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IONIZATION OF EXCITED ATOMIC HYDROGEN BY FAST ELECTRONS

KAZEM OMIDVAR

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IONIZATION OF EXCITED ATOMIC HYDROGEN BY FAST ELECTRONS

K. Omidvar

Laboratory for Theoretical Studies

NASA, Goddard Space Flight Center, Greenbelt, Maryland, USA

ABSTRACT

Electron impact ionization cross section, energy distribution and the average energy of the ejected electrons for the first five principal quantum numbers of atomic hydrogen, and all the azimuthal quantum numbers are calculated within the Born approximation. Calculations are extended to a range of 100 to 900 threshold units of energy. Regions of agreement and disagreement between the high energy quantal and classical calculations are analyzed. Validity of the Born approximation for excitation and ionization for a single particle model is given. An energy spectrum of the secondary electrons due to the passage of an energetic electron in a hydrogen atom gas is found.

1. INTRODUCTION

Ionization of the ground and excited states of atomic hydrogen by electron collison has a number of applications in plasma physics and astrophysical problems. While there has been an extensive study for the ionization of the ground state, little has been done for the excited states. Among studies for the ground state ionization we can mention the early calculations by Bethe (1930), and Massey and Mohr (1933) within the Born approximation; measurement of the cross section by Fite and Brackman (1958), and Boksenberg (1960); measurement of the cross section at the threshold by McGowan et al. (1968); study of the wave function for e-H ionization by Peterkop (1962); distorted-wave calculation by Veldre and Vinkalns (1963), and Burke and Taylor (1965); and study of the threshold of ionization by Wannier (1953), Geltman (1956), Rudge and Seaton (1965), and Temkin (1966).

Here we are concerned with ionization of the excited states. In a previous paper (Omidvar 1965) a calculation on impact ionization of the excited atomic hydrogen was reported in which the cross section and other related values were given for wave functions in parabolic coordinates. In the present paper these values are given for wave functions in spherical coordinates. In problems related to radiation, these are more suitable coordinates. Similarly, in more complicated calculations than the Born approximation, spherical coordinates are more often used. For these reasons the present calculation will have a wider range of applicability.

In the present paper, calculation is extended to much higher incident energies than used in the previous paper. For principal quantum numbers $n = 1, 2, 3$, calculation has been extended to 900 threshold units; for $n = 4$, to 225 threshold units; and for $n = 5$, to 100 units. The numerical results presented here are more accurate than the previous calculation. Finally, in this paper, energies are expressed in threshold units, and scaling law has been used for other quantities. Thus it has been possible to study more precisely the variation in cross section and other physical quantities in terms of n and the azimuthal quantum number l.

On the other hand, values for different magnetic quantum numbers m are not reported here. In this paper the axis of spatial quantization is taken along the momentum of the ejected electron, while in the previous paper this axis was along the momentum transfer of the incident electron. Values for a given m in the two cases naturally do not correspond. Unless one is interested in the ionization cross section and related values for a particular momentum transfer, or for a particular direction of the ejected electron, the m dependent values serve no useful purpose. Values related to a given n and l are listed here after an integration is carried out with respect to both the direction of the ejected electron and the direction of the momentum transfer.

An analysis is also made for the validity of the Born approximation and its relation to the Bethe approximation. Also a comparison is made between

high-energy quantal and classical calculations, and it is shown that as n increases in accordance with the correspondence principle, the quantal results approach those given by the classical calculation.

2. DERIVATION OF THE IONIZATION AMPLITUDE

The analysis must start with the evaluation of the Born amplitude for ionization for any given state. For this it is necessary to specify the states of the atom before and after ionization. Atomic units are used in which $\hbar$ and the electronic mass and charge are set equal to unity, and energy is expressed throughout in rydbergs. If $\mathbf{p}$ and ϵ specify the momentum and the energy of a particle, and $\mathbf{k}$, its propagation vector, it then follows that $\mathbf{p} = \mathbf{k}$ and $\epsilon = k^2$. In this way energy takes the dimension of inverse of the length squared, but numerically its value is given in rydbergs.

