Spring 1984

Partial Radiative Recombination Cross Sections for Excited States of Hydrogen

Patricia M. Fazio
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PARTIAL RADIATIVE RECOMBINATION CROSS SECTIONS
FOR EXCITED STATES OF HYDROGEN

by

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A Thesis Submitted to the Faculty of
Old Dominion University in Partial Fulfillment of the
Requirements for the degree of

DOCTOR OF PHILOSOPHY

APPLIED PHYSICS

OLD DOMINION UNIVERSITY

May 1984

Approved by:

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Patricia M. Fazio
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Thesis Advisor: Dr. Gary Copeland

ABSTRACT

In calculating the radiative recombination cross sections for interstellar H II regions usually only the electric dipole term in the expansion of the interaction Hamiltonian is kept. However, conditions present in these regions permit recombination into highly excited states and the "effective size" of the atom is not much less than the wavelength of the emitted photon. These physical conditions do not meet the requirements for making the dipole approximation. A higher order approximation is to keep an additional term in the expansion of the Hamiltonian, and, therefore, to include contributions of quadrupole transitions in the calculation of the partial recombination cross sections. The dipole and quadrupole transition strengths in closed analytical form are calculated using the

Coulomb wave functions because results for any electron energy and for recombination into any angular momentum state of hydrogen are needed.

Several interesting effects are found. First, the transition probabilities are maximum for recombination into specific intermediate angular momentum states at low energies ($w < 2\text{eV}$) and where the free state angular momentum is greater than that of the bound state. Further, that specific intermediate angular momentum state depends on the kinetic energy of the free electron. This behavior is in contrast to the "normal" behavior of the transition strengths where recombination into s states is greatest and decreases with increasing angular momentum. Second, the quadrupole matrix elements vanish for certain velocities of the free electron. This leads to minima in the corresponding quadrupole cross sections when plotted as a function of the free electron's kinetic energy. Finally, the partial cross sections for highly excited states are greater than previously calculated because of the additional effects of the quadrupole transitions.

ACKNOWLEDGEMENTS

I would like to express my appreciation to Dr. Gary E. Copeland, my thesis advisor, for his help and guidance in this research. I am also fortunate to have benefitted from suggestions rendered by the members of my dissertation committee and, therefore, thank Dr. James L. Cox, Dr. Govind S. Khandelwal, and Dr. Wynford L. Harries of the Department of Physics, as well as Dr. Robert L. Ake, Chairman of the Department of Chemical Sciences.

I would like to acknowledge the computer centers of both Old Dominion University and the University of Virginia for their kind help in the implementation of the programs that were necessary for this dissertation.

My warmest thanks go to Dr. John E. Sipe of the University of Toronto, Toronto, Ontario, who made many valuable and insightful suggestions.

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I. INTRODUCTION

In the region near a very hot star, such as an O, B, A or Wolf-Rayet star, there are concentrations of ionized hydrogen atoms known as H II clouds which are constantly recombining with free electrons to form neutral hydrogen [1-3]. The densities of these clouds range from ten ions per cubic centimeter in the outer regions to three thousand ions per cubic centimeter near the star. At densities below 10^8 ions per cubic centimeter, however, collisions between ions are rare. As a consequence, the dominant mechanism for recombination in these low density clouds is radiative electron capture (radiative recombination) in which energy and momentum conservation are maintained by an outgoing photon. An additional consequence of a low collision rate is that an electron that recombines into a very highly excited state has time to cascade to lower levels radiatively. Moreover, the temperatures of H II clouds vary from 3000 to 15000 K, corresponding to free electron kinetic energies of a few electron volts. Radiative capture, therefore, of low energy electrons and subsequent radiative decay to lower energy levels are dominant processes in H II regions.

Recombination transitions for these unusual physical conditions in H II regions have not been adequately described in previous treatments. Normally, the function

describing the electromagnetic wave is expanded in a Taylor series, and assuming that the wavelength of the emitted radiation is much larger than the size of the radiator, only the first term is kept. This is the dipole approximation in which $\exp(i\vec{k}\cdot\vec{r})$ is set equal to 1. This condition is not met, however, for capture into highly excited states, as can be understood by considering the wavelength of the emitted photon, $\lambda = hc/(w + Ry/n^2)$, where w is the kinetic energy of the electron, n is the principle quantum number for the bound state, and Ry is the ionization potential of hydrogen. For a given energy w the wavelength of the photon approaches a maximum as n increases, while the radius of the atom grows as n^2 . Clearly the dipole approximation fails because the "effective size" of the radiating system grows as n increases, becoming significantly in error as n approaches 20. We make the next order approximation by keeping an additional term in the expansion of $\exp(i\vec{k}\cdot\vec{r})$: that is, we put $\exp(i\vec{k}\cdot\vec{r}) = 1 + i\vec{k}\cdot\vec{r}$. The first term yields dipole transitions and the second leads to transitions which, in classical electromagnetic theory, involve electric quadrupole and magnetic dipole moments. In atomic physics they are simply called "quadrupole transitions" [4].

We calculate exact transition strengths (the square of the matrix elements) in closed analytical form for dipole and quadrupole transitions into all bound states up to $n=20$ and $l=19$. Since we use exact Coulomb wave functions to describe the unbound state the results are valid for any

energy of the free electron. We find that at energies greater than 15eV recombination into s states is preferred, while probabilities for transitions into states of higher angular momentum decrease with increasing l . A decrease in transition probability with increasing l is also found at low energies when $l' \leq l$, where l' labels the angular momentum of the free state, except when the angular momentum of the initial state of the hydrogen atom is greater than that of the final state. In that case, the preferred recombination is into a state that has an intermediate value of l .

In addition to this ordering of the transition strengths, we have also found that there are certain energies at which the transition strengths for quadrupole transitions vanish. This vanishing occurs when the free state of the hydrogen atom has two units of angular momentum more than the final state and when the final state is one of low angular momentum. These zeros, in turn, have the effect of producing minima in the corresponding quadrupole cross sections. These minima are analagous to the Cooper minima which occur in the photo-ionization cross sections for some multi-electron systems [5]. We are able to predict a maximum number of zeros by inspection of the formulas for transition strength, but we can only show their detailed behavior by plotting them as functions of the kinetic energy of the free electron. We show that, as expected, the relative importance of the quadrupole transitions with respect to the dipole grows with n for any fixed energy,

thus increasing the values of the partial recombination cross sections.

In Chapter II, we supply a brief description of the Coulomb wave functions, both bound and free, and of the perturbation theory used to calculate the transition probabilities. We give a brief historical review of the theory of radiative recombination in Chapter III and discuss the cross section formulas for photo-ionization and radiative recombination, including their relationship through the principle of detailed balancing, in Chapter IV. Chapter V presents the derivation of the general formula for the transition strength. In chapters VI and VII we present the results of this dissertation in the form of sample matrix elements, transition strengths, and cross sections and discuss their implications.

II. MATHEMATICAL AND PHYSICAL BACKGROUND

The solutions of the Schrodinger equation for an electron in the field of a nucleus of charge Ze and infinite mass are products of spherical harmonics and solutions of the radial wave equation

$$\frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} + 2 \left[E + \frac{Z}{r} \right] R - \frac{l(l+1)}{r^2} R = 0 , \quad (2-1)$$

where the energy E is positive if the electron is unbound (called "free") and negative if it is bound [6]. The energy eigenfunctions thus found are called Coulomb wave functions and span both negative and positive energies. Thus, when these wave functions are used to describe the system, the distinction between ionized hydrogen and neutral hydrogen is purely formal. Therefore, both bound and free state wave functions are written as products of spherical harmonics and the appropriate solution of the radial wave equation (2-1). For a recombination process the electron is initially free so the initial state function is

$$| i \rangle = | n'l'm' \rangle = R(wl') Y(l'm') ,$$

where E is positive, continuous, and related to the quantum number n' by the formula $w=E=Ry/n'^2$. These energy levels

are infinitely degenerate in l' and m' . The final state for recombination is a bound state:

$$|f\rangle = |n\ l\ m\rangle = R(nl) Y(lm) ,$$

where E is negative and the energy levels are discrete, n -degenerate in l , and $2l+1$ -degenerate in m .

In constructing the solutions to Equation (2-1), we follow the treatment of Bethe and Salpeter [6]. A general solution to the wave equation (2-1), which remains finite as r becomes infinitely large, is of the form

$$R(r) = e^{-\epsilon r} f(r) .$$

Here $\epsilon = \sqrt{-2E}$, and $f(r)$ is a power series which can be generated by a recurrence relation

$$f(r) = r^\lambda \sum_{v=0}^{\infty} a_v r^v .$$

For bound solutions, E is negative and substitution of $f(r)$ into the wave equation leads to the possibilities $\lambda=1$ or $\lambda=-1-1$. With the condition that $f(r)$ remain finite at $r=0$, $\lambda=1$ is required, and the corresponding recursion formula is

$$a_v = 2 a_{v-1} \frac{(1+v) - Z}{(1+v)(1+v+1) - 1(1+1)} .$$

If we require $\epsilon=Z/n$ then the series will terminate.

Otherwise, $f(r) \approx \exp(2\epsilon r)$, with the consequence that $R(\rho) \approx \exp(\epsilon r)$, which diverges as r becomes infinitely large. With this requirement, the recurrence relation is

$$a_v = -2\epsilon a_{v-1} \frac{(n-1-v)}{(2l+1+v)}.$$

With $\rho = 2\epsilon r = 2Zr/n$, the bound state radial wave functions can be written in terms of a confluent hypergeometric function:

$$R(\rho) = C (2\epsilon)^{3/2} e^{-\rho/2} \rho^l F(-(n-l-1), 2l+1, \rho),$$

where

$$F(a, b, x) = 1 + \frac{a}{b} x + \frac{a(a+1)}{b(b+1)} \frac{x^2}{2!} + \dots$$

$R(\rho)$ can also be written in terms of associated Laguerre polynomials:

$$L_{\lambda}^{\mu}(\rho) = \frac{d^{\mu}}{d\rho^{\mu}} L_{\lambda}(\rho); \quad L_{\lambda}(\rho) = \frac{e^{\rho} d^{\lambda} e^{-\rho}}{d\rho^{\lambda}}. \quad (2-2)$$

By carrying out the indicated differentiations one can identify $\lambda = n+1$ and $\mu = 2l+1$. The resulting formula for the radial wave function in terms of the Laguerre polynomials is

$$R(\rho) = -C \frac{(2\varepsilon)^{3/2} (2l+1)! (n-l-1)!}{(n+1)!} e^{-\rho/2} L_{n+1}^{2l+1}(\rho). \quad (2-3a)$$

Normalizing the wave functions to unity in the usual manner yields the constant C:

$$C = \sqrt{\frac{(n+1)!}{(n-l-1)! 2n}} \frac{1}{(2l+1)!}. \quad (2-3b)$$

For the free state, $\varepsilon = i\sqrt{2E} = ik$, and the series $f(r)$ no longer needs to terminate through a choice of ε because the factors $\exp(\pm \varepsilon r)$ in the solution for $R(r)$ remain finite. Unfortunately λ is not an integer, and the solutions $R(r)$ cannot be written in terms of the Laguerre polynomials when these polynomials are defined according to Equation (2-2). By the use of Cauchy's theorem, however, an integral representation of the Laguerre polynomials can be found which admits generalization for non-integral λ and, thus, makes possible a representation of the free solutions to the radial wave equation:

$$R(wl') = \frac{C}{2\pi} (i\rho)^{-l'-1} \oint e^{-\rho\xi} (\xi + 1/2)^{-in'-l'-1} (\xi - 1/2)^{in'-l'-1} d\xi. \quad (2-4)$$

Figure 2-1. In this figure the contour of Equation (2-4) is represented. In addition, path b represents an asymptotic incoming wave while path c represents the outgoing wave.

This integral representation can be cast into two forms of infinite hypergeometric series. One form is good for all ρ but is slowly convergent and another form is rapidly convergent but good for only small ρ [6].

Now that we have described the initial and final states of the hydrogen atom we must discuss the interaction Hamiltonian responsible for the transitions between the free and bound states.

An electron in a radiation field is described by

$$H' = \frac{1}{2m} \left[\bar{p} - \frac{e\bar{A}}{c} \right]^2 - e\Phi,$$

where $\bar{A}$ and Φ are the vector and scalar potentials of the electromagnetic field, e is the charge on the electron, $\bar{p}$ the canonical momentum of the electron, m is the reduced

mass of the system, and c the speed of light. The pure radiation field which perturbs the atom can be described in terms of the vector potential alone in the Coulomb gauge in which $\nabla \cdot \bar{A} = 0$. In this gauge, Φ satisfies the Poisson equation

$$\nabla^2 \Phi = 4\pi Ze \delta(\bar{r}) ,$$

where $-Ze$ is the charge of the nucleus, and this implies that

$$\Phi = \frac{-Ze}{r} .$$

The radiation field is then described by a homogeneous wave equation for $\bar{A}$:

$$\nabla^2 \bar{A} - \frac{1}{c^2} \frac{\partial^2 \bar{A}}{\partial t^2} = 0 .$$

Thus, the Hamiltonian can be written as follows:

$$H = \frac{\bar{p}^2}{2m} - \frac{Ze^2}{r} + \frac{e}{mc} \bar{A} \cdot \bar{p} + \frac{e^2 \bar{A}^2}{2mc} .$$

The first two terms comprise the unperturbed Hamiltonian and the last two terms the interaction Hamiltonian that accounts for the perturbation of the electromagnetic field. For a

single photon process the term containing $\bar{A} \cdot \bar{p}$ is much larger than the term containing $\bar{A}^2$. Consequently, the term containing $\bar{A}^2$ is ignored in the interaction Hamiltonian. Therefore, the interaction between the atom and the electromagnetic field becomes

$$H(\text{rad}) = \frac{e}{mc} \bar{A} \cdot \bar{p} \quad . \quad (2-5)$$

The transition probability per unit time, according to Fermi's Golden Rule, is

$$W = \frac{2\pi}{\hbar} \rho(\hbar\omega) \left| \langle f | H(\text{rad}) | i \rangle \right|^2 \delta(E(i) - E(f) - \hbar\omega) \quad .$$

where $\rho(\hbar\omega)$ is the density of final states and the delta function specifies the energy of the photon emitted for the process connecting states $|i\rangle$ and $|f\rangle$. In order to find the transition probability per unit time, therefore, the matrix element $\langle f | H(\text{rad}) | i \rangle$ must be calculated between the initial and final states. In order to calculate the matrix elements, $\bar{A}$ becomes the electromagnetic field operator and $\bar{p}$ the momentum operator. The matrix element containing $\bar{A} \cdot \bar{p}$ can be related to the matrix element containing $\bar{A} \cdot \bar{r}$ through the commutation relationship $[H, \bar{r}] = -i\hbar\bar{p}/m$ if the unperturbed Hamiltonian is of the form $H_0 = p^2/2m + V_0$, and if V_0 commutes with $\bar{r}$ [7]. The number of photon modes for each polarization per unit energy interval is given by

$$\rho(E) = \frac{\omega^2 L^3 d\Omega}{8\pi^3 \hbar c^3}.$$

The transition probability per unit time for spontaneous emission of light into the solid angle $d\Omega$ is then

$$W = \frac{2\pi \omega^2 L^3 d\Omega}{\hbar 8\pi^3 c^3} |\langle f | H(\text{rad}) | i \rangle|^2 \delta(E(i) - E(f) - \hbar\omega),$$

where the initial and final states are direct products of the hydrogenic wave functions and the photon wave functions:

$$\begin{aligned} |i\rangle &= |n' l' m'\rangle |N\rangle; \\ |f\rangle &= |n l m\rangle |N+1\rangle. \end{aligned}$$

The electromagnetic field operator for the emission of a photon is

$$\bar{A} = \left[\frac{\hbar}{\omega L^3} \right]^{1/2} c \left(a + \hat{e}_{\vec{k}}^{(\lambda)} \hat{e}^{i\vec{k} \cdot \vec{r}} \right),$$

where $a |N\rangle = N+1 |N+1\rangle$ and $\langle N | N \rangle = 1$. By combining these expressions together, the equation for the transition probability per unit time is as follows:

$$W = \frac{2\pi L^3 d\Omega}{\hbar 8\pi^3 c^4} |\langle n l m | \langle N+1 | i e^{i\vec{k} \cdot \vec{r}} \bar{A} | N \rangle | n' l' m' \rangle|^2 \delta(E(i) - E(f) - \hbar\omega).$$

since

$$\langle N+1 | \bar{A} | N \rangle = \langle N+1 | \left[\frac{\hbar}{\omega L} \right]^{1/2} c \hat{e}_{\vec{k}}^{(\lambda)} e^{i\vec{k} \cdot \vec{r}} | N \rangle ,$$

one can finally write

$$W = \frac{\omega^3}{(2\pi) c} \frac{d\Omega}{2} |\langle nlm | (\hat{e}_{\vec{k}}^{(\lambda)} \cdot \vec{r}) e^{i\vec{k} \cdot \vec{r}} | n'l'm' \rangle|^2 \delta(E(i) - E(f) - \hbar\omega) .$$

(2-6)

This result is used below to derive the partial cross section formula for radiative recombination of electrons and protons.

