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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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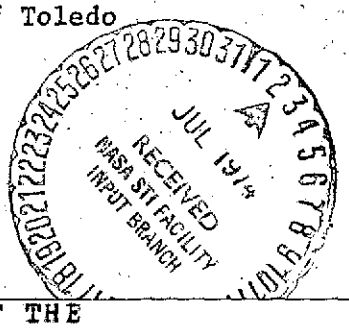

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INTRODUCTION

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 °K. 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 °K, .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 → 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).[2] 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 $\psi_{n\ell m} = R_{n\ell}(r)Y_{\ell m}(\Omega)$ where $R_{n\ell}(r)$ is a Slater radial wave function and $Y_{\ell m}(\Omega)$ is a spherical harmonic. In one type which will be referred to as Slater Wave Functions I (SWFI), the ℓ-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:[3]

$$R_1(r) = N_1 \exp(-Z_1 r/a_o)$$

$$R_2(r) = N_2\left[r \exp(-Z_2 r/2a_o) + A_{21}R_1(r)\right]$$

$$R_3(r) = N_3\left[r^2 \exp(-Z_3 r/3a_o) + A_{32}R_2(r) + A_{31}R_1(r)\right]$$

$$\vdots$$

$$R_n(r) = N_n\left[r^{n-1} \exp(-Z_n r/na_o) + \sum_{j=1}^{n-1} A_{nj}R_j(r)\right]$$

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,

$$A_{nj} = N_j\left[\sum_{i=1}^{j-1} A_{ni}A_{ji} - (n+j)!\left(\frac{a_o}{\frac{Z_j}{j}+\frac{Z_n}{n}}\right)^{n+j+1}\right] \quad j \le n-1$$

and

$$N_j = \left[(2j)!\left(\frac{ja_o}{2Z_j}\right)^{2j+1} - \sum_{n=1}^{j-1} A_{jn}^2\right]^{-\frac{1}{2}}$$

To make the radial integrations simpler the radial wave functions may be rewritten in the following form,

$$R_n(r) = N_n \sum_{j=1}^{n} F_{n,n+1-j}\, r^{n-j} \exp\left(-\frac{Z_{n+1-j}}{n+1-j}\,\frac{r}{a_o}\right) \qquad (1)$$

where the $F_{n,j}$'s can be determined from

$$F_{n,j} = N_j \sum_{K=1}^{n+1-j} F_{n,n+1-K}\, A_{n+1-K,j} \qquad (2)$$

and we choose $F_{n,n} = 1$, $A_{n,n} = 0$. (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 ℓ-dependence in the radial function. This is accomplished by writing different radial functions with different ℓ-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:

$$R_{10} = N_{10} \exp(-Z_1 r/a_o)$$

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

$$R_{21} = N_{21} \left[r \exp(-Z_2 r/2a_o)\right]$$

$$\vdots$$

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

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

$$\langle R_{n\ell}, F_{n'\ell} \rangle = \delta_{nn'} \quad .$$

$$A_{n\ell n'} = -N_{n'\ell} \left[(n+n')! \left(\frac{a_o}{\frac{Z_{n'}}{n'} + \frac{Z_n}{n}}\right)^{n+n'+1} - \sum_{K=1}^{n'-1} A_{n\ell K} A_{n'\ell K}\right] \quad n>n'>\ell$$

and

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

Here again the radial functions can be put into a form which make the radial integrations simpler. Thus

$$R_{n\ell}(r) = N_{n\ell} \sum_{j=1}^{n-\ell} F_{n,\ell,n+1-j}\, r^{n-j} \exp\left(\frac{Z_{n+1-j}\, r}{(n+1-j)\, a_o}\right) \qquad (3)$$

where $F_{n,\ell,j} = N_{j\ell} \sum_{K=1}^{n+1-j} F_{n,\ell,n+1-K}\, A_{n+1-K,\ell,j}$ and $A_{n,\ell,j}=0$ if $n \leq j \leq \ell$

and we choose $F_{n,\ell,n}=1$.

BORN APPROXIMATION

The Schrodinger equation for the atom plus incident electron is

$$\left[\frac{\hbar^2}{2m} \nabla_r^2 + \frac{\hbar^2}{2m} \sum_{i=1}^{Z} \nabla_i^2 + E_T + \frac{Ze^2}{r} + \sum_{j=1}^{Z} \frac{Ze^2}{r_j} - \sum_{i \neq j}^{Z} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} - \right.$$

$$\left. - \sum_{j=1}^{Z} \frac{e^2}{|\vec{r} - \vec{r}_j|} \right] \Psi(\vec{r}, \vec{r}_e) = 0 \qquad (4)$$

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,

$\vec{r}_e = (r_1 \ldots \vec{r}_2)$.

Now expand $\Psi(\vec{r}, \vec{r}_e)$ in terms of a complete set of orthonormal atomic wave functions $\psi_n(\vec{r}_e)$ satisfying the equation

$$\left[\frac{\hbar 2}{2m} \sum_{i=0}^{Z} \nabla_i^2 + \sum_{j=1}^{Z} \frac{Ze^2}{r_j} - \sum_{i \neq j}^{Z} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} + E_n \right] \psi_n(\vec{r}_e) = 0 \qquad (5)$$

where E_n are the associated eigenenergies. Now, set

$$\Psi(\vec{r}, \vec{r}_e) = S_\ell F_\ell(\vec{r}) \quad \psi_\ell(\vec{r}_e) \qquad (6)$$

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

Substitute equation (6) into equation (4), multiply by $\psi_n^*(\vec{r}_e)$ and integrate with respect to $\vec{r}_e$ to obtain

$$\int \left\{ \frac{\hbar^2}{2m} \nabla_r^2 + \frac{\hbar^2}{2m} \sum_{i=1}^{Z} \nabla_i^2 + E_T + \frac{Ze^2}{r} + \sum_{j=1}^{Z} \frac{Ze^2}{r_j} - \sum_{i \neq j}^{Z} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} - \cdots \right.$$

$$\left. - \sum_{j=1}^{Z} \frac{e^2}{|\vec{r} - \vec{r}_j|} \right\} S_\ell F_\ell(\vec{r}) \quad \psi_\ell(\vec{r}_e) \times \psi_n^*(\vec{r}_e) \quad d\vec{r}_e = 0 \qquad (7)$$

Now use equation (5) to obtain

$$\frac{\hbar^2}{2m} \left[\nabla_r^2 + K_n^2 \right] F_n(\vec{r}) = \int \psi_n^*(\vec{r}_e) \, V(\vec{r},\vec{r}_e) \, \Psi(\vec{r},\vec{r}_e) \, d\vec{r}_e \qquad (8)$$

where

$$V(\vec{r},\vec{r}_e) = -\frac{Ze^2}{r} + \sum_{j=1}^{Z} \frac{e^2}{|\vec{r} - \vec{r}_j|} \qquad (9)$$

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

$$K_n^2 = \frac{2m}{\hbar^2} (E_T - E_n)$$

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

$$F_f(\vec{r}') \sim e^{i\vec{K}_i \vec{r}'} \delta_{fi} + \frac{e^{iK_f r'}}{r'} f_f(\theta,\phi) \qquad (10)$$

where $f_f(\theta,\phi)$ is the scattering amplitude corresponding to the excitation of the fth state of the atom and θ,ϕ are the polar angles of $\vec{r}$ referred to the direction of incidence as polar axis.

Consider the equation for the Green's function

$$\left[\nabla^2 + K_n^2 \right] G(\vec{r},\vec{r}') = \delta(\vec{r} - \vec{r}')$$

then the solution to equation (8) can be written as

$$F_f(\vec{r}') = e^{i\vec{K}_i\cdot\vec{r}'}\,\delta_{fi} + \frac{2m}{\hbar^2}\iint G(\vec{r},\vec{r}')\,\psi_f^*(\vec{r}_e)\,V(\vec{r},\vec{r}_e)\,\Psi(\vec{r},\vec{r}_e)\,d\vec{r}_e d\vec{r} \qquad (11)$$

In order that F_f should have the correct asymptotic form given by equation (10) we find[5],

$$G(r,r') = -\frac{e^{iK_f|\vec{r}-\vec{r}'|}}{4\pi|\vec{r}-\vec{r}'|}\,. \qquad (12)$$

where $\vec{K}_f$ is a wave vector in the direction of $\vec{r}$.

Now

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

So for large r'

$$\frac{1}{|\vec{r}-\vec{r}'|} \sim \frac{1}{r'} \qquad (13)$$

and

$$K_f|\vec{r}-\vec{r}'| \sim K_f r'\left[1 - \frac{r}{r'}\cos\theta\right] = K_f r' - \vec{K}_f\cdot\vec{r} \qquad (14)$$

Then

$$G(\vec{r},\vec{r}') \sim -\frac{e^{iK_f r'}\,e^{-i\vec{K}_f\cdot\vec{r}}}{4\pi r'} \qquad (15)$$

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

$$F_f(\vec{r}') = e^{i\vec{K}_i\cdot\vec{r}'}\,\delta_{fi} - \frac{m}{2\pi\hbar^2}\,\frac{e^{iK_f r'}}{r'}\iint e^{-i\vec{K}_f\cdot\vec{r}}\,\psi_f^*(\vec{r}_e)\,V(\vec{r},\vec{r}_e)\Psi(\vec{r},\vec{r}_e)\,d\vec{r}_e d\vec{r} \qquad (16)$$

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

$$f_f(\theta,\phi) = -\frac{m}{2\pi\hbar^2}\iint e^{-i\vec{K}_f\cdot\vec{r}}\,\psi_f^*(\vec{r}_e)\,V(\vec{r},\vec{r}_e)\,\Psi(\vec{r},\vec{r}_e)\,d\vec{r}_e d\vec{r} \qquad (17)$$

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 $e^{i\vec{K}_i\vec{r}}$ 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 $K_i a \gg 1$ where a is the range of the electron-atom interaction. With the above assumption substitute

$$\Psi(\vec{r},\vec{r}_e) = e^{i\vec{K}_i\vec{r}}\,\psi_i(\vec{r}_e)$$

into equation (17) Then

$$f_f(\theta,\phi) = -\frac{m}{2\pi\hbar^2}\int e^{i(\vec{K}_i - \vec{K}_f)\cdot\vec{r}}\, V_{fi}(\vec{r})\,d\vec{r} \qquad (18)$$

where

$$V_{fi}(\vec{r}) = \int \psi_f^*(\vec{r}_e)\, V(\vec{r},\vec{r}_e)\, \psi_i(\vec{r}_e)\, d\vec{r}_e \qquad (19)$$

Now substitute equation (9) and equation (19) into equation (18) and use Bethe's integral[6]

$$\int \frac{e^{i\vec{K}\cdot\vec{r}_2}}{|\vec{r}_1-\vec{r}_2|}\, d\vec{r}_2 = \frac{4\pi}{K^2}\, e^{i\vec{K}\cdot\vec{r}_1}$$

to obtain

$$f_f(\theta,\phi) = \frac{2Zm}{K^2\hbar^2}\int \psi_f^* (\vec{r}_e)\, \psi_i (\vec{r}_e)\, e^{i\vec{K}\cdot\vec{r}}\, d\vec{r}_e$$

$$- \frac{2m}{K^2\hbar^2} \sum_{j=1}^{Z} \int \psi_f^* (\vec{r}_e)\, e^{i\vec{K}\cdot\vec{r}_j}\, \psi_i (\vec{r}_e)\, d\vec{r}_e$$

where $\vec{K} = \vec{K}_i - \vec{K}_f$ and $\hbar\vec{K}$ 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)

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

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

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

and

$$\psi_i(\vec{r}_e) = \psi_i(\vec{r}_1 \ldots \vec{r}_Z) = (Z!)^{-\frac{1}{2}}\, \varepsilon_{\ell m\ldots n}\, \psi_\ell(\vec{r}_1)\, \psi_m(\vec{r}_2) \ldots \psi_n(\vec{r}_Z)$$

