A thesis

entitled

Calculation of the Total Electron Excitation Cross Section in the Born Approximation Using Slater Wave Functions for the Li (2s + 2p), Li' (2s + 3p), Na (3s + 4p), Mg (3p + 4s), Ca (4s + 4p) and K (4s + 4p) Excitations

by

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INTRODUCTION

Galactic nebulae which show emission-line spectrum are of two types, that is, diffuse and planetary nebulae. The diffuse nebulae are normally irregular, often of low density and surface brightness, and sometimes extensive; whereas, planetary nebulae are generally symmetrical and compact and usually have a higher surface brightness and density than the diffuse bright nebulae. The spectra of these gaseous nebulae as well as those of certain stars, including the Sun, show strong emission lines owing to allowed and forbidden transitions of a number of "heavy" elements (atoms and ions other than H and He), such as N, O, Ne, S, Cl, Ar, P, Fe, Ca, Mn, Cr, V, Ca and Ni in various stages of ionization. In addition Mg I lines have been observed and Na and K are known to exist in planetary nebulae although not in great abundance.¹

Interpretation of gaseous nebulae requires proper evaluation of their geometrical structure, physical state, and chemical composition. One must be able to interpret the spectra quantitatively in terms of physical parameters and chemical composition of the emitting medium. Consequently, collisional cross-sections for allowed and forbidden transitions and line intensities are necessary for the proper interpretation of the properties of gaseous nebulae. One type of excitation mechanism which is possible is \( e + A \rightarrow e + A^* \).

This paper considers excitations of neutral atoms by inelastic scattering of incident electrons. Simple antisymmetrized product Slater
Wave functions describing the initial and final states of the atom are used. Total cross-sections using the Born Approximation are calculated for the following excitations: Li(2s → 2p), Li(2s → 3p), Na(3s → 4p), Mg(3p → 4s), Ca(4s → 4p) and K(4s → 4p). Since intensities of the emitted radiation are also of importance in interpreting gaseous nebulae, the line strength of the Na(3s → 3p) transition is calculated using Slater Wave functions and compared to an experimental result.

Typical electron temperatures in gaseous nebulae are $10^4$ oK. If a Maxwell distribution is assumed the average kinetic energy at this temperature is about .8 ev. This is below the threshold energy of all of the transitions calculated here. There are of course electrons with energies higher than this average and these appear in the tail of the velocity distribution. In particular for a Maxwell distribution at $10^4$ oK, .9% of the total number of electrons have energies higher than 5 ev. This is above the threshold of all the transitions considered here, the largest threshold being 3.75 ev.

Due to the relatively low abundance in planetary nebulae of the elements for which the total cross sections are calculated here, the particular cross sections given may not be of great interest to those studying these nebulae. However, by using either of the programs given in the Appendix it is relatively simple to obtain cross sections for any desired $s \rightarrow p$ transition. All one needs are the threshold energies and the configuration of the atom to allow the determination of the effective atomic numbers. These effective atomic numbers are calculated
using Slater's rules which are given in the next section. Any determination of the effective atomic numbers using these rules takes only a few minutes.

The reason for choosing Li, Na and K was so that a comparison could be made with another readily available calculation, i.e. (Vainshtein, Opykhtin, Presnyakov). Ca and Mg were chosen because they were originally thought to be of importance in the emission spectra of comets.

The method is not expected to yield reliable results near threshold but should give answers within a factor of 2-7 for incident electron energies about 3-4 times threshold.
WAVE FUNCTIONS

Two types of wave functions are used. Both have the general form $\psi_{n\ell m} = R_{n\ell}(r)Y_{\ell m}(\theta)$ where $R_{n\ell}(r)$ is a Slater radial wave function and $Y_{\ell m}(\theta)$ is a spherical harmonic. In one type which will be referred to as Slater Wave Functions I (SWFI), the $\ell$-dependence of the $R_{n\ell}(r)$'s was deleted. This is equivalent to setting $\ell = 0$ in the radial function for all $n$. The general form of the SWFI is given by the following:

$$R_1(r) = N_1 \exp(-Z_1 r/a_0)$$
$$R_2(r) = N_2 \left[ r \exp(-Z_2 r/2a_0) + A_{21} R_1(r) \right]$$
$$R_3(r) = N_3 \left[ r^2 \exp(-Z_3 r/3a_0) + A_{32} R_2(r) + A_{31} R_1(r) \right]$$
$$\vdots$$
$$R_n(r) = N_n \left[ r^{n-1} \exp(-Z_n r/na_0) + \sum_{j=1}^{n-1} A_{nj} R_j(r) \right]$$

The $N_n$'s and $A_{nj}$'s are constants and are determined from the orthonormality conditions $\langle R_i, R_j \rangle = \delta_{ij}$. Thus,

$$A_{nj} = N_j \left[ \prod_{i=1}^{j-1} A_{ni} A_{ji} - (n+j)! \left( \frac{a_0}{Z_n \frac{1}{j} + \frac{Z_n}{n}} \right)^{n+j+1} \right] \quad j \leq n-1$$

and

$$N_j = \left[ (2j)! \left( \frac{ja_0}{2Z_j} \right)^{2j+1} - \sum_{n=1}^{j-1} A_{jn} \right]^{-1/2}$$
To make the radial integrations simpler the radial wave functions may be rewritten in the following form,

\[ R_n(r) = N \sum_{j=1}^{n} F_{n,n+1-j} r^{n-j} \exp\left(-\frac{Z_{n+1-j}}{n+1-j} \frac{r}{a_0}\right) \tag{1} \]

where the \( F_{n,j} \)'s can be determined from

\[ F_{n,j} = N \sum_{K=1}^{n,n+1-K} F_{n,n+1-K} A_{n+1-K,j} \tag{2} \]

and we choose \( F_{n,n} = 1, A_{n,n} = 0. \) \tag{2'}

The \( Z_n \)'s are effective atomic numbers which are determined by the following Slater rules. 4

"For determining \( Z_n = Z-s \), the electrons are divided into the following groups, each having a different shielding constant: 1s; 2s,p; 3s,p; 3d; 4s,p; 4d; etc. (The s and p are grouped together but the d and f are separated.) The shells are considered to be arranged from the inside out in the order named. The shielding constant s for any group is found as follows,

1. Nothing from any shell outside the one considered.

2. An amount 0.35 from each other electron in the group considered (except in the 1s group, where 0.30 is used instead).

3. If the shell considered is an s,p shell an amount 0.85 for each electron with total quantum number less by one, and an amount 1.00 from each electron still further in; but if the shell is a d or f, an amount 1.00 from every electron inside it."
The second type of wave functions which are used allow for an \( \ell \)-dependence in the radial function. This is accomplished by writing different radial functions with different \( \ell \)-values for the same \( n \). These radial wave functions are referred to as Slater Wave Function II (SWF II) and are given by the following:

\[
R_{10} = N_{10} \exp \left(-\frac{Z_1 r}{a_0}\right)
\]

\[
R_{20} = N_{20} \left[r \exp \left(-\frac{Z_2 r}{2a_0}\right) + A_{201} R_{10}\right]
\]

\[
R_{21} = N_{21} \left[r \exp \left(-\frac{Z_2 r}{2a_0}\right)\right]
\]

\[
\vdots
\]

\[
R_{n\ell} = N_{n\ell} \left[r^{n-1} \exp \left(-\frac{Z_n r}{na_0}\right) + \sum_{n'=\ell+1}^{n-1} A_{n\ell n'} R_{n'\ell} \right]
\]

The \( A_{n\ell n'} \)'s are the amount of the \( R_{n'\ell} \)'s with \( n' \leq n - 1 \) which must be added to \( R_{n\ell} \) to make the \( R_{n\ell} \)'s orthonormal. The \( N_{n\ell} \)'s and the \( A_{n\ell n'} \)'s are again determined from the orthonormality conditions

\[
< R_{n\ell}, R_{n'\ell} > = \delta_{nn'}
\]

\[
A_{n\ell n'} = -N_{n'\ell} \left[(n+n')!\right] \left(\frac{a}{n'}^n + \frac{Z_n}{n}\right)^{n+n'+1} - \sum_{k=1}^{n'-1} A_{n\ell k} A_{n'\ell k} \sum_{n>n'>\ell}^{n'\ell} A_{n'\ell n''}
\]

\[
N_{n\ell} = \left[(2n)!\right] \left(\frac{a}{Z_n^2} \right)^{2\ell+1} - \sum_{j=1}^{n-1} A_{n\ell j} \sum_{\ell}^{2\ell} \left[ A_{n\ell j} \right]^{-\ell^2}
\]

Here again the radial functions can be put into a form which make the radial integrations simpler. Thus...
\[ R_{n \ell} (r) = N \sum_{n \ell} \sum_{j=1}^{n-l} F_{n, \ell, n+l-j} r^{n-j} \exp \left( \frac{Z_{n+l-j} r}{(n+l-j) a_0} \right) \] (3)

where \( F_{n, \ell, j} = N_{n \ell} \sum_{k=1}^{n+l-j} F_{n, \ell, n+l-k} A_{n+l-k, \ell, j} \) and \( A_{n, \ell, j} = 0 \) if \( n \leq j \leq \ell \)

and we choose \( F_{n, \ell, n} = 1 \).
The Schrödinger equation for the atom plus incident electron is

\[
\left[ \frac{\hbar^2}{2m} \nabla^2 + \frac{\lambda^2}{2m} \sum_{i=1}^{Z} \nabla_i^2 + E_T + \sum_{j=1}^{Z} \frac{Ze_i^2}{r_j} - \sum_{i\neq j} \frac{e^2}{|r_i - r_j|} - \sum_{j=1}^{Z} \frac{e^2}{|r - r_j|} \right] \psi(r, r_e) = 0
\]

where \( E_T \) is the total energy,
\( \vec{r} \) refers to the position of the incident electron,
\( \vec{r}_j \) refers to the position of the incident atomic electrons,
\( \vec{r}_e = (r_1 \ldots r_2) \).

