l & m_s & -m_j\end{bmatrix}\epsilon_{nl\Lambda s}(R) . \qquad (18)$$

For the proton-impact excitation of the fine-structure levels of O^{3+}, $\epsilon_{nl\Lambda s}(R)$ are the $^2\Sigma$ and $^2\Pi$ interaction potentials $\epsilon_\Sigma(R)$ and $\epsilon_\Pi(R)$ of OH^{4+}.

The coupling matrix element occurring in the Coulomb-Born approximation is

$$V^J_{L'3/2L1/2}(R)=(-1)^{L'+L}[1-(-1)^{L'+L+2J}](2L'+1)^{1/2}(2L+1)^{1/2} \times \begin{bmatrix} L' & \frac{3}{2} & J \\ O & \frac{1}{2} & -\frac{1}{2} \end{bmatrix} \begin{bmatrix} L & \frac{1}{2} & J \\ O & \frac{1}{2} & \frac{1}{2} \end{bmatrix} \frac{\sqrt{2}}{3}[\epsilon_\Sigma(R)-\epsilon_\Pi(R)] \quad (19)$$

If the relative nuclear velocity is less than the electron orbital velocities, the elastic approximation[19] may be useful. According to it, the transition is regarded as occurring as the ions scatter elastically along adiabatic electronic potential-energy surfaces. Transitions are a direct result of recoupling of the scattered molecular states to produce a different final superposition of ionic fine-structure states. The approximation has been applied in studies of fine-structure transitions in neutral systems by Bottcher *et al.*[20] and Harel *et al.*,[21] although Reid and Rankin[22] have argued that it is not a reliable procedure.

By neglecting spin-orbit splittings and T_R couplings, we obtain a set of elastic adiabatic nuclear scattering equations. Upon recoupling to the appropriate asymptotic representation, inelastic cross sections can be expressed in terms of the adiabatic elastic phase shifts. For ${}^2P_{1/2}\rightarrow{}^2P_{3/2}$ transitions, the formula is[20]

$$\sigma(\tfrac{3}{2}\leftarrow\tfrac{1}{2})=\frac{8\pi}{9k^2}\sum_L(2L+1)\sin^2[\delta_L(\Pi)-\delta_L(\Sigma)]\ , \quad (20)$$

where $\delta_L(\Pi)$ and $\delta_L(\Sigma)$ are the partial wave phase shifts for elastic scattering along the ${}^2\Pi$ and ${}^2\Sigma$ molecular surfaces, respectively.

III. APPLICATION TO O^{3+} (${}^2P_{1/2}\rightarrow{}^2P_{3/2}$)

We calculated potential-energy curves for the ${}^2\Pi$ and ${}^2\Sigma^+$ states of OH^{4+} using single-configuration self-consistent-field wave functions. For the basis set we used the O^{3+} Hartree-Fock wave function of Clementi and Roetti[23] augmented with oxygen $3s,3d,4s,4d$ polarization functions as well as oxygen $3p,4p$ and hydrogen $1s,2s,2p,3s,3p$ functions. Table I is a list of the calculated potential energies. The corresponding O^{3+} quadrupole moment $q=\frac{2}{5}\langle r\rangle^2=0.4044a_0^2$. The dipole polarizabilities of O^{3+} may be determined from the OH^{4+} wave functions.[24] We obtained $\alpha_\Sigma=1.31a_0^3$ and $\alpha_\Pi=1.44a_0^3$ for the ${}^2\Sigma$ and ${}^2\Pi$ states, respectively. The corresponding asymptotic limits

$$\epsilon_\Sigma(R)\sim\frac{3}{R}-\frac{q}{R^3}-\frac{\alpha_\Sigma}{2R^4}+\cdots \quad (21)$$

and

$$\epsilon_\Pi(R)\sim\frac{3}{R}+\frac{q}{2R^3}-\frac{\alpha_\Pi}{2R^4}+\cdots \quad (22)$$

are accurate representations of the molecular potential curves to within a few tenths of a percent into R as small as $3.0a_0$. For the scattering calculations, we used the calculated molecular potential curves inside $5a_0$ and the asymptotic forms at longer distances. The calculations include the effects of polarization and of penetration of the O^{3+} electron distribution.