States of the atom are specified by the Coulomb functions. The initial state is given by $|nlm\rangle$, where n, l, and m are the principal, the azimuthal, and the absolute value of the magnetic quantum numbers. This state is related to the states in the parabolic coordinates, $|nn_1m\rangle$, by the unitary transformation

$$|nlm\rangle = \sum_{n_1=0}^{n-m-1} |nn_1m\rangle \langle nn_1m|nlm\rangle \quad , \qquad (1)$$

where $\langle nn_1 m \mid nlm \rangle$ are elements of the transformation matrix. In this transformation n and m remain fixed, n_1 ranges from 0 to n-m -1, and l ranges from m to n-1. The recursion relation and the specific values of $\langle nn_1 m \mid nlm \rangle$ for n = 0 to 5 and all possible values of m are given elsewhere (Omidvar, 1967). Barut and Kelinert (1967), and Hughes (1967) have shown independently that these elements are related to the Clebsch-Gordan coefficients through

$$\langle nn_1 m \mid nlm \rangle = (-)^m (2l+1)^{1/2} \begin{pmatrix} 1/2\,(n-1) & 1/2\,(n-1) & l \\ 1/2\,(m-n_1+n_2) & 1/2\,(m+n_1-n_2) & -m \end{pmatrix}$$

$$= C \left(\frac{n-1}{2} \quad \frac{n-1}{2} \; l; \quad \frac{m-n_1+n_2}{2} \quad \frac{m+n_1-n_2}{2} \quad m \right) \qquad (2)$$

where $\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{pmatrix}$ are Wigner's $3j$, and $C(j_1 j_2 j; m_1 m_2 m)$ are the Clebsch-Gordan, coefficients (Edmonds 1957)*.

In (2) the integer n_2 is given by $n_2 = n-1-m-n_1$. The normalized hydrogenic state $\mid nn_1 m \rangle$ corresponding to a nuclear charge Z is given by Bethe and Salpeter (1967)

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*Equation (2) is given by Barut et al. If we write A_{ln_1} for $\langle nn_1 m \mid nlm \rangle$, then it can be shown directly that $A^B_{ln_1} = (-)^{n_2} A^H_{ln_1} = (-)^{n_2+l} A_{ln_1}$, where $A^B_{ln_1}$, $A^H_{ln_1}$, and A_{ln_1} are the matrices of Barut et al., Hughes, and this author, respectively. These phase differences have no effect on the calculation.

$$|nn_1m\rangle = N_{n_1n_2m}\, e^{-\frac{1}{2}\alpha(\xi+\eta)}\,(\xi\eta)^{\frac{1}{2}m}\, L^m_{n_1+m}(\alpha\xi)\, L^m_{n_2+m}(\alpha\eta)\, e^{im\varphi} \quad ,$$

$$N_{n_1n_2m} = \frac{1}{\sqrt{2\pi}}\left(\frac{2}{n}\right)^{\frac{1}{2}} \alpha^{m+3/2} \frac{\left[n_1!\,n_2!\right]^{\frac{1}{2}}}{\left[(n_1+m)!\,(n_2+m)!\right]^{3/2}} \quad , \alpha = \frac{Z}{na_0} \quad . \tag{3}$$

In this equation ξ, η, φ, are the parabolic coordinates of the atomic electron related to the spherical coordinates by $\xi = r(1+\cos\theta)$, $\eta = r(1-\cos\theta)$ and $\varphi = \varphi$; and a_0 is the Bohr radius.

The final atomic state is the state of an ejected electron in the field of a nucleus of charge Z, and is given by a Coulomb function with outgoing waves. If $\mathbf{k}$ represents the propagation vector of the ejected electron and at the same time the direction of the z-axis of the coordinate system, this function is given by (Landau and Lifshitz 1958)

$$|\mathbf{k}\rangle = \Psi_{\mathbf{k}}^{+}(\mathbf{r}) = N_c\, e^{i\mathbf{k}\cdot\mathbf{r}}\, F(i\beta, l, ik\eta) \quad ,$$

$$N_c = \frac{1}{2\pi}\left[\frac{\beta}{1-\exp(-2\pi\beta)}\right]^{\frac{1}{2}} ,$$

$$\beta = \frac{Z}{ka_0} , \tag{4}$$

where $F(a, b, z)$ is the confluent hypergeometric function which is regular at the origin. $\psi^{+}(\mathbf{r})$ is normalized such that