Now expand \( \psi(r, r_e) \) in terms of a complete set of orthonormal atomic wave functions \( \psi_n(r_e) \) satisfying the equation

\[
\left[ \frac{\hbar^2}{2m} \sum_{i=0}^{Z} \nabla_i^2 + \sum_{j=1}^{Z} \frac{Ze_i^2}{r_j} - \sum_{i\neq j} \frac{e^2}{|r_i - r_j|} + E_n \right] \psi_n(r_e) = 0
\]

where \( E_n \) are the associated eigenenergies. Now, set

\[
\psi(r, r_e) = S \int \psi_n(r_e) \ \psi_n(r_e)
\]

where \( S \) denotes a summation over the discrete states and an integration over the continuum states.

Substitute equation (6) into equation (4), multiply by \( \psi_n(r_e) \) and integrate with respect to \( r_e \) to obtain
\[
\int \left[ \frac{\hbar^2}{2m} \nabla^2 + \frac{\pi^2}{2m} \sum_{i=1}^{Z} \right] \psi_i^2 + \frac{Ze^2}{r} + \sum_{j=1}^{Z} \frac{Ze^2}{r_j} - \sum_{i \neq j}^{Z} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \cdots
\]

\[
- \frac{2}{\mathbf{r}} \cdot \frac{e^2}{|\mathbf{r} - \mathbf{r}_j|} \right] \right) S_{x \ell} F_{\ell} (\mathbf{r}) \quad \psi_x (\mathbf{r}_e) \times \psi_n^* (\mathbf{r}_e) \ d\mathbf{r}_e = 0 \quad (7)
\]

Now use equation (5) to obtain

\[
\frac{\hbar^2}{2m} \left[ \nabla^2 + \frac{K_n^2}{r} \right] \psi_n (\mathbf{r}) = \int \psi_n (\mathbf{r}_e^+) V (\mathbf{r}, \mathbf{r}_e) \psi (\mathbf{r}, \mathbf{r}_e^+) \ d\mathbf{r}_e \quad (8)
\]

where

\[
V (\mathbf{r}, \mathbf{r}_e^+) = - \frac{Ze^2}{r} + \sum_{j=1}^{Z} \frac{e^2}{|\mathbf{r} - \mathbf{r}_j|} \quad (9)
\]

is the interaction energy between the incident electron and an atom composed of \(Z\) electrons and protons, and the wave number \(K_n\) is given by

\[
K_n^2 = \frac{2m}{\hbar^2} (E_T - E_n) \quad (10)
\]

Now suppose the incident electron has wave vector \(\mathbf{k}_i\) and impinges on an atom in state with energy \(E_i\). Then the asymptotic behavior of \(F_{\ell} (\mathbf{r})\) for larger \(\mathbf{r}\) has the form

\[
F_{\ell} (\mathbf{r}') \sim e^{iK_x' \mathbf{r}'} \delta_{fi} + \frac{e^{iK_x' \mathbf{r}'}}{\mathbf{r}'} f_{\ell} (\theta', \phi') \quad (10)
\]

where \(f_{\ell} (\theta, \phi)\) is the scattering amplitude corresponding to the excitation of the \(\ell\)th state of the atom and \(\theta, \phi\) are the polar angles of \(\mathbf{r}\) referred to the direction of incidence as polar axis.

Consider the equation for the Green's function

\[
\left[ \nabla^2 + K_n^2 \right] G (\mathbf{r}, \mathbf{r}') = \delta (\mathbf{r} - \mathbf{r}')
\]
then the solution to equation (8) can be written as

\[ F_f(\hat{r}') = e^{i K_f \cdot \hat{r}'} \delta_{fi} + \frac{2m}{\hbar^2} \int G(\hat{r}, \hat{r}') \psi^*_f(\hat{r}_e) \psi(\hat{r}, \hat{r}_e) \, d\hat{r}_e \, d\hat{r} \]  

(11)

In order that \( F_f \) should have the correct asymptotic form given by equation (10) we find,

\[ G(\hat{r}, \hat{r}') = -\frac{e^{i K_f \cdot \hat{r}'} \delta_{fi} + \frac{2m}{\hbar^2} \int G(\hat{r}, \hat{r}') \psi^*_f(\hat{r}_e) \psi(\hat{r}, \hat{r}_e) \, d\hat{r}_e \, d\hat{r}}{4\pi |\hat{r} - \hat{r}'|} . \]  

(12)

where \( \hat{K}_f \) is a wave vector in the direction of \( \hat{r} \).

Now

\[ |\hat{r} - \hat{r}'| = (\hat{r}^2 + \hat{r}'^2 - 2\hat{r}\hat{r}' \cos \theta)^{1/2} = \hat{r}' \left[ (\frac{\hat{r}}{\hat{r}'})^2 + 1 - \frac{2\hat{r}}{\hat{r}'} \cos \theta \right]^{1/2} . \]

So for large \( \hat{r}' \)

\[ \frac{1}{|\hat{r} - \hat{r}'|} \sim \frac{1}{\hat{r}'} . \]  

(13)

and

\[ K_f \cdot |\hat{r} - \hat{r}'| \sim K_f \hat{r}' \left[ 1 - \frac{\hat{r}}{\hat{r}'} \cos \theta \right] = K_f \hat{r}' - K_f \hat{r}' \]  

(14)

Then

\[ G(\hat{r}, \hat{r}') \sim \frac{e^{i K_f \cdot \hat{r}'} e^{-i K_f \cdot \hat{r}'}}{4\pi \hat{r}'} . \]  

(15)

Substitute equation (15) into Equation (11) to obtain

\[ F_f(\hat{r}') = e^{i K_f \cdot \hat{r}'} \delta_{fi} - \frac{e^{i K_f \cdot \hat{r}'}}{2\pi n^2} \int e^{-i K_f \cdot \hat{r}'} \psi^*_f(\hat{r}_e) \psi(\hat{r}, \hat{r}_e) \, d\hat{r}_e \, d\hat{r} \]  

(16)

Comparing equation (16) with equation (10), we see that

\[ f_f(\theta, \phi) = -\frac{e^{-i K_f \cdot \hat{r}'} \psi^*_f(\hat{r}_e) \psi(\hat{r}, \hat{r}_e) \, d\hat{r}_e \, d\hat{r}}{2\pi n^2} . \]  

(17)
To obtain the Born scattering amplitude make the assumption that the incident electron interacts only slightly with the target atom so that its wave function may be closely approximated by the plane wave $e^{ik_1 \cdot \mathbf{r}}$ which would be the correct wave function in the absence of all interaction. This approximation should be valid when the speed of the electron is great in comparison to that of the electron in the target atom. This is essentially equivalent to the requirement that $k_1 a \gg 1$ where $a$ is the range of the electron-atom interaction. With the above assumption substitute

$$v(r, r_e) = e^{ik_1 \cdot \mathbf{r}} \psi_1(r_e)$$

into equation (17). Then

$$f_x(\theta, \phi) = -\frac{m}{2\pi\hbar^2} \int e^{i(k_1 - k_F) \cdot \mathbf{r}} v_f(r) dr$$

(18)

where

$$v_f(r) = \int \psi_x^*(r_e) v(r, r_e) \psi_1(r_e) dr_e$$

(19)

Now substitute equation (9) and equation (19) into equation (18) and use Bethe's integral

$$\int \frac{e^{iK_1 \cdot \mathbf{r}_2}}{|r_1 - r_2|} dr_2 = \frac{4\pi}{K^2} e^{-iK_1 \cdot \mathbf{r}_1}$$

to obtain


\[ f_f(\theta, \phi) = \frac{2Zm}{K^2n^2} \int \psi_f^*(\hat{r}_e) \psi_i(\hat{r}_e) \left( e^{i\hat{K}\cdot\hat{r}} \right) d\hat{r}_e \]

\[ -\frac{2m}{K^2n^2} \sum_{j=1}^{Z} \int \psi_f^*(\hat{r}_e) e^{i\hat{K}\cdot\hat{r}_j} \psi_i(\hat{r}_e) d\hat{r}_e \]

where \( \hat{K} = \hat{K}_1 - \hat{K}_f \) and \( \hat{\Delta K} \) is the momentum change of the incident electron.