III. HISTORICAL BACKGROUND

The first approach to the study of recombination was, of course, a classical one, put forth in 1923. Kramers based his approximate formula for cross sections on the classical radiation of a free electron colliding with a bare nucleus [8]. It was shown by Gaunt to be valid in the region of large quantum numbers [9]. The classical calculations yielded oscillator strengths given by the following formula:

$$f(nn') = \frac{2^6}{3\sqrt{3}} \frac{1}{\omega_n} \left[\frac{1}{n+n'} \right]^2 \frac{1}{nn'},$$

where ω_n is the ratio of the statistical weights of the bound and free states. So near to agreement are the classical and quantum mechanical calculations that it was found convenient to write $f(nn') = g_{II} f'(nn')$, where $f(nn')$ and $f'(nn')$ are the classical and quantum mechanical oscillator strengths, respectively. Here g_{II} is a correction factor, known as the Gaunt factor. It is dependent on the bound and free state principal quantum numbers and is usually close to unity. The quantum mechanical cross sections can be related to the Kramers-Gaunt factor $g_{II}(n, k/2)$ by the formula

$$\sum_l \frac{(2l+1)}{n} \sigma_{nl}^c(Z, k^2) = \frac{n}{Z^2} \left[\frac{g_{II}(n, k/2)}{1 + \left(\frac{nka}{Z}\right)^2} \right]^3,$$

where $\sigma_{nl}^c(Z, k^2)$ is the cross section and k is related to the energy of the electron by the formula $w = k^2/2$.

The earliest quantum mechanical calculations of the matrix elements and transition strengths necessary for calculating the cross sections were carried out in the late 1920's and early 30's by Suguria [10], Mott [11], Oppenheimer [12,13], Gordon [14], Gaunt [9], Wessel [15] and Morse and Stukelberg [16]. These early papers presented general evaluations of the necessary matrix elements and the results are in terms of hypergeometric functions. Applications of the general formulas, to obtain closed analytic expressions, were only made for the very lowest values of n (i.e. Suguria and Oppenheimer), or in certain limiting cases; Mott presented asymptotic expressions for the integrals at low and high energies and Morse and Stukelberg presented results for up to $n=5$, based on Mott's asymptotic expressions. All cross sections were calculated without regard to the azimuthal quantum number l . Oppenheimer also evaluated the matrix elements in closed analytical form by putting the wave functions in parabolic coordinates, a procedure which also does not retain information on l .

Bates, Buckingham, Massey and Anwin [17] carried out extensive calculations for total capture cross sections for thermal electrons, but again the dependence on angular momentum is not explicitly calculated.

Other early researchers such as Maue [18], Cillie [19,20], Menzel and Pekeris [21], and Baker and Menzel [22] extended the results of Gaunt [9]. For example, Menzel and Pekeris expanded the hypergeometric function in an asymptotic series and applied the method of steepest descents to obtain results in certain limiting cases. The general formula for oscillator strength, as given by Menzel and Pekeris, for bound-free transitions where n and n' are the bound and free state respectively is

$$f(n,n') = \frac{2^5 e^{-4n' \arctan(n/n')}}{3n^2 n'n} \left[\frac{2}{n+n'} \right]^2 \frac{|\Delta(n',n)|}{(1-e^{-2\pi n'})},$$

where

$$|\Delta(n',n)| = \left[F(-n'+1, -n, 1, -4nn'/(n'-n)^2) \right]^2 - \left[F(-n+1, -n', 1, -4nn'/(n'-n)^2) \right]^2,$$

and where F is the ordinary hypergeometric function:

$$F(a,b,c,x) = 1 + \frac{abx}{c} + \frac{a(a+1)b(b+1)x^2}{c(c+1)} + \dots$$

The Kramers-Gaunt factor, g_{II} , can then be identified as

$$g_{II} = \frac{3}{(n' + n)^2} \frac{nn' e^{-4n' \arctan(n/n')}}{(1 - e^{-2nn'})} \left| \Delta(in', n) \right| .$$

When n is large the exact analytic equations become somewhat cumbersome but g_{II} can be expanded in an asymptotic series:

$$g_{II} = 1 + \frac{0.1728(n k/Z - 1)^2}{n^{3/2} (n k/Z + 1)^{3/2}} - \frac{0.0496(n k^2/Z + 4k/6 + 1)^2}{n^{4/3} (n k/Z + 1)^{4/3}} + \dots$$

The asymptotic method employed by Menzel and Pekeris kept only the first term in this expansion.

In the late 1950's new interest appeared in the study of the recombination spectrum for hydrogen generated, perhaps, by two incidents. New data became available to the scientific community because of the advent of radio astronomy and more numerical calculative procedures became possible because of the increased availability of powerful computers.

Green, Rush and Chandler [23] calculated Gaunt factors to six figures for n up to 30. Burgess used the method of steepest descents to obtain an asymptotic expansion for the hydrogen dipole matrix elements involving l explicitly [24]. He obtained poor results for n greater than 5. Searle [25] calculated transition probabilities for n up to 10 but,

again, the calculations are based on approximate expressions. In essence, all three of these papers included methods that involved keeping higher order terms in the expansion of g_{II} . The results of Burgess and Searle showed that the population following recombination is far from the statistical weight and, according to Leonard Searle "The derivation of accurate relative line intensities in hydrogen nebula requires the calculation of exact recombination cross sections at several energies for all n, l up to at least 20. This remains a formidable problem."

Pengelley did an exact treatment of the capture cascade problem for all n, l up to five. He used the hydrogen transition probabilities tabulates by Green, Rush and Chandler [23] and the recombination coefficients of Burgess [27]. For n larger than five he resorted to an extrapolation procedure [26]. In 1964 Burgess calculated the transition matrix elements in the most exact and accurate way thus far presented [27]. He used a numerical technique to calculate recombination coefficients and photo-ionization cross sections for all l up to $n=20$. He chose a suitable hypergeometric function for the representaton of the bound and free states and expressed the resulting matrix elements in terms of hypergeometric functions. This result had already been presented in a general form by several authors, e.g. Gordon [14] and Alder and Winther [28]. The resulting hypergeometric series terminates after a finite number of terms; however, the

procedure is not suitable in general because of the large number of terms occurring in the series when $n-1$ is large. Also, for some ranges of parameters there is gross cancellation between terms. Burgess circumvented these problems by calculating the terms for a given n where $l=n-1$ and $n-2$, since they are the simplest, and then used a numerical technique employing a recurrence relation for hypergeometric series to calculate the matrix elements for smaller l 's. The only drawback is that for large n , severe scaling problems may arise due to rapid variations in the recurrence relation with n . Calculations were performed over a variety of electron temperatures, but step size is presented in such a way that though for $n=1$ he spans an energy range from 0 to 40.96 eV by the time $n=20$ is reached the energy range is limited from 0 to 1.39 eV. Burgess carried out extensive checks for his calculations and claims an accuracy of seven figures for low n , and high n and high l , but loses accuracy, because of a build up error, to six figures. His tables are presented to five significant figures.

In 1971 Brockelhurst [29] applied the method of Burgess in studying the level populations for hydrogenic ions and claims a build up error that reduces accuracy to at least four figures.

In review, the early works on electron-proton radiative recombination and photo-ionization did not explicitly calculate the dependence on the angular momentum quantum number l . This information is of importance because the lifetimes increase not only with principal quantum number n but with azimuthal quantum number l . Also, the various simplifying assumptions which were made limited their range of applicability. The few papers that presented the squares of the matrix elements in closed analytic form did so only for the lowest of the bound states. Burgess developed the best numerical method for calculation of the bound-free transition strengths, but lost accuracy at high n and low l . There is no work that addresses the failure of the dipole approximation for recombination or photo-ionization from highly excited states of hydrogen when the kinetic energy of the electron is low.

IV. THE CROSS SECTION

In Chapter II we presented a description of the bound and continuum states of the hydrogen atom along with the interaction Hamiltonian which describes the perturbation that causes the transition between states. With this information, a general formula for the transition probability per unit time for spontaneous transitions between initial free states and final bound states was presented (Equation (2-7)). In this chapter we discuss the partial cross sections (cross sections for recombination into a state described by both n and l) for the radiative recombination process, which are dependent on the transition probabilities.

Since the processes of radiative recombination and photo-ionization are related through the principle of detailed balancing, we will begin this section with the relationship between the two formulas. Then we expand the interaction Hamiltonian and write a general partial cross section formula for any order transition. Finally, by keeping the first two terms in this expansion (because we wish to investigate the importance of quadrupole transitions to the partial cross sections), we write a formula for partial cross sections that is dependent on both the dipole and quadrupole transitions.

The principle of detailed balancing [30,31] states that transition rates for excitations are equal to transition rates for decays between the same two levels. Therefore, the cross sections for photo-ionization and radiative recombination are related through the following formula:

$$\bar{p}_e^2 \sigma_{nl}^c = \bar{p}_{ph}^2 \sigma_{nl}^{pi}, \quad (4-1)$$

where $\bar{p}$ is momentum and the subscripts e and ph are for the electron and the photon respectively. The superscripts label the capture (c) and photo-ionization (pi) processes while n and l are the quantum numbers of the bound state. The kinetic energy of the electron is related to the principal quantum number n' and the momentum of the electron as follows:

$$w = \frac{\hbar\omega}{n'^2} = \frac{\bar{p}_e^2}{2m},$$

where m is the mass of the electron and $\hbar\omega$ is the energy of the emitted photon. The momentum of the emitted photon can be related to the principal quantum numbers n and n' by the equation

$$\bar{p}_{ph} = \frac{\hbar\omega}{c} \left[\frac{1}{n'^2} + \frac{1}{n^2} \right].$$

The ratio of the momenta is

$$\frac{\bar{p}}{p_e} = \frac{\alpha}{2} \frac{n'}{n} \left[\frac{1}{n^2} + \frac{1}{n'^2} \right]^2, \quad (4-2)$$

where α is the fine structure constant.

In terms of the radial matrix elements, the cross section [6] for photo-ionization from a bound state with quantum numbers n and l is

$$\sigma_{nl}^{pi} = (2\pi)^2 \alpha (\hbar\omega) \left| \langle f | e^{i\vec{k} \cdot \vec{r}} \vec{r} \cdot \hat{e} | i \rangle \right|^2 \frac{a_0^3}{e^2},$$

where the factor a_0^3/e^2 has been inserted to convert from atomic units to cgs units.

Substituting the photo-ionization cross section formula and Equation (4-2) into Equation (4-1) yields the partial cross section formula for radiative recombination:

$$\sigma_{nl}^c = \frac{(na_0)^2}{2} \alpha^3 \left[\frac{n^2 + n'^2}{6n n'} \right]^3 \left| \langle f | e^{i\vec{k} \cdot \vec{r}} \vec{r} \cdot \hat{e} | i \rangle \right|^2, \quad (4-3)$$

where the identities $e^2/a_0 = 2\hbar\omega_1$ and $e^2 = \alpha\hbar c$ have been used to simplify the formula.

When the wavelength of the emitted radiation is large compared to the size of the radiator, it is sufficient to expand $\exp(i\vec{k}\cdot\vec{r})$ as $(1 + i\vec{k}\cdot\vec{r} + \dots)$ and keep only the first term. This is called the dipole approximation.

For transitions between bound states, and transitions from free states to low lying states, this condition is satisfied. However, the size of the hydrogen atom increases as the square of the principle quantum number n and rapidly approaches the wavelength of the emitted radiation ($\lambda_n = hc/(w + Ry/n^2)$). It can be seen from the ratio $2\pi r_n/\lambda_n$ (see Figure 4-1) that the dipole approximation fails as n increases and a significant error results as n approaches 20.

For an exact treatment the matrix elements as they are expressed in Equation (4-3) should be calculated. The extreme complexity of this derivation, however, prohibits such a direct method. We have developed an alternate approach.

Since our interests are in low energy recombinations, the effect of the Coulomb field of the proton on the electron cannot be ignored. We, therefore, describe the electron with Coulomb wave functions. We do not wish to make the dipole approximation, but do expand the exponential term in the interaction Hamiltonian in a Taylor series:

Figure 4-1. The ratio of the radius of the final size of the hydrogen atom to the wavelength of the emitted photon is presented.

$$e^{i\vec{k} \cdot \vec{r}} = 1 + \frac{(i\vec{k} \cdot \vec{r})}{1!} + \frac{(i\vec{k} \cdot \vec{r})^2}{2!} + \dots = \sum_{q=0} \frac{(i\vec{k} \cdot \vec{r})^q}{q!}.$$

Then, substituting the series into Equation (4-3) the matrix element becomes

$$\begin{aligned} \langle n \ l \ m | e^{i\vec{k} \cdot \vec{r}} \vec{r} \cdot \hat{e} | n' l' m' \rangle \\ = \langle n \ l \ m | \sum_{q=0} \frac{(i\vec{k} \cdot \vec{r})^q}{q!} \vec{r} \cdot \hat{e} | n' l' m' \rangle. \end{aligned}$$

There have been no demands made on the geometry and we are free to take the wave vector $\vec{k}$ of the photon to lie along the z axis. The angle between $\vec{r}$ and $\vec{k}$ is θ so that $\vec{k} \cdot \vec{r} = kr \cos \theta$. Pulling terms that are independent of the integration variables outside the matrix element yields

$$\sum_{q=0} \frac{(ik)^q}{q!} \langle n \ l \ m | r^{q+1} \cos^q \theta (\sin \theta \cos \theta + \sin \theta \sin \theta) | n' l' m' \rangle,$$

where $\vec{r} \cdot \hat{e} = r(\sin \theta \cos \theta + \sin \theta \sin \theta)$ and includes the sum over the two polarizations of the photon. Having written the matrix element in this manner, the angular integrals can be separated from the radial integrals:

$$\sum_{q=0} \frac{(ik)^q}{q!} \langle n \ l \ m | r^{q+1} | n' l' \rangle$$

$$\cdot \langle 1 m | \cos\theta (\sin\theta \cos\theta + \sin\theta \sin\theta) | 1' m' \rangle \quad . \quad (4-4)$$

We have already indicated that the dipole approximation is not sufficient to describe the capture of an electron into highly excited states of hydrogen because the size of the final state of the system is no longer much smaller than the wavelength of the radiation emitted during the transition. Inclusion of this form for the matrix element would allow any degree of accuracy required by keeping additional terms in the sum. As a first example and as a means of demonstrating the importance of additional terms in the expansion, we keep two of the terms in Equation (4-4). The matrix element becomes

$$\langle n l m | e^{i\vec{k} \cdot \vec{r}} \hat{r} \cdot \hat{e} | n' l' m' \rangle \approx$$

$$\langle n l | r | n' l' \rangle \langle 1 m | \sin\theta \cos\theta + \sin\theta \sin\theta | 1' m' \rangle +$$

$$\frac{i\omega}{c} \langle n l | r | n' l' \rangle \langle 1 m | \cos\theta (\sin\theta \cos\theta + \sin\theta \sin\theta) | 1' m' \rangle .$$

Squaring this yields

$$|\langle n l m | e^{i\vec{k} \cdot \vec{r}} \hat{r} \cdot \hat{e} | n' l' m' \rangle|^2 =$$

$$|\langle n l | r | n' l' \rangle \langle 1 m | \sin\theta \cos\theta + \sin\theta \sin\theta | 1' m' \rangle|^2 +$$

$$\left(\frac{\omega}{c}\right)^2 |\langle n l | r | n' l' \rangle \langle 1 m | \cos\theta (\sin\theta \cos\theta + \sin\theta \sin\theta) | 1' m' \rangle|^2$$

$$\begin{aligned}
& + \frac{i}{c} \langle n \, l \, | r \, | \, n' \, l' \rangle \langle n \, l \, | r \, | \, n' \, l' \rangle^* \\
& \quad \cdot \langle l \, m \, | \sin \theta \cos \theta + \sin \theta \sin \theta \, | \, l' \, m' \rangle^* \\
& \quad \cdot \langle l \, m \, | \cos \theta (\sin \theta \cos \theta + \sin \theta \sin \theta) \, | \, l' \, m' \rangle^* \\
& - \frac{i}{c} \langle n \, l \, | r \, | \, n' \, l' \rangle \langle n \, l \, | r \, | \, n' \, l' \rangle^* \\
& \quad \cdot \langle l \, m \, | \sin \theta \cos \theta + \sin \theta \sin \theta \, | \, l' \, m' \rangle^* \\
& \quad \cdot \langle l \, m \, | \cos \theta (\sin \theta \cos \theta + \sin \theta \sin \theta) \, | \, l' \, m' \rangle^* .
\end{aligned}
\tag{4-5}$$

The angular integrals can be evaluated using the Wigner-Eckhart theorem (see Appendix B). The selection rules are found upon performing the angular integration. For dipole transitions ($q=0$) they are $\Delta l = \pm 1$ and for quadrupole transitions ($q=1$) they are $\Delta l = 0, \pm 2$ but $l=0 \rightarrow 0$. This implies that when one of the integrals in a cross term is non-zero the other must necessarily be zero. Consequently, the cross terms in Equation (4-5) vanish. The m and m' substates can be summed over if information concerning the polarization of radiation is not required. The derivation of the formulas for the squares of the angular parts of the matrix element are presented in Appendix B. By substituting these angular integrals into Equation (4-5) the formula for the bound-free transition strengths are found to be

$$\begin{aligned}
& \sum_{mm'} \left| \langle n \, l \, m \, | e^{i \vec{k} \cdot \vec{r}} \hat{r} \cdot \hat{e} \, | \, n' \, l' \, m' \rangle \right|^2 = \\
& \frac{2}{3} \left[1 \, | \langle n \, l \, | r \, | \, n' \, l-1 \rangle |^2 + (l+1) \, | \langle n \, l \, | r \, | \, n' \, l+1 \rangle |^2 \right]
\end{aligned}$$

$$\begin{aligned}
& + \left(\frac{\omega}{c}\right)^2 [A(l) |\langle n \ l \ | r^2 | n' \ l+2 \rangle|^2 \\
& B(l) |\langle n \ l \ | r^2 | n' \ l \rangle|^2 + C(l) |\langle n \ l \ | r^2 | n' \ l-2 \rangle|^2] , \\
& \hspace{25em} (4-6a)
\end{aligned}$$

where $A(l)$, $B(l)$, and $C(l)$ are the squares of the angular parts of the quadrupole matrix elements summed over all m and m' substates and over the two polarizations of the photon:

$$\begin{aligned}
A(l) &= \frac{(l+1)(l+2)}{(3l+3)} \delta(l'-l-2) \\
B(l) &= \frac{2}{3} \frac{l(l+1)}{(2l+3)(2l-1)} \delta(l'-l) \\
C(l) &= \frac{l(l-1)}{(2l-1)} \delta(l'-l+2) . \\
& \hspace{25em} (4-6b)
\end{aligned}$$

In the next section, RADIAL MATRIX ELEMENTS, we derive a formula for the transition strengths and, in conjunction with the algebraic software package REDUCE2 [32], generate the free-bound transition strengths for allowed dipole and quadrupole transitions into all bound states up to $n=20$ and $l=19$.