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

$$\sum_{t=1}^{Z}\int \psi_f^* (\vec{r}_e)\ e^{i\vec{K}\cdot\vec{r}_t}\ \psi_i(\vec{r}_e)d\vec{r}_e$$

$$= \sum_{t=1}^{Z}\int d\vec{r}_1\ldots d\vec{r}_Z\ \psi_f^* (\vec{r}_1\ldots\vec{r}_Z)\ e^{i\vec{K}\cdot\vec{r}_t}\ \psi_i(\vec{r}_1\ldots\vec{r}_Z)$$

$$= \frac{1}{Z}\sum_{t=1}^{Z} \varepsilon_{ij\ldots K}\,\varepsilon_{\ell m\ldots n}\int d\vec{r}_1\ldots d\vec{r}_Z\ \psi_i^*(\vec{r}_1)\ldots\psi_K^*(\vec{r}_Z)\ e^{i\vec{K}\cdot\vec{r}_t}\ \psi_\ell(\vec{r}_1)\ldots\psi_n(\vec{r}_Z) \quad (21)$$

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

Then equation (21) becomes

$$= \frac{1}{Z!}\ \varepsilon_{ij\ldots K}\,\varepsilon_{\ell m\ldots n}\int d\vec{r}_1\ \psi_i^*(\vec{r}_1)\ e^{i\vec{K}\cdot\vec{r}_1}\ \psi_\ell(\vec{r}_1)\ \delta_{jm}\ldots\delta_{Kn}$$

where $\psi_i(r_1)$ is the final state wave function that does not appear in the initial state wave functions.

$$= \frac{1}{Z!}\ \varepsilon_{ij\ldots K}\,\varepsilon_{\ell j\ldots K}\int d\vec{r}_1\psi_i^*(\vec{r}_1)\ e^{i\vec{K}\cdot\vec{r}_1}\ \psi_\ell(\vec{r}_1) \quad (22)$$

Now use the relation $\varepsilon_{\alpha\beta\gamma\ldots\pi}\,\varepsilon_{\alpha'\beta\gamma\ldots\pi} = (P-1)!\ \delta_{\alpha\alpha'}$, where P is the number of subscripts on the $\varepsilon_{\alpha\beta\gamma\ldots\pi}$'s.

Then equation (22) becomes

$$= \frac{1}{Z!}\ (Z-1)!\delta_{i\ell}\int d\vec{r}_1\psi_i^*(\vec{r}_1)\ e^{i\vec{K}\cdot\vec{r}_1}\ \psi_\ell(\vec{r}_1)$$

$$= \frac{1}{Z}\int d\vec{r}_1\psi_i^*(\vec{r}_1)\ e^{i\vec{K}\cdot\vec{r}_1}\ \psi_i(\vec{r}_1)$$

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

$$\int d\vec{r} \quad \psi_f^*(\vec{r}) \quad e^{i\vec{K}\cdot\vec{r}} \quad \psi_i(\vec{r})$$

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

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

$$f(\theta,\phi) = -\frac{2}{K^2} \int dr\, r^2 R_{n_f \ell_f}(r)\, R_{n_i \ell_i}(r) \langle \ell_f m_f | e^{i\vec{K}\cdot\vec{r}} | \ell_i m_i \rangle$$

where

$$\langle \ell_f m_f | e^{i\vec{K}\cdot\vec{r}} | \ell_i m_i \rangle = \int d\Omega\, Y^+_{\ell_f m_f}(\Omega)\, e^{i\vec{K}\cdot\vec{r}}\, Y_{\ell_i m_i}(\Omega)$$

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

$$e^{i\vec{K}\cdot\vec{r}} = \sum_{\nu=0}^{\infty} i^{\nu} \left[4\pi(2\nu+1)\right]^{\frac{1}{2}} j_\nu(Kr) Y_{\nu o}(\Omega)$$

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

For an s → p excitation the angular integral becomes

$$\langle 1\ m_f \ | e^{i\vec{K}\cdot\vec{r}} \ | \ oo \rangle = i\sqrt{3}\, j_1(Kr)$$

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 → p excitation becomes (for SWF I)

$$f(K) = \frac{2\sqrt{3}\, N_{n_f} N_{n_i}}{K^4 i} \sum_{\substack{j=1\ldots n_f \\ K=1\ldots n_i}} F_{n_f, n_f+1-j}\, F_{n_i, n_i+1-K}\, \frac{(a_{jK}-2)!}{\rho_{jK}^{a_{jK}}}$$

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

where

$$a_{jK} = n_f + n_i + 2 - j - K, \quad (23)$$

$$b_{jK} = \left[\frac{Z_{n_f+1-j}}{n_f+1-j} + \frac{Z_{n_i+1-K}}{n_i+1-K} \right], \quad (24)$$

$$\theta_{jK} = \tan^{-1} \left(\frac{K}{b_{jK}} \right) \quad \text{and} \quad \rho_{jK} = \sqrt{b_{jK}^2 + K^2}$$

For an s → p excitation the angular integral remains the same when SWF II are used. In this case use equation (3) for $R_{n_f \ell_f}(r)$ and $R_{n_i \ell_i}(r)$.

So for an s → p excitation with SWF II

$$f(K) = \frac{2\sqrt{3}N_{n_f\ell_f}N_{n_i\ell_i}}{K^4 i} \sum_{\substack{j=1\ldots n_f-\ell_f \\ K=1\ldots n_i-\ell_i}} F_{n_f,\ell_f,n_f+1-j}\, F_{n_i,\ell_i,n_i+1-K}$$

$$\frac{(a_{jK}-2)!}{\rho_{jK}^{a_{jK}}} \left\{ K(a_{jK}-1)\sin(a_{jK}\theta_{jK}-\pi/2) + \rho_{jK}\cos\left[(a_{jK}-1)\theta_{jK}-\pi/2\right] \right\} \quad (25)$$

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

$$V(|\vec{r}-\vec{r}'|) = -\frac{e^{-C\,K^2|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}$$

In dimensionless units

$$V(|\vec{r}-\vec{r}'|) = -\frac{e^{-C(\frac{1}{a_o})^2(Ka_o)^2(\frac{|\vec{r}-\vec{r}'|}{a_o})\,a_o}}{|\vec{r}-\vec{r}'|}$$

$$V(\vec{r}-\vec{r}') = -\frac{e^{-(\frac{C}{a_o})\,K'^2\,(|\vec{r}-\vec{r}'|)'}}{|\vec{r}-\vec{r}'|} \quad .$$

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

$$f(K) = f_{Born}(K)/(1 + Z^2E_T^2K^2)$$

TOTAL CROSS SECTION

The total cross-section is given by

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

Since our $V(\vec{r})$ has azimuthal symmetry

$$d\Omega = 2\pi \sin\theta d\theta$$

the total cross section becomes

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

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

$$K^2 = K_i^2 + K_f^2 - 2K_iK_f \cos\theta$$

where $h\vec{K}$ is the momentum transfer and θ is the angel between $\vec{K}_i$ and $\vec{K}_f$.
Then

$$2KdK = 2K_iK_f \sin\theta d\theta$$

or

$$\sin\theta d\theta = \frac{KdK}{K_iK_f} \quad .$$

Now at $\theta = 0$

$$(K_{min})^2 = (K_i - K_f)^2 \quad \text{or} \quad K_{min} = K_i - K_f$$

and at $\theta = \pi$

$$(K^{max})^2 = (K_i + K_f)^2 \quad \text{or} \quad K^{max} = K_i + K_f \ .$$

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

$$K_{min}^{max} = K_i \pm K_f = (E_i)^{\frac{1}{2}} \pm (E_f)^{\frac{1}{2}} = (E_i)^{\frac{1}{2}} \left[1 \pm \left(1 - \frac{E_T}{E_i}\right)^{\frac{1}{2}}\right]$$

And so the integral for the total cross section becomes

$$\sigma_T = \frac{2\pi}{K_i^2} \int_{K_{min}}^{K_{max}} dK \; K|f(K)|^2 \qquad (26)$$

Slaters' rules are used to determine the effective atomic numbers Z_n's. These values are used to calculate the orthonormality constants A_{nj}'s and N_n's for the SWF I and the $A_{n\ell n}$'s and $N_{n\ell}$'s for SWF II. The $F_{n\ell}$'s and $F_{n\ell j}$'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 → 2p), Li(2s → 3p), Na(3s → 4p), Mg(3p → 4s), Ca(4s → 4p) and K(4s → 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 the b_{jK}'s equation (24) are calculated. Next, the F_{nn}'s equation (2') and the A_{nn}'s equation (2') are initialized to 1 and 0 respectively. The N_j's and A_{nj}'s are calculated next. These must be calculated together since they depend upon each other. Then using the calculated N_j's and A_{nj}'s the F_{nj}'s equation (2) are calculated. Finally the last part of the program calculates the scattering amplitude f(K) equation (22) squares it and integrates $|f(K)|^2$ 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 $A_{nj\ell}$'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.

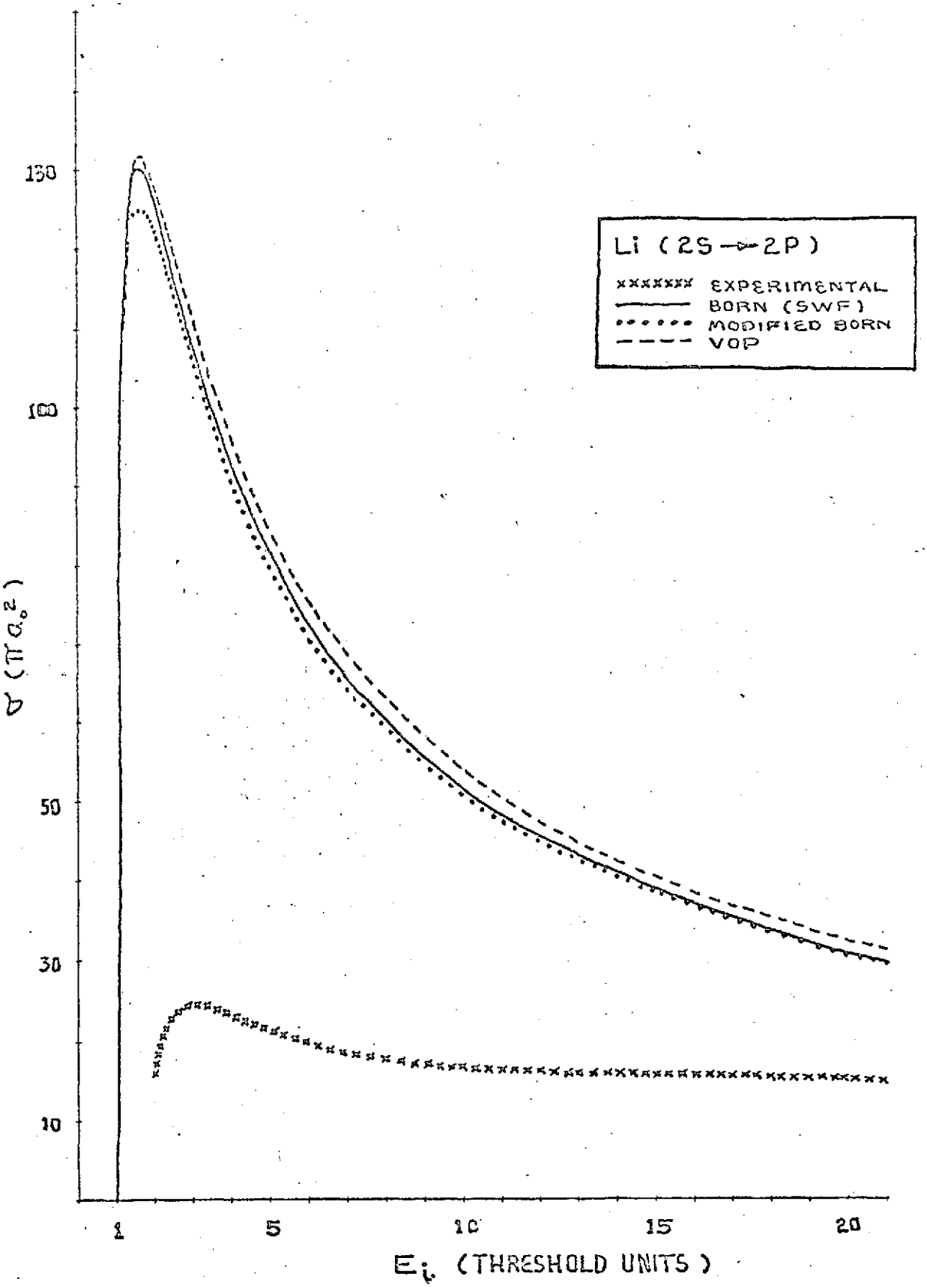
The results of the calculations are given in graphic form on the following pages. These results are compared with the calculations of Vainshtein, Opykhtin, and Presnyakov (VOP) and with experimental data where available. It was found that the difference in using SWF I and SWF II for all of the calculated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