The first term vanishes due to the orthogonality of the atomic wave function.

So (in atomic units)

\[ f_f(\theta, \phi) = -\frac{2}{K^2} \sum_{j=1}^{Z} \int \psi_f^*(\hat{r}_e) e^{i\hat{K}\cdot\hat{r}_j} \psi_i(\hat{r}_e) d\hat{r}_e \quad (20). \]

Equation (20) can be simplified by writing \( \psi_f(\hat{r}_e) \) and \( \psi_i(\hat{r}_e) \) in terms of antisymmetric product wave functions. Thus

\[ \psi_f(\hat{r}_e) = \psi_f(\hat{r}_1 \ldots \hat{r}_Z) = (Z!)^{-\frac{1}{2}} \varepsilon_{ij\ldots K} \psi_i(\hat{r}_1) \psi_j(\hat{r}_2) \ldots \psi_K(\hat{r}_Z) \]

and

\[ \psi_i(\hat{r}_e) = \psi_i(\hat{r}_1 \ldots \hat{r}_Z) = (Z!)^{-\frac{1}{2}} \varepsilon_{km\ldots n} \psi_k(\hat{r}_1) \psi_m(\hat{r}_2) \ldots \psi_n(\hat{r}_Z) \]

where \( \varepsilon_{ij\ldots K} \) is the permutation symbol

\[ \varepsilon_{ij\ldots K} = \begin{cases} +1 & \text{even permutation} \\ 0 & \text{any two indices the same} \\ -1 & \text{odd permutation} \end{cases} \]
Consider the expression

\[ \sum_{t=1}^{Z} \int \psi^*_f (r_e) e^{iK\cdot r_t} \psi_i (r_e) dr_e \]

\[ = \sum_{t=1}^{Z} \int d\mathbf{r}_1 \ldots d\mathbf{r}_Z \psi^*_f (\mathbf{r}_1 \ldots \mathbf{r}_Z) e^{iK\cdot r_t} \psi_i (\mathbf{r}_1 \ldots \mathbf{r}_Z) \]

\[ = \frac{1}{Z} \sum_{t=1}^{Z} \epsilon_{ij} \ldots K \epsilon_{m \ldots n} \int d\mathbf{r}_1 \ldots d\mathbf{r}_Z \psi^*_f (\mathbf{r}_1) \ldots \psi^*_k (\mathbf{r}_Z) e^{iK\cdot r_t} \psi_l (\mathbf{r}_1) \ldots \psi_n (\mathbf{r}_Z) \tag{21} \]

In order to simplify equation (21) consider the case \( t = 1 \).

Then equation (21) becomes

\[ = \frac{1}{Z} \sum_{t=1}^{Z} \epsilon_{ij} \ldots K \epsilon_{m \ldots n} \int d\mathbf{r}_1 \psi^*_f (\mathbf{r}_1) e^{iK\cdot r_1} \psi_i (\mathbf{r}_1) \delta_{jm} \ldots \delta_{kn} \]

where \( \psi_i (\mathbf{r}_1) \) is the final state wave function that does not appear in the initial state wave functions.

\[ = \frac{1}{Z!} \epsilon_{ij} \ldots K \epsilon_{jl} \ldots K \int d\mathbf{r}_1 \psi^*_f (\mathbf{r}_1) e^{iK\cdot r_1} \psi_i (\mathbf{r}_1) \tag{22} \]

Now use the relation

\[ \epsilon_{a\beta \gamma \ldots \pi} \epsilon_{a' \beta' \gamma' \ldots \pi'} = (P-1)! \delta_{aa'} \]

where \( P \) is the number of subscripts on the \( \epsilon_{a\beta \gamma \ldots \pi} \)'s.

Then equation (22) becomes

\[ = \frac{1}{Z!} (Z-1)! \delta_{il} \int d\mathbf{r}_1 \psi^*_f (\mathbf{r}_1) e^{iK\cdot r_1} \psi_i (\mathbf{r}_1) \]

\[ = \frac{1}{Z} \int d\mathbf{r}_1 \psi^*_f (\mathbf{r}_1) e^{iK\cdot r_1} \psi_i (\mathbf{r}_1) \]
But this shows that all of the terms in the sum in equation (21) are equal. And since there are Z terms in the sum equation (21) becomes

$$\int d\mathbf{r} \psi^*_f(\mathbf{r}) e^{i\mathbf{K}\cdot\mathbf{r}} \psi_i(\mathbf{r})$$

where $\psi_f(\mathbf{r})$ and $\psi_i(\mathbf{r})$ are the final and initial state wave functions of the excited electron.

Using Slater Wave functions the expression for the Born scattering amplitude becomes

$$f(\theta, \phi) = -\frac{Z_0}{K^2} \int d\mathbf{r} r^2 R_n^2(\mathbf{r}) R_{n_1}^2(\mathbf{r}) \langle \ell_f \! m_f | e^{i\mathbf{K}\cdot\mathbf{r}} | \ell_i \! m_i \rangle$$

where

$$\langle \ell_f \! m_f | e^{i\mathbf{K}\cdot\mathbf{r}} | \ell_i \! m_i \rangle = \int d\Omega Y^\ell_{\ell_f \! m_f} (\Omega) e^{i\mathbf{K}\cdot\mathbf{r}} Y_{\ell_i \! m_i} (\Omega)$$

To do the angular integral choose $\mathbf{K}$ to be along the z-axis and use the expansion

$$e^{i\mathbf{K}\cdot\mathbf{r}} = \sum_{\nu=0}^{\infty} i^\nu \left[ \frac{2\pi (2\nu+1)}{\nu!} \right]^{\frac{1}{2}} j_\nu(Kr) Y_{\nu\nu} (\Omega)$$

where $j_\nu(Kr)$ is a spherical Bessel function of the first kind.

For an $s + p$ excitation the angular integral becomes

$$\langle 1 \! m_f | e^{i\mathbf{K}\cdot\mathbf{r}} | oo \rangle = i \sqrt{3} j_1(Kr)$$
To do the radial integral for SWF I use equation (1) which gives the \( R_n \)'s in the terms of the \( F \)'s.

Finally the scattering amplitude for an \( s \rightarrow p \) excitation becomes (for SWF I)

\[
f(K) = \frac{2^{1/2} N_n N_i}{K_{i}^{K_{i}}} \sum_{j=1\ldots n_{i}}^{n_{f}} \frac{F_{n_{f_{i}}n_{f_{i}} + 1 - j} F_{n_{i_{i}}n_{i_{i}} + 1 - K}}{a_{jK}} \frac{(a_{jK} - 2)!}{\rho_{jK}}
\]

\[
\left\{ K(a_{jK} - 1) \sin \theta_{jK} - \pi/2) + \rho_{jK} \cos \left[ (a_{jK} - 1) \theta_{jK} - \pi/2 \right] \right\} (22)
\]

where

\[
a_{jK} = n_{f} + n_{i} + 2 - j - K,
\]

\[
b_{jK} = \left[ \frac{Z_{n_{f} + 1 - j}}{n_{f} + 1 - j} + \frac{Z_{n_{i} + 1 - K}}{n_{i} + 1 - K} \right],
\]

\[
\theta_{jK} = \tan^{-1} \left( \frac{K_{i}}{b_{jK}} \right) \text{ and } \rho_{jK} = \sqrt{b_{jK}^{2} + K_{i}^{2}}
\]

For an \( s \rightarrow p \) excitation the angular integral remains the same when SWF II are used. In this case use equation (3) for \( R_{n_{f_{f}}f} \) and \( R_{n_{i_{i}}l_{i}} \).

So for an \( s \rightarrow p \) excitation with SWF II
\[
f(K) = \frac{2N\sqrt{\delta}}{K^2_i} \sum_{j=1}^{n_f-\delta \frac{N}{f_i}} \sum_{K=1}^{n_i-n_l} \frac{F_{n_f,j,n_i+1-j}}{F_{n_i,j,n_i+1-K}} \ 
\]

Total cross sections were also calculated using an effective potential of the form

\[
V(|r - r'|) = -\frac{e^{-C K^2 |r - r'|}}{|r - r'|}
\]

In dimensionless units

\[
V(|\hat{r} - \hat{r}'|) = -\frac{e^{-\frac{C}{a_o} K^2 (|\hat{r} - \hat{r}'|)}}{|\hat{r} - \hat{r}'|}
\]

Now choose

\[
\frac{C}{a_o} = Z^2 E_T^2
\]

where \(Z\) is the atomic number of the target atom and \(E_T\) is numerically equal to the threshold energy in Rydbergs. The effective potential has an overall effect of replacing the Born scattering amplitude by

\[
f(K) = f_{\text{Born}}(K) / (1 + Z^2 E_T K^2)
\]
TOTAL CROSS SECTION

The total cross-section is given by

\[ \sigma_T = \frac{K_f}{K_i} \int |f(\theta, \phi)|^2 \, d\Omega . \]

Since our \( V(r) \) has azimuthal symmetry

\[ d\Omega = 2\pi \sin \theta \, d\theta \]

the total cross section becomes

\[ \sigma_T = \frac{2\pi K_f}{K_i} \int_0^{\pi} |f(\theta)|^2 \sin \theta \, d\theta . \]

Now from conservation of momentum (\( \vec{h}K \) is momentum vector) we get

\[ \vec{K}^2 = \vec{K}_i^2 + \vec{K}_f^2 - 2\vec{K}_i \cdot \vec{K}_f \cos \theta \]

where \( \vec{h}K \) is the momentum transfer and \( \theta \) is the angle between \( \vec{K}_i \) and \( \vec{K}_f \).