V. THE RADIAL MATRIX ELEMENTS

In order to calculate the values of the radial matrix elements of Equation (4-4) it is necessary to evaluate integrals of the form

$$\int_0^{\infty} R(nl)^* r^{q+1} R(wl') r^2 dr, \quad (5-1)$$

which have been of interest since the early years of quantum mechanics. Previously this integral has been evaluated for a general value of q in terms of hypergeometric functions [28]. However, it has been possible to express these results in terms of elementary functions only for the lowest bound states [12,13], or for higher n but only for $l=(n-1)$ and $(n-2)$ [27], and under certain simplifying assumptions because the algebra involved in the calculations of the matrix elements is prohibitively laborious. In this dissertation, the integrals are presented in a form that, with the aid of the REDUCE2 package, permits the generation of the matrix elements or the transition strengths for bound-free transitions into any state. The derivation of this formula follows.

The bound state wave functions (Equation (2-2)), labelled by principal quantum number n and angular momentum quantum number l and with atomic number Z , can be written in

a finite series representation (see Appendix B):

$$R(nl;r) = \frac{(-1)^{\frac{n+1}{2}} \frac{n+1/2}{n}}{(n+1)! \frac{1/2}{(n-1-1)!} \frac{1/2}{n+1}} \cdot \left\{ \sum_{j=0}^{n-1-1} \frac{1}{j!} \left(\frac{-n}{2Z} \right)^j \prod_{i=0}^{j-1} (n+1-i)(n-1-1-i) \cdot e^{-Zr/n} r^{n-1-j} \right\}. \quad (5-2a)$$

The terms independent of the variables of integration can be represented by $C(nl)$, and

$$R(nl,r) = C(nl) e^{-Zr/n} r^{n-1-j}. \quad (5-2b)$$

For the free state we have chosen an integral representation with normalization on the energy scale [6]. The kinetic energy of the electron is related to the free state principal quantum number n' by the formula $w=Z^2/2n'^2$ au, where au is twice the ionization potential of hydrogen. Like the energy, n' is continuous, and it is a good quantum number. By using the relationship $\mathbf{p}=2ikr=2iZn/n'$, the free state radial wave functions can be written as

$$R(wl'; r) = \frac{(-1)^{l'+1}}{(1 - e^{-2\pi n'})^{1/2}} \prod_{s=0}^{l'} (s^2 + n'^2)^{1/2} \left(\frac{n'}{2Z} \right)^{l'+1},$$

$$\cdot \frac{r}{2\pi} \oint_c e^{-2iZr\xi/n'} (\xi+1/2)^{-in'-l'-1} (\xi-1/2)^{in'-l'-1} d\xi, \quad (5-3a)$$

where c is a contour taken around the two branch points (see Figure 2-1). Again, for integration purposes, all terms independent of r and ξ can be represented by the constant $C(n'l')$, and

$$R(wl'; r) = C(n'l') r^{-(l'+1)} \frac{1}{2\pi} \oint_c e^{-2iZr\xi/n'} (\xi+1/2)^{-in'-l'-1} (\xi-1/2)^{in'-l'-1} d\xi. \quad (5-3b)$$

By substituting Equations (5-3b) and (5-2b) into (5-1) and interchanging the order of integration it is found that

$$\begin{aligned} & \langle n \, l \mid r^{q+1} \mid n' \, l' \rangle \\ &= C(nl)C(n'l) \frac{1}{2\pi} \oint_c d\xi (\xi+1/2)^{-in'-l'-1} (\xi-1/2)^{in'-l'-1} \\ & \quad \cdot \int_0^\infty dr \, r^{q+n+1-j-l'} e^{-(2iZ\xi/n' + Z/n)r}. \end{aligned}$$

By representing the integral in this manner it can be seen that the integration on r is simply the definite integral

$$\int_0^{\infty} x^n e^{-ax} dx = n! a^{-(n+1)} \quad (a > 0, n \text{ positive integer}),$$

where $x=r$, $n=q+n-l'-1+1$, and $a = (2iZ\xi/n' + Z/n)$. After some algebraic manipulation the matrix element takes the form

$$\begin{aligned} \langle n \ 1 \ | r^{q+1} \ | w \ 1' \rangle &= \frac{C(n)C(n'1')}{(2iZ/n')} \frac{(q+n-l'-j+1)!}{q+n-l'-j+2} \\ &\quad \frac{1}{2\pi} \oint_c d\xi \frac{(\xi+1/2)^{-in'-l'-1} (\xi-1/2)^{in'-l'-1}}{(\xi - in'/2n)^{q+n-l'-j+2}}. \end{aligned} \quad (5-4)$$

The contour integral must be taken around the two branch points $\xi=+1/2$ and $\xi=-1/2$ (see Figure 5-1). Since the integrand goes to zero as ξ raised to the $(-q-n-l'-4+j)$ th power, which is less than ξ to the negative sixth power, the contour may be extended to infinity. Also, since the contour goes around the pole $\xi=in'/2$ in the negative sense, the result of the integration is simply the residue at that pole. The pole is not simple, but is of the order $q+n-l'-j+2$ which shall be referred to as p .

Figure 5-1. In this figure the contour of Equation (5-4) is represented.

The residue for a pole of order p is [33]

$$\text{Res} = \frac{1}{(p+1)!} \left[\frac{d^{p-1}}{dz^{p-1}} [(Z-Z_0)^p f(Z)] \right]_{Z=Z_0}$$

which for this case becomes

$$\frac{1}{(p+1)!} \left[\frac{d^{p-1}}{d\xi^{p-1}} \frac{(\xi - in'/2n)^p (\xi + 1/2)^{-in'-1'-1} (\xi - 1/2)^{in'-1'-1}}{(\xi - in'/2n)^p} \right]_{\xi = in'/2n}$$

or

$$\frac{1}{(p+1)!} \left[\frac{d^{p-1}}{d\xi^{p-1}} (\xi + 1/2)^{-in'-1'-1} (\xi - 1/2)^{in'-1'-1} \right]_{\xi = in'/2n} \quad (5-5)$$

A derivation for a series representation of

$$\frac{d}{d\xi} \frac{\xi^{p-1}}{\xi^{p-1}} \frac{(\xi+1/2)^{-in'-l'-1}}{(\xi-1/2)^{in'-l'-1}}$$

is presented in Appendix D. By use of this formula, evaluated at the pole, the residue becomes

$$\sum_{m=1}^p \frac{(\xi+1/2)^{-in'-l'-m}}{(m-1)!} \frac{(\xi-1/2)^{in'-l'-p+m-1}}{(p-m)!} \cdot \prod_{k=1}^{m-1} (-in'-l'-k) \prod_{k=1}^{p-m} (in'-l'-k) \quad (5-6)$$

In the interest of developing the most symmetric algorithm for use in programming, we use the identity [34]

$$\left(\frac{in'/n - 1}{in'/n + 1} \right)^{in'} = e^{-2n' \operatorname{arccot}(n'/n)}$$

to write the following form for the residue:

$$\begin{aligned} \text{RES} &= (2n)^{2l'+p+1} e^{-2n' \operatorname{arccot}(n'/n)} \\ &\cdot \sum_{m=1}^p \frac{(\xi+n)^{-l'-m}}{(p-m)!} \frac{(\xi-n)^{-l'-p+m-1}}{(m-1)!} \end{aligned}$$

$$\cdot \prod_{k=1}^{m-1} (-in'-l'-k) \prod_{kk=1}^{p-m} (in'-l'-kk) , \quad (5-7)$$

where $p=q+n-l'-j+2$. Finally, substituting $2i(\text{RES})$ for the value of the contour integral, along with the constants $C(nl)$ and $C(n'l')$ given by Equations (3-5a) and (3-6a), into Equation (5-4) gives

$$\begin{aligned} \langle n l | r^{q+1} | n' l' \rangle &= \frac{(-1)^{1/2} e^{-2n' \arccot(n'/n)} (n+1)!}{(n-1-1)! (1-e^{-2\pi n'})^{1/2}} \\ &\quad \frac{\frac{2}{i} \frac{n+l'+1}{q+n-l'+1} \frac{n^{q+1+2}}{z^{q+2}} \frac{n^{q+n+3}}{n'}}{\prod_{s=0}^{l'} \left(s^2 + n'^2 \right)^{1/2}} \\ &\quad \cdot \left\{ \sum_{j=0}^{n-l-1} \left(\frac{i}{2n'} \right)^j \frac{(q+n-l'-j+1)!}{j!} \prod_{i=0}^{j-1} (n+l-i)(n-l-1-i) \right. \\ &\quad \cdot \sum_{m=1}^p \frac{(in'+n)^{-l'-m}}{(p-m)! (m-1)!} \frac{(in'-n)^{-l'-p+m-1}}{(p-m)! (m-1)!} \\ &\quad \cdot \left. \prod_{k=1}^{m-1} (-in'-l'-k) \prod_{kk=1}^{p-m} (in'-l'-kk) \right\} , \quad (5-8) \end{aligned}$$

which, when squared and simplified, yields

$$|\langle n l | r^{q+1} | n' l' \rangle|^2 = \frac{2^{2(n+l'+1)} e^{-4n' \arccot(n'/n)}}{z^{2(q+2)} \frac{2}{n'} + n^2 \frac{2}{2(n+q+2)} (1 - e^{-2\pi n'})}$$

$$\begin{aligned}
& \cdot \prod_{s=1}^{l'} \left(s^2 + n'^2 \right) \frac{2(q+l'+2)}{(n+l)!} \frac{(q+n+3)}{(n-l-1)!} \\
& \cdot \left\| \sum_{j=0}^{n-l-1} \left(\frac{i}{2n'} \right)^j \left(n'^2 + n^2 \right)^j \frac{(q+n-l'-j+1)!}{j!} \prod_{i=0}^{j-1} (n+l-i)(n-l-1-i) \right. \\
& \cdot \sum_{m=1}^p \frac{(in'+n)^{p-m} (in'-n)^{m-1}}{(p-m)! (m-1)!} \prod_{k=1}^{p-m} (-in'-l'-k) \prod_{k=1}^{m-1} (in'-l'-k) \left. \right\|^2.
\end{aligned}
\tag{5-9}$$

The dimensions for the transition strengths are those of area raised to the $(q+1)$ th power divided by energy; in atomic units the dimensions are a^{2q+3}/e^2 . An alternate way to express the same formula is in terms of a factor inversely proportional to the free state quantum number $x=1/n'$ or $w=x^2 Ry$:

$$\begin{aligned}
& |\langle n \ l \ | r^{q+1} \ | \ n' \ l' \rangle|^2 = \\
& \frac{2^{2(l'+n+1)} n^{2(q+l'+2)} e^{-4 \arctan(xn)/x}}{2^{2(q+2)} (n+l)! (n-l-1)! (1 - e^{-2n/x})^2 (x n + 1)^{2(q+n+2)}} \prod_{s=1}^{l'} \left(x^2 s^2 + 1 \right) \\
& \left\| \sum_{j=0}^{n-l-1} \frac{i^j}{2} x^{j-n-1-q+l'} \left(1 + x^2 n^2 \right)^j \frac{(p-1)!}{j!} \prod_{i=0}^{j-1} (n+l-i)(n-l-1-i) \right. \\
& \sum_{m=1}^p \frac{(i+nx)^{p-m} (i-nx)^{m-1}}{(p-m)! (m-1)!} \prod_{k=1}^{p-m} (-i-l'-x-kx) \prod_{k=1}^{m-1} (i-xl'-kx) \left. \right\|^2
\end{aligned}
\tag{5-10}$$

where $p=q+n-l'-j+2$.

It is this final form that is used, in conjunction with the REDUCE2 package, to generate analytic forms for the matrix elements and transition strengths. To study higher energies, application of Equation (5-9) would be more convenient.

The REDUCE program used to generate the radial matrix elements and their squares is contained in Appendix E along with the FORTRAN programs that were used to generate the values for the allowed dipole and quadrupole transition strengths and the cross sections for recombination into all bound states up to $n=7$ and $l=6$. Additional matrix elements can be obtained either by use of the REDUCE program or by request from the author.

VI. RESULTS

1. Overview

We have calculated exact transition strengths, in closed analytical form, for dipole and quadrupole transitions into all bound states up to $l=19$ and $n=20$ using the general formula (Equation (5-10)) derived in the last section and the REDUCE2 program (see Appendix C). These formulas were then used to calculate the partial cross sections for the radiative recombination of an electron-proton system.

The information contained in this chapter is in several parts. First, we present sample matrix elements and their corresponding transition strengths for both dipole and quadrupole transitions. We choose a relatively simple case -- all the angular momentum states of $n=4$ -- but one that exhibits both curve crossings and vanishing transition strengths. We present analytic forms for the matrix elements and transition strengths in addition to plotting them as a function of the kinetic energy of the incoming electron (Figures 6-1 through 6-4). Second, since the transition strengths with free state angular momentum greater than bound state angular momentum ($l' > l$) show the most interesting behavior, we present them, plotted as a function of kinetic energy of the free electron, for all

angular momentum states up to $n=10$ (Figure 6-5a through 6-5j). Third, we present dipole and quadrupole radiative recombination cross sections for all angular momentum states up to $l=19$ and $n=20$ (Figures 6-6a through 6-6s). This is done because, for the recombination process as it occurs in interstellar H II regions, information on the angular momentum distributions of states is required. The cross sections exhibit both the curve crossing behavior and minima due to the zeros of the transition strengths. Fourth, we discuss the behavior of the transition strengths and cross sections, offering a possible explanation for the zeros and curve crossings, a comparison with Cooper minima, and a comparison of the relative importance of the quadrupole to the dipole transitions.

2. The Matrix Elements

The following relationships exist between the REDUCE programs of Appendix C, and the matrix elements.

A) The dipole matrix element is

$$\langle n \ l \ | \ r \ | \ n' \ l' \rangle = \frac{e^{-2\arctan(xn)/x} (n \ l \ | \ r \ | \ n' \ l')}{(1 - e^{-2\pi/x})^{1/2}},$$

where $(n \ l \ | \ r \ | \ n' \ l')$ is generated with the aid of the REDUCE program XMAT(n, l). Sample dipole matrix elements for bound-free transitions into all angular momentum states of

Figure 6-1. The radial part of the dipole matrix elements, $\langle n'l'|r|n'l \rangle$, for all angular momentum states of $n=4$ are presented. The transitions represented are from angular momentum states $l'=l+1$ (top) -- note the curve crossings at low energy -- and $l'=l-1$ (bottom).