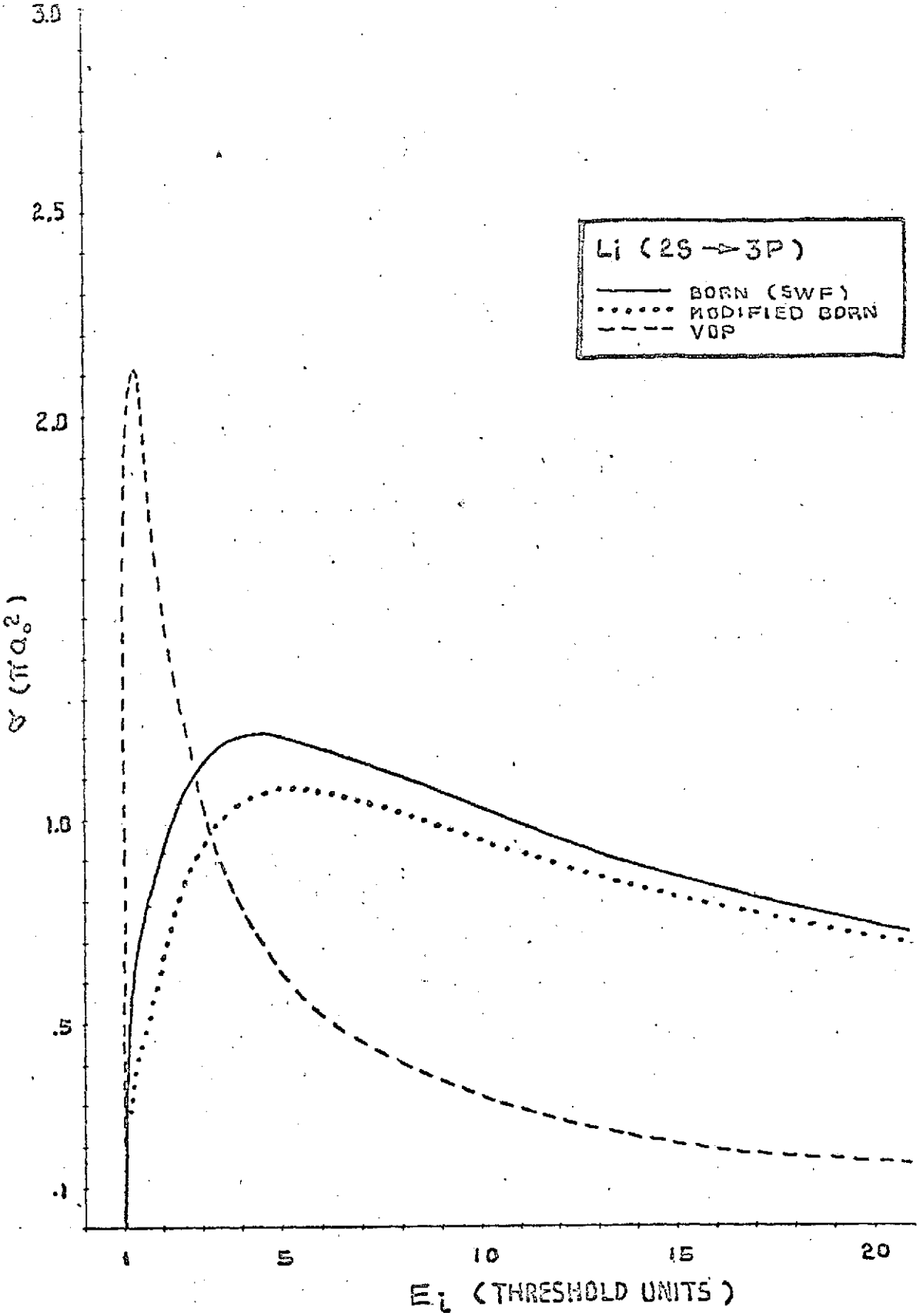
Agreement with VOP is very good for the Li(2s → 2p) transition. Both calculations are high with respect to the experimental data given in reference (9). Agreement with VOP for the Li(2s → 3p) transition

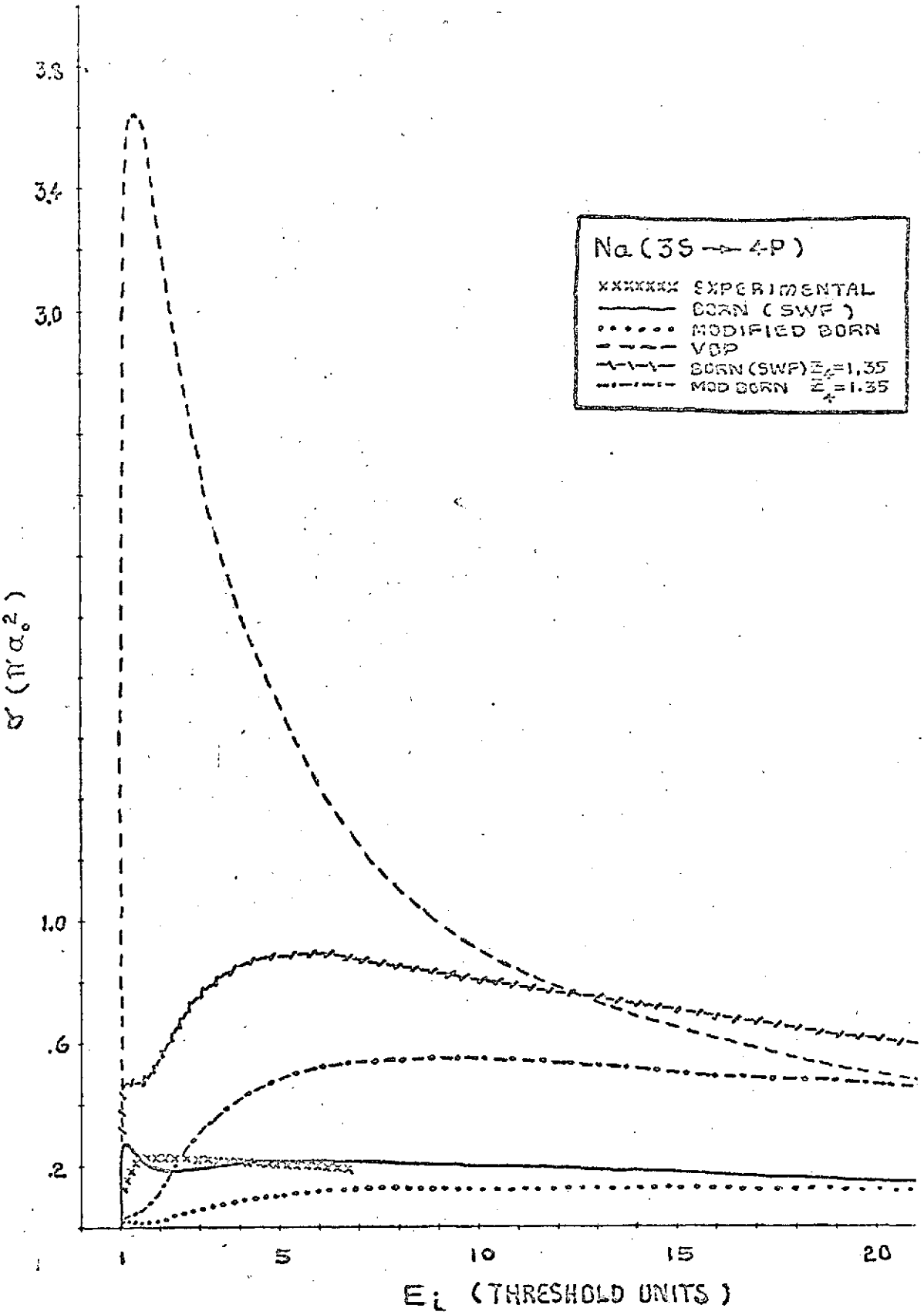
is not as good with VOP obtaining a peak cross section which is more than 3/2 times and at a lower energy than the SWF result. No experimental data could be found for this transition. The SWF result for the Na(3s → 4p) is about an order of magnitude smaller than the VOP calculation up to 5 threshold 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 → 4s) and Ca(4s → 4p) transitions. Good agreement with VOP is obtained for the K(4s → 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.

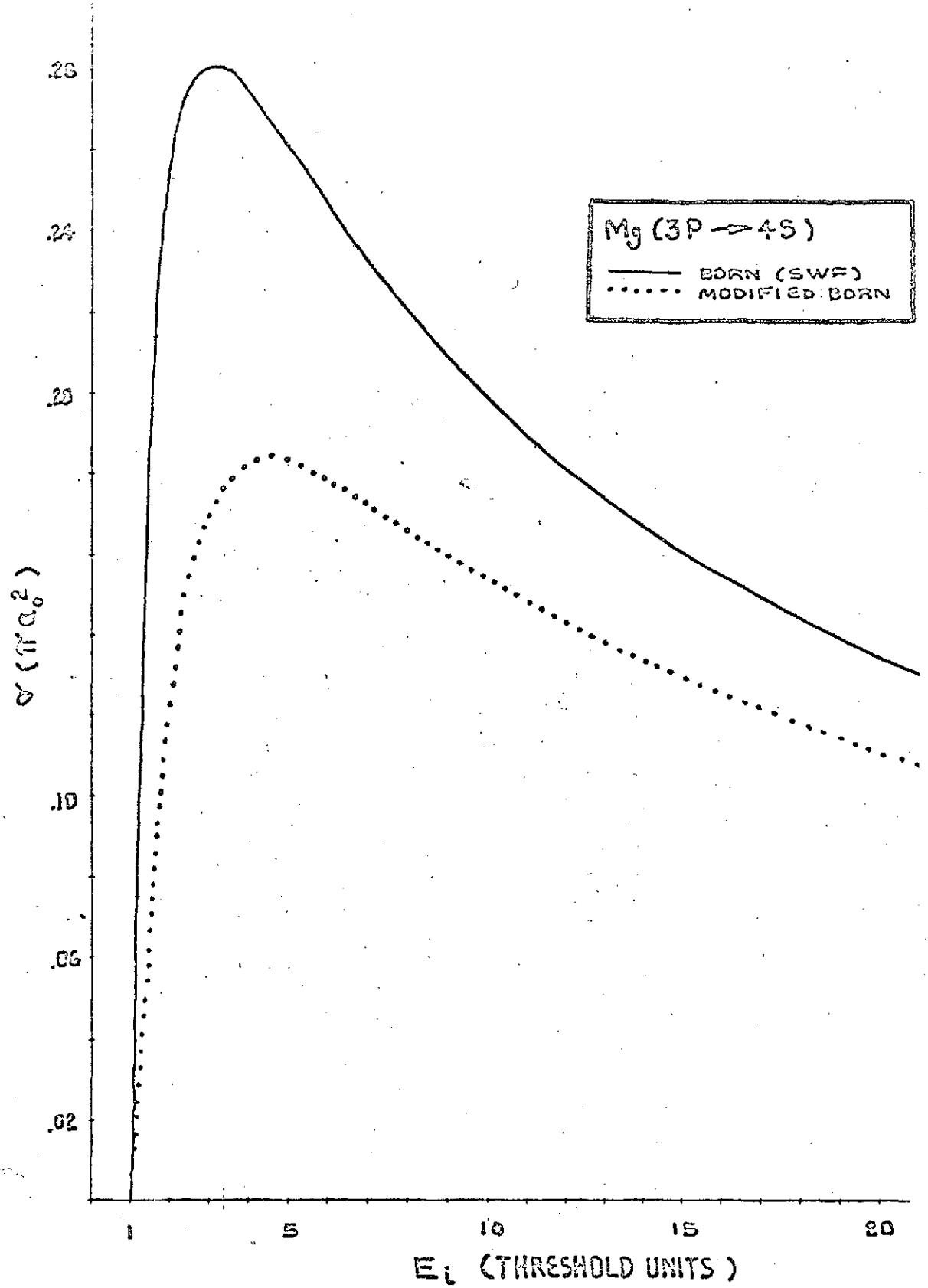
All of the Modified Born results show the expected behavior of a lower cross-section at the lower energies with the approach to the same value as the Born Approximation at the high energies.