Then

\[ 2K_d\vec{K} = 2\vec{K}_i \cdot \vec{K}_f \sin \theta \, d\theta \]

or

\[ \sin \theta \, d\theta = \frac{K_d\vec{K}}{\vec{K}_i \cdot \vec{K}_f} \]

Now at \( \theta = 0 \)

\[ (K_{\min})^2 = (\vec{K}_i - \vec{K}_f)^2 \quad \text{or} \quad K_{\min} = \vec{K}_i - \vec{K}_f \]
and at $\theta = \pi$

$$(k_{\text{max}})^2 = (k_i + k_f)^2 \quad \text{or} \quad k_{\text{max}} = k_i + k_f.$$ 

From $E = k^2$ and $E_f = E_i - E_T$ where $E_f$ is the energy of the scattered electron, $E_i$ is the incident electron energy and $E_T$ is the threshold energy we get

$$k_{\text{min}}^{\text{max}} = k_i \pm k_f = (E_i)^{\frac{1}{2}} \pm (E_f)^{\frac{1}{2}} = (E_i)^{\frac{1}{2}} \left[ 1 \pm \left( 1 - \frac{E_T}{E_i} \right)^{\frac{1}{2}} \right]$$

And so the integral for the total cross section becomes

$$\sigma_T = \frac{2\pi}{k_i^2} \int_{k_{\text{min}}^{\text{max}}}^{} dK |\phi(K)|^2$$

(26)

Slater's rules are used to determine the effective atomic numbers $Z_n$'s. These values are used to calculate the orthonormality constants $A_{n,l,j}$'s and $N_n$'s for the SWF I and the $A_{n,l,j}$'s and $N_{n,k}$'s for SWF II. The $F_{n,k}$'s and $F_{n,l,j}$'s are in turn calculated from these orthonormality constants. These results are then substituted into equation (22) for SWF I and into equation (25) for SWF II. The scattering amplitude thus obtained must be squared and integrated over the momentum transfer according to equation (26).

The following cross sections were calculated using both SWF I and SWF II: Li(2s $\rightarrow$ 2p), Li(2s $\rightarrow$ 3p), Na(3s $\rightarrow$ 4p), Mg(3p $\rightarrow$ 4s), Ca(4s $\rightarrow$ 4p) and K(4s $\rightarrow$ 4p). Two computer programs which were written to do the calculations are given in the Appendix. The first program calculates the
total cross section using SWF I as follows: First the a_{jK}'s given by

equation (23) are calculated. The b_{jK}'s equation (24) are calcu-
lated. Next, the F_{nn}'s equation (2') and the A_{nn}'s equation (2') are
initialized to 1 and 0 respectively. The N_{nj}'s and A_{nj}'s are calcu-
rated next. These must be calculated together since they depend upon
each other. Then using the calculated N_{nj}'s and A_{nj}'s the F_{nj}'s
equation (2) are calculated. Finally the last part of the program cal-
culates the scattering amplitude f(K) equation (22) squares it and in-
tegrates \( |f(K)|^2 \) over the momentum transfer using Simpson's rule as an
approximation to the integral.

The second program calculates the total cross section using
SWF II. This program calculates the radial integral in addition to
the integral over the momentum transfer. Thus, the N_{nj}'s and the A_{nj}'s
are calculated first. Then the radial integration is done and finally
integral over the momentum transfer is done. Simpson's rule is again
used for both of these integrations.

The results of the calculations are given in graphic form on
the following pages. These results are compared with the calculations
of Vainshtein, Opykhtin, and Presnyakov (VOP) and with experimental data
where available. It was found that the difference in using SWF I and
SWF II for all of the calculated excitations was less than about 5%.
The data are therefore only plotted for one set of wave functions.

Agreement with VOP is very good for the Li(2s \rightarrow 2p) transition.
Both calculations are high with respect to the experimental data given
in reference (9). Agreement with VOP for the Li(2s \rightarrow 3p) transition
is not as good with VOP obtaining a peak cross section which is more than
3/2 times and at a lower energy than the SWF result. No experimental
data could be found for this transition. The SWF result for the
Na(3s \rightarrow 4p) is about an order of magnitude smaller than the VOP calculation up to 5 threshold units and a factor of 3-8 smaller for the higher energies. However, the SWF cross section for this transition has an
oscillation in it. More will be said about this oscillation and attempts
to understand it ($Z_4 = 1.35$ curve) in the conclusions. As can be seen
from the graph the SWF cross-section is closer to the experimental values
given in reference (9). No other calculations or experimental data could
be found for the Mg(3p \rightarrow 4s) and Ca(4s \rightarrow 4p) transitions. Good agreement
with VOP is obtained for the K(4s \rightarrow 4p) transition. The cross section
peaks at roughly the same energy but the VOP peak is about 50% larger
and does not tail off as fast.

All of the Modified Born results show the expected behavior
of a lower cross-section at the lower energies with the approach to the
same value as the Born Approximation at the high energies.

These data are presented in tabular form in Tables I and II on
pages 27, 28 and 29.
Li (2S → 2P)

**Graph:**
- Experimental
- Born (SWF)
- Modified Born
- VOP

**Axes:**
- $Y$ (in $\text{I} \cdot \text{cm}^2$)
- $E_t$ (Threshold Units)

**Legend:**
- Experimental
- Born (SWF)
- Modified Born
- VOP
<table>
<thead>
<tr>
<th>E (threshold units)</th>
<th>Li (2s + 2p)</th>
<th>Li (2s \rightarrow 3p)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Born (SWF)</td>
<td>Mod. Born VOP(7) CC(8) Exp. (9)</td>
</tr>
<tr>
<td>1.16</td>
<td>.101(3) .961(2) .998(2) .284(2) --</td>
<td>.551(0) .399(0) .201(1)</td>
</tr>
<tr>
<td>1.64</td>
<td>.130(3) .125(3) .131(3) .564(2) --</td>
<td>.788(0) .518(0) .187(1)</td>
</tr>
<tr>
<td>2.00</td>
<td>.127(3) .122(3) .129(3) a --</td>
<td>.159(2)</td>
</tr>
<tr>
<td>2.44</td>
<td>.119(3) .115(3) .122(3) a --</td>
<td>.230(2)</td>
</tr>
<tr>
<td>3.56</td>
<td>.995(2) .966(2) .103(3) --</td>
<td>.239(2)</td>
</tr>
<tr>
<td>5.00</td>
<td>.818(2) .797(2) .850(2) a --</td>
<td>.213(2)</td>
</tr>
<tr>
<td>6.76</td>
<td>.674(2) .659(2) .692(2) a --</td>
<td>.186(2)</td>
</tr>
<tr>
<td>11.24</td>
<td>.475(2) .465(2) .501(2) --</td>
<td>.161(2)</td>
</tr>
<tr>
<td>17.00</td>
<td>.351(2) .345(2) .375(2) a --</td>
<td>.156(2)</td>
</tr>
<tr>
<td>24.04</td>
<td>.271(2) .266(2) .298(2) a --</td>
<td>.144(2)</td>
</tr>
</tbody>
</table>

a - Graphically interpolated
TABLE I
(cont.)

<table>
<thead>
<tr>
<th>Na (3s → 4p)</th>
<th>Mg (3s → 4p)</th>
<th>K (4s → 4p)</th>
<th>Ca (4s → 4p)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Born (SWF)</td>
<td>Mod. Born</td>
<td>VOP (7)</td>
<td>Exp (9)</td>
</tr>
<tr>
<td>.266(0)</td>
<td>.211(-1)</td>
<td>.320(1)</td>
<td>--</td>
</tr>
<tr>
<td>.211(0)</td>
<td>.187(-1)</td>
<td>.360(1)</td>
<td>.232(0)</td>
</tr>
<tr>
<td>.194(0)</td>
<td>.245(-1)</td>
<td>.347(1)</td>
<td>.234(0)</td>
</tr>
<tr>
<td>.194(0)</td>
<td>.381(-1)</td>
<td>.311(1)</td>
<td>.230(0)</td>
</tr>
<tr>
<td>.209(0)</td>
<td>.740(-1)</td>
<td>.222(1)</td>
<td>.223(0)</td>
</tr>
<tr>
<td>.219(0)</td>
<td>.103(0)</td>
<td>.170(1)</td>
<td>.214(0)</td>
</tr>
<tr>
<td>.219(0)</td>
<td>.120(0)</td>
<td>.132(1)</td>
<td>.193(0)</td>
</tr>
<tr>
<td>.196(0)</td>
<td>.124(0)</td>
<td>.839(0)</td>
<td>--</td>
</tr>
<tr>
<td>.169(0)</td>
<td>.120(0)</td>
<td>.585(0)</td>
<td>--</td>
</tr>
<tr>
<td>.144(0)</td>
<td>.109(0)</td>
<td>.426(0)</td>
<td>--</td>
</tr>
</tbody>
</table>

a - Graphically interpolated

b - Additional points calculated, n = 1.02, σ = 0.148; n = 1.04, σ = 0.195; n = 1.08, σ = 0.241.
TABLE II

ELECTRON EXCITATION CROSS SECTIONS FOR Na (3s → 4p) USING Z_{41} = 1.35.