$$\int \psi^{+*}_{\mathbf{k}'}(\mathbf{r})\, \psi^{+}_{\mathbf{k}}(\mathbf{r})\, d\mathbf{r} = \delta(\mathbf{k}-\mathbf{k}') = 2k^{-1}\, \delta(\epsilon-\epsilon')\, \delta(\hat{\mathbf{k}}-\hat{\mathbf{k}}') \quad , \tag{5}$$

with ϵ and ϵ' the energy of the ejected electrons in rydbergs. The asymptotic form of $\psi^{+}(\mathbf{r})$ is given by

$$\psi^{+}(\mathbf{r}) \sim (2\pi)^{-3/2} e^{i\mathbf{k}\cdot\mathbf{r}} \tag{6}$$

In some application it is more useful to use an integral representation for $\psi^{+}(\mathbf{r})$ which originally was given by Sommerfeld (1931). This is

$$\psi^{+}_{\mathbf{k}}(\mathbf{r}) = N_c \frac{e^{ikr}}{\Gamma(1-i\beta)} \int_0^{\infty} e^{-u} u^{-i\beta} J_0(2\sqrt{iukr}) \, du \quad . \tag{7}$$

However, in this paper we use the form given by (5).

With the atomic states so defined and with $\mathbf{k}_1$ and $\mathbf{k}_1$ the propagation vectors of the incident and the scattered electrons, the ionization cross section per unit energy range of the ejected electrons is given by

$$\frac{dQ}{d\epsilon} = \frac{1}{4\pi a_0^2 k_1^2} \int k \, d\hat{k} \int_{k_1 - k_2}^{k_1 + k_2} |T(i,f)|^2 \, q \, dq, \tag{8}$$

where the transition amplitude $T(i,f)$ is defined by

$$T(i,f) = \frac{4\pi}{q^2} < f | e^{i\mathbf{q}\cdot\mathbf{r}} | i > , \tag{9}$$

with $\mathbf{q} = \mathbf{k}_1 - \mathbf{k}_2$; and the total cross section defined by

$$Q = \int_0^{\epsilon_{max}} \frac{dQ}{d\epsilon} \, d\epsilon \quad . \tag{10}$$

The values of k_2, ϵ , and ϵ_{max} are related to the incident energy k_1^2 by conservation of energy through

$$k_1^2 - Z^2/n^2 a_0^2 = k_2^2 + \epsilon = \epsilon_{max} \quad , \tag{11}$$

with n being the principal quantum number of the initial state. To have a clear account of the dimensions involved notice that with reference to (3) and (4), $T(i,f)$ has the dimension of $[l]^{7/2}$. Then $dQ/d\epsilon$ and Q have the dimensions of the fourth and the second powers of length respectively.

The rest of formulation consists of evaluation of $T(i,f)$ given by (9). We take $|i>$ and $|f>$ to be the states given by (3) and (4). For simplification in evaluation of $T(i,f)$, we take the z -axis of the coordinate system not along $\mathbf{k}_1$, as is customary, but along $\mathbf{k}$. We represent the spherical coordinates of $\mathbf{q}$ in this system, by q, θ_1, φ_1, and the parabolic coordinates of $\mathbf{r}$ by ξ, η, φ. The φ-dependent integral in (9) and its value are then given by

$$\int_0^{2\pi} e^{(i\mathbf{q}\cdot\mathbf{r} + im\varphi)} d\varphi$$
$$= 2\pi \exp\left[\tfrac{1}{2} i q (\cos\theta_1)(\xi - \eta) + i m (\varphi_1 + \tfrac{1}{2}\pi)\right] J_m(q \sin\theta_1 \sqrt{\xi\eta}) \quad , \tag{12}$$

where $J_m(x)$ is the Bessel's function with argument x. Using this expression we can write

$$T(nn_1 m, \mathbf{k}) = \frac{-2\pi^2}{q^2} e^{im(\varphi_1 + \frac{\pi}{2})} N_{n_1 n_2 m} N_c \frac{\partial U}{\partial p} , \tag{13}$$

$$U = \int_0^\infty d\eta \left[e^{-(p-s)\eta} \eta^{\frac{1}{2}m} L^m_{n_2+m}(\alpha\eta) F(-i\beta, 1, -ik\eta) \right]$$

$$\times \int_0^\infty d\xi \left[e^{-(p+s)\xi} \xi^{\frac{1}{2}m} L^m_{n_1+m}(\alpha\xi) J_m(q \sin\theta_1 \sqrt{\xi\eta}) \right] ,$$

$$p = \tfrac{1}{2}\alpha \quad , \; s = -\tfrac{1}{2} i (q \cos\theta_1 - k) \quad . \tag{14}$$