$n=4$ follow. Note that some are purely real and some purely imaginary. These matrix elements are plotted, in Figure 6-1, as a function of the kinetic energy of the incoming electron, but with the i suppressed if the element is imaginary. All the curves are labeled by the angular momentum quantum number of the bound state.

$$(4,0 |r| X,1)$$

$$= [\frac{4096}{24} \frac{(1/2)}{6} \frac{(1/2)}{(16 X^2 + 1)^6}]$$

$$\cdot [(X^2 + 1)^{(1/2)}]$$

$$\cdot [8 (- 12288 X^6 - 5376 X^4 - 656 X^2 - 23)]$$

$$(4,1 |r| X,2)$$

$$= [\frac{32768}{120} \frac{(1/2)}{2} \frac{(1/2)}{(16 X^2 + 1)^6}]$$

$$\cdot [(X^2 + 1)^{(1/2)} (4 X^2 + 1)^{(1/2)}]$$

$$\cdot [4 i (1280 X^4 + 224 X^2 + 9)]$$

$$(4,1 |r| X,0)$$

$$= [\frac{512}{120} \frac{(1/2)}{2} \frac{(1/2)}{(16 X^2 + 1)^6}]$$

$$\cdot [16 i (- 20480 X^6 - 11008 X^4 - 1520 X^2 - 57)]$$

$$(4,2 \mid r \mid X,3)$$

$$= [262144/(720^{(1/2)} (16 X^2 + 1)^6)] \\ \cdot [(X^2 + 1)^{(1/2)} (9 X^2 + 1)^{(1/2)} (4 X^2 + 1)^{(1/2)}] \\ \cdot [8 (16 X^2 + 1)]$$

$$(4,2 \mid r \mid X,1)$$

$$= [4096/(720^{(1/2)} (16 X^2 + 1)^6)] \\ \cdot [(X^2 + 1)^{(1/2)}] \\ \cdot [16 (- 768 X^4 - 160 X^2 - 7)]$$

$$(4,3 \mid r \mid X,4)$$

$$= [2097152/(5040^{(1/2)} (16 X^2 + 1)^6)] \\ \cdot [(X^2 + 1)^{(1/2)} (9 X^2 + 1)^{(1/2)} (16 X^2 + 1)^{(1/2)}] \\ \cdot [(4 X^2 + 1)^{(1/2)}] \\ \cdot [- 2 i]$$

$$(4,3 \mid r \mid X,2)$$

$$= [32768/(5040^{(1/2)} (16 X^2 + 1)^6)] \\ \cdot [(X^2 + 1)^{(1/2)} (4 X^2 + 1)^{(1/2)}] \\ \cdot [16 i (16 X^2 + 1)]$$

B) The quadrupole matrix element is

$$\langle n \ l \ | \ r \ | \ n' \ l' \rangle = \frac{e^{-2\arctan(xn)/x} (n \ l \ | \ r \ | \ n' \ l')}{(1 - e^{-2\pi/x})^{1/2}},$$

where $(n \ l \ | \ r \ | \ n' \ l')$ is generated with the aid of the REDUCE2 program QMAT(n,l). Following, are sample quadrupole bound-free matrix elements for all angular momentum states of $n=4$. As in the dipole case, some are real and some imaginary, but there is an additional feature. The $l=0$ curve (Figure 6-2 top), representing the matrix element with bound state $|4,0\rangle$ and free state $|w,2\rangle$, is positive at low energy, changes sign to have a negative value, and finally approach zero from below the axis.

$$(4,0 \ | \ r \ | \ X,2)$$

$$= [131072/(24^{(1/2)} 6^{(1/2)} (16 X^2 + 1)^7)] \\ \cdot [(4 X^2 + 1)^{(1/2)} (X^2 + 1)^{(1/2)}] \\ \cdot [64 (- 3072 X^6 - 384 X^4 + 4 X^2 + 1)]$$

$$(4,1 \ | \ r \ | \ X,3)$$

$$= [1048576/(2^{(1/2)} 120^{(1/2)} (16 X^2 + 1)^7)] \\ \cdot [(4 X^2 + 1)^{(1/2)} (X^2 + 1)^{(1/2)} (9 X^2 + 1)^{(1/2)}] \\ \cdot [8 i (1280 X^4 + 96 X^2 + 1)]$$

Figure 6-2. The radial part of the quadrupole matrix elements, $\langle n l | r^2 | n' l' \rangle$, for all angular momentum states of $n=4$ are presented. The transitions represented are from angular momentum states $l'=l+2$ (top), -- note the curve representing transitions into the bound s state crosses zero -- $l'=l$ (center), and $l'=l-2$ (bottom).

$$\begin{aligned}
& (4,1 \mid r \mid X,1) \\
&= [16384/(2^{(1/2)} 120^{(1/2)} (16 X^2 + 1)^7)] \\
&\quad \cdot [(X^2 + 1)^{(1/2)}] \\
&\quad \cdot [32 i (20480 X^6 + 7936 X^4 + 880 X^2 + 29)]
\end{aligned}$$

$$\begin{aligned}
& (4,2 \mid r \mid X,4) \\
&= [8388608/(720^{(1/2)} (16 X^2 + 1)^7)] \\
&\quad \cdot [(4 X^2 + 1)^{(1/2)} (X^2 + 1)^{(1/2)} (16 X^2 + 1)^{(1/2)}] \\
&\quad \cdot [(9 X^2 + 1)^{(1/2)}] \\
&\quad \cdot [8 (32 X^2 + 1)]
\end{aligned}$$

$$\begin{aligned}
& (4,2 \mid r \mid X,2) \\
&= [131072/(720^{(1/2)} (16 X^2 + 1)^7)] \\
&\quad \cdot [(4 X^2 + 1)^{(1/2)} (X^2 + 1)^{(1/2)}] \\
&\quad \cdot [32 (768 X^4 + 128 X^2 + 5)]
\end{aligned}$$

$$\begin{aligned}
& (4,2 \mid r \mid X,0) \\
&= [2048/(720^{(1/2)} (16 X^2 + 1)^7)] \\
&\quad \cdot [128 (- 49152 X^6 - 18176 X^4 - 1888 X^2 - 59)]
\end{aligned}$$

$$(4,3 \mid r^2 \mid X,5)$$

$$= [67108864/(5040^{(1/2)} (16 X^2 + 1)^7)] \\ \cdot [(25 X^2 + 1)^{(1/2)} (4 X^2 + 1)^{(1/2)} (X^2 + 1)^{(1/2)} \\ \cdot (16 X^2 + 1)^{(1/2)} (9 X^2 + 1)^{(1/2)}] \\ \cdot [-4 i]$$

$$(4,3 \mid r^2 \mid X,3)$$

$$= [1048576/(5040^{(1/2)} (16 X^2 + 1)^7)] \\ \cdot [(4 X^2 + 1)^{(1/2)} (X^2 + 1)^{(1/2)} (9 X^2 + 1)^{(1/2)}] \\ \cdot [32 i (-16 X^2 - 1)]$$

$$(4,3 \mid r^2 \mid X,1)$$

$$= [16384/(5040^{(1/2)} (16 X^2 + 1)^7)] \\ \cdot [(X^2 + 1)^{(1/2)}] \\ \cdot [64 i (3328 X^4 + 480 X^2 + 17)]$$

3. Transition Strengths

The following relationships exist between the REDUCE programs of Appendix C and the transition strengths.

A) The dipole transition strengths are

$$|\langle n \ l \ | \ r \ | \ n' \ l' \rangle|^2 = \frac{e^{-4 \arctan(xn)/x} |\langle n \ l \ | \ r \ | \ n' \ l' \rangle|^2}{(1 - e^{-2\pi/x})},$$

where $|\langle n \ l \ | \ r \ | \ n' \ l' \rangle|^2$ is generated with the aid of the the REDUCE program NEQN(n,l). The dipole bound-free transition strengths, or squares of the matrix elements, for all angular momentum states of $n=4$ are presented next. They are plotted as a function of the kinetic energy of the free electron in Figures 6-3 and 6-5. Note that all transition strengths are positive and real. Note also that, for the cases with $l'=l-1$ (Figure 6-3 bottom), or the free state angular momentum less than the bound state, the value of the transition strengths is always greatest for the lowest angular momentum state. But, when the free state angular momentum is greater than the bound state, $l'=l+1$ (Figure 6-3 top and Figures 6-5a through j), the curves cross each other. The result of this crossing is that, at very low energies, the transition strength for the greatest angular momentum curve ($l=n-1$) is greatest and decreases with decreasing angular momentum.

Figure 6-3. The radial part of the dipole transition strengths, $|\langle n'l | r | n'l' \rangle|^2$, for all angular momentum states of $n=4$ are presented. The transitions represented are from angular momentum states $l'=l+1$ (top) -- note the total curve crossing at low energy -- and $l'=l-1$ (bottom).

$$\begin{aligned}
& |(4,3|r|X,4)|^2 \\
&= [274877906944/(315 (16 X^2 + 1)^{12})] \\
&\cdot [(16 X^2 + 1) (X^2 + 1) (4 X^2 + 1) (9 X^2 + 1)] \\
&\cdot [4]
\end{aligned}$$

$$\begin{aligned}
& |(4,3|r|X,2)|^2 \\
&= [67108864/(315 (16 X^2 + 1)^{12})] \\
&\cdot [(X^2 + 1) (4 X^2 + 1)] \\
&\cdot [256 (256 X^4 + 32 X^2 + 1)]
\end{aligned}$$

$$\begin{aligned}
& |(4,2|r|X,3)|^2 \\
&= [4294967296/(45 (16 X^2 + 1)^{12})] \\
&\cdot [(X^2 + 1) (4 X^2 + 1) (9 X^2 + 1)] \\
&\cdot [64 (256 X^4 + 32 X^2 + 1)]
\end{aligned}$$

$$\begin{aligned}
& |(4,2|r|X,1)|^2 \\
&= [1048576/(45 (16 X^2 + 1)^{12})] \\
&\cdot [X^2 + 1] \\
&\cdot [256 (589824 X^8 + 245760 X^6 + 36352 X^4 + 2240 X^2 + 49)]
\end{aligned}$$

$$\begin{aligned}
& |(4,1|r|X,2)|^2 \\
&= [67108864 / (15 (16 X^2 + 1)^{12})] \\
&\quad \cdot [(X^2 + 1) (4 X^2 + 1)] \\
&\quad \cdot [16 (1638400 X^8 + 573440 X^6 + 73216 X^4 + 4032 X^2 + 81)]
\end{aligned}$$

$$\begin{aligned}
& |(4,1|r|X,0)|^2 \\
&= [16384 / (15 (16 X^2 + 1)^{12})] \\
&\quad \cdot [256 (419430400 X^{12} + 450887680 X^{10} + 183435264 X^8 \\
&\quad + 35799040 X^6 + 3565312 X^4 + 173280 X^2 + 3249)]
\end{aligned}$$

$$\begin{aligned}
& |(4,0|r|X,1)|^2 \\
&= [1048576 / (9 (16 X^2 + 1)^{12})] \\
&\quad \cdot [X^2 + 1] \\
&\quad \cdot [64 (150994944 X^{12} + 132120576 X^{10} + 45023232 X^8 \\
&\quad + 7618560 X^6 + 677632 X^4 + 30176 X^2 + 529)]
\end{aligned}$$

B) The quadrupole transition strengths are

$$| \langle n \ 1 \mid r \mid n' \ 1' \rangle |^2 = \frac{e^{-4 \arctan(xn)/x} | \langle n \ 1 \mid r \mid n' \ 1' \rangle |^2}{(1 - e^{-2\pi/x})},$$

where $| \langle n \ 1 \mid r \mid n' \ 1' \rangle |^2$ is generated by using the REDUCE2 program QNEQN(n,l). Note, the polynomial in the transition strength connecting $|4,0\rangle$ to $|n'2\rangle$ has two sign changes. According to "Descartes rule of signs" the maximum possible number of real positive roots equals the number of sign changes. By comparison of Figures 6-2 and 6-4 it can be seen that the zero in transition strength occurs at the same energy as the sign change in the matrix element.

$$\begin{aligned} | \langle 4,3 \mid r \mid X,5 \rangle |^2 \\ = [281474976710656 / (315 (16 X^2 + 1)^{14})] \\ \cdot [(16 X^2 + 1) (X^2 + 1) (4 X^2 + 1) (9 X^2 + 1) (25 X^2 + 1)] \\ \cdot [16] \end{aligned}$$

$$\begin{aligned} | \langle 4,3 \mid r \mid X,3 \rangle |^2 \\ = [68719476736 / (315 (16 X^2 + 1)^{14})] \\ \cdot [(X^2 + 1) (4 X^2 + 1) (9 X^2 + 1)] \\ \cdot [1024 (256 X^4 + 32 X^2 + 1)] \end{aligned}$$

Figure 6-4. The radial part of the quadrupole transition strengths, $|\langle n1|r^2|n'1'\rangle|^2$, for all angular momentum states of $n=4$ are presented. The transitions represented are from angular momentum states $l'=l+2$ (top), - note the zeros caused by the sign change in the matrix element -- $l'=1$ (center), and $l'=l-2$ (bottom).

$$|(4,3|r|X,1)|^2$$

$$= [16777216 / (315 (16 X^2 + 1)^{14})]$$

$$\cdot [X^2 + 1]$$

$$\cdot [4096 (11075584 X^8 + 3194880 X^6 + 343552 X^4 + 16320 X^2 + 289)]$$

$$|(4,2|r|X,4)|^2$$

$$= [4398046511104 / (45 (16 X^2 + 1)^{14})]$$

$$\cdot [(16 X^2 + 1) (X^2 + 1) (4 X^2 + 1) (9 X^2 + 1)]$$

$$\cdot [64 (1024 X^4 + 64 X^2 + 1)]$$

$$|(4,2|r|X,2)|^2$$

$$= [1073741824 / (45 (16 X^2 + 1)^{14})]$$

$$\cdot [(X^2 + 1) (4 X^2 + 1)]$$

$$\cdot [1024 (589824 X^8 + 196608 X^6 + 24064 X^4 + 1280 X^2 + 25)]$$

$$|(4,2|r|X,0)|^2$$

$$= [262144 / (45 (16 X^2 + 1)^{14})]$$

$$\cdot [16384 (2415919104 X^{12} + 1786773504 X^{10} + 515964928 X^8 + 74432512 X^6 + 5709312 X^4 + 222784 X^2 + 3481)]$$

$$\begin{aligned}
 & |(4,1|r|X,3)|^2 \\
 &= [68719476736 / (15 (16 X^2 + 1)^{14})] \\
 &\quad \cdot [(X^2 + 1) (4 X^2 + 1) (9 X^2 + 1)] \\
 &\quad \cdot [64 (1638400 X^8 + 245760 X^6 + 11776 X^4 + 192 X^2 + 1)]
 \end{aligned}$$

$$\begin{aligned}
 & |(4,1|r|X,1)|^2 \\
 &= [16777216 / (15 (16 X^2 + 1)^{14})] \\
 &\quad \cdot [X^2 + 1] \\
 &\quad \cdot [1024 (419430400 X^{12} + 325058560 X^{10} + 99024896 X^8 \\
 &\quad \quad 15155200 X^6 + 1234688 X^4 + 51040 X^2 + 841)]
 \end{aligned}$$

$$\begin{aligned}
 & |(4,0|r|X,2)|^2 \\
 &= [1073741824 / (9 (16 X^2 + 1)^{14})] \\
 &\quad \cdot [(X^2 + 1) (4 X^2 + 1)] \\
 &\quad \cdot [4096 (9437184 X^{12} + 2359296 X^{10} + 122880 X^8 - 9216 X^6 \\
 &\quad \quad - 752 X^4 + 8 X^2 + 1)]
 \end{aligned}$$

Figure 6-5a. The dipole (top) and quadrupole (bottom) transition strengths for all angular momentum states of $n=1$ for transitions from free states of angular momentum greater than the bound state are presented.

Figure 6-5b. The dipole (top) and quadrupole (bottom) transition strengths for all angular momentum states of $n=2$ for transitions from free states of angular momentum greater than the bound state are presented.

Figure 6-5c. The dipole (top) and quadrupole (bottom) transition strengths for all angular momentum states of $n=3$ for transitions from free states of angular momentum greater than the bound state are presented.

Figure 6-5d. The dipole (top) and quadrupole (bottom) transition strengths for all angular momentum states of $n=4$ for transitions from free states of angular momentum greater than the bound state are presented.

Figure 6-5e. The dipole (top) and quadrupole (bottom) transition strengths for all angular momentum states of $n=5$ for transitions from free states of angular momentum greater than the bound state are presented.

Figure 6-5f. The dipole (top) and quadrupole (bottom) transition strengths for all angular momentum states of $n=6$ for transitions from free states of angular momentum greater than the bound state are presented.

Figure 6-5g. The dipole (top) and quadrupole (bottom) transition strengths for all angular momentum states of $n=7$ for transitions from free states of angular momentum greater than the bound state are presented.

Figure 6-5h. The dipole (top) and quadrupole (bottom) transition strengths for all angular momentum states of $n=8$ for transitions from free states of angular momentum greater than the bound state are presented.

Figure 6-5i. The dipole (top) and quadrupole (bottom) transition strengths for all angular momentum states of $n=9$ for transitions from free states of angular momentum greater than the bound state are presented.

Figure 6-5j. The dipole (top) and quadrupole (bottom) transition strengths for all angular momentum states of $n=10$ for transitions from free states of angular momentum greater than the bound state are presented.