(Units of \( \pi a_0^2 \)).

<table>
<thead>
<tr>
<th>E (Threshold units)</th>
<th>1.16</th>
<th>1.64</th>
<th>2.00</th>
<th>2.44</th>
<th>3.56</th>
<th>5.00</th>
<th>6.76</th>
<th>11.24</th>
<th>17.00</th>
<th>24.04</th>
</tr>
</thead>
<tbody>
<tr>
<td>Born (SWF)</td>
<td>.469(0)</td>
<td>.477(0)</td>
<td>.555(0)</td>
<td>.657(0)</td>
<td>.818(0)</td>
<td>.883(0)</td>
<td>.878(0)</td>
<td>.781(0)</td>
<td>.664(0)</td>
<td>.563(0)</td>
</tr>
<tr>
<td>Mod. Born</td>
<td>.313(-1)</td>
<td>.581(-1)</td>
<td>.119(0)</td>
<td>.202(0)</td>
<td>.367(0)</td>
<td>.478(0)</td>
<td>.532(0)</td>
<td>.537(0)</td>
<td>.489(0)</td>
<td>.433(0)</td>
</tr>
</tbody>
</table>
LINE STRENGTH OF $\text{Na}(3s \rightarrow 3p)$ LINE

The line strength for spontaneous emission in the dipole approximation is given by \( ^{10} \)

\[
S = \sum_{i,K} \left| \tilde{R}_{i,m}^{n} \right|^2 \tag{27}
\]

where \( i \) and \( K \) number the degenerate sublevels of the upper state \( n \) and lower state \( m \); and where the summation is over all possible combinations of the sublevels of the upper state with those of the lower state; and where

\[
\tilde{R}_{nm} = \langle n | \tilde{r} | m \rangle \tag{28}
\]

It will now be shown how \( S \) is related to the Einstein coefficient for spontaneous emission. This will be done semiclassically in the sense that the \( E \) and \( M \) field is treated classically while the particles are treated quantum mechanically. A correct quantum electrodynamical treatment leads to the same results \(^{11} \).

Maxwell's equations of motion for the electromagnetic field are in gaussian units

\[
\nabla \cdot \mathbf{E} = 4\pi \rho \tag{29}
\]

\[
\nabla \times \mathbf{E} - \frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} = \frac{4\pi}{c} \mathbf{J} \tag{30}
\]

\[
\nabla \times \mathbf{B} + \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} = 0 \tag{31}
\]

\[
\nabla \cdot \mathbf{B} = 0 \tag{32}
\]
From equation (32), we see $\ddot{H} = \dot{V} \times \dot{A}$. If this is substituted into equation (31) and the order of the spatial and time derivatives is interchanged we obtain

$$\dot{V} \times (\dot{E} + \frac{1}{c} \frac{\partial \dot{A}}{\partial t}) = 0.$$  

Thus

$$\dot{E} + \frac{1}{c} \frac{\partial \dot{A}}{\partial t} = - \dot{V} \phi$$

or

$$\dot{E} = - \frac{1}{c} \frac{\partial \dot{A}}{\partial t} - \dot{V} \phi$$

Substitution of the equations for $\dot{E}$ and $\dot{H}$ into equations (29) and (30)

$$\dot{V} \left( \ddot{\phi} + \frac{1}{c} \frac{\partial \phi}{\partial t} + \frac{V^2 A}{c^2} + \frac{\partial^2 A}{\partial t^2} \right) = \frac{4\pi}{c} \frac{3}{3}$$

(33)

$$\frac{1}{c} \frac{\partial}{\partial t} \frac{\partial}{\partial t} \dot{V} \cdot \dot{A} + V^2 \phi = - 4\pi \rho$$

(34)

where $\dot{V} \times (\dot{V} \times \dot{A}) = \dot{V} (\ddot{V} \cdot \dot{A}) - V^2 \dot{A}$ has been used. Now choose the Lorentz gauge so that

$$\dot{V} \cdot \dot{A} + \frac{1}{c} \frac{\partial \phi}{\partial t} = 0$$

Then equations (33) and (34) become

$$V^2 \ddot{A} - \frac{1}{c^2} \frac{\partial^2 A}{\partial t^2} = - \frac{4\pi}{c} \frac{3}{3}$$

(35)

$$V^2 \phi - \frac{1}{c^2} \frac{\partial^2 \phi}{\partial t^2} = 4\pi \rho$$

(36)
Now, taking the curl of equation (35) we obtain

\[ \nabla^2 \mathbf{H} - \frac{1}{c^2} \frac{\partial^2 \mathbf{H}}{\partial t^2} = - \frac{4\pi}{c} \nabla \times \mathbf{J} \]  \hspace{1cm} (37)

Assume that the three cartesian components of \( \mathbf{J} \) vary harmonically in time with the same angular frequency \( \omega \) but not necessarily with the same phase:

\[ \mathbf{J}_x (\mathbf{r}, t) = 2 |\mathbf{J}_x (\mathbf{r})| \cos (\omega t - \phi_x) = \mathbf{J}_x (\mathbf{r}) e^{-i\omega t} + \mathbf{J}_x^* (\mathbf{r}) e^{i\omega t} \]  \hspace{1cm} (38)

where

\[ \mathbf{J}_x (\mathbf{r}) = |\mathbf{J}_x (\mathbf{r})| e^{i\theta_x} \]

with similar equations for the y and z components. We are interested only in the solutions for \( \mathbf{E} \) and \( \mathbf{H} \) that have the same frequency \( \omega \). Thus the x-components are given by

\[ E_x (\mathbf{r}, t) = 2 |E_x (\mathbf{r})| \cos (\omega t - \phi_x) = E_x (\mathbf{r}) e^{i\omega t} + E_x^* (\mathbf{r}) e^{-i\omega t} \]  \hspace{1cm} (39)

\[ H_x (\mathbf{r}, t) = 2 |H_x (\mathbf{r})| \cos (\omega t - \alpha_x) = H_x (\mathbf{r}) e^{-i\omega t} + H_x^* (\mathbf{r}) e^{i\omega t} \]  \hspace{1cm} (40)

where

\[ E_x (\mathbf{r}) = |E_x (\mathbf{r})| e^{i\phi_x} \quad \text{and} \quad H_x (\mathbf{r}) = |H_x (\mathbf{r})| e^{i\alpha_x} \]

Using equation (30) \( \mathbf{H} \) is given in terms of \( \mathbf{H} \) in a vacuum by

\[ \mathbf{E} (\mathbf{r}) = \frac{ic}{\omega} \nabla \times \mathbf{H} (\mathbf{r}) . \]  \hspace{1cm} (41)
Substituting the expressions for $\mathbf{J}$, $\mathbf{H}$ and $\mathbf{E}$ into the wave equation for $\mathbf{H}$, equation (37), we obtain,

$$(\nabla^2 + K^2) \mathbf{H}(\mathbf{r}) = -\frac{4\pi}{c} \mathbf{\nabla} \times \mathbf{J}(\mathbf{r}) \quad K = \omega/c \quad (42)$$

The retarded solution of the above equation is given by

$$\mathbf{H}(\mathbf{r}) = \frac{1}{c} \int \frac{\mathbf{\nabla} \times \mathbf{J}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \ e^{iK|\mathbf{r} - \mathbf{r}'|} \ d^3r' \quad (43)$$

Now

$$e^{iK|\mathbf{r} - \mathbf{r}'|} \sim \frac{1}{r} \quad (44)$$

where $\theta$ is the angle between $\mathbf{r}$ and $\mathbf{r}'$.