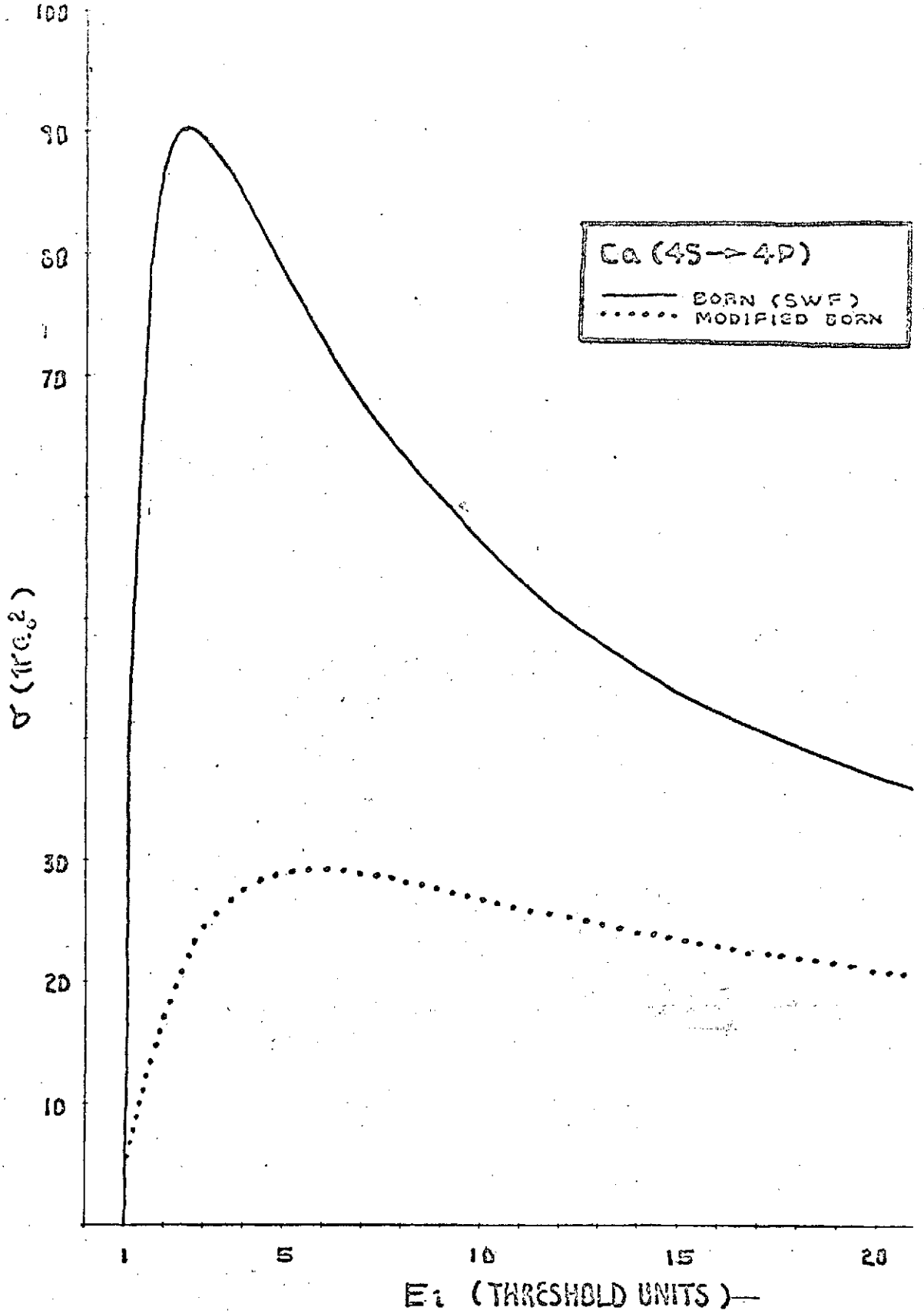
These data are presented in tabular form in Tables I and II on pages 27, 28 and 29.


Li (2S → 2P)
EXPERIMENTAL
BORN (SWF)
MODIFIED BORN
VOP
Q (πa₀²)
100
50
30
10
1
5
10
15
20
Eᵢ (THRESHOLD UNITS)


Li (2S → 3P)
BORN (SWF)
MODIFIED BORN
VOP
3.0
2.5
2.0
1.0
.5
.1
σ (πa₀²)
1
5
10
15
20
Ei (THRESHOLD UNITS)


Na (3S → 4P)
EXPERIMENTAL
BORN (SWF)
MODIFIED BORN
VBP
BORN (SWF) E_i=1.35
MOD BORN E_i=1.35
3.8
3.4
3.0
1.0
.6
.2
σ (πa₀²)
1
5
10
15
20
E_i (THRESHOLD UNITS)


Mg (3P → 4S)
BORN (SWF)
MODIFIED BORN
.28
.24
.20
.10
.06
.02
σ (πa₀²)
1
5
10
15
20
E_i (THRESHOLD UNITS)


Ca (4S → 4P)
BORN (SWF)
MODIFIED BORN
σ (πa₀²)
100
90
80
70
30
20
10
1
5
10
15
20
Ei (THRESHOLD UNITS)

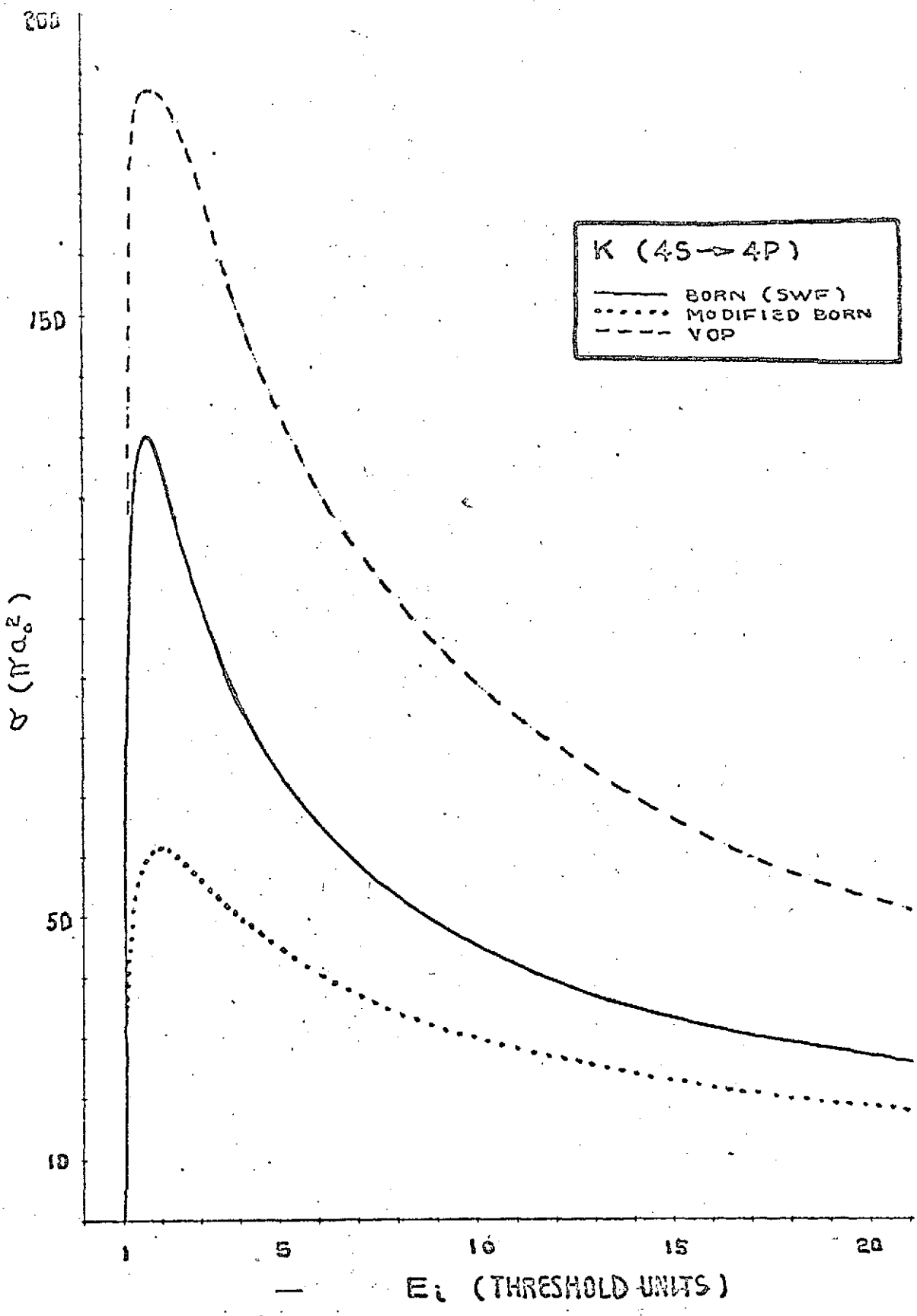

200
150
50
10
σ (πa₀²)
K (4S → 4P)
BORN (SWF)
MODIFIED BORN
VOP
1
5
10
15
20
E_i (THRESHOLD UNITS)

TABLE I

ELECTRON EXCITATION CROSS SECTIONS

(Units of πa_o^2)

	Li (2s → 2p)					Li (2s → 3p)		
E (threshold units)	Born (SWF)	Mod. Born	VOP[7]	CC[8]	Exp.[9]	Born (SWF)	Mod. Born	VOP[7]
1.16	.101(3)	.961(2)	.998(2)	.284(2)	--	.551(0)	.399(0)	.201(1)
1.64	.130(3)	.125(3)	.131(3)	.564(2)	--	.788(0)	.518(0)	.187(1)
2.00	.127(3)	.122(3)	.129(3)[a]	--	.159(2)	.917(0)	.667(0)	.151(1)[a]
2.44	.119(3)	.115(3)	.122(3)[a]	--	.230(2)	.102(1)	.813(0)	.127(1)[a]
3.56	.995(2)	.966(2)	.103(3)	--	.239(2)	.118(1)	.101(1)	.891(0)
5.00	.818(2)	.797(2)	.850(2)[a]	--	.213(2)	.120(1)	.107(1)	.631(0)[a]
6.76	.674(2)	.659(2)	.692(2)[a]	--	.186(2)	.115(1)	.105(1)	.477(0)[a]
11.24	.475(2)	.465(2)	.501(2)	--	.161(2)	.976(0)	.911(0)	.288(0)
17.00	.351(2)	.345(2)	.375(2)[a]	--	.156(2)	.809(0)	.765(0)	.190(0)[a]
24.04	.271(2)	.266(2)	.298(2)[a]	--	.144(2)	.675(0)	.643(0)	.133(0)[a]

a - Graphically interpolated

TABLE I

(cont.)

Na (3s → 4p)				Mg (3s → 4p)		K (4s → 4p)			Ca (4s → 4p)	
Born[b] (SWF)	Mod. Born	VOP[7]	Exp[9]	Born (SWF)	Mod. Born	Born (SWF)	Mod. Born	VOP[7]	Born (SWF)	Mod. Born
.266(0)	.211(-1)	.320(1)	--	.753(-1)	.195(-1)	.103(3)	.417(2)	.135(3)	.411(2)	.294(1)
.211(0)	.187(-1)	.360(1)	.232(0)	.214(0)	.842(-1)	.130(3)	.597(2)	.187(3)	.774(2)	.112(2)
.194(0)	.245(-1)	.347(1)	.234(0)	.253(0)	.119(0)	.125(3)	.611(2)	.186(3)[a]	.866(2)	.161(2)
.194(0)	.381(-1)	.311(1)	.230(0)	.273(0)	.148(0)	.115(3)	.596(2)	.182(3)[a]	.902(2)	.205(2)
.209(0)	.740(-1)	.222(1)	.223(0)	.279(0)	.178(0)	.931(2)	.529(2)	.159(3)	.873(2)	.264(2)
.219(0)	.103(0)	.170(1)	.214(0)	.261(0)	.183(0)	.746(2)	.452(2)	.135(3)[a]	.786(2)	.288(2)
.219(0)	.120(0)	.132(1)	.193(0)	.236(0)	.175(0)	.604(2)	.383(2)	.114(3)[a]	.690(2)	.289(2)
.196(0)	.124(0)	.839(0)	--	.187(0)	.148(0)	.414(2)	.280(2)	.821(2)	.526(2)	.261(2)
.169(0)	.120(0)	.585(0)	--	.149(0)	.122(0)	.301(2)	.212(2)	.595(2)[a]	.409(2)	.225(2)
.144(0)	.109(0)	.426(0)	--	.121(0)	.102(0)	.230(2)	.166(2)	.457(2)[a]	.326(2)	.193(2)

a - Graphically interpolated

b - Additional points calculated, $n = 1.02$, $\sigma = 0.148$; $n = 1.04$, $\sigma = 0.195$; $n = 1.08$, $\sigma = 0.241$.