4. The Cross Sections

For the cross sections we substitute Equation (4-6) into Equation (4-3) and identify the partial cross section as a sum of dipole and quadupole terms:

$$\sigma_{nl} = \sigma_{nl}^{(d)} + \sigma_{nl}^{(q)}$$

Therefore, the formula for cross sections for dipole transitions is

$$\begin{aligned} \sigma_{nl}^{(d)} = & \frac{(\pi a_0)^2}{2} \alpha^3 \frac{(n'^2 + n^2)}{n n'} \\ & \cdot \left[\frac{2}{3} \frac{1}{3} |\langle n \ 1 | r | n' \ 1-1 \rangle|^2 \right. \\ & \left. + \frac{2(1+1)}{3} |\langle n \ 1 | r | n' \ 1+1 \rangle|^2 \right], \end{aligned} \quad (6-1)$$

and the cross section formula for quadrupole transistons, using the identity $\omega = \omega_1(n^2 + n'^2)/(nn')^2$, becomes

$$\begin{aligned} \sigma_{nl}^{(q)} = & \frac{(\pi a_0)^2}{2} \alpha^5 \frac{(n'^2 + n^2)}{n n'} \\ & \cdot \left[A(1) |\langle n \ 1 | r^2 | n' \ 1+2 \rangle|^2 + \right. \\ & \left. B(1) |\langle n \ 1 | r^2 | n' \ 1 \rangle|^2 + C(1) |\langle n \ 1 | r^2 | n' \ 1-2 \rangle|^2 \right], \end{aligned} \quad (6-2)$$

where we have simplified by using the identities $e^2/a_0 = 2\hbar\omega_1$ and $e^2 = \alpha\hbar c$ so that ω_1/c is written $\alpha/2a_0$.

In Figures 6-6a through 6-6t we plot the cross sections for recombination into all bound states up to $|20,19\rangle$ as a function of the kinetic energy of the incoming electron. The curve crossing behavior of the transition strengths for free state angular momentum greater than bound state ($l' > l$) is exhibited by the cross sections. This is because the transition strengths with the zeros make an important contribution to the partial cross section. The zeros from the quadrupole transition strengths cause zeros in the quadrupole cross sections for bound s states because there is only one allowed quadrupole transition into an $l=0$ state. The remaining zeros, however, cause minima in the cross sections because they are added to other transition strengths which do not have zeros.

Figure 6-6a. The dipole (top) and quadrupole (bottom) cross sections for recombination into all angular momentum states of $n=1$ are presented.

Figure 6-6b. The dipole (top) and quadrupole (bottom) cross sections for recombination into all angular momentum states of $n=2$ are presented.

Figure 6-6c. The dipole (top) and quadrupole (bottom) cross sections for recombination into all angular momentum states of $n=3$ are presented.

Figure 6-6d. The dipole (top) and quadrupole (bottom) cross sections for recombination into all angular momentum states of $n=4$ are presented.

Figure 6-6e. The dipole (top) and quadrupole (bottom) cross sections for recombination into all angular momentum states of $n=5$ are presented.

Figure 6-6f. The dipole (top) and quadrupole (bottom) cross sections for recombination into all angular momentum states of $n=6$ are presented.

Figure 6-5g. The dipole (top) and quadrupole (bottom) cross sections for recombination into all angular momentum states of $n=7$ are presented.

Figure 6-6h. The dipole (top) and quadrupole (bottom) cross sections for recombination into all angular momentum states of $n=8$ are presented.

Figure 6-6i. The dipole (top) and quadrupole (bottom) cross sections for recombination into all angular momentum states of $n=9$ are presented.

Figure 6-6j. The dipole (top) and quadrupole (bottom) cross sections for recombination into all angular momentum states of $n=10$ are presented.

Figure 6-6k. The dipole (top) and quadrupole (bottom) cross sections for recombination into all angular momentum states of $n=11$ are presented.

Figure 6-61. The dipole (top) and quadrupole (bottom) cross sections for recombination into all angular momentum states of $n=12$ are presented.

Figure 6-6m. The dipole (top) and quadrupole (bottom) cross sections for recombination into all angular momentum states of $n=13$ are presented.

Figure 6-6n. The dipole (top) and quadrupole (bottom) cross sections for recombination into all angular momentum states of $n=14$ are presented.

Figure 6-60. The dipole (top) and quadrupole (bottom) cross sections for recombination into all angular momentum states of $n=15$ are presented.

Figure 6-6p. The dipole (top) and quadrupole (bottom) cross sections for recombination into all angular momentum states of $n=16$ are presented.

Figure 6-6q. The dipole (top) and quadrupole (bottom) cross sections for recombination into all angular momentum states of $n=17$ are presented.

Figure 6-6r. The dipole (top) and quadrupole (bottom) cross sections for recombination into all angular momentum states of $n=18$ are presented.

Figure 6-6s. The dipole (top) and quadrupole (bottom) cross sections for recombination into all angular momentum states of $n=19$ are presented.

Figure 6-6t. The dipole (top) and quadrupole (bottom) cross sections for recombination into all angular momentum states of $n=20$ are presented.

5. Physical Interpretation

At high energy, the transition strengths for zero angular momentum have the greatest value and decrease with increasing angular momentum quantum number l . This order is also followed, at low energy, by the transition strengths that have a free state angular momentum less than or equal to the bound state. However, for transitions with the free state angular momentum greater than the bound state ($l'=l+1$ for the dipole case and $l'=l+2$ for the quadrupole) the order of the curves reverse as the energy of the free electron approaches zero. They reverse because the transition strengths with the greatest angular momentum increase more rapidly, with decreasing energy, thereby crossing over the curves of lower angular momentum. This behavior can be seen most readily in Figures 6-5b through 6-5j where the transition strengths as a function of the free electron kinetic energy are plotted. For $n=2$ (Figure 6-5b) there are only two curves and the crossing takes place at about 10 eV. For $n=3$ (Figure 6-5c) the first crossing takes place, again, at about 10 eV with two more at lower energies. Through $n=4$ (Figure 6-5d) for the quadrupole transition strengths and $n=3$ (Figure 6-5c) for the dipole transition strengths the reversal is complete; for states of higher principal quantum number the curve crossing is incomplete, but only because the complete reversal appears at energies lower than the lowest energy displayed. The pattern, that can be seen by inspection of the rest of the curves for transition

strengths, is (a) the higher the principal quantum number the lower the energy required to exhibit complete curve reversal, and (b) states of high angular momentum cross at lower energies. The quadrupole transition strengths also exhibit curve reversal at low energies; indeed, they are in a more advanced stage than for the dipole transition strengths. For example, the dipole transition strength curves for $n=7$ (Figure 6-5g top) and $l=5$ and $l=6$ states have not, as of 0.01 eV, yet completely crossed the lower angular momentum curves, while, for the quadrupole case (Figure 6-5a bottom) only the $l=6$ state curve is left to cross $l=4$ and 5 at 0.01 eV.

In addition, at energies less than 2 eV, some quadrupole transition strengths vanish for certain values of the free electron kinetic energy, and this has the effect of producing minima in the corresponding cross sections at those values of w . The maximum number of these zeros can be determined by inspection of the formulas for the transition strengths. The detailed behavior, however, can only be determined by calculating their numerical values as a function of the kinetic energy of the incoming electron. The first zero occurs for the bound-free transition into $|3,0\rangle$ from $|W,2\rangle$, and other zeros occur at higher values of n and l .

In an attempt to account for the curve crossings and the zeros we offer the following heuristic argument -- an argument which is based on the angular momentum relationships between the bound and the free states.

A transition is most probable if the bound and free state wave functions have a large overlap. This is true, in general, at low energies. Then, as the kinetic energy of the free electron increases -- the free state wave function contracts -- positive and negative contributions to the radial integral cancel each other causing the matrix elements to decrease in value. Thus, matrix elements have maximum absolute values at zero energy of the free electron and decrease monotonically to zero as energy increases (see Figures 6-1 and 6-3). This is always the case for the dipole matrix elements of hydrogen. We now extend this argument to include information on angular momentum. When the free state has a greater angular momentum than the bound state, the centrifugal barrier causes the free state wave function to be located farther from the origin than the bound state. This decreases the region of greatest overlap and causes the matrix element to have a smaller value. The separation of the free state from the bound state has a more pronounced effect for lower angular momentum final bound states because the bound state wave function is more localized about the nucleus. This is what causes the lower angular momentum curves to decrease in relative importance as energy decreases. Furthermore, the free state for a

quadrupole transition ($l'=l+2$) is even further from the bound state than would be the corresponding free state for the dipole transition. Thus, decreased values of the matrix elements are exhibited by both the dipole and quadrupole transition strengths, but the quadrupole curve crossings happen sooner (at higher energies), because the free states for quadrupole transitions are further from the origin than are the free states for the dipole transitions.

In addition to the increased centrifugal barrier, the quadrupole matrix elements have an extra multiplicative value of r . This weights the matrix elements away from the origin. If other "conditions" are right a sign change for the value of the matrix element can occur. Then, as energy increases and the continuum wave function contracts the value of the matrix element sweeps through a zero, has a maximum absolute value and finally decays toward zero in a "normal" hydrogenic fashion. Again, as in the case of curve crossings, the zeros occur for transitions into bound states with the lowest angular momentum, those concentrated near the nucleus, and come from free states that are concentrated farthest away -- these are the "conditions" necessary for the sign change in the matrix element to occur.

Although the above argument qualitatively accounts for both curve crossing and zeros, it is clear, that they are rather distinct: curve crossings exist for the dipole transitions, while zeros do not; they both exist for

quadrupole transitions. In order to account for the zeros a full wave-mechanical treatment must be used, but a simple classical argument can be used to account for the curve crossings. At low energy and high angular momentum particles are excluded from the region near the nucleus by the centrifugal barrier; thereby, reducing contact with the bound state and making a transition into that state less probable. If the kinetic energy of the particle is increased, it can penetrate the barrier further making more probable the transition. Thus, at high energies the transition probabilities for s states take their "normal" dominant values and probabilities decrease with increasing angular momentum.

We would like to note, at this point, that there are multi-electron systems where zeros occur in the bound-free and bound-bound dipole transition strengths. These zeros produce the well known Cooper minima. The reason these zeros appear is that the matrix element has a zero value for some kinetic energy of the free electron. These zeros are attributed to the departure of the wave functions from a purely hydrogenic behavior.

As a means of comparison we would like to discuss, in more detail, the phenomenon of Cooper minima which occurs during the process of photo-ionization. Zeros occur in the dipole matrix elements for photo-ionization from ground and excited states of multi-electron systems in both the $1 \rightarrow 1+1$

and $l \rightarrow l-1$ transitions [5,35-41]. These zeros do not occur in the dipole matrix elements for hydrogen ground or excited states. Thus, this behavior is due to the deviation of the atomic wave functions from a purely hydrogenic description. The zeros appear, at specific w , because positive and negative contributions to the matrix elements exactly cancel each other. The partial cross section for photo-ionization is given by [6]

$$\sigma(w) = \frac{4\pi\alpha}{3} a_0 N(nl) \frac{(w-w_{nl})^2}{(2l+1)}$$

$$[1 \left| \langle n l | r | n' l-1 \rangle \right|^2 + (l+1) \left| \langle n l | r | n' l+1 \rangle \right|^2],$$

where w_{nl} and w are the binding energy and photoelectron energy respectively and w is related to the free state quantum number n' by the formula $w=Ry/n'^2$. α is the fine structure constant, a_0 is the Bohr radius and $N(nl)$ is the number of electrons in the subshell. A minimum can appear in the cross section if one of the transition strengths has a zero. These minima are known as Cooper minima, and quite a number have been found both theoretically and experimentally.

Because the "final size" of the hydrogen atom grows to approach the wavelength of the emitted radiation (see Figure 4-1), we were lead to examine the relative contributions of quadrupole transitions to the recombination process. In Figure 6-7 we plot the ratios of quadrupole to dipole cross

Figure 6-7. Ratios of the quadrupole to dipole cross sections for $n = 5, 10, 15$ and 20 as a function of energy are presented.

sections as a function of the kinetic energy of the incoming electron for all angular momentum states of $n = 5, 10, 15$ and 20 . We see that the relative contributions increase, as expected, with n ; we also see that the relative contributions increase with l . This is, perhaps, not totally expected because the "final size" of hydrogen decreases with increasing angular momentum -- as can be seen by examination of the formula for the mean value of r [6]:

$$\langle r \rangle = \frac{1}{2Z} [3n^2 - l(l+1)] .$$

At first this may seem a paradox, but it is not difficult to explain. We have been using the "final size" of the hydrogen atom in our qualitative arguments for the importance of quadrupole transitions, whereas we should have been using the "size of the radiating system"; radiating systems with larger angular momenta have larger impact parameters ($l = m v b$ -- with v constant) and, therefore, are larger during the radiation process.

In the energy range of one to ten electron volts, based on our qualitative argument of the relative size of the hydrogen atom to the wavelength of the emitted radiation, we were expecting quadrupole transitions into states with principle quantum numbers greater than 15 to have a relative importance which could be called significant (greater than one one-hundredth -- this figure was arrived at because of the accuracies reported by Burgess [27] in his work on

recombination coefficients and photo-ionization cross sections). We can see, by examination of Figure 6-7, that this is, indeed, true for the higher angular momentum states of $n=15$, and does approach one tenth for $n=20$.

In review, we have calculated the partial radiative recombination cross sections for all bound states of hydrogen up to $n=20$ including contributions from dipole and quadrupole transitions. This was done because, for recombination into highly excited states, the wavelength of the emitted photon is not much larger than the "effective size" of the radiator. In order to calculate these cross sections we generated the transition strengths, in closed analytical form, using the Coulomb wave functions for the description of, not only the bound, but the free state because for low energy recombinations the Coulomb field of the proton, on the electron, cannot be ignored. The transition strengths, or the matrix elements, have only been presented in this form for the lowest bound states because of the extreme complexity of the derivations. We have been able to overcome this problem using the algebraic programming package REDUCE2, and the accuracy of our results is limited only by the accuracy of the constants we used -- eight significant figures. Values of the transition strengths were compared with the values presented by Burgess [27]. When rounded to five significant figures the two methods agree over 90% of the time. The disagreement is due to error propagation in Burgess' numerical method.

Also, as a means of comparison, we sum the partial cross sections for our exact solutions over the angular momentum states of $n=1$ and $n=3$ and plot these curves (see Figure 6-8) along with the values from an approximate formula [6]

$$\sigma_n = \frac{1.96 \pi^2 e^2 \hbar^2 \omega_1^2}{m^2 c^3 \omega(\omega - \omega_n)} \cdot \frac{1}{n^3} .$$

This formula is good for low energy, and, as can be seen by inspection of the curves, it is most accurate in the energy range between one and 100 eV.

Figure 6-8. A comparison of the exact solution (dashed line) -- summed over angular momentum states -- to an approximate solution (solid line) for the cross sections as a function of energy of the incoming electron are presented.

VII. CONCLUSIONS AND COMMENTS

The method we have developed for the study of the recombination process as it occurs in interstellar H II regions was in response to a hypothesis that higher multipole transitions would become increasingly more important as the final size of the hydrogen atom increased. We have found this to be true. Indeed, we have found that the relative importance of quadrupole transitions into high angular momentum states ($l > 15$) is several orders of magnitude greater than for lower angular momentum states. An important application of this result would be for the calculation of the so-called "recombination spectrum" from interstellar H II clouds. This spectrum results from the electron cascade which, in fact, follows the recombination process. If the quadrupole transitions are included for the recombination process the initial population distribution will be modified. It will have more electrons in higher angular momentum states. The resulting cascade spectrum will have more photons emitted at lower energies than in the case where only dipole transitions were included for the recombination process. Further, the effects of still higher order multipole transitions should be investigated for a complete examination of the capture-cascade problem in interstellar H II regions because recombination into states of very high quantum numbers ($n=250$) have been observed.

Of particular interest are the Cooper-like minima shown to exist in the quadrupole cross sections for atomic hydrogen, where there are no minima in the dipole cross sections. The fact that zeros exist in dipole matrix elements for atomic systems is well known. There has been some recent work on the existence of zeros in quadrupole matrix elements of multi-electron atomic systems [39,42-47]. For instance, Wang and Pratt [42] discuss zeros in the $ns_{1/2}$ subshells of uranium with a given potential; they suggest that zeros should be a general feature for all multipole matrix elements, all subshells, all potentials and all elements. We can now say that we have found zeros in the simplest possible multipole transitions -- those for excited states of hydrogen.

We note, however, that although the occurrence of zeros in the dipole transition strengths of atomic systems is attributed to the deviation of their wave functions from a purely hydrogenic description, a clear physical interpretation of the absence of zeros in the dipole transition strengths of atomic hydrogen has not been presented. We see from this work that even atomic hydrogen has zeros in higher multipole transition strengths. It would be interesting if zeros could be understood in a more general way, which might lead to a better understanding of when and in what systems Cooper-like minima will be significant.

Future work in this area, in addition to the capture-cascade problem, might include the study of the angular distribution of photo-electrons for "forbidden" transitions. The angular distribution of photo-electrons is dependent on the type of transition [48]. If the photo-ionized electron is observed at an angle where dipole allowed electrons are not ejected, observation of "forbidden" transitions may be possible. This would be one way to detect the vanishing of transition strengths that occur for quadrupole transitions. For example, we find that the transition strength connecting the bound $|3,0\rangle$ with $|w,2\rangle$ has a zero at about 0.25 eV. This state can be easily populated using two lasers, and a third could photo-ionize the hydrogen. Sweeping the energy of the third laser past the zero would yield a drop in the number of ejected electrons.