The Poynting vector is

$$\mathbf{P}(\mathbf{r},t) = \frac{c}{4\pi} \left[ \mathbf{E}(\mathbf{r},t) \times \mathbf{H}(\mathbf{r},t) \right]$$

Using equations (39) and (40) for $\mathbf{E}$ and $\mathbf{H}$, we see that the average over a period of oscillation has a $z$ component

$$P_z(\mathbf{r}) = \frac{c}{\pi} \left\{ |E_x(\mathbf{r})| \ \ |H_y(\mathbf{r})| \ \left[ \cos(\omega t - \phi_x) \ \cos(\omega t - \alpha_y) \right]_{\text{time ave}} \right.$$

$$- |E_y(\mathbf{r})| \ \ |H_x(\mathbf{r})| \ \left[ \cos(\omega t - \phi_y) \ \cos(\omega t - \alpha_x) \right]_{\text{time ave}}$$

$$P_z(\mathbf{r}) = \frac{c}{2\pi} \left[ E_x(\mathbf{r}) \ \ |H_y(\mathbf{r})| \ \cos(\phi_x - \alpha_y) - E_y(\mathbf{r}) \ \ E_x(\mathbf{r}) \ \ cos(\alpha_x - \phi_y) \right]$$
Then

$$\mathcal{P}(\mathbf{r}) = \frac{c}{2\pi} \text{Re} \left[ \mathcal{E}(\mathbf{r}) \times \mathcal{H}(\mathbf{r}) \right] \quad (45)$$

Now we are only interested in those terms in the energy flux that fall off as $1/r^2$ since only these correspond to radiated energy. Choose the $z$-axis along the vector $\mathbf{r}$ which goes from the center of the charge-current distribution to the point at which the field is measured.

Using equations (41), (43), and (44) we obtain

$$\begin{align*}
\mathcal{H}_x &= -\frac{iK}{rc} e^{iKr} \int J_y(\mathbf{r'}) e^{-iKz'} d^3r' \\
\mathcal{H}_y &= \frac{iK}{rc} e^{iKr} \int J_x(\mathbf{r'}) e^{-iKz'} d^3r' \\
\mathcal{H}_z &= 0 \quad (46)
\end{align*}$$

$$\begin{align*}
\mathcal{E}_x &= \frac{iK}{rc} e^{iKr} \int J_y(\mathbf{r'}) e^{-iKz'} d^3r' \\
\mathcal{E}_y &= \frac{iK}{rc} e^{iKr} \int J_y(\mathbf{r'}) e^{-iKz'} d^3r' \\
\mathcal{E}_z &= 0
\end{align*}$$

Partial integration has been used to get rid of the derivatives of the integrand of $\mathcal{H}$. The above equations show that the asymptotic fields are transverse to the direction of propagation. They also show that only the component of the current perpendicular to the direction of propagation contributes to the radiated energy.
Substituting these fields into equation (45) we obtain

\[ P_z = \frac{K^2}{2\pi r^2 c} \left[ \left| \int J_x e^{iKz'} d^3r' \right|^2 + \left| \int J_y e^{-iKz'} d^3r' \right|^2 \right] \]

Generalizing the above equation to give the average energy flux in the direction of \( \hat{K} \) we obtain

\[ P_z = \frac{K^2}{2\pi r^2 c} \left| \int J_{\perp K}(r') e^{i\hat{K}\cdot\hat{r}'} d^3r' \right|^2 \]

where \( J_{\perp K} \) is the component of \( \vec{J} \) perpendicular to \( \hat{K} \).

In most cases of practical interest the wavelength of the radiation is many times greater than the linear dimensions of the current-charge distribution. This means that \( R\cdot r' \ll 1 \) and \( e^{-iK\cdot r'} \) can be replaced by 1 in the integrand of the equation for \( P_z \). Then

\[ P_z = \frac{K^2}{2\pi r^2 c} \left| \int J_{\perp K}(r') d^3r' \right|^2 \tag{47} \]

From equation (46) with the same approximation it is apparent that the polarization of the radiation is determined by the total current vector

\[ \vec{J}_o = \int \vec{J}(r') d^3r' \]

With \( \vec{J}_o \) linearly polarized the integral in equation (47) can be replaced by \( |\vec{J}_o|^2 \sin^2 \theta \) where \( \theta \) is the angle between \( \hat{K} \) and \( \vec{J}_o \). Then the total power radiated is

\[ P = \frac{K^2}{2\pi r^2 c} |\vec{J}_o|^2 \int_0^{2\pi} \int_0^\pi r^2 \sin^3 \theta \, d\theta d\phi \]

\[ = \frac{4K^2}{3c} |\vec{J}_o|^2 \]

\tag{48}
Equation (48) is also valid for non-linear polarizations.

To convert to quantum theory the classical expression for $\mathbf{J}$ must be replaced by its quantum analog. We want to replace $\mathbf{J}$ by a current density that is associated with an initial upper state $u_K$ and a final lower state $u_n$, since energy is radiated during the transition from $K$ to $n$. It is natural to represent the current density as a product of a charge density and a velocity and to take for the velocity the momentum operator divided by the mass: $-(i\hbar/m)\hat{\mathbf{V}}$. The charge density for a stationary state is expected to be the charge of the particle times its position probability density i.e., $e|\psi|^2$. However, we are concerned here with a transition between states and so replace this by $e u_n^* u_K$. Thus we can replace $\mathbf{J}(\mathbf{r})$ by

$$\mathbf{J}(\mathbf{r}) - \frac{ie\hbar}{m} u_n^* \hat{\mathbf{V}} u_K(\mathbf{r})$$

To get $J_0$ we must integrate the above expression for $\mathbf{J}(\mathbf{r})$ over the coordinates.

Thus

$$J_0 = -\frac{ie\hbar}{m} \int u_n^* \hat{\mathbf{V}} u_K d^3r$$

or

$$J_0 = e \int u_n^* \hat{\mathbf{P}} u_K d^3r$$

or

$$J_0 = e \frac{\mathbf{P}}{m} \langle n | \mathbf{P} | K \rangle.$$ 

(49)
The matrix element of \( \hat{P} \) is \( \hat{P} = m \frac{d}{dt} . \)

So
\[
\frac{1}{m} \langle n | \hat{P} | K \rangle = \frac{d}{dt} \langle n | \hat{r} | K \rangle . \quad (50)
\]

If an energy representation in the Schrodinger picture is used we have

\[
\langle n(t) | \hat{r} | K(t) \rangle = \langle n(o) | \hat{r} | K(o) \rangle e^{i \omega_{nK} t}
\]

where \( \omega_{nK} = \frac{E_n - E_K}{\hbar} \).

So
\[
\frac{d}{dt} \langle n(t) | \hat{r} | K(t) \rangle = \frac{d}{dt} \langle n(o) | \hat{r} | K(o) \rangle e^{i \omega_{nK} t}
\]

\[
= i \omega_{nK} \langle n(o) | \hat{r} | K(o) \rangle e^{i \omega_{nK} t}
\]

\[
= i \omega_{nK} \langle n(t) | \hat{r} | K(t) \rangle . \quad (51)
\]

Substituting equation (51) into equation (50) we obtain

\[
\frac{1}{m} \langle n | \hat{r} | K \rangle = i \omega_{nK} \langle n | \hat{r} | K \rangle . \quad (52)
\]

Substituting equation (52) into equation (49) we obtain

\[
\hat{J}_o = i e \omega_{nK} \langle n | \hat{r} | K \rangle . \quad (53)
\]

Substitution of equation (53) into equation (48) gives the radiated power.

We can interpret this power as the product of the spontaneous rate of transition from \( n \) to \( K \) and the quantum energy \( \omega_{nK} = E_K - E_n \) given off in each transition.
Thus

\[ p = \frac{4K^2}{3c} e^{2\omega_{nK}} |<n|\hat{r}|K>|^2 \]

and the transition probability per unit time for spontaneous emission (Einstein probability coefficient) becomes

\[ A_{nk} = \frac{4K^2 e^{2\omega_{nK}}}{3\hbar c} |<n|\hat{r}|K>|^2 \]

Using \(\omega_{nK} = \hbar c\) we obtain

\[ A_{nk} = \frac{4e^{2\omega_{nK}}}{3\hbar c^3} |<n|\hat{r}|K>|^2 \]

The line strength is the sum over all possible combinations of the (possibly) degenerate sublevels with those of the lower state of the matrix element in the expression for \(A_{nk}\).

To calculate the line strength of the Na(3p \rightarrow 3s) line we need the effective atomic numbers \(Z_n\) for sodium. Using Slater's rules we find: \(Z = 10.7\), \(Z_2 = 6.85\) and \(Z_3 = 2.20\). From these values the \(A\)'s and \(N\)'s can be found and substituted in Slater's radial wave functions. The same result is obtained for the line strength of the Na(3p \rightarrow 3s) if either SWF I or SWF II are used.

Thus we obtain (in atomic units)

for \(m = 0\)

\[ \int \psi_n^* \hat{r} \psi_K d^3r = 2.76 \hat{e}_z \]

for \(m = 1\)

\[ \int \psi_n^* \hat{r} \psi_K d^3r = .799 / \sqrt{6} |\hat{e}_x + i\hat{e}_y| \]
\[ \text{for } m = 1 \quad \int \psi_n^* \mathbf{r} \psi_{\mathbf{k}} \, d^3 \mathbf{r} = 0.799\sqrt{6} \left( e_x + ie_y \right). \]

When these results are substituted into the expression for \( S \) the answer is (in atomic units)

\[ S = 22.9. \]

This compares reasonably well with an experimental value of 19 atomic units given in reference 2.