TABLE II

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

(Units of πa_o^2)

E (Threshold units)	1.16	1.64	2.00	2.44	3.56	5.00	6.76	11.24	17.00	24.04
Born (SWF)	.469(0)	.477(0)	.555(0)	.657(0)	.818(0)	.883(0)	.878(0)	.781(0)	.664(0)	.563(0)
Mod. Born	.313(-1)	.581(-1)	.119(0)	.202(0)	.367(0)	.478(0)	.532(0)	.537(0)	.489(0)	.433(0)

LINE STRENGTH OF Na(3s → 3p) LINE

The line strength for spontaneous emission in the dipole approximation is given by[10]

$$S = \sum_{i,K} |\vec{R}^{n_i m_K}|^2 \qquad (27)$$

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

$$\vec{R}^{nm} = \langle n|\vec{r}|m\rangle \qquad (28)$$

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 electrodynamic treatment leads to the same results[11].

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

$$\vec{\nabla} \cdot \vec{E} = 4\pi\rho \qquad (29) \qquad \vec{\nabla} \times \vec{H} - \frac{1}{c}\frac{\partial \vec{E}}{\partial t} = \frac{4\pi}{c}\vec{J} \qquad (30)$$

$$\vec{\nabla} \times \vec{E} + \frac{1}{c}\frac{\partial \vec{H}}{\partial t} = 0 \qquad (31) \qquad \vec{\nabla} \cdot \vec{H} = 0 \qquad (32)$$

From equation (32) we see $\vec{H} = \vec{\nabla} \times \vec{A}$. If this is substituted into equation (31) and the order of the spatial and time derivatives is interchanged we obtain

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

Thus $$\vec{E} + \frac{1}{c} \frac{\partial \vec{A}}{\partial t} = - \vec{\nabla} \phi$$

or $$\vec{E} = - \frac{1}{c} \frac{\partial \vec{A}}{\partial t} - \vec{\nabla} \phi$$

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

$$\vec{\nabla} (\vec{\nabla} \cdot \vec{A} + \frac{1}{c} \frac{\partial \phi}{\partial t}) - \nabla^2 \vec{A} + \frac{1}{c^2} \frac{\partial^2 \vec{A}}{\partial t^2} = \frac{4\pi}{c} \vec{J} \qquad (33)$$

$$\frac{1}{c} \frac{\partial}{\partial t} \vec{\nabla} \cdot \vec{A} + \nabla^2 \phi = - 4\pi\rho \qquad (34)$$

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

$$\vec{\nabla} \cdot \vec{A} + \frac{1}{c} \frac{\partial \phi}{\partial t} = 0$$

Then equations (33) and (34) become

$$\nabla^2 \vec{A} - \frac{1}{c^2} \frac{\partial^2 \vec{A}}{\partial t^2} = - \frac{4\pi}{c} \vec{J} \qquad (35)$$

$$\nabla^2 \phi - \frac{1}{c^2} \frac{\partial^2 \phi}{\partial t^2} = 4 \pi\rho \qquad (36)$$

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

$$\nabla^2 \vec{H} - \frac{1}{c^2} \frac{\partial^2 \vec{H}}{\partial t^2} = - \frac{4\pi}{c} \vec{\nabla} \times \vec{J} \qquad (37)$$

Assume that the three cartesian components of $\vec{J}$ vary harmonically in time with the same angular frequency ω but not necessarily with the same phase:

$$J_x (\vec{r}, t) = 2 \left|J_x(\vec{r})\right| \cos (\omega t - \theta_x) = J_x (\vec{r}) \, e^{-i\omega t} + J_x^* (\vec{r}) \, e^{i\omega t} \qquad (38)$$

where

$$J_x(\vec{r}) = \left|J_x(\vec{r})\right| \, e^{i\theta_x}$$

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

$$E_x(\vec{r},t) = 2\left|E_x(\vec{r})\right| \cos (\omega t - \phi_x) = E_x(\vec{r}) \, e^{i\omega t} + E_x^* (\vec{r}) \, e^{-i\omega t} \qquad (39)$$

$$H_x(\vec{r},t) = 2\left|H_x(\vec{r})\right| \cos(\omega t - \alpha_x) = H_x(\vec{r}) \, e^{-i\omega t} + H_x^* (\vec{r}) e^{i\omega t} \qquad (40)$$

where

$$E_x(\vec{r}) = \left|E_x(\vec{r})\right| \, e^{i\phi_x} \qquad \text{and} \qquad H_x(\vec{r}) = \left|H_x(\vec{r}\right| \, e^{i\alpha_x}$$

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

$$\vec{E}(\vec{r}) = \frac{ic}{\omega} \vec{\nabla} \times \vec{H} (\vec{r}). \qquad (41)$$

Substituting the expressions for $\vec{J}$, $\vec{H}$ and $\vec{E}$ into the wave equation for $\vec{H}$, equation (37), we obtain,

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

The retarded solution of the above equation is given by

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

Now

$$\frac{e^{iK|\vec{r} - \vec{r}'|}}{|\vec{r} - \vec{r}'|} \xrightarrow[r \to \infty]{} \frac{1}{r}\ e^{iK(r - r' \cos\theta)} \qquad (44)$$

where θ is the angle between $\vec{r}$ and $\vec{r}'$.

The Poynting vector is

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

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

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

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

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

Then

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

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 $\vec{r}$ 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

$$H_x \to -\frac{iK}{rc} e^{iKr} \int J_y(\vec{r}') e^{-iKz'} d^3r'$$

$$H_y \to \frac{iK}{rc} e^{iKr} \int J_x(\vec{r}') e^{-iKz'} d^3r'$$

$$H_z \to 0 \qquad (46)$$

$$E_x \to \frac{iK}{rc} e^{iKr} \int J_y(\vec{r}') e^{-iKz'} d^3r'$$

$$E_y \to \frac{iK}{rc} e^{iKr} \int J_y(\vec{r}') e^{-iKz'} d^3r'$$

$$E_z \to 0$$

Partial integration has been used to get rid of the derivatives of J in the integrand of $\vec{H}$. 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 $\vec{K}$ we obtain

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

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

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 $e^{-iK\cdot\vec{r}'}$ can be replaced by 1 in the integrand of the equation for P_z. Then

$$P_z = \frac{K^2}{2\pi r^2 c} \left| \int J_{\perp K}(\vec{r}') \, d^3r' \right|^2 \qquad (47)$$

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

$$\vec{J}_o = \int \vec{J}(\vec{r}') \, d^3r'$$

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

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

$$= \frac{4K^2}{3c} |\vec{J}_o|^2 \qquad (48)$$

Equation (48) is also valid for non-linear polarizations.

To convert to quantum theory the classical expression for $\vec{J}$ must be replaced by its quantum analog. We want to replace $\vec{J}$ 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: $-(i\hbar/m)\vec{\nabla}$. 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 $eu_n^* u_K$. Thus we can replace $\vec{J}(\vec{r})$ by

$$\vec{J}(\vec{r}) \rightarrow -\frac{ie\hbar}{m} \quad u_n^*(\vec{r})\vec{\nabla}u_K(\vec{r})$$

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

Thus

$$\vec{J}_o = -\frac{ie\hbar}{m}\int u_n^* \ \vec{\nabla} \ u_K d^3r$$

or

$$\vec{J}_o = \frac{e}{m}\int \quad u_n^* \ \vec{P} \ \ u_K \ d^3r$$

or

$$\vec{J}_o = \frac{e}{m} \quad \langle n \ |\vec{P}| \ K\rangle \ . \qquad (49)$$

The matrix element of $\vec{P}$ is $\vec{P} = m\frac{d\vec{r}}{dt}$.

$$\text{So} \qquad \frac{1}{m} \langle n|\vec{P}|K\rangle = \frac{d}{dt} \langle n\ |\vec{r}|K\rangle. \tag{50}$$

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

$$\langle n(t)\ |\vec{r}|\ K(t)\rangle = \langle n(o)\ |\vec{r}|\ K(o)\rangle\ e^{i\omega_{nK}t}$$

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

So

$$\frac{d}{dt} \langle n(t)\ |\vec{r}|\ K(t)\rangle = \frac{d}{dt}\ \langle n(o)\ |\vec{r}|\ K(o)\rangle\ e^{i\omega_{nK}t}$$

$$= i\omega_{nK}\langle n(o)\ |\vec{r}|\ K(o)\rangle\ e^{i\omega_{nK}t}$$

$$= i\omega_{nK}\langle n(t)\ |\vec{r}|\ K(t)\rangle \tag{51}$$

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

$$\frac{1}{m} \langle n|\vec{P}|K\rangle = i\omega_{nK}\ \langle n|\vec{r}|K\rangle\ . \tag{52}$$

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

$$\vec{J}_o = ie\omega_{nK}\ \langle n|\vec{r}|K\rangle \tag{53}$$

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 $\hbar\omega_{nK} = E_K - E_n$ given off in each transition.

Thus

$$P = \frac{4K^2}{3c} \quad e^2\omega^2_{nK} \quad |\langle n|\vec{r}|K\rangle|^2$$

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

$$A_{nk} = \frac{4K^2e^2\omega_{nK}}{3\hbar c} \quad |\langle n|\vec{r}|K\rangle|^2$$

Using $\omega_{nK} = Kc$ we obtain

$$A_{nK} = \frac{4e^2\omega^3_{nK}}{3\hbar c^3} \quad |\langle n|\vec{r}|K\rangle|^2$$

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 → 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 → 3s) if either SWF I or SWF II are used.

Thus we obtain (in atomic units)

$$\text{for } m = 0 \qquad \int \psi^*_n \, \vec{r} \, \psi_K \, d^3r = 2.76 \, \hat{e}_z$$

$$\text{for } m = 1 \qquad \int \psi^*_n \, \vec{r} \, \psi_K \, d^3r = .799 \sqrt{6} \, |-\hat{e}_x + i\hat{e}_y|$$

$$\text{for } m = 1 \qquad \int \psi_n^* \vec{r}\, \psi_K \, d^3r = .799\sqrt{6}\,[\hat{e}_x + i\hat{e}_y] \,.$$