APPENDIX A

THE BOUND STATE RADIAL WAVE FUNCTIONS

The bound state radial wave functions, written in terms of the Laguerre polynomials [6,49], are

$$R_{nl}(r) = \frac{(-1)^{l+1} (n-l-1)!}{(n+l)!} \left(\frac{2Z}{n} \right)^{1+3/2} e^{-Zr/n} r^l L_{n+l}^{2l+1}(2Zr/n)$$

where n is the principle quantum number, l is the angular momentum quantum number, Z the atomic number and L_{n+l}^{2l+1} are the Laguerre polynomials which can be represented by the series form [50]

$$L_n^m(x) = \frac{(-1)^m n!}{(n-m)!} \left[x^{n-m} - \frac{n(n-m)}{1!} x^{n-m-1} + \frac{n(n-1)(n-m)(n-m-1)}{2!} x^{n-m-2} + \dots \right]$$

which is a finite series and can also be written in the form

$$L_n^m(x) = \frac{(-1)^m n!}{(n-m)!} \left[\sum_{j=0}^{n-m} \frac{(-1)^j}{j!} x^{n-m-j} \prod_{i=0}^{j-1} (n-i)(n-m-i) \right]$$

Letting $n \rightarrow n+1$, $m \rightarrow 2l+1$ and $x \rightarrow 2Zr/n$ the Laguerre polynomial can be written in terms of the bound state radial wave function, and finally in the form that we use for our derivation of the general form for the matrix element.

$$R(nl) = \frac{(-1)^{n+1+1} \frac{n}{2} Z^{n+1/2} e^{-Zr/n} r^{n-1}}{(n+1)!^{1/2} (n-1-1)!^{1/2} n^{n+1}}$$

$$\sum_{j=0}^{n-1-1} \frac{1}{j!} \left(\frac{-n}{2Zr} \right)^j \prod_{i=0}^{j-1} (n+1-i)(n-1-1-i)$$

APPENDIX B THE ANGULAR MATRIX ELEMENTS

The squares of the angular parts of the matrix elements summed over the m and m' substates can be written in the general form

$$\sum_{mm'} |\langle l m | \cos^q \theta (\sin \theta \cos \theta + \sin \theta \sin \theta) | l' m' \rangle|^2 \quad (B-1)$$

The angular operators can be written in terms of spherical harmonics

$$\sin \theta \cos \theta + \sin \theta \sin \theta = \sqrt{\frac{4\pi}{3}} \sqrt{\frac{1}{2}} \left[(i-1) Y_{11} + (i+1) Y_{1-1} \right],$$

and

$$\cos^q \theta = \left(\frac{4\pi}{3} \right)^{q/2} Y_{10}^q.$$

Substitution of these identities into the matrix elements of Equation (B-1) and squaring gives

$$\sum_{mm'} |\langle l m | \cos^q \theta (\sin \theta \cos \theta + \sin \theta \sin \theta) | l' m' \rangle|^2$$

$$= \left(\frac{4\pi}{3}\right) \left[\sum_{mm'} |\langle 1 m | Y_{10}^q | 1' m' \rangle|^2 + \sum_{mm'} |\langle 1 m | Y_{10}^q | 1' m' \rangle|^2 \right] \quad (B-2)$$

It can be seen, during the derivation of this formula, that the cross terms cancel because the integral product of three spherical harmonics is always real.

For the dipole case $q=0$ and

$$\begin{aligned} & \sum_{mm'} |\langle 1 m | \sin\theta \cos\theta + \sin\theta \sin\theta | 1' m' \rangle|^2 \\ &= \left(\frac{4\pi}{3}\right) \left[\sum_{mm'} |\langle 1 m | Y_{11} | 1' m' \rangle|^2 + \sum_{mm'} |\langle 1 m | Y_{1-1} | 1' m' \rangle|^2 \right]. \end{aligned} \quad (B-3)$$

These angular integrals can be done using the Gaunt Formula, which is a formula for the integral product of three spherical harmonics. The Gaunt formula [51] is

$$\langle 1 m | Y_{LM} | 1' m' \rangle = -1 \sqrt{\frac{(2L+1)(2L'+1)(2L+1)}{4\pi}} \begin{pmatrix} 1 & L & 1' \\ -m & M & m' \end{pmatrix} \begin{pmatrix} 1 & L & 1' \\ 0 & 0 & 0 \end{pmatrix}, \quad (B-4)$$

where the $3j$ symbols, the terms in the parentheses are subject to the triangle conditions $-m+M+m'=0$, $1'+1+L$ is an even integer and $1'+L-1$, $1'-L+1$ and $-1'+L+1$ must all be greater than zero. Application of the triangle conditions give the selection rules for transitions.

The squares of matrix elements, required to find the angular part of the transition strengths are;

$$\sum_{mm'} |\langle 1 m | Y_{11} | 1' m' \rangle|^2 = \frac{(2l+1)(2l'+1)3}{4} \sum_{mm'} \begin{pmatrix} 1 & 1 & 1' \\ -m & 1 & m' \end{pmatrix}^2 \begin{pmatrix} 1 & 1 & 1' \\ 0 & 0 & 0 \end{pmatrix}^2,$$

with the conditions that $(-m+1+m=0)$ and $\Delta l = \pm 1$, and

$$\sum_{mm'} |\langle 1 m | Y_{1-1} | 1' m' \rangle|^2 = \frac{(2l+1)(2l'+1)3}{4} \sum_{mm'} \begin{pmatrix} 1 & 1 & 1' \\ -m-1 & m' \end{pmatrix}^2 \begin{pmatrix} 1 & 1 & 1' \\ 0 & 0 & 0 \end{pmatrix}^2,$$

with the conditions that $(-m-1+m=0)$ and $\Delta l = \pm 1$. Hence,

$$\begin{aligned} & \sum_{mm'} |\langle 1 m | \sin\theta \cos\theta + \sin\theta \sin\theta | 1' m' \rangle|^2 \\ &= (2l+1)(2l'+1) \sum_{mm'} \begin{pmatrix} 1 & 1 & 1' \\ -m & 1 & m' \end{pmatrix}^2 \begin{pmatrix} 1 & 1 & 1' \\ 0 & 0 & 0 \end{pmatrix}^2 [\delta(-m+1+m')] \\ & \quad \times [\delta(l'-l-1) + \delta(l'-l+1)] \\ &+ (2l+1)(2l'+1) \sum_{mm'} \begin{pmatrix} 1 & 1 & 1' \\ -m-1 & m' \end{pmatrix}^2 \begin{pmatrix} 1 & 1 & 1' \\ 0 & 0 & 0 \end{pmatrix}^2 [\delta(-m-1+m')] \\ & \quad \times [\delta(l'-l-1) + \delta(l'-l+1)]. \end{aligned} \quad (B-5)$$

Using the identity for the 3j symbols [51]:

$$\sum_{mM} \begin{pmatrix} 1 & L & 1' \\ m & M & m' \end{pmatrix} \begin{pmatrix} 1 & L & 1'' \\ m & M & m'' \end{pmatrix} = \frac{\delta(l'1'') \delta(m'm'')}{2l'+1},$$

and setting $l'=l''$ and $m'=m''$ the identity takes the form

$$\sum_{mM} \begin{pmatrix} 1 & L & 1' \\ m & M & m' \end{pmatrix}^2 = \frac{1}{2l'+1}.$$

This formula can be used in Equation (B-5) in the form

$$\sum_{mm'} \begin{pmatrix} 1 & L & 1' \\ -m & M & m' \end{pmatrix} = \frac{1}{2L+1},$$

where a permutation identity on the $3j$ symbol has been used. For the dipole case L equals 1 and the sum over the m and m' substates is $1/3$. Therefore, Equation (B-5) simplifies to

$$\sum_{mm'} |\langle 1 \ m | \sin\theta \cos\theta + \sin\theta \sin\theta | 1' m' \rangle|^2 = \frac{2}{3} \left[(2l+1)(2l'+1) \begin{pmatrix} 1 & 1 & 1' \\ 0 & 0 & 0 \end{pmatrix}^2 [\delta(l'-l-1) + \delta(l'-l+1)] \right]. \quad (B-6)$$

This formula has non zero values for two cases. First when $l'=l+1$:

$$\begin{aligned} \sum_{mm'} |\langle 1 \ m | \sin\theta \cos\theta + \sin\theta \sin\theta | l+1, m' \rangle|^2 \\ = \frac{2}{3} (2l+1)(2l+3) \begin{pmatrix} 1 & 1 & l+1 \\ 0 & 0 & 0 \end{pmatrix}^2, \end{aligned}$$

and, second, when $l'=l-1$:

$$\begin{aligned} \sum_{mm'} |\langle 1 \ m | \sin\theta \cos\theta + \sin\theta \sin\theta | l-1, m' \rangle|^2 \\ = \frac{2}{3} (2l+1)(2l-1) \begin{pmatrix} 1 & 1 & l-1 \\ 0 & 0 & 0 \end{pmatrix}^2. \end{aligned}$$

By using the formulas for special cases of $3j$ symbols

$$\begin{pmatrix} 1 & 1 & l+1 \\ 0 & 0 & 0 \end{pmatrix}^2 = \frac{1}{(2l+3)} \quad \text{and} \quad \begin{pmatrix} 1 & 1 & l-1 \\ 0 & 0 & 0 \end{pmatrix}^2 = \frac{1}{(2l+1)(2l-1)},$$

the final results are

$$\sum_{mm'} |\langle l m | \sin\theta \cos\theta + \sin\theta \sin\theta | l+1, m' \rangle|^2 = \frac{2(2l+1)}{3},$$

and

$$\sum_{mm'} |\langle l m | \sin\theta \cos\theta + \sin\theta \sin\theta | l+1, m' \rangle|^2 = \frac{2l}{3}.$$

For the quadrupole integrals ($q=1$) Equation (B-1) becomes

$$\begin{aligned} & \sum_{mm'} |\langle l m | \cos\theta (\sin\theta \cos\theta + \sin\theta \sin\theta) | l' m' \rangle|^2 \\ &= \left(\frac{4\pi}{3}\right)^2 \left[\sum_{mm'} |\langle l m | Y_{10} Y_{11} | l' m' \rangle|^2 + \sum_{mm'} |\langle l m | Y_{10} Y_{1-1} | l' m' \rangle|^2 \right]. \end{aligned}$$

By use of the identity [6]

$$\cos\theta Y_{lm} = \sqrt{\frac{(l+m+1)(l-m+1)}{(2l+1)(2l+3)}} Y_{l+1,m} + \sqrt{\frac{(l+m)(l-m)}{(2l+1)(2l-1)}} Y_{l-1,m}$$

the operators can be written as

$$Y_{10} Y_{11} = \sqrt{\frac{3}{4\pi}} \sqrt{\frac{1}{5}} Y_{21} \quad \text{and} \quad Y_{10} Y_{1-1} = \sqrt{\frac{3}{4\pi}} \sqrt{\frac{1}{5}} Y_{2-1}.$$

Thus, the square of the quadrupole angular matrix elements can be written as follows:

$$\begin{aligned} & \sum_{mm'} |\langle l m | \cos\theta (\sin\theta \cos\theta + \sin\theta \sin\theta) | l' m' \rangle|^2 \\ &= \frac{4\pi}{15} \left[\sum_{mm'} |\langle l m | Y_{21} | l' m' \rangle|^2 + \sum_{mm'} |\langle l m | Y_{2-1} | l' m' \rangle|^2 \right] \end{aligned}$$

Following the same procedure as in the dipole case the Gaunt formula is used in Equation (B-4) to get the results in terms of the 3j symbols. Then, by using the special formulas for 3j symbols [52,53];

$$\begin{pmatrix} 1 & 2 & 1+2 \\ 0 & 0 & 0 \end{pmatrix}^2 = \frac{3}{2} \frac{(1+1)(1+2)}{(2+1+5)(2+1+1)(2+1+3)},$$

$$\begin{pmatrix} 1 & 2 & 1 \\ 0 & 0 & 0 \end{pmatrix}^2 = \frac{1(1+1)}{(2+1+3)(2+1+1)(2+1-1)},$$

and,

$$\begin{pmatrix} 1 & 2 & 1-2 \\ 0 & 0 & 0 \end{pmatrix}^2 = \frac{3}{2} \frac{1(1-1)}{(2+1-3)(2+1-1)(2+1+1)}$$

the final result can be found. For the quadrupole matrix elements the selection rules on l are $\Delta l = 0, \pm 2$ where $l' = 0 \nrightarrow l = 0$. The squares of the angular matrix elements summed on the m and m' substates are:

$$\sum_{mm'} |\langle lm | \cos\theta(\sin\theta\cos\theta + \sin\theta\sin\theta) | l+2, m' \rangle|^2 = \frac{(1+1)(1+2)}{(2+1+3)} \delta(l'-l-2)$$

$$\sum_{mm'} |\langle l m | \cos\theta(\sin\theta\cos\theta + \sin\theta\sin\theta) | l m' \rangle|^2 = \frac{2l(1+1)}{3(2+1+3)(2+1-1)} \delta(l'-l)$$

$$\sum_{mm'} |\langle l m | \cos\theta(\sin\theta\cos\theta + \sin\theta\sin\theta) | l-2, m' \rangle|^2 = \frac{1(1-1)}{(2+1-1)} \delta(l'-l+2)$$

APPENDIX C

PROGRAMS

This section contains the REDUCE2 programs used to generate the matrix elements and the transition strengths, and the FORTRAN programs that use these transition strengths to generate the cross section curves for all angular momentum states up to $n=7$ as a function of energy.

The first group of REDUCE2 procedures will generate the dipole and quadrupole matrix elements. The program XMAT(n,l) (also the command to execute the program) returns the dipole matrix elements for bound free transitions when the bound state is described by the quantum numbers n and l . The program QMAT(n,l), when executed, will return the quadrupole matrix elements for bound-free transitions for bound states described by the quantum numbers n and l .

The second group of REDUCE2 procedures will generate the dipole and quadrupole transition strengths. The program NEQN(n) returns the dipole transition strengths for all angular momentum states of the quantum number n . The program QNEQN(n) will generate the quadrupole transition strengths for all angular momentum states of the bound quantum state n .

The last two programs are FORTRAN programs. They contain the formulas for the dipole and quadrupole transition strengths for all bound states up to $n=7$ and $l=6$. When executed, they build data files for the partial cross sections.

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```

N:=NINIT$
Q:=1$
L2:      LP:=L+2$
        X7:=N*10000+L*100+LP$
WRITE X7,"  CONTINUE";
OFF EXP;
WRITE Y1:=#NONE(N,L,X,LP,Q);
WRITE Y2:=#MTWO(N,L,X,LP,Q);
ON EXP;
WRITE Y3:=#MTHREE(N,L,X,LP,Q);
WRITE"  GO TO 20";
LP:=L$
IF L=0 THEN GO TO L3;
X7:=N*10000+L*100+LP$
WRITE X7,"  CONTINUE";
OFF EXP;
WRITE Y1:=#NONE(N,L,X,LP,Q);
WRITE Y2:=#MTWO(N,L,X,LP,Q);
ON EXP;
WRITE Y3:=#MTHREE(N,L,X,LP,Q);
WRITE"  GO TO 35";
IF L=1 THEN GO TO L3;
LP:=L-2$
X7:=N*10000+L*100+LP$
WRITE X7,"  CONTINUE";
OFF EXP;
WRITE Y1:=#NONE(N,L,X,LP,Q);
WRITE Y2:=#MTWO(N,L,X,LP,Q);
ON EXP;
WRITE Y3:=#MTHREE(N,L,X,LP,Q);
WRITE"  GO TO 60";
L3:  END;

```

```

COMMENT PROCEDURES TO GENERATE THE TRANSITION STRENGTHS FOR$
COMMENT THE DIPOLE AND QUADRUPOLE CASES$
COMMENT NEQN(N) RETURNS ALL DIPOLE TRANSITION STRENGTHS$
COMMENT FOR A GIVEN N WHILE ONEQN(N) RETURNS ALL QUADRUPOLES$
COMMENT TRANSITION STRENGTHS FOR A GIVEN N$
COMMENT $
COMMENT FAC(N) RETURNS THE FACTORIAL OF N$
INTEGER PROCEDURE FAC(N);
BEGIN  INTEGER M$
      N:=1$
      L1: IF N=0 THEN RETURN M;
      M:=M*N$
      N:=N-1$
      GO TO L1
END;
COMMENT $
COMMENT PROCEDURE FOR THE SUM ON P$
PROCEDURE SUMMP(N,L,X,LP,P);
BEGIN  SCALAR TKK,TK,A1,A;
      SUMPH:=0$
      N:=1$
      L1:      MM1:=M-1$
              PMH:=P-M$
              TKK:=1-LP*X-KK*X$

```