The value obtained for the Einstein probability coefficient is

\[ A_{nK} = 2.256 \times 10^6 \text{ sec}^{-1}. \]
CONCLUSIONS

With the exception of Na(3s → 4p) cross section the SWF cross sections are roughly with a factor of 3-4 of VOP's results. In particular, there is very good agreement with VOP for the Li(2s → 3p) cross section. One should realize that comparing one theoretical calculation with another does not establish the validity of either.

The oscillation in the Na(3s → 4p) cross section is disconcerting. Normally such oscillations come from the interference of coupled states, but couplings have not been included in the SWF calculation and so it was first thought to be a programming error. A second program was written to serve as an independent check on the results of the first program. In this program the radial integration was also done on the computer. Numerous excitation levels of hydrogen using hydrogen wave functions were calculated with both programs. Both gave the same results and agreed with the results given in VOP. When SWF's were used the programs also calculated the A and N parameters. Both programs used the same routine for calculating these parameters. So it was concluded that the oscillation in the Na(3s → 4p) cross section was real.

By setting all of the A's individually equal to zero it was found that only $A_{413}$ significantly affects the cross-section. In particular by setting $A_{413}$ equal to 90% of its calculated value the oscillation is removed. However, the cross-sections increase by about 60%.

Using the orthonormality conditions $\langle \mathbf{R}_n, \mathbf{R}_{n'} \rangle = \delta_{nn'}$ it can be shown that
Thus, the absolute value of $A_{413}$ can be reduced by using a different value for $Z_4$ than that given by Slater's rules. The value obtained for $Z_4$ by using Slater's rules is $Z_4 = 1.00$. By setting $Z_4 = 1.35$ the oscillation is removed. However, this increases the cross section to 3-4 times the original calculated value and the peak shifts toward higher energy. This rather large change in the cross section should be expected since the A's, N's and F's all depend on $Z_4$ and these appear in the expression for the scattering amplitude $f(K)$.

Thus it appears that the absolute value of $A_{413}$ is too large. This could be due to too large an overlap between $R_{31}$ and the characteristic part of $R_{41}$ which is the factor in brackets in the above expression for $A_{413}$.
APPENDIX A

The following programs were used to do most of the calculations related to this work. The first program does both the radial integral and the integral over the momentum transfer using Simpson's rule as an approximation to the integrals. The first part of the program down to and including statement 10 calculates the \( N_n \)'s and \( A_{n,j} \)'s. Then the radial integration is done and finally the integral over the momentum transfer is done.

The second program as given uses the SWF I. Only minor modifications are required to use SWF II. In this program only the integral over the momentum transfer is done as equation (1) is used for \( f(K) \). This program will work for any \( s \rightarrow p \) transition for which \( n_f \geq n_i \). If \( n_f < n_i \) enough \( N_j \)'s, \( A_{n,j} \)'s and \( F_{n,j} \)'s may not be calculated. Only the statements marked * need be changed to calculate the total cross-section for other than \( s \rightarrow p \) transitions for which \( n_f \geq n_i \).
// EXAMPLE JOB 016722.6, PAUL SINGEL
// EXEC FORTEC5, PARCHG
// FORTECSYS DD *
DIMENSION T[N], XSUM(N), X(N), A(N), FX(N), XANS(N), SIGMA(N)
DIMENSION PFX(N), RIFA(210), R(225), RFX(225)
DIMENSION C(4,4), AA(4,4,4), R(4,4,225), T(4)
READ 20, M, NF, T(1,1:1,1)
20 FORMAT (212, 10F5.2)
READ(5,50) (A(I), I=1,5), (T(I), I=1,10)
50 FORMAT (5(F5.2, 2X), 10(F6.2, 2X))
24 FORMAT (F16.9, 4X, 11, 4X, 11)
34 FORMAT (F16.9, 4X, 11, 4X, 11, 4X, 11)
77 = 11, **
TF = 2.7503
AA = 1.722
CC = 8.1784
XRF = 1.00
NX = XR + 1.
RN = 20.0
NP = RN + 1.
DO 1 J=1, NF
DO 1 K=1, NF
AA(I, J, K) = 0.006
1 CONTINUE
DO 10 J=1, NF
DO 12 L=1, NF
10 IF (J+L = 10, 15, 15)
15 ASQR = 0.0
IF (J = 2) 4, 2, 2
2  K=J-1
   DO 3  I=1,K
3   ASQR=ASQR+AA(J,L,I)**2
   S=S*J+1
   G=G
   C(J,L)=1./SORT(GAMMA(S)*(S/(2.*Z(J)))**(2*J+1)-ASQR))
   WRITE (6,24) C(J,L), J, L
   DO 9  N=2,NF
   IF (N-J) 9,9,5
5   ASUM=C,J
   IF (J-2) 8,6,5
   LL=J-1
   DO 7  I=1,LL
7   ASUM=ASUM+AA(N,L,I)*AA(J,L,I)
8   SA=N*J+1
   H=J
   G=G
   AA(N,L,J)=C(J,L)*ASUM- GAMMA(SA)*(1./(Z(J)/H+Z(N)/G))**(N+J+1))
   AA(4,2,3)=.95*AA(4,2,3)
   WRITE (6,34) AA(N,L,J), N, L, J
9   CONTINUE
10  CONTINUE
   PRINT 400
400  FORVRA (1=1)
   ALTR=0
   BLIR=56.*3
   DLIR=(BLIR-ALTR)/EN
   Y=ALTR-DLIR
   DO 60  I=1,2-1
60   DO 60  N=1,45
DO 60 L=1,4
60 R(N,L,1)=C(0,0)
   R(1,1,1)=C(1,1)
   IF (N-2) 65, 62, 62
62 R(2,1,1)=C(2,1)*AA(2,1,1)*C(1,1)
   IF (N-3) 65, 63, 63
63 R(3,1,1)=C(3,1)*AA(3,1,2)*C(2,1)*AA(2,1,1)*C(1,1)+AA(3,1,1)*C(1,1)
   IF (N-4) 65, 64, 64
64 R(4,1,1)=C(4,1)*AA(4,1,3)*C(3,1)*AA(3,1,2)*C(2,1)*AA(2,1,1)*C(1,1)+AA(4,1,2)*C(2,1)*AA(2,1,1)*C(1,1)+AA(4,1,1)*C(1,1)
65 Y=Y+DELDP
   DO 70 J=2, NF
   X=Y+DELQ
   DO 80 K=1, NF
   M1=N-1
   IF (J-35) 82, 40, 40
40 IF (N-1) 80, 30, 83
60 IF (J-30) 82, 41, 41
41 IF (N-2) 80, 30, 82
82 DO 81 K=L, M1
81 R(R,L,J)=R(N,L,J)+C(N,L)*AA(N,L,K)*R(K,L,J)
   IF (N-1) 84, 34, 85
94 R(N,L,J)=C(N,L)*EXP(-Z(N)*Y/N)+R(N,L,J)
   GO TO 86
95 R(N,L,J)=C(N,L)*(Y**(N-1)*EXP(-Z(N)*Y/N))+R(N,L,J)
86 CONTINUE
   R1(J)=R(3,1,J)
70 RE(J)=R(4,2,J)
DO 21 I = 1, 10
BLIM = SQRT(TET*TN(I)) *(1.0 - SQRT(1.0 - I / TN(I)))
ALIM = SQRT(TET*TN(I)) *(1.0 - SQRT(1.0 - I / TN(I)))
KX = 1
DO 25 IN = 1, 6
25 XSUM(IN) = 0
DELX = (BLIM - ALIM)/XN
X = ALIM + DELX
DO 54 IX = 1, 14
X = X + DELX
KY = -XY
K2 = 1
R SUM = 0
Y = ALIM + DELY
DO 300 IR = 1, NR
Y = Y + DELY
KP = -XY
ANG = SIN(X*Y) / X**2 - Y*COS(X*Y) / X
RIFA(IR) = R1(IR) * RF(1R) * ARG
IF ((IR-1) * (1R-NF) * KP) 100, 300, 200
100 R SUM = R SUM + 2.0 * RIFA(IR)
200 R SUM = R SUM + RIFA(IR)
300 R SUM = R SUM + RIFA(IR)
RAN5 = DELP * R SUM / 3.
6X = (RAN5 * RANS) / (X*Y*Y)
DO 53 IN = 1, 5
AX(IN) = 1.0 / (1.0 + (27*A(IN) * X)**2)**2
FX(IN) = GY*AX(IN)
PFX(IN) = CC + IF*FX(IN)
IF ((IX-1) * (IX-NX) * KY) = 1, 52, 32
51  XSUM(I)=XSUM(I)+2.*FX(I)
52  XSUM(I)=XSUM(I)+Y(I)
53  XSUM(I)=XSUM(I)+F(I)
54  CONTINUE
60  DO 56 J=1,5
61  XANS(J)=DEL X*XSUM(J)/3.
56  SIGMA(J)=CC*XANS(J)/TR(I)
60   WRITE(6,11) ((SIGMA(K),A(K)),K=1,5),TR(I),1
11  FORMAT(5(E12.8,A32),6X,TN=6.2X,1=913,/) 
21  CONTINUE
END