To evaluate (14) we use the identity

$$L^m_n(z) = \frac{(-)^m n!}{(n-m)!} e^z z^{-m} \frac{d^{n-m}}{dz^{n-m}} (e^{-z} z^n) \quad . \tag{15}$$

Then by direct differentiation

$$L^m_{n_1+m}(\alpha\xi) = (-)^m . \frac{(n_1+m)!}{n_1!} \sum_{\nu_1=0}^{n_1} \binom{n_1}{\nu_1} \frac{(n_1+m)!}{(\nu_1+m)!} (-\alpha\xi)^{\nu_1} \quad . \tag{16}$$

With this form for $L^m_{n_1+m}(\alpha\xi)$, the ξ-integral in (14) can be evaluated and its value is given by

$$(-)^m . \frac{(n_1+m)!}{n_1!} \sum_{\nu_1=0}^{n_1} \binom{n_1}{\nu_1} \frac{(n_1+m)!}{(\nu_1+m)!} \alpha^{\nu_1}$$

$$\times \frac{d^{\nu_1}}{dP^{\nu_1}} \left[\frac{2 (q \sin\theta_1)^m \eta^{\frac{1}{2}m}}{(2P)^{m+1}} \exp\left(\frac{-q^2 \sin^2\theta_1 \eta}{4P} \right) \right] , \; P = p + s.$$

When this is substituted for the ξ-integral in (14) we obtain

$$U = (-)^m \frac{(n_1 + m)!}{n_1!} \sum_{\nu_1 = 0}^{n_1} \binom{n_1}{\nu_1} \frac{(n_1 + m)!}{(\nu_1 + m)!} \alpha^{\nu_1} \frac{d^{\nu_1}}{dP^{\nu_1}} \left\{ \frac{2\,(q \sin\theta_1)^m}{(2P)^{m+1}} I \right\}, \tag{17}$$

$$I = \int_0^\infty d\eta \left[e^{-\lambda\eta} \eta^m L^m_{n_2 + m}(\alpha\eta)\, F(-i\beta, 1, -ik\eta) \right], \tag{18}$$

$$\lambda = p - s + q^2 \sin^2\theta_1 \Big/ 4P.$$

Evaluation of the integral in (17) is accomplished by expanding $L^m_{n_2+m}(\alpha\eta)$ according to (16). The integral can then be evaluated by standard methods (Landau and Lifshitz 1958). The result is

$$I = \frac{(n_2 + m)!}{n_2!} \sum_{\nu_2 = 0}^{n_2} \binom{n_2}{\nu_2} \frac{(n_2 + m)!}{(\nu_2 + m)!} \alpha^{\nu_2} \sum_{\mu_2 = 0}^{m + \nu_2} \binom{m + \nu_2}{\mu_2}$$

$$\times \frac{(-i\beta - 1)!\,(i\beta)!}{(-i\beta - 1 - m - \nu_2 + \mu_2)!\,(i\beta - \mu_2)!} \times \frac{(\lambda + ik)^{i\beta - \mu_2}}{\lambda^{i\beta + 1 + m + \nu_2 - \mu_2}}. \tag{19}$$

By some manipulation and using the properties of the binomial coefficients, this can be written

$$I = \frac{[(n_2+m)!]^2}{n_2!} \sum_{\nu_2=0}^{n_2} \binom{n_2}{\nu_2} \alpha^{\nu_2} \sum_{\mu_2=0}^{m+\nu_2} (-)^{m+\nu_2-\mu_2} \binom{-i\beta-1}{\mu_2}$$

$$\times \binom{m+\nu_2}{\mu_2} \frac{(\lambda+ik)^{i\beta-m-\nu_2} (ik)^{\mu_2}}{\lambda^{i\beta+1+\mu_2}} \quad . \tag{20}$$