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 $\langle R_{n\ell}, R_{n'\ell} \rangle = \delta_{nn'}$ it can be shown that

$$A_{413} = -\int_0^\infty drr^2 R_{31}(r) \quad [r^3 \exp(-Z_4 r/4)]$$

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 $N_{n\ell}$'s and $A_{n\ell j}$'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 → p transition for which $n_f \geq n_i$. If $n_f < n_i$ enough N_j's, A_{nj}'s and F_{nj}'s may not be calculated. Only the statements marked * need be changed to calculate the total cross-section for other than s → p transitions for which $n_f \geq n_i$.

```
//CRSECT   JOB #16722  #,#PAUL SIMSIC          #,MSGL VEL=)#,CL
// EXEC FORT#CLG,PARM=NOMAP
//FORT.SYSIN DD *
      DIMENSION TN(10),XSUM(5),AX(5),A(5),FX(5),XANS(5),SIGMA(5)
      DIMENSION PFX(5),RIFA(210),RI(205),RF(205)
      DIMENSION C(4,4), AA(4,4,4), R(4,4,205),Z(4),
      READ 30, NI, NF, (Z(I),I=1,NF)
   30 FORMAT (2I2, 10F5.2)
      READ(5,50) (A(I),I=1,5),(TN(I),I=1,10)
   50 FORMAT(5(F5.2,2X)/10(F6.2,2X))
   24 FORMAT (F16.8,4X,I1,4X,I1)
   34 FORMAT (F16.8,4X,I1,4X,I1,4X,I1)
      ZZ=11.00
      TF=.27503
      AAA=1.732
      CC=8.*AAA**2/TF
      XN=100.
      NX=XN+1.
      RN=200.
      NR=RN+1.
      DO 1 I=1,NF
      DO 1 J=1,NF
      DO 1 K=1,NF
      AA(I,J,K)=0.00
    1 CONTINUE
      DO 10 J=1,NF
      DO 10 L=1,NF
      IF (J+1-L) 10,10,15
   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
    4 S=2*J+1
      G=J
      C(J,L)=1./( SQRT( GAMMA(S)*(G/(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=0.0
      IF (J-2) 8,6,6
    6 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
      Q=N
      AA(N,L,J)=C(J,L)*(ASUM- GAMMA(SA)*(1./(Z(J)/H+Z(N)/Q))**(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 FORMAT (1H1)
      ALIMR=.0
      BLIMR=50.0
      DELR=(BLIMR-ALIMR)/RN
      Y=ALIMR-DELR
      DO 60 I=1,201
      DO 60 N=1,NF
```

```
      DO 60 L=1,NF
   60 R(N,L,I)=0.000
      R(1,1,1)=C(1,1)
      IF (NF-2) 65,62,62
   62 R(2,1,1)=C(2,1)*AA(2,1,1)*C(1,1)
      IF (NF-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
     1))
      IF (NF-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
     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+DELP
      DO 70 J=2,NP
      Y=Y+DELP
      DO 80 L=1,2
      DO 80 N=1,NF
      N1=N-1
      IF (J-35) 82,40,40
   40 IF (N-1) 80,80,83
   83 IF (J-80 ) 82,41,41
   41 IF (N-2) 80,80,82
   82 DO 81 K=L,N1
   81 R(N,L,J)=R(N,L,J)+C(N,L)*AA(N,L,K)*R(K,L,J)
      IF (N-1) 94,94,95
   94 R(N,L,J)=C(N,L)*EXP(-Z(N)*Y/N) +R(N,L,J)
      GO TO 80
   95 R(N,L,J)=C(N,L)*(Y**(N-1)*EXP(-Z(N)*Y/N))+R(N,L,J)
   80 CONTINUE
      RI(J)=R(3,1,J)
   70 RE(J)=R(4,2,J)
```

```
      DO 21 I=1,10
      BLIM=SQRT(TE*TN(I))*(1.+SQRT(1.-1./TN(I)))
      ALIM=SQRT(TE*TN(I))*(1.-SQRT(1.-1./TN(I)))
      KX=1
      DO 25 IN=1,5
   25 XSUM(IN)=.0
      DELX=(BLIM-ALIM)/XN
      X=ALIM-DELX
      DO 54 IX=1,NX
      X=X+DELX
      KY=-KX
      KR=1
      RSUM=.0
      Y=ALIMR-DELR
      DO 300 IR=1,NR
      Y=Y+DELR
      KR=-KR
      ANG=SIN(X*Y)/X**2-Y*COS(X*Y)/X
      RIFA(IR)=RI(IR)*RF(IR)*ANG
      IF((IR-1)*(IR-NR )*KR) 100,300,200
  100 RSUM=RSUM+2.*RIFA(IR)
  200 RSUM=RSUM+RIFA(IR)
  300 RSUM=RSUM+RIFA(IR)
      RANS=DELR*RSUM/3.
      GX=(RANS*RANS)/(X*X*X)
      DO 53 IM=1,5
      AX(IM)=1./(1.+(ZZ*A(IM)*X)**2)**2
      FX(IM)=GX*AX(IM)
      PFX(IM)=CC*TE*FX(IM)
      IF((IX-1)*(IX-NX )*KX) 51,55,52
```

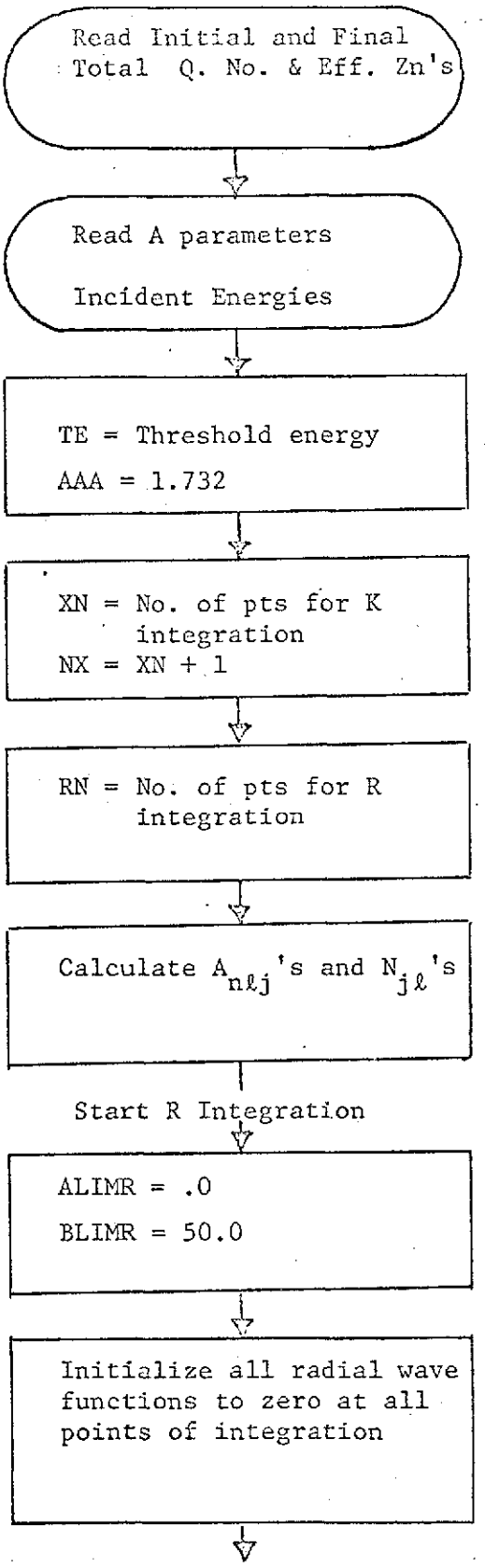
```
      51 XSUM(IM)=XSUM(IM)+2.*FX(IM)
      52 XSUM(IM)=XSUM(IM)+FX(IM)
      53 XSUM(IM)=XSUM(IM)+FX(IM)
      54 CONTINUE
         DO 56 J=1,5
         XANS(J)=DEL X*XSUM(J)/3.
      56 SIGMA(J)=CC*XANS(J)/TN(I)
         WRITE(6,11) ((SIGMA(K),A(K)),K=1,5),TN(I),I
      11 FORMAT(5(@ SIGMA=@E8.3,2X,@ A=@F4.2,2X)/@ TN=@F6.2,2X,@ I=@I3,//)
      21 CONTINUE
         END
/*
//GO.SYSIN DD *
 3 410.7 6.85 2.20 1.35
+0.00  +0.10  +0.15  +0.20  +0.28
+ 1.16  + 1.64  + 2.00  + 2.44  + 3.56  + 5.00  + 6.76  +11.24  +17.00  +24.34
/*
```

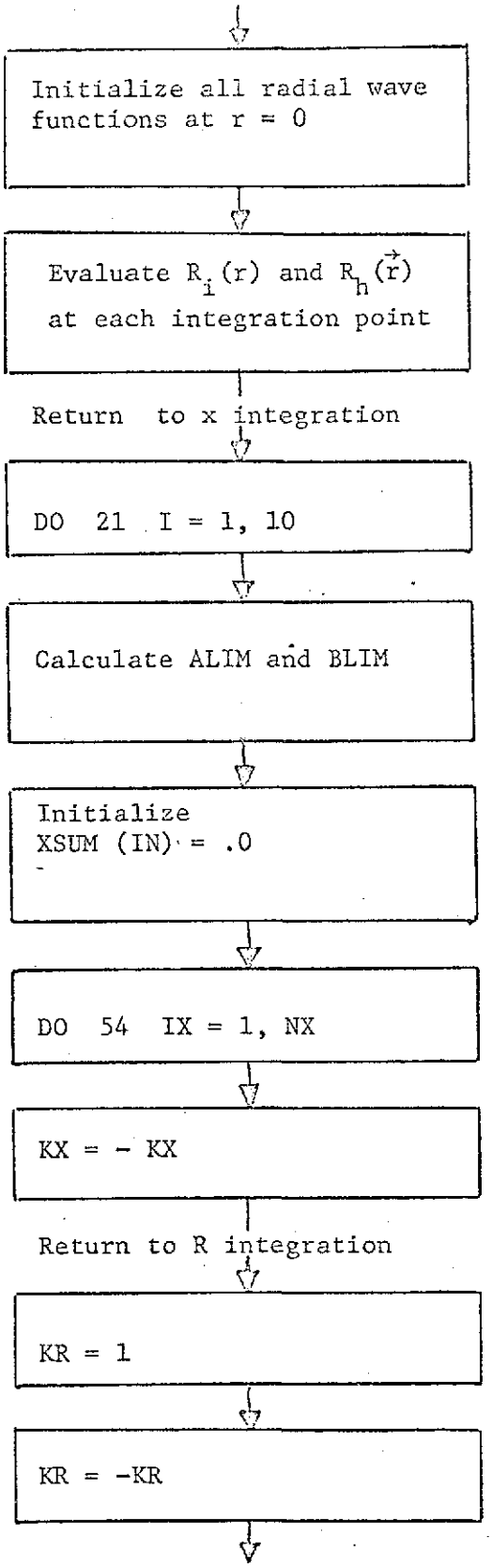
```
//CRSECT   JOB @16722  @,@PAUL SIMSIC          @,MSGLEVEL=)@,@
// EXEC FORTGCLG,PARM=NOMAP
//FORT.SYSIN DD *
      DIMENSION A(10,10), RHO(10,10), THET(10,10), B(10,10), F(10,10),
     1Z(10), C(10), AA(10,10)
      READ 30, NI, NF, (Z(I),I=1,NF)
   30 FORMAT (212, 10F5.2)
   34 FORMAT (E 16.8,4X,I1,4X,I1)
      DO 40 J=1,NF
      DO 40 K=1,NI
      A(J,K)=NF+NI+2-J-K
   40 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 1 M=1,NF
      F(M,M)=1.
    1 AA(M,M)=0.
      DO 10 J=1,NF
      ASQR=0.0
      IF (J-2) 4,2,2
    2 K=J-1
      DO 3 I=1,K
    3 ASQR=ASQR+AA(J,I)**2
    4 S=2*J+1
      G=J
      C(J)=1./(SQRT(GAMMA(S)*(G/(2.*2(J)))**(2*J+1)-ASQR))
```