```

      TK:=1-LP*X-KK*X$
      A:=(1-H*X)**PMH*((1-H*X)**MM1)/FAC(PMH)/FAC(MM1)$
      IF PMH<1 THEN GO TO L2$
      A1:=FOR JJ:=1:PMH PRODUCT(SUB(KK=JJ,TKK))$
      A:=A*A1$
L2:      IF MM1<1 THEN GO TO L3$
      A1:=FOR J:=1:MM1 PRODUCT(SUB(K=J,TK))$
      A:=A*A1$
L3:      SUMPH:=SUMPH+A$
      IF M=P THEN RETURN SUMPH;
      M:=M-1$
      GO TO L1
END;
COMMENT $
COMMENT PROCEDURE FOR THE SUM ON J$
PROCEDURE SUMJ(N,L,X,LP,Q);
BEGIN  SCALAR NNP,TNP,REXP,TERM,A1;
      JSUMJ:=0$
      NNP:=1-X*X*N*N$
      PPJ:=Q-N-LP+2$
      NML1:=N-L-1$
      REXPR:=(N-L-II )*(N-L-1-II)$
      J:=0$
      L1:      P:=PPJ-J$
      TERM:=2**(-J)*(X**((J-N-1-Q*LP)))*(I**J)*(NNP**J)*FAC(P-1)$
      TERM:=TERM/FAC(J)$
      A1:=FOR JJ:=0:(J-1) PRODUCT(SUB(II=JJ,REXP))$
      TERM:=TERM*A1*SUMP(N,L,X,LP,P)$
      JSUMJ:=JSUMJ+TERM$
      IF J=NML1 THEN RETURN JSUMJ;
      J:=J+1$
      GO TO L1
END;
COMMENT $
COMMENT THE FOLLOWING THREE PROCEDURES ARE EACH PARTS$
COMMENT OF THE TOTAL TRANSITION STRENGTHS$
COMMENT THEY ARE EACH CALLED BY NEQN AND ONEQN$
COMMENT WHICH GENERATE ALL MATRIX ELEMENTS FOR DIPOLES$
COMMENT AND QUADRUPOLE CASES RESPECTIVELY$
PROCEDURE SQNONE(N,L,X,LP,Q);
BEGIN  SCALAR JJJ;
      Z:=1$
      NNP:=1-N*N*X*X$
      OFF EXP;
      X1:=2**((2*(LP+N+1))*N**((2*(Q+LP+2)))/(Z**((2*(Q+2)))/NNP**((2*(Q+N+2))$
      X1:=X1/FAC(N+L)/FAC(N-L-1);
      RETURN X1;
END;
PROCEDURE SQMTWO(N,L,X,LP,Q);
BEGIN  SCALAR JJJ;
      Z:=1$
      SNP:=S**2*X*X+1$
      OFF EXP;
      K2:=(FOR SS:=1:LP PRODUCT(SUB(S=SS,SNP)));
      RETURN X2;
END;
PROCEDURE SQMTHREE(N,L,X,LP,Q);
BEGIN  SCALAR JJJ;
      Z:=1$
      ON EXP;

```

```

      JJJ:=SUMJ(N,L,X,LP,Q)$
      X3:=JJJ*SUB(I=-I,JJJ);
      RETURN X3;
      END;
      COMMENT $
      COMMENT PROCEDURE FOR GENERATION OF THE DIPOLE TRANSITION STRENGTHS $
      PROCEDURE NEQN(NINIT);
      BEGIN INTEGER N,L,LP,Y7;
      Q:=0$
      N:=NINIT$
      L:=NINIT-1$
      L2:      LP:=L+1$
              Y7:=N*10000*L*100+LP$
      WRITE Y7,"      CONTINUE";
      OFF EXP;
      WRITE Y1:=SQMONE(N,L,X,LP,Q);
      WRITE Y2:=SQMTWO(N,L,X,LP,Q);
      ON EXP;
      WRITE Y3:=SQMTHREE(N,L,X,LP,Q);
      WRITE"      GO TO 20";
      IF L=0 THEN GO TO L3;
      LP:=L-1$
      Y7:=N*10000*L*100+LP$
      WRITE Y7,"      CONTINUE";
      OFF EXP;
      WRITE Y1:=SQMONE(N,L,X,LP,Q);
      WRITE Y2:=SQMTWO(N,L,X,LP,Q);
      ON EXP;
      WRITE Y3:=SQMTHREE(N,L,X,LP,Q);
      WRITE"      GO TO 60";
      L:=L-1$
      GO TO L2;
      L3:      END;
      COMMENT $
      COMMENT PROCEDURE FOR GENERATION OF QUADRUPOLE TRANSITION STRENGTHS $
      PROCEDURE QNEQN(NINIT);
      BEGIN INTEGER N,L,LP,X7;
      Q:=1$
      N:=NINIT$
      L:=NINIT-1$
      L2:      LP:=L+2$
              X7:=N*10000*L*100+LP$
      WRITE X7,"      CONTINUE";
      OFF EXP;
      WRITE Y1:=SQMONE(N,L,X,LP,Q);
      WRITE Y2:=SQMTWO(N,L,X,LP,Q);
      ON EXP;
      WRITE Y3:=SQMTHREE(N,L,X,LP,Q);
      WRITE"      GO TO 20";
      LP:=L$
      IF L=0 THEN GO TO L3;
      X7:=N*10000*L*100+LP$
      WRITE X7,"      CONTINUE";
      OFF EXP;
      WRITE Y1:=SQMONE(N,L,X,LP,Q);
      WRITE Y2:=SQMTWO(N,L,X,LP,Q);
      ON EXP;
      WRITE Y3:=SQMTHREE(N,L,X,LP,Q);
      WRITE"      GO TO 35";
      IF L=1 THEN GO TO L4;

```

```

      LP:=L-2$
      X7:=N*10000*L*100+LP$
      WRITE X7,"      CONTINUE";
      OFF EXP;
      WRITE Y1:=SQMONE(N,L,X,LP,Q);
      WRITE Y2:=SQMTWO(N,L,X,LP,Q);
      ON EXP;
      WRITE Y3:=SQMTHREE(N,L,X,LP,Q);
      WRITE"      GO TO 60";
      L4:      L:=L-1$
      GO TO L2;
      L3:      END;

```

[illegible]

[illegible]

```

40100 CONTINUE
Y1=16384.D0/(15.D0*(16.D0*X2+1.D0)**12)
Y2=X2+1.D0
Y3=625.D0*((137391015655.D0*X116+1318359375000.D0*X114+
& 91366787500.D0*X12+106078125000.D0*X10+12733843750.D0*X8+
& 3579940.D0*X6+3565312.D0*X4+173280.D0*X2+3247.D0)
GO TO 20
40001 CONTINUE
Y1=1048576.D0/(9.D0*(16.D0*X2+1.D0)**12)
Y2=X2+1.D0
Y3=64.D0*((150994944.D0*X12+132120576.D0*X10+45023232.D0*X8+
& 7618560.D0*X6+677632.D0*X4+30176.D0*X2+529.D0)
GO TO 20
50005 CONTINUE
Y1=4000000000000.D0/(567.D0*(25.D0*X2+1.D0)**14)
Y2=(25.D0*X2+1.D0)*(X2+1.D0)*(4.D0*X2+1.D0)*(9.D0*X2+1.D0)
& *(16.D0*X2+1.D0)
Y3=4.D0
GO TO 20
50003 CONTINUE
Y1=400000000000.D0/(567.D0*(25.D0*X2+1.D0)**14)
Y2=X2+1.D0*(4.D0*X2+1.D0)*(9.D0*X2+1.D0)
Y3=625.D0*(625.D0*X4+50.D0*X2+1.D0)
GO TO 20
50304 CONTINUE
Y1=400000000000.D0/(63.D0*(25.D0*X2+1.D0)**14)
Y2=(X2+1.D0)*(4.D0*X2+1.D0)*(9.D0*X2+1.D0)*(16.D0*X2+1.D0)
Y3=100.D0*(625.D0*X4+50.D0*X2+1.D0)
GO TO 20
50302 CONTINUE
Y1=400000000.D0/(63.D0*(25.D0*X2+1.D0)**14)
Y2=X2+1.D0*(4.D0*X2+1.D0)
Y3=625.D0*(390625.D0*X6+93750.D0*X4+8125.D0*X2+300.D0*X2+4.D0)
GO TO 20
50203 CONTINUE
Y1=16000000000.D0/(63.D0*(25.D0*X2+1.D0)**14)
Y2=X2+1.D0*(4.D0*X2+1.D0)*(9.D0*X2+1.D0)
Y3=25.D0*(1940625.D0*X8+3937500.D0*X6+298750.D0*X4
& +9900.D0*X2+121.D0)
GO TO 20
50201 CONTINUE
Y1=16000000.D0/(63.D0*(25.D0*X2+1.D0)**14)
Y2=X2+1.D0
Y3=2500.D0*(4306640625.D0*X12+2280468750.D0*X10+474484375.D0*X8+
& 49502500.D0*X6+2736975.D0*X4+76270.D0*X2+841.D0)
GO TO 20
50102 CONTINUE
Y1=160000000.D0/(27.D0*(25.D0*X2+1.D0)**14)
Y2=X2+1.D0*(4.D0*X2+1.D0)*(9.D0*X2+1.D0)
Y3=25.D0*(5831640625.D0*X12+23730468750.D0*X10+4121484375.D0*X8
& +368062500.D0*X6+17839375.D0*X4+445550.D0*X2+4489.D0)
GO TO 20
50100 CONTINUE
Y1=16000.D0/(27.D0*(25.D0*X2+1.D0)**14)
Y2=1.D0
Y3=10000.D0*(1373291015625.D0*X16+162597652500.D0*X14+
& 760195312500.D0*X12+182573437500.D0*X10+24847093750.D0*X8+
& 1979337500.D0*X6+90964500.D0*X4+2220100.D0*X2+22201.D0)
GO CONTINUE
50001 CONTINUE
Y1=8000000.D0/'9.D0*(25.D0*X2+1.D0)**14)

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60102  CONTINUE
Y1=127401884.D0/(35.D0*(36.D0*X2-1.D0)**6)
Y1=X1/((36.D0*X2-1.D0)**10)
Y2=(4.D0*X2+1.D0)*(X2-1.D0)
Y3=49.D0*(697549921.D0*X8+67295228.D0*X6+2415406.D0*X4
& +38220.D0*X2+225.D0)
GO TO 20
70403  CONTINUE
Y1=3305778854.D0/(22275.D0*(49.D0*X2-1.D0)**8)
Y1=X1/((49.D0*X2-1.D0)**10)
Y2=(X2+1.D0)*(4.D0*X2+1.D0)
Y3=196.D0*(4.D0*X2+1.D0)*(9.D0*X2+1.D0)
& +186983783025.D0*X12+8731309946580.D0*X10+
& 737381460711.D0*X8+32257002820.D0*X6+70968303.D0*X4+9550590.D0*
& X2+47961.D0)
GO TO 60
70304  CONTINUE
Y1=64793042714624.D10/(6075.D0*(49.D0*X2-1.D0)**8)
Y1=X1/((49.D0*X2-1.D0)**10)
Y2=(X2+1.D0)*(4.D0*X2+1.D0)
Y3=49.D0*(2802860582025.D0*X12+44957440619950.D0*X10+
& 359610054415.D0*X8+13715520420.D0*X6+289635031.D0*X4+3213518.D0*
& X2+4494.D0)*1.D-10
GO TO 60
70302  CONTINUE
Y1=1686616064.D10/(6075.D0*(49.D0*X2+1.D0)**8)
Y1=X1/((49.D0*X2+1.D0)**10)
Y2=(4.D0*X2+1.D0)*(X2-1.D0)
Y3=153664.D0*(1373401722519225.D0*X16+504514918476450.D0*X14+
& 7780972188395.D0*X12+6575564916120.D0*X10+33268910611.D0*X8+
& 10397698570.D0*X6+195221733.D0*X4+2020060.D0*X2+8836.D0)*1.D-10
GO TO 60
70203  CONTINUE
Y1=16528378272.D10/(1215.D0*(49.D0*X2+1.D0)**8)
Y1=X1/((49.D0*X2+1.D0)**10)
Y2=(X2+1.D0)*(4.D0*X2+1.D0)
Y3=196.D0*(131901501430746369.D0*X16+3993458159759832.D0*X14+
& 5169720769573500.D0*X12+372128373428616.D0*X10+16321339180096.D0*
& X8+446697726632.D0*X6+7465448508.D0*X4+69618808.D0*X2+
& 277729.D0)*1.D-10
GO TO 20
70201  CONTINUE
Y1=302592.D10/(1215.D0*(49.D0*X2+1.D0)**8)
Y1=X1/((49.D0*X2+1.D0)**10)
Y2=X2+1.D0
Y3=49.D0*(58169563130950148729.D0*X20
& +330030601852762974.D0*X18+10562029481731844245.D0*X16
& +161822064919647688.D0*X14+
& 15319506901175554.D0*X12+939068960196636.D0*X10+
& 373349653283650.D0*X8+9978602156824.D0*X6+16423282981.D0*X4+
& 1511787530.D0*X2+6165289.D0)*1.D-10
GO TO 60
70102  CONTINUE
Y1=843308032.D10/(675.D0*(49.D0*X2+1.D0)**8)
Y1=X1/((49.D0*X2+1.D0)**10)
Y2=(X2+1.D0)*(4.D0*X2+1.D0)
Y3=196.D0*(131901501430746369.D0*X16+3993458159759832.D0*X14+
& 5169720769573500.D0*X12+372128373428616.D0*X10+16321339180096.D0*
& X8+446697726632.D0*X6+7465448508.D0*X4+69618808.D0*X2+
& 277729.D0)*1.D-10
GO TO 20
70100  CONTINUE
Y1=12695943672066304.D0/(22275.D0*(49.D0*X2+1.D0)**8)
Y1=X1/((49.D0*X2+1.D0)**10)

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Y1=21952.D10/(.675.D0*(49.D0*X2+1.D0)**8)
Y1=X1/((49.D0*X2+1.D0)**10)
Y2=1.D0
Y3=153664.D0*((4310577706062743240225.D0*X12)*X12+
& 5630423095955027905600.D0*X2+3018370450610881400850.D0*X20+
& 8787347814470519269880.D0*X18+159134562030057173235.D0*X16+
& 180064286057420607360.D0*X14+1328092542939.D0*X12+
& 73541148095197056340.D0*X10+69673405500511.D0*X4+8348695683246.D0*X2+
& 92756481.D0)*1.D-10
& 92756481.D0)*1.D-10
GO TO 60
70001 CONTINUE
Y1=17210368.D10/(2025.D0*(49.D0*X2+1.D0)**8)
Y1=X1/((49.D0*X2+1.D0)**10)
Y2=X2+1.D0
Y3=(2401.D0*((3879519935546999162025.D0*X12)*X12+
& 4170415641578661559700.D0*X2+1833061863525600850.D0
& X20+6071184922118837283260.D0*X18+52351994022024768204.D0*X12+
& 51654232384489093.D0*X10+8517433440744951.D0*X8+
& 193036678278596.D0*X6+27795350731546.D0*X4+232676087812.D0*X2
& 854562829.D0))*1.D-10/4.D0
GO TO 20
3000 CONTINUE
CLOSE(UNIT=21)
END

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C      W=-2.0000000000000000
CC     STEP=0.005000000000
C      DO 1000 I=1, IEND
C      X2=(10*W)/RY
C      EN=X2*PI*0.000000000000
STEP=0.5000000000000000
IF(L-LE-150)STEP=0.0500000000000000
IF(L-LE-150)STEP=0.0100000000000000
IF(L-LE-75)STEP=0.0010000000000000

C      EN=EN+STEP
X2=EN/RY
X=DSORT(X2)
X4=X2*X2
X6=X4*X2
X8=X6*X2
X10=X8*X2
X12=X10*X2
IF(X-1.0000000-10)XXX=1.0000000-10
UP=DEXP(-4./XXX*DATA(N*XXX))
CONTINUE
333  IF(X-LT-0.08)DEN=1.000000000
IF(X-LT-0.08)GO TO 222
DEN=1.000000000-DEXP(-2.000000000*P3.141592654D0/X)
CONTINUE
222  FNNP=UP/DEN
NORM=(X2*FN2+1.000000000000)**5/X2/FN10
C      IF(NP.EQ.10002)GO TO 10002
IF(NP.EQ.10002)GO TO 20002
IF(NP.EQ.20103)GO TO 20103
IF(NP.EQ.30002)GO TO 30002
IF(NP.EQ.30103)GO TO 30103
IF(NP.EQ.30204)GO TO 30204
IF(NP.EQ.40002)GO TO 40002
IF(NP.EQ.40103)GO TO 40103
IF(NP.EQ.40204)GO TO 40204
IF(NP.EQ.40305)GO TO 40305
IF(NP.EQ.50002)GO TO 50002
IF(NP.EQ.50103)GO TO 50103
IF(NP.EQ.50204)GO TO 50204
IF(NP.EQ.50305)GO TO 50305
IF(NP.EQ.50406)GO TO 50406
IF(NP.EQ.60002)GO TO 60002
IF(NP.EQ.60103)GO TO 60103
IF(NP.EQ.60204)GO TO 60204
IF(NP.EQ.60305)GO TO 60305
IF(NP.EQ.60406)GO TO 60406
IF(NP.EQ.60507)GO TO 60507
IF(NP.EQ.70002)GO TO 70002
IF(NP.EQ.70103)GO TO 70103
IF(NP.EQ.70204)GO TO 70204
IF(NP.EQ.70305)GO TO 70305
IF(NP.EQ.70406)GO TO 70406
IF(NP.EQ.70507)GO TO 70507
IF(NP.EQ.70608)GO TO 70608
GO TO 3000
CONTINUE