Substitution of I in (17) and evaluation of U and $\partial U/\partial p$ is straight forward algebra. By inserting the value of $\partial U/\partial p$ in (13) we find that

$$T(nn_1 m, \mathbf{k}) = \frac{-4\pi}{q^2} \cdot \frac{(2\alpha)^{m+3/2}}{\sqrt{2\pi n}} \left[\frac{(n_2+m)!}{(n_1+m)!\, n_1!\, n_2!} \right]^{1/2} e^{im(\varphi_1 + \frac{\pi}{2})}$$

$$\times \left(\frac{\beta}{1-e^{-2\pi\beta}} \right)^{1/2} q^m \, [1-(\hat{\mathbf{q}}\cdot\hat{\mathbf{k}})^2]^{m/2} \, A^{-m+i\beta} B^{-1-i\beta} \sum , \tag{21}$$

$$\sum = \sum_{\mu_1}^{n_1} \sum_{\mu_2}^{\mu_1} \sum_{\mu_3}^{\mu_2} \sum_{\mu_4}^{\mu_3} \sum_{\nu_1}^{n_2} \sum_{\nu_2}^{m+\nu_1} (-)^{\mu_2+\mu_4+\nu_1} (2\alpha)^{\mu_1+\nu_1} C(\mu_4, \mu_3)$$

$$\times \binom{n_1}{\mu_1} \binom{n_2}{\nu_1} \binom{m+\nu_1}{\nu_2} \binom{\mu_1}{\mu_2} \binom{\mu_2}{\mu_3} \frac{(m+n_1)!}{(m+\mu_1)!} \frac{(\nu_1+\nu_2)!\, \mu_4!}{(\nu_1+\nu_2-\mu_1+\mu_2)!}$$

$$\times \frac{(m+\nu_1+\nu_2+\mu_2-\mu_3)!}{(m+\nu_1+\nu_2)!} \binom{\nu_2+i\beta}{\nu_2} \binom{-m-\nu_1+i\beta}{\mu_4}$$

$$\times (2ik)^{\mu_4+\nu_2} q^{2\mu_4} \left[1-(\hat{\mathbf{q}}\cdot\hat{\mathbf{k}})^2\right]^{\mu_4} \cdot F , \tag{22}$$

with

$$F = A^{-\mu_4 - \nu_1} B^{-\mu_2 - \nu_2} D^{\mu_2 - \mu_4} D^{*\,-\mu_1 + \mu_2 + \nu_1 + \nu_2}$$

$$\times \left[-\frac{2(\alpha + ik)(m + \mu_4 + \nu_1 - i\beta)}{A} - \frac{2\alpha(1 + \mu_2 + \nu_2 + i\beta)}{B} + \frac{\mu_2 - \mu_4}{D} + \frac{-\mu_1 + \mu_2 + \nu_1 + \nu_2}{D^*} \right] , \quad (23)$$

where D^* is the complex conjugate of D. In (22) the lower limits of the variable integers are zero, and in (23) $A, B,$ and D are defined as

$$A = (\alpha + ik)^2 + q^2 , \; B = \alpha^2 + (\mathbf{q} - \mathbf{k})^2 , \; D = \alpha + i\hat{\mathbf{k}} \cdot (\mathbf{q} - \mathbf{k}) . \quad (24)$$

In this way, in the expression for $T(n n_1 m, \mathbf{k})$ all symbols are defined except $C(\mu_4, \mu_3)$. This coefficient arises from the following consideration.

Suppose

$$U(P) = \frac{AP}{-BP + C} , \quad (25)$$

where A, B, and C are constants. Then the lth derivative of $y = y(u)$ with respect to P is given by

$$\frac{d^l y}{dP^l} = (Bg)^l \sum_{\lambda=1}^{l} C(\lambda,l) \left(\frac{AC}{B}g\right)^{\lambda} y^{\lambda}(u), \quad g = \frac{1}{-BP+C} \quad , \tag{26}$$

where $y^{\lambda}(u)$ is the λth derivative of y with respect to u, and $C(\lambda, l)$ are numbers depending on λ and l. Differentiating equation (26) on one hand with respect to P, and, on the other hand, substituting $l+1$ for l in this equation and equating the resulting expressions, we find the recursion relation for $C(\lambda, l)$ is

$$C(\lambda, l) = (l-1+\lambda)\ C(\lambda, l-1) + C(\lambda-1, l-1), \ \lambda \leqslant l. \tag{27}$$

We also note from (26) that $C(1,1) = 1$; and we put $C(\lambda, l) = 0$ for $\lambda > l$. These conditions and (27) are sufficient to determine all $C(\lambda, l)$.