//GOUT.DIN DB *
3 412.6 6.85 2.2 1.96
+0.06 +0.16 +0.16 +0.3  +0.28
+ 1.16 + 1.64 + 2.00 + 2.44 + 3.56 + 5.00 + 6.76 +11.24 +17.60 +24.04
// EXEC  FORTGLO, PARM=ROSA
//FORT, SYSIN DO *
DIVERSION A(10,10), RHO(10,10), THET(10,10), B(10,10), F(10,10),
1Z(10), C(10), AA(10,10)
READ 30, NI, NF, (Z(I), I=1, NI)
30 FORMAT (212, 10F5.2)
34 FORMAT (E 16.9, 4X, 11, 4X, 11)
DO 40 J=1, NF
DO 40 K=1, NI
A(J,K) = NF+NI+2-J-K

CONTINUE
DO 41 J=1, NF
DO 41 K=1, NI
T= NF+1-J
U= NI+1-K
B(J,K)= Z(NF+1-J)/T+Z(NI+1-K)/U
41 CONTINUE
DO 42 M=1, NF
F(J,M) = 1
1 AA(V,W)= 
DO 10 J=1, MF
ASQR= 0.
IF (J-Z) 4, 2, 2
2 K=J-1
DO 31 J=1, K
3 ASQR = ASQR+AA(J,1)*Z
4 S= Z+1
C= J
C(J)= 1./ (SQRT(GAMMA(S)*((C/(2.*J**3))**2*(2*J+1)-ASQR)))
DO 9 N=2, M
9 IF (N-J) 9, 6, 6
A=SUM+*C
IF (J-2) 8, 6, 6
L=J-1
DO 7 1=1, L
7 ASUM=ASUM+AA(N, J)*AA(J, 1)
8 SA=N+J+1
P=J
Q=N
AA(N, J)=C(J)*ASUM/GAMMA(SA)*(N*(N+1)/(J*(J+1))/(N+Z(N)/Q))#(K+J+1)
WRITE (6, 54) AA(N, J), N, J
CONTINUE
DO 10 NF=1, M
J=NF
NF=NF-1
NF1=N+1-NF
DO 13 1=1, NF1
13 M=1, NF1
M1=M-1
JM=J-M
IF (M1-JM) 13, 13, 11
F(SUM)=G
L=M1-JM
DO 12 K=1, L
H(K)=K+1-K
12 F(SUM)=F(SUM)+F(N), H(K)*AA(N, K, J)
F(N), J=J+C(J)*F(SUM)
13 CONTINUE

**50** FORMAT (122H1) CALCULATION OF ELECTRON EXCITATION CROSS SECTION FOR
1THE 1S-2P TRANSITION IN HYDROGEN IN THE BORN APPROXIMATION USING
2G/113H SLATER WAVE FUNCTIONS. E1 IS THE INCIDENT ENERGY IN THRESHOL
31D UNITS AND XNCA IS THE TOTAL CROSS SECTION IN UNITS/ 97TH OF PI 1

AINES THE BORN RADIUS SQUARED.

100 READ 191, XN, E1, ET, FZ

101 FORMAT (12 + 8.5)

ALIM=STRT(E1*ET)*(1.-STRT(1.1.0/E1))

BLIM=STRT(E1*ET)*(1.+STRT(1.1.0/E1))

JX=XX/1.

XX=1

XSUM=*F

DELY=(ALIM-ALIM)/XN

X=ALIM-DELY

DO 105 IX=1,JX.

X=X+DELY

XSUM=X

DO 102 X=1,N1

DO 102 J=1,NF.

RHO(J,K)=STRT(B*(J,K)*+2*X**2)

THET(J,K)=ATAN(X/Z(J,K))

*102 XSUM=XSUM+F(NF,N1+1-J)*F(MN,1+1-K)*GAMMA(A(J,K)-1.0)/(RHO(J,K)**

1A(J,K)*(X*A(J,K)-1.0)**1B(A(J,K)*THET(J,K)-1.573756)+RHO(J,K)**

2COS((A(J,K)-1.0)*1BTHET(J,K)-1.573756))

* EX=(XSUM**2)/X**7

XX=EX

= ((IX-1)/**((IX-JX)**XX)) 103, JX+1,N0.
103 XSSM=XSUM+2.*FX
104 XSUM=XSUM+FX
105 XSUM=XSUM+FX
   XANS=DELX*XSUM/2.
* XANS=24.*((C(N1)**2)*(C(NF)**2)/(EI*ET))*XANS
   WRITE (6,106) EI,XANS
106 FORMAT (50X,4H EI=, F9.4, 5X, 7H SIGMA=, F9.4)
   IF(FZ) 100,108,100
108 CALL EXIT
END
/*
//go_lysin dd *
  1 21.00 1.00
100.000 1.04    .74979 10.0000
100.000 1.16    .74979 10.0000
100.000 1.36    .74979 10.0000
100.000 1.64    .74979 10.0000
100.000 2.44    .74979 10.0000
100.000 3.56    .74979 10.0000
100.000 5.29    .74979 10.0000
100.000 6.76    .74979 10.0000
100.000 8.24    .74979 10.0000
100.000 12.00   .74979 10.0000
100.000 24.04   .74979 10.0000
/
Read Initial and Final Total Q. No. & Eff. Zn's

Read A parameters
Incident Energies

TE = Threshold energy
AAA = 1.732

XN = No. of pts for K integration
NX = XN + 1

RN = No. of pts for R integration

Calculate \( A_{\nu j} \)'s and \( N_{j} \)'s

Start R Integration

ALIMR = .0
BLIMR = 50.0

Initialize all radial wave functions to zero at all points of integration
Initialize all radial wave functions at $r = 0$

Evaluate $R_1(r)$ and $R_n(r)$ at each integration point

Return to x integration

DO 21 I = 1, 10

Calculate $ALIM$ and $BLIM$

Initialize $XSUM(IN) = 0$

DO 54 IX = 1, NX

$XX = -XX$

Return to R integration

$KR = 1$

$KR = -KR$
\[ \text{ANG} = \frac{\sin(x^2y)}{x} - \frac{y \cos(x^2y)}{x} \]

\[ \text{RIFA (IR)} = \text{RI (IR)} \times \text{RF(IR)} \times \text{ANG} \]

What is the relationship between: (IR, NR, KR)

and what is the sign of KR

\[ \text{RSUM} = \text{RSUM} + 2 \times \text{RIFA (IR)} \]

\[ \text{RSUM} = \text{RSUM} + \text{RIFA (IR)} \]

\[ \text{RSUM} = \text{RSUM} + \text{RIFA (IR)} \]

\[ \text{RANS} = \text{DELR} \times \frac{\text{RSUM}}{3} \]

Return to x integration
\[ GX = \frac{(RANS \ast RANS)}{(X \ast X \ast X)} \]

\[ \text{DO 53 IM} = 1,5 \]

\[ AX(IM) = \frac{1}{(1. + (ZZ \ast A(IM) \ast X)^2)^2} \]

What is the relationship between (IX, NX, KX) and what is the sign of KR

\[ XSUM(IM) = XSUM(IM) + 2 \ast FX(IM) \]

\[ XSUM = XSUM(IM) + FX(IM) \]

\[ XSUM = XSUM(IM) + FX(IM) \]

\[ XANS(J) = DELX \ast XSUM(J)/3. \]
\[
\sigma(j) = \frac{cc \cdot \text{ANS}(j)}{\text{TN}(i)}
\]

WRITE \(\sigma(k)\), A(R), TN(I), I

END
Read Initial and Final total Q. No.'s & Eff Z_n's

Calculate a_{jk}'s

Calculate b_{jk}'s

Initialize F_{mn}'s=1. and A_{nn}'s = 0.

Calculate N_j's, A_{nj}'s

WRITE N(J) and A(N,J), N, J

Calculate F(N,J)'s

WRITE F(N1, JM) N1, JM

101

READ XN, EI, ET, FX

Start Integration
Start Integration

Calculate A LIM, B LIM

KX = 1

Calculate YSUM

FX = (YSUM **2)/X**7

KX = - KX

What is relationship between (IX, JX, KX) and what is sign of KX

<0

XSUM = XSUM + 2.*FX

> 0
\[ X_{\text{SUM}} = X_{\text{SUM}} + F_X \]

104

\[ X_{\text{ANS}} = \frac{\Delta L \times X_{\text{SUM}}}{3}. \]

\[ X_{\text{ANS}} = 24 \times \frac{(C/NI)^2 \times (C(NF)^2)}{(E_I \times E_T)^{\Delta N}} \]

WRITE EI, XANS

What is FA

<0

>0

= 0

END
REFERENCES