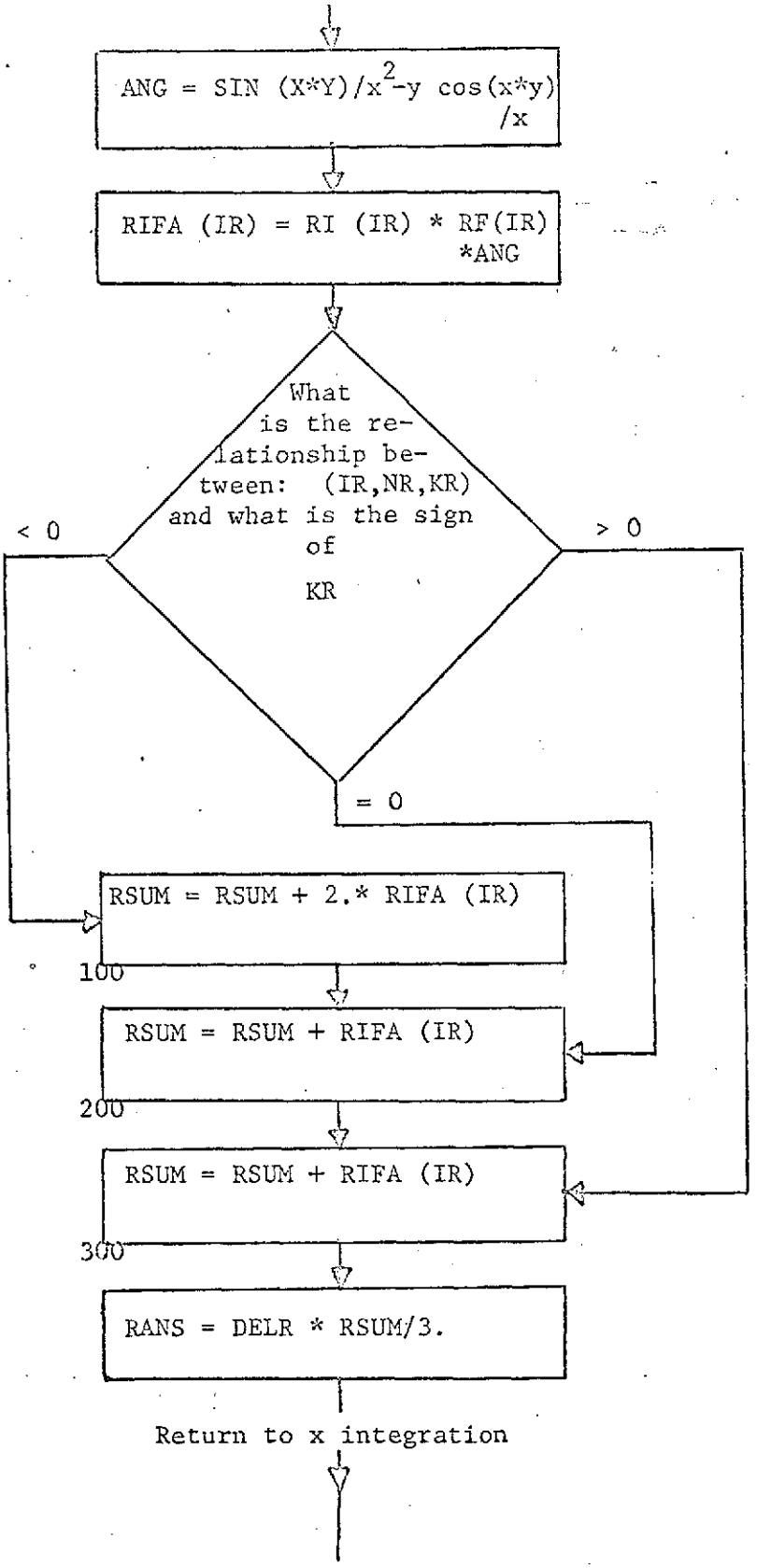
```
      WRITE (6,24) C(J), J
      DO 9 N=2,NF
      IF (N-J) 9,9,5
    5 ASUM=0.0
      IF (J-2) 8,6,6
    6 L=J-1
      DO 7 I=1,L
    7 ASUM=ASUM+AA(N,I)*AA(J,I)
    8 SA=N+J+1
      R=J
      Q=N
      AA(N,J)=C(J)*(ASUM- GAMMA(SA)*(1./(Z(J)/R+Z(N)/Q))**(N+J+1))
      WRITE (6,34) AA(N,J), N,J
    9 CONTINUE
   10 CONTINUE
      N=NF+1
      J=NF
      NF1=NF-1
      NF1N1=NF+1-N1
      DO 13 I=1,NF1N1
      DO 13 M=1,NF1
      N1=N-1
      JM=J-M
      IF (N1-JM) 13,13,11
   11 FSUM=0.0
      L=N1+1-JM
      DO 12 K=1,L
      N1K=N1+1-K
   12 FSUM=FSUM+F(N1,N1K)*AA(N1K,JM)
      F(N1,JM)=C(JM)*FSUM
```

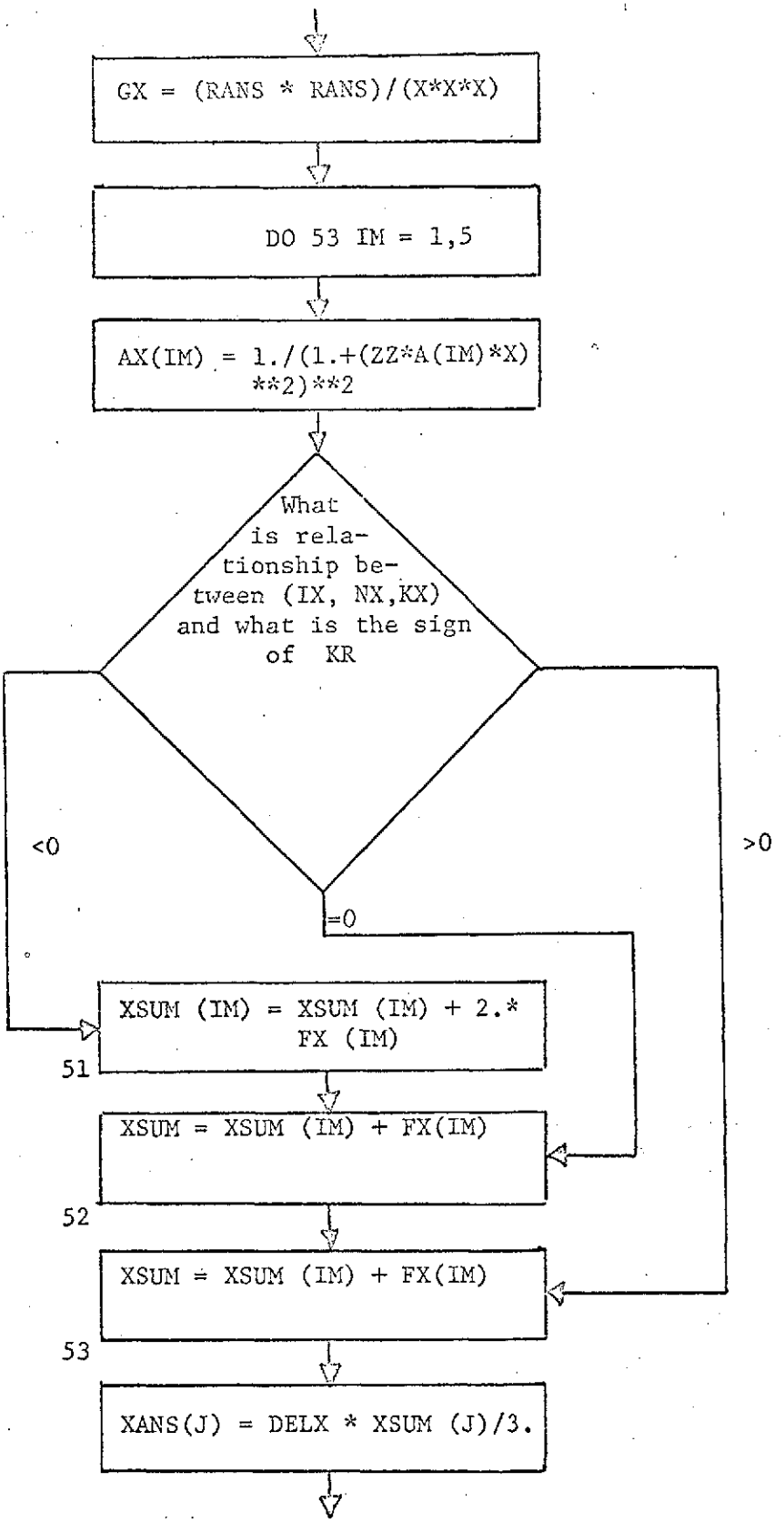
```
      WRITE (6,34) F(N1,JM), N1,JM
   13 CONTINUE
      PRINT 50
   50 FORMAT(1H1 CALCULATION OF ELECTRON EXCITATION CROSS SECTION FOR
     1THE 1S TO 2P TRANSITION IN HYDROGEN IN THE BORN APPROXIMATION US
     2G/113H SLATER WAVE FUNCTIONS. EI IS THE INCIDENT ENERGY IN THRESHO
     3LD UNITS AND XANS IS THE TOTAL CROSS SECTION IN UNITS/ 97H OF PI T
     4IMES THE BOHR RADIUS SQUARED.)
  100 READ 101, XN, EI, ET, FZ
  101 FORMAT (10 F 8.5)
      ALIM=SQRT(EI*ET)*(1.-SQRT(1.-1.0/EI))
      BLIM=SQRT(EI*ET)*(1.+SQRT(1.-1.0/EI))
      JX=XN+1.
      KX=1
      XSUM=.0
      DELX=(BLIM-ALIM)/XN
      X=ALIM-DELX
      DO 105 IX=1,JX
      X=X+DELX
      YSUM=0.0
      DO 102 K=1,NI
      DO 102 J=1,NF
      RHO(J,K)=SQRT(B(J,K)**2+X**2)
      THET(J,K)=ATAN(X/B(J,K))
*102 YSUM=YSUM+F(NF,NF+1-J)*F(NI,NI+1-K)*GAMMA(A(J,K)-1.0)/(RHO(J,K)**
     1A(J,K))*(X*(A(J,K)-1.0)*SIN(A(J,K)*THET(J,K)-1.570796)+RHO(J,K)*
     2COS((A(J,K)-1.0)*THET(J,K)-1.570796))
     * FX=(YSUM**2)/X**7
      KX=-KX
      IF ((IX-1)*(IX-JX)*KX) 103,105,104
```

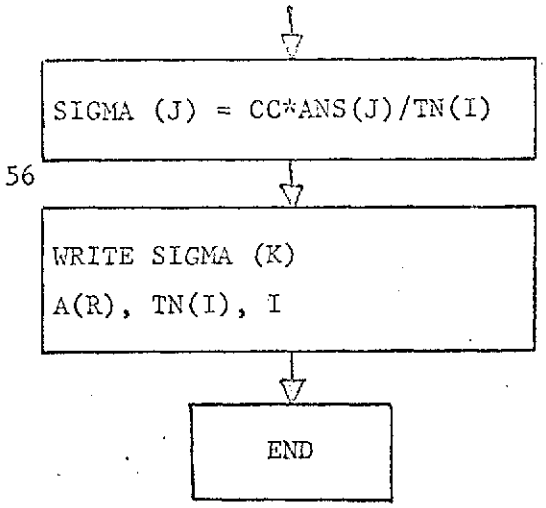
```
  103 XSUM=XSUM+2.*FX
  104 XSUM=XSUM+FX
  105 XSUM=XSUM+FX
      XANS=DELX*XSUM/3.
     * XANS=24.*(C(NI)**2)*(C(NF)**2)/(EI*ET)*XANS
      WRITE (6,106) EI,XANS
  106 FORMAT (50X, 4H EI=, E9.4, 5X, 7H SIGMA=, E9.4)
      IF(FZ) 100,108,100
  108 CALL EXIT
      END
/*
//GO.SYSIN DD *
 1 21.00 1.00
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 5.00     .74979   10.0000
100.000 6.76     .74979   10.0000
100.000 11.24    .74979   10.0000
100.000 17.00    .74979   10.0000
100.000 24.04    .74979   10.0000
/*
```