It is convenient to define $C(0, l) = \delta(0, l)$. Then (26) can be written in a more general form

$$\frac{d^l y}{dP^l} = (Bg)^l \sum_{\lambda=o}^{l} C(\lambda, l) \left(\frac{AC}{B}g\right)^{\lambda} y^{\lambda}(U), \tag{26a}$$

with g defined as before. The use of $C(\lambda, l)$ becomes necessary when in (17) differentiation with respect to P is carried out to evaluate U. A numerical table for $C(\lambda, l)$ is given elsewhere (Omidvar 1965).

The expression given here for $T(nn_1 m, \mathbf{k})$, is also given elsewhere (Omidvar and Sullivan, 1967)*.

Since the transition amplitude is linear with respect to the initial state wave function, from (1) the transition amplitude in spherical coordinates, $T(nlm, \mathbf{k})$, is given by

$$T(nlm, \mathbf{k}) = \sum_{n_1 = 0}^{n-m-1} \langle nn_1 m \mid nlm \rangle \, T(nn_1 m, \mathbf{k}). \tag{28}$$

This completes the evaluation of the transition matrices.

3. VALIDITY OF THE BORN APPROXIMATION AND BETHE APPROXIMATION

In collision of a charged particle with an atomic system, the use of the first Born approximation amounts to two separate approximations. One is the assumption that the atomic system has only one mode of excitation or ionization. The second assumption is that the incident particle moves in a force-free field and is not affected by the atomic potential. Physically there are infinite modes of atomic excitations or ionization, virtual or real, depending on the energy of the incident particle. The validity of the first assumption then depends on how

*The phase $exp\,[im\,(\varphi_1 + \frac{1}{2}\pi)]$ does not multiply $T(nn_1 m, \mathbf{k})$ in this reference. This phase becomes important when we consider the effect of the electron exchange.

strongly the excited mode in question is coupled to the neglected modes of excitation. Mathematically, its validity depends on the convergence, and the rapidity of the convergence, of the higher order of the Born approximation (Moiseiwitsch and Smith, 1968).

The second approximation is analoguous to the scattering of a particle by a single center of force, and similar to the case of the single center of force, a criterion for its validity can be derived. This will be done here.

By designating the position vectors of the bound and the incident electrons by $\mathbf{r}_1$ and $\mathbf{r}_2$, the exact transition matrix will be given by

$$T^{E}(1,2) = \langle \phi_2(\mathbf{r}_1)\, e^{i\mathbf{k}_2 \cdot \mathbf{r}_2} \left| \frac{1}{r_{12}} - \frac{Z}{r_2} \right| \Psi(\mathbf{r}_1, \mathbf{r}_2) \rangle \tag{29}$$

where *1* and *2* refer to the initial and final states, $\Psi(\mathbf{r}_1, \mathbf{r}_2)$ is the total wave function of the system, and $\phi_2(\mathbf{r}_1)$ is the final state atomic wave function. The two approximations mentioned previously consist of the replacement of $\Psi(\mathbf{r}_1, \mathbf{r}_2)$ by $\Psi_1(\mathbf{r}_1)\, exp(i\mathbf{k}_1, \mathbf{r}_2)$. Thus when integration is carried out with respect to $\mathbf{r}_1$, (9) ensues. However, without carrying out the integration, (29), with this replacement, can be written

$$T(1,2) = \int V(\mathbf{r})\, e^{i\mathbf{q}\cdot\mathbf{r}}\, d\mathbf{r} \quad , \tag{30}$$

$$V(\mathbf{r}_2) = \langle \phi_2(\mathbf{r}_1) \left| \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \right| \phi_1(\mathbf{r}_1) \rangle , \tag{31}$$

where the Z/r_2 is dropped on account of the orthogonality of ϕ_1 and ϕ_2. (30) is the scattering amplitude of a potential $V(\mathbf{r})$ in the Born approximation (Schiff 1955). Corresponding to this amplitude the scattered-electron wave function, $u(\mathbf{r})$, is given by

$$u(\mathbf{r}) = e^{i\mathbf{k}_1 \cdot \