The Coulomb-Born approximation is accurate in the high-energy limit and in the small-interaction limit. For collisions between positive ions, the interaction is small at low energies and for large angular momenta. At low energies the Coulomb repulsion and for large angular momenta the centrifugal barrier restrict the nuclei to the weak-interaction region. Coulomb-Born results for individual partial cross sections are illustrated in Figs. 1 and 2 for proton-impact energies of 3 and 30 eV, respectively. Solutions of the close-coupled radial scattering equations were calculated using the log-derivative method of Johnson[25] and the cross sec-

TABLE I. Potential energies of the lowest ${}^2\Sigma$ and ${}^2\Pi$ states of OH^{4+} in a.u.

$R\,(a_0)$	${}^2\Sigma$	${}^2\Pi$
0.050	140.378 04	140.395 77
0.075	88.196 76	88.325 52
0.100	62.711 88	62.778 13
0.125	47.843 72	47.942 31
0.150	38.218 21	38.352 28
0.175	31.531 65	31.702 41
0.2	26.638 04	26.844 11
0.3	15.656 65	15.943 42
0.4	10.417 20	10.708 18
0.5	7.435 12	7.716 49
0.6	5.598 20	5.869 62
0.8	3.606 82	3.861 00
1.0	2.663 70	2.894 93
1.25	2.077 34	2.269 56
1.5	1.759 17	1.907 96
2	1.391 19	1.469 46
3	0.974 88	0.997 67
4	0.740 84	0.750 24
5	0.595 64	0.600 45

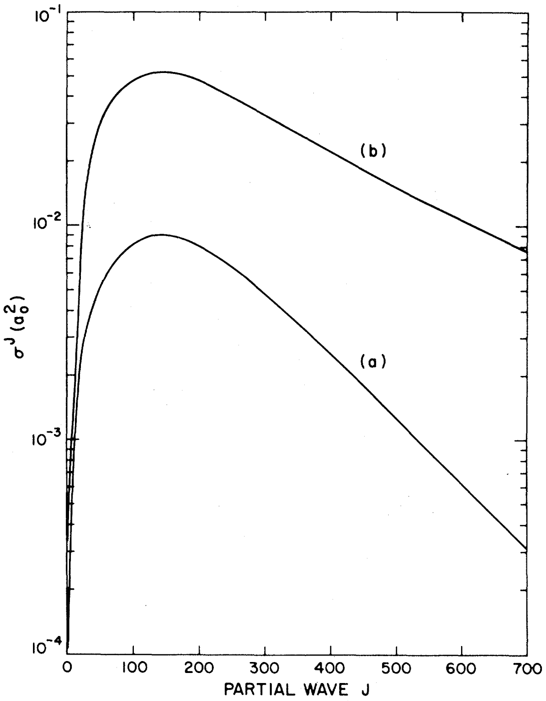

FIG. 1. Partial-wave contributions $\sigma^J=(\pi/2k^2)\times\sum_{L,L'}(2J+1)\,|S_{3/2,1/2}|^2$ at a total energy of 7 eV. (a) Close-coupled and Coulomb-Born, (b) elastic approximation.

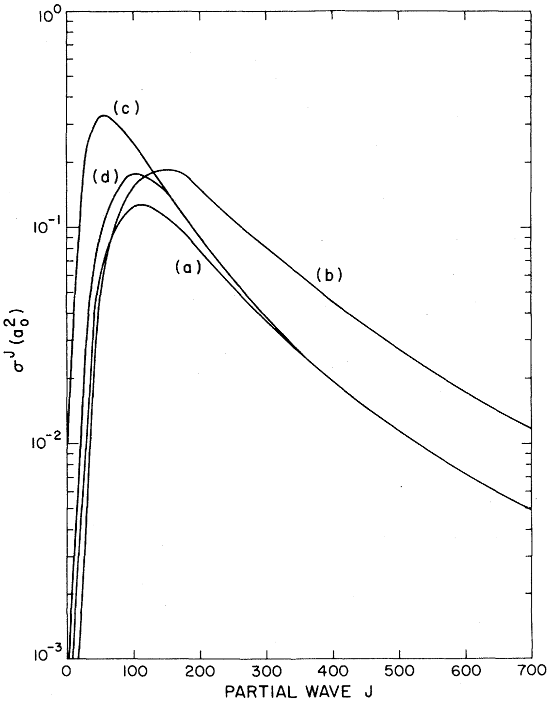

FIG. 2. Partial-wave contributions σ^J at a total energy of 27 eV. (a) Close-coupled, (b) elastic, (c) Coulomb-Born, and (d) unitarized Coulomb-Born approximation.