C      Y=X1Y2*Y3
ONE=Y
IF(L.EQ.0)TWO=0.0
IF(L.EQ.0)GO TO 3535
IF(MZ.EQ.20101)GO TO 20101
IF(MZ.EQ.30101)GO TO 30101
IF(MZ.EQ.30202)GO TO 30202
IF(MZ.EQ.40101)GO TO 40101
IF(MZ.EQ.40202)GO TO 40202
IF(MZ.EQ.40303)GO TO 40303
IF(MZ.EQ.50101)GO TO 50101
IF(MZ.EQ.50202)GO TO 50202
IF(MZ.EQ.50303)GO TO 50303
IF(MZ.EQ.50404)GO TO 50404
IF(MZ.EQ.60101)GO TO 60101
IF(MZ.EQ.60202)GO TO 60202
IF(MZ.EQ.60303)GO TO 60303
IF(MZ.EQ.60404)GO TO 60404
IF(MZ.EQ.60505)GO TO 60505
IF(MZ.EQ.70101)GO TO 70101
IF(MZ.EQ.70202)GO TO 70202
IF(MZ.EQ.70303)GO TO 70303
IF(MZ.EQ.70404)GO TO 70404
IF(MZ.EQ.70505)GO TO 70505
IF(MZ.EQ.70606)GO TO 70606
GO TO 3000
CONTINUE
35  TWO=Y
Y=X1Y2*Y3
CONTINUE
3535 C
IF(L-LE-0)THREE=0.0
IF(L-LE-1)GO TO 70
IF(MM.EQ.30200)GO TO 30200
IF(MM.EQ.40200)GO TO 40200
IF(MM.EQ.50200)GO TO 50200
IF(MM.EQ.50301)GO TO 50301
IF(MM.EQ.50402)GO TO 50402
IF(MM.EQ.60200)GO TO 60200
IF(MM.EQ.60301)GO TO 60301
IF(MM.EQ.60402)GO TO 60402
IF(MM.EQ.60503)GO TO 60503
IF(MM.EQ.70200)GO TO 70200
IF(MM.EQ.70301)GO TO 70301
IF(MM.EQ.70402)GO TO 70402
IF(MM.EQ.70503)GO TO 70503
IF(MM.EQ.70604)GO TO 70604
GO TO 3000
Y=X1Y2*Y3
60  THREE=Y
70  CROSS=(ANG1*ONE+ANG2*TWO+ANG3*THREE)*FNNP*NORM*CON
C70  CROSS=(ONE)*FNNP*ANG1
WRITE(21,21)EN, CROSS
21  FORMAT(1X,F.3X,1E)
W=W+STEP
1000 CONTINUE
C      TYPE N
4  FORMAT(1X,'DO YOU WISH TO CONTINUE? ANSWER 1=YES, OPEN

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1 NEW DATA FILE. 2: YES, SAME DATA FILE. 3: NO, END*')
ACCEPT #, IANS
X=0.0
Y1=0.0, Y2=0.0, Y3=0.0
IF(IANS.EQ.1)CLOSE(UNIT=21)
IF(IANS.EQ.1)GO TO 4000
IF(IANS.EQ.2)GO TO 2000
GO TO 3000
10002 CONTINUE
Y1=256.D0/(X2+1.D0)**8
Y2=(4.D0*X2+1.D0)*(X2+1.D0)
Y3=16.D0
GO TO 20
20103 CONTINUE
Y1=6388608.D0/(3.D0*(4.D0*X2+1.D0)**10)
Y2=(X2+1.D0)*(4.D0*X2+1.D0)*(9.D0*X2+1.D0)
Y3=16.D0
GO TO 20
20101 CONTINUE
Y1=32768.D0/(3.D0*(4.D0*X2+1.D0)**10)
Y2=X2+1.D0
Y3=256.D0*(16.D0*X4+8.D0*X2+1.D0)
GO TO 35
20002 CONTINUE
Y1=272388.D0/(4.D0*X2+1.D0)**10
Y2=(X2+1.D0)*(4.D0*X2+1.D0)
Y3=1024.D0*X4
GO TO 20
30204 CONTINUE
Y1=13060698016.D0/(5.D0*(9.D0*X2+1.D0)**12)
Y2=(9.D0*X2+1.D0)*(X2+1.D0)*(4.D0*X2+1.D0)*(16.D0*X2+1.D0)
Y3=16.D0
GO TO 20
30202 CONTINUE
Y1=10077696.D0/(5.D0*(9.D0*X2+1.D0)**12)
Y2=(4.D0*X2+1.D0)*(X2+1.D0)
Y3=576.D0*(81.D0*X4+18.D0*X2+1.D0)
GO TO 35
30200 CONTINUE
Y1=1776.D0/(5.D0*(9.D0*X2+1.D0)**12)
Y2=1776.D0*(2916.D0*X8+1620.D0*X6+333.D0*X4+30.D0*X2+1.D0)
Y3=331776.D0
GO TO 60
30103 CONTINUE
Y1=362797056.D0/(9.D0*X2+1.D0)**12
Y2=(4.D0*X2+1.D0)*(X2+1.D0)*(9.D0*X2+1.D0)
Y3=16.D0*(729.D0*X4+54.D0*X2+1.D0)
GO TO 20
30101 CONTINUE
Y1=279936.D0/(9.D0*X2+1.D0)**12
Y2=X2+1.D0
Y3=2304.D0*(6561.D0*X8+4374.D0*X6+1053.D0*X4+108.D0*X2+4.D0)
GO TO 20
30002 CONTINUE
Y1=20155392.D0/(9.D0*X2+1.D0)**12
Y2=(X2+1.D0)*(4.D0*X2+1.D0)
Y3=36.D0*(59049.D0*X8+8748.D0*X6+162.D0*X4+36.D0*X2+1.D0)
GO TO 20
40305 CONTINUE
Y1=281474976710656.D0/(315.D0*(16.D0*X2+1.D0)**14)
Y2=(X2+1.D0)*(16.D0*X2+1.D0)*(9.D0*X2+1.D0)*(9.D0*X2+1.D0)*(9.D0*X2+1.D0)
Y3=(16.D0*X2+1.D0)
GO TO 20
40303 CONTINUE
Y1=68719476736.D0/(315.D0*(16.D0*X2+1.D0)**14)
Y2=(X2+1.D0)*(4.D0*X2+1.D0)*(9.D0*X2+1.D0)
Y3=1024.D0*(256.D0*X4+32.D0*X2+1.D0)
GO TO 35
40301 CONTINUE
Y1=16777216.D0/(315.D0*(16.D0*X2+1.D0)**14)
Y2=X2+1.D0
Y3=4096.D0*(11075584.D0*X8+3194880.D0*X6+343552.D0*X4
& +16320.D0*X2+289.D0)
GO TO 60
40204 CONTINUE
Y1=43968051104.D0/(45.D0*(16.D0*X2+1.D0)**14)
Y2=(X2+1.D0)*(4.D0*X2+1.D0)*(9.D0*X2+1.D0)*(9.D0*X2+1.D0)
Y3=64.D0*(1024.D0*X4+64.D0*X2+1.D0)
GO TO 20
40202 CONTINUE
Y1=1073741824.D0/(45.D0*(16.D0*X2+1.D0)**14)
Y2=(X2+1.D0)*(4.D0*X2+1.D0)
Y3=1024.D0*(589824.D0*X8+196608.D0*X6+24064.D0*X4
& +1280.D0*X2+25.D0)
GO TO 35
40200 CONTINUE
Y1=20214.D0/(45.D0*(16.D0*X2+1.D0)**14)
Y2=20214.D0
Y3=15384.D0*(2815919104.D0*X12+176673504.D0*X10+515964928.D0*X8
& +7432512.D0*X6+5709312.D0*X4+222784.D0*X2+3481.D0)
GO TO 60
40103 CONTINUE
Y1=68719476736.D0/(15.D0*(16.D0*X2+1.D0)**14)
Y2=(X2+1.D0)*(4.D0*X2+1.D0)*(9.D0*X2+1.D0)
Y3=64.D0*(1638400.D0*X8+245760.D0*X6+11776.D0*X4+192.D0*X2+1.D0)
GO TO 20
40101 CONTINUE
Y1=16777216.D0/(15.D0*(16.D0*X2+1.D0)**14)
Y2=X2+1.D0
Y3=1024.D0*(419430400.D0*X12+325058560.D0*X10+99024896.D0*X8
& +1515520.D0*X6+123488.D0*X4+51040.D0*X2+841.D0)
GO TO 35
40002 CONTINUE
Y1=1073741824.D0/(9.D0*(16.D0*X2+1.D0)**14)
Y2=(X2+1.D0)*(4.D0*X2+1.D0)
Y3=4096.D0*(9437184.D0*X12+2359296.D0*X10+122880.D0*X8
& +9216.D0*X6+752.D0*X4+8.D0*X2+1.D0)
GO TO 20
50406 CONTINUE
Y1=1000000000000000.D0/(567.D0*(25.D0*X2+1.D0)**6)
Y1=Y1/(25.D0*X2+1.D0)**10
Y2=(X2+1.D0)*(4.D0*X2+1.D0)*(9.D0*X2+1.D0)*(16.D0*X2+1.D0)
& *(36.D0*X2+1.D0)*(25.D0*X2+1.D0)
Y3=16.D0
GO TO 20
50404 CONTINUE
Y1=1000000000000000.D0/(567.D0*(25.D0*X2+1.D0)**6)
Y1=Y1/((25.D0*X2+1.D0)**10)
Y2=(X2+1.D0)*(4.D0*X2+1.D0)*(9.D0*X2+1.D0)*(16.D0*X2+1.D0)

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& 530406250.D0*X6+20577525.D0*X4+434620.D0*X2+3844.D0)*1.D-10
GO TO 35
CONTINUE
50002 Y1=2000000000.D10/(9.D0*(25.D0*X2+1.D0)**16)
Y2=X2+1.D0)*(4.D0*X2+1.D0)
Y3=100.D0*(343227390625.D0*X8)*X8+(10966328125000.D0*X4)*X10+
& 393353537500.D0*X2+12*(117875000.D0*X10-372656250.D0*X8
& 393353537500.D0*X4+3617500.D0*X2+405000.D0*X2+6561.D0)*1.D-10
GO TO 20
CONTINUE
60507 Y1=4731070277129322466.D10/(1925.D0*(36.D0*X2+1.D0)**8)
Y1=X1/((36.D0*X2+1.D0)**10)
Y2=(9.D0*X2+1.D0)*(16.D0*X2+1.D0)*(25.D0*X2+1.D0)*(36.D0*X2+1.D0)
& *(49.D0*X2+1.D0)*(X2+1.D0)*(4.D0*X2+1.D0)
Y3=16.D-10
GO TO 20
CONTINUE
60505 Y1=228252171473536.D10/(1925.D0*(36.D0*X2+1.D0)**8)
Y1=X1/((36.D0*X2+1.D0)**10)
Y2=(16.D0*X2+1.D0)*(25.D0*X2+1.D0)*(X2+1.D0)*(4.D0*X2+1.D0)
& *(9.D0*X2+1.D0)
Y3=23.D0*(1296.D0*X4+72.D0*X2+1.D0)*1.D-10
GO TO 35
CONTINUE
60503 Y1=110075314176.D10/(1925.D0*(36.D0*X2+1.D0)**8)
Y1=X1/((36.D0*X2+1.D0)**10)
Y2=(X2+1.D0)*(4.D0*X2+1.D0)*(9.D0*X2+1.D0)
Y3=746496.D0*(10969344.D0*X8+1324800.D0*X6+59872.D0*X4+1200.D0*X2
& +9.D0)*1.D-10
GO TO 60
CONTINUE
60406 Y1=324683126824509184.D10/(175.D0*(36.D0*X2+1.D0)**8)
Y1=X1/((36.D0*X2+1.D0)**10)
Y2=16.D0*(16.D0*X2+1.D0)*(25.D0*X2+1.D0)*(36.D0*X2+1.D0)
& *(X2+1.D0)*(4.D0*X2+1.D0)
Y3=256.D0*(2916.D0*X4+108.D0*X2+1.D0)*1.D-10
GO TO 20
CONTINUE
60404 Y1=15850845241344.D10/(175.D0*(36.D0*X2+1.D0)**8)
Y1=X1/((36.D0*X2+1.D0)**10)
Y2=(X2+1.D0)*(4.D0*X2+1.D0)*(9.D0*X2+1.D0)*(16.D0*X2+1.D0)
Y3=2304.D0*(41990400.D0*X8+5598720.D0*X6+277344.D0*X4+6048.D0*X2
& +9.D0)*1.D-10
GO TO 35
CONTINUE
60402 Y1=228252171473536.D10/(175.D0*(36.D0*X2+1.D0)**8)
Y1=X1/((36.D0*X2+1.D0)**10)
Y2=(X2+1.D0)*(4.D0*X2+1.D0)
Y3=11843936.D0*(1360888600.D0*X12+3426416640.D0*X10
& +348706944.D0*X8+18377280.D0*X6+530512.D0*X4
& +7980.D0*X2+49.D0)*1.D-10
GO TO 60
CONTINUE
60305 Y1=228252171473536.D10/(35.D0*(36.D0*X2+1.D0)**8)
Y1=X1/((36.D0*X2+1.D0)**10)
Y2=(4.D0*X2+1.D0)*(9.D0*X2+1.D0)*(16.D0*X2+1.D0)*(25.D0*X2+1.D0)
& *(16.D0*X2+1.D0)*(136048896.D0*X8+11757312.D0*X6+370656.D0*X4
& +5040.D0*X2+25.D0)*1.D-10
GO TO 20

```


[illegible]

```

Y1=X1/(49.D0*X2+1.D0)*5
Y1=X1/(49.D0*X2+1.D0)*5
Y1=X1/(49.D0*X2+1.D0)*5
Y2=(X2+1.D0)*(4.D0*X2+1.D0)
Y2=X2*(1.D0*(38795193345646989162025.D0*X12)*X12+
& (38795193345646989162025.D0*X10)+
& (240214617889160923005.D0*X10)*X10
& +(13951788513296584020.D0*X10)*X8-
& (29848750036271881025.D0*X8)*X8-
& (8148364070510829400.D0*X4)*X10-398339614481545716.D0*X12-
& 12650323126887.0.D0*X10+601714730835127.D0*X8+26693055122020.D0*
& X6+546339268314.D0*X4+5660166820.D0*X2+23961025.D0)*1E-10
GO TO 20
3000      CLOSE(UNIT=21)
          END

```

APPENDIX D
THE SERIES REPRESENTATION OF THE DERIVATIVE
IN THE RESIDUE

$$\frac{d^{(p-1)}}{d\xi^{(p-1)}} \left(\xi + \frac{1}{2} \right)^{-in'-l'-1} \left(\xi - \frac{1}{2} \right)^{in'-l'-1} \quad (D-1)$$

let $n=p-1$, $x=\xi$, $y=(\xi + 1/2)$, $z=(\xi - 1/2)$, $a=-in'-l'-1$
and $b=in'-l'-1$ then we can write equation (D-1) as

$$\begin{aligned} & \frac{d^n}{dx^n} y^a z^b \\ &= \sum_{m=0}^n \frac{n!}{(n-m)!m!} \frac{d^m}{dx^m} y^a \frac{d^{n-m}}{dx^{n-m}} z^b \end{aligned} \quad (D-2)$$

The derivatives can also be written in a series form [50]

$$\frac{d^m}{dx^m} y^a = \prod_{k=0}^{m-1} (a-k) y^{a-m}$$

substituting this and a similar series for the $(n-m)$ th derivative of z into equation (D-2) yields

$$\sum_{m=0}^n \frac{n!}{(n-m)!m!} y^{a-m} z^{b-n+m} \prod_{k=0}^{m-1} (a-k) \prod_{k=0}^{n-m-1} (b-k)$$

identifying y , z , a , and n along with letting $m \rightarrow m+1$ yields

$$\sum_{m=1}^{p-1} \frac{(p-1)!}{(p-m)!(m-1)!} (\xi + 1/2)^{-in'-l'-m} (\xi - 1/2)^{in'-l'-1-p+m}$$

$$\prod_{k=0}^{m-1} (-in'-l'-k) \prod_{k=0}^{p-m} (in'-l'-k)$$

(D-3)

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Patricia Marie Fazio was born in Brooklyn, New York in 1952. She received her undergraduate education at Adelphi University in Garden City, New York. After graduating in 1974 with a B.A. in Physics, she entered the United States Air Force. As a Second Lieutenant, she was stationed at the NORAD Cheyenne Mountain Complex as a Space Systems Analyst. In 1976 she entered graduate school at Old Dominion University, Norfolk, Virginia. She received a Masters degree in Physics in 1979, with a thesis on the numerical calculations of Frank-Condon Factors and R-Centroids for diatomic molecules. She remained at Old Dominion University to enter the Ph.D. program in Applied Physics under the supervision of Dr. Gary E. Copeland. She was supported mainly by assistantships and fellowships, and held the position of part time instructor, at Adelphi University, for two summers. She is scheduled to graduate in May 1984, with a thesis on the partial cross sections for radiatively recombining electrons and protons.