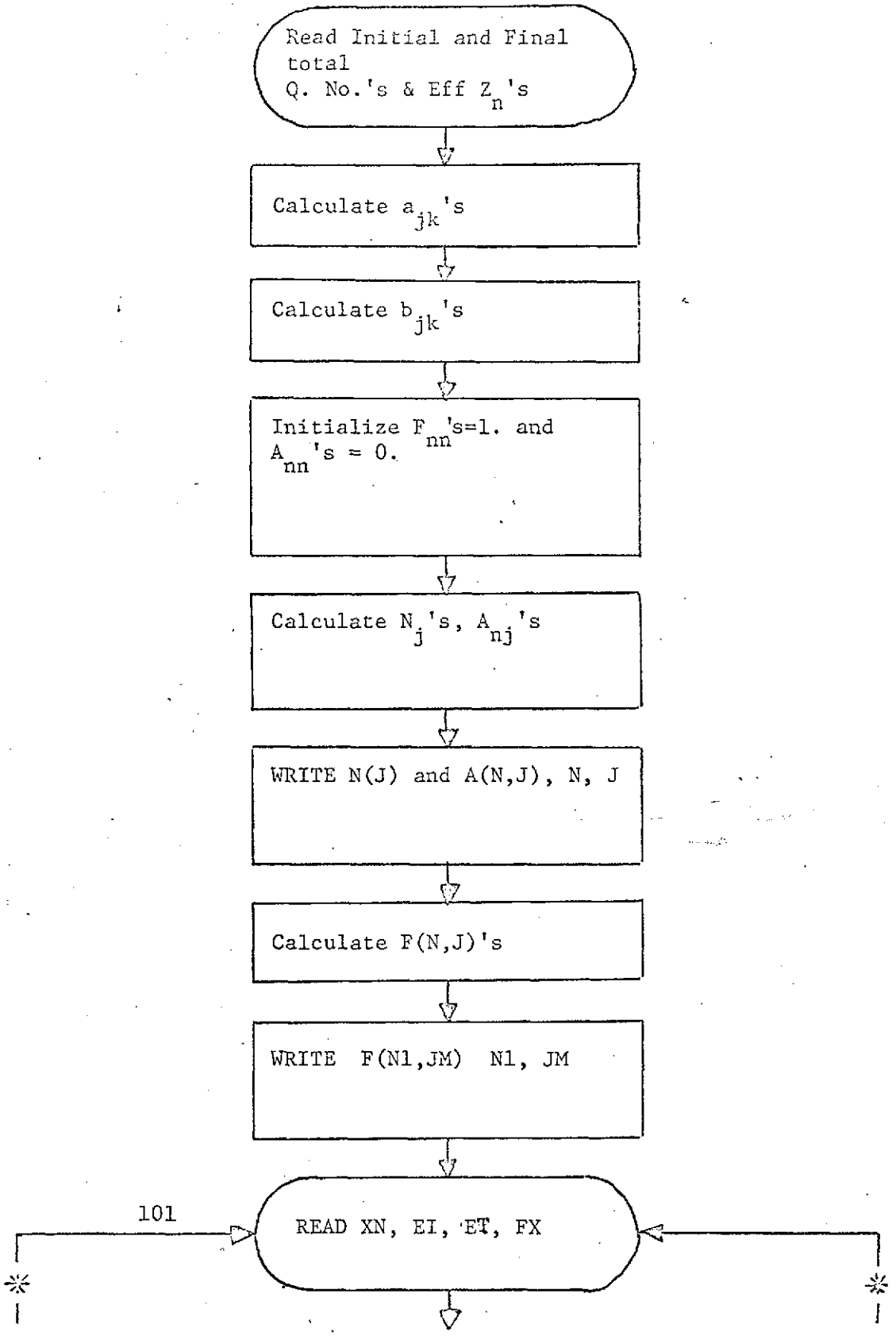

Read Initial and Final Total Q. No. & Eff. Zn's
Read A parameters
Incident Energies
TE = Threshold energy
AAA = 1.732
XN = No. of pts for K integration
NX = XN + 1
RN = No. of pts for R integration
Calculate $A_{n\ell j}$'s and $N_{j\ell}$'s
Start R Integration
ALIMR = .0
BLIMR = 50.0
Initialize all radial wave functions to zero at all points of integration


Initialize all radial wave functions at r = 0
Evaluate $R_i(r)$ and $R_h(\vec{r})$ 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
KX = - KX
Return to R integration
KR = 1
KR = -KR

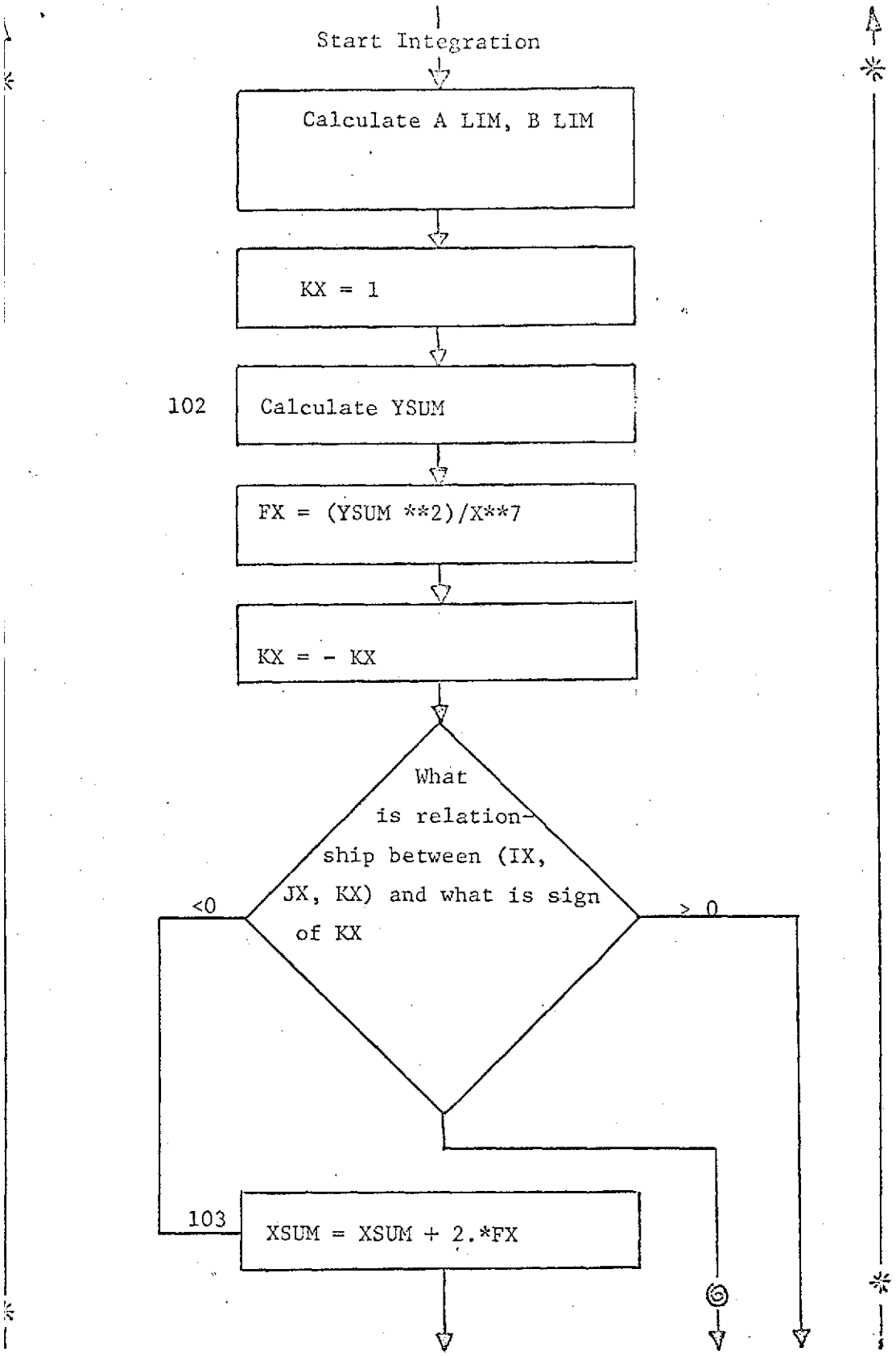

ANG = SIN (X*Y)/x2-y cos(x*y)
/x
RIFA (IR) = RI (IR) * RF(IR)
*ANG
What is the relationship between: (IR,NR,KR) and what is the sign of KR
< 0
> 0
= 0
RSUM = RSUM + 2.* RIFA (IR)
100
RSUM = RSUM + RIFA (IR)
200
RSUM = RSUM + RIFA (IR)
300
RANS = DELR * RSUM/3.
Return to x integration

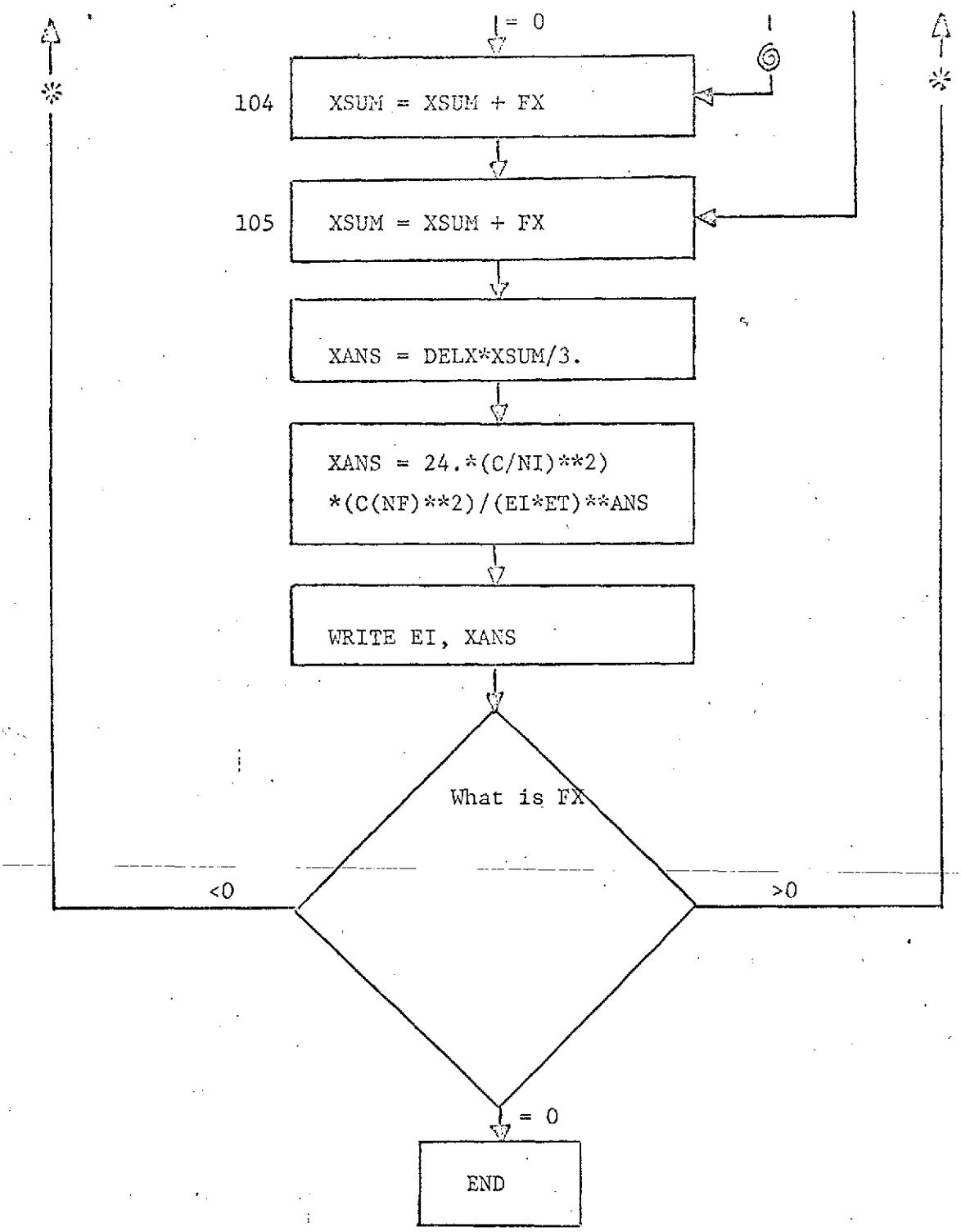

GX = (RANS * RANS)/(X*X*X)
DO 53 IM = 1,5
AX(IM) = 1./(1.+(ZZ*A(IM)*X)**2)**2
What is relationship between (IX, NX,KX) and what is the sign of KR
<0
>0
=0
XSUM (IM) = XSUM (IM) + 2.* FX (IM)
51
XSUM = XSUM (IM) + FX(IM)
52
XSUM = XSUM (IM) + FX(IM)
53
XANS(J) = DELX * XSUM (J)/3.


SIGMA (J) = CC*ANS(J)/TN(I)
56
WRITE SIGMA (K)
A(R), TN(I), I
END



Start Integration


Start Integration
Calculate A LIM, B LIM
KX = 1
102
Calculate YSUM
FX = (YSUM **2)/X**7
KX = - KX
What is relation-ship between (IX, JX, KX) and what is sign of KX
<0
> 0
103
XSUM = XSUM + 2.*FX


= 0
104
XSUM = XSUM + FX
105
XSUM = XSUM + FX
XANS = DELX*XSUM/3.
XANS = 24.*(C/NI)**2)
*(C(NF)**2)/(EI*ET)**ANS
WRITE EI, XANS
What is FX
<0
>0
= 0
END

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