tions are included in Figs. 1 and 2. The Coulomb-Born and close-coupled partial cross sections are indistinguishable for $E=3$ eV, but significant differences occur at low angular momenta for $E=30$ eV. The Coulomb-Born approximation violates unitarity and overestimates the partial cross section in the strong-interaction region. Unitarity can be imposed in several ways. We chose to set $|S^J(\alpha,\alpha')|^2=0.5$ whenever the Coulomb-Born estimate exceeded 0.5. The results are shown in Fig. 2. Despite the arbitrary nature of our simple procedure, there is a marked and systematic improvement.

Partial cross sections calculated using the elastic approximation are presented in Figs. 1 and 2. The approximation overestimates the cross sections for all except the low-J partial waves, the discrepancies becoming more severe as the angular momentum increases. The elastic approximation assumes that the recoupling of the atomic states to form the ${}^2\Sigma$ and ${}^2\Pi$ molecular states takes place in the limit of large internuclear distances whereas in practice it will occur at some intermediate distance where the electrostatic interaction is comparable to the spin-orbit interaction. A detailed analysis of the elastic approximation in neutral particle fine-structure excitation has been carried out by Reid and Rankin[22] who argue that it is generally unreliable. Their results demonstrate that the approximation is inadequate at intermediate values of J but gives good agreement with the close-coupled partial cross sections at low and high J values.

In the low-energy limit the cross section for process (1) is zero because of the Coulomb repulsion. At a collision energy of 3 eV, corresponding to a classical turning point $R_c=30a_0$, the cross section

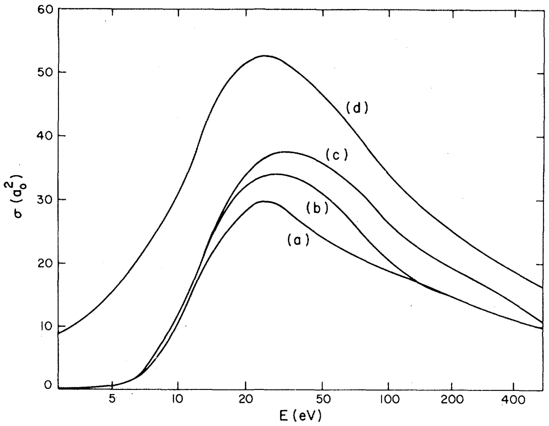

FIG. 3. Total cross section $\sigma(\frac{3}{2}\leftarrow\frac{1}{2})$ versus energy. (a) Close-coupled, (b) hybrid elastic Coulomb-Born, (c) unitarized Coulomb-Born, and (d) elastic approximations.

is $10^{-4}a_0^2$. It rises to a maximum of $30a_0^2$ for a collision energy of 30 eV for which $R_c = 3a_0$. The Coulomb-Born and close-coupled results agree closely at energies up to 7 eV. At energies above 7 eV, the particles enter the strong-interaction region and the Coulomb-Born approximation loses accuracy. At $E = 30$ eV, the Coulomb-Born cross section is $54a_0^2$. The simple unitarity correction reduces the cross section to $37a_0^2$. The elastic approximation overestimates the cross section at all energies. A hybrid approach, in which the elastic approximation is used for low-order partial waves, where $|S_{\alpha'\alpha}|^2 > 0.5$ and the Coulomb-Born approximation elsewhere is computationally very rapid and produces much improved results.

Figure 3 illustrates the cross sections obtained by the full solution of the coupled equations and by the unitarized Coulomb-Born, elastic, and hybrid approximation. Their accuracy is a reflection of the computational burden of the calculations. Given reliable interaction potentials, the use of close-coupling solutions at low J giving way at high J to the Coulomb-Born approximation as it becomes accurate provides a rapid procedure without loss of precision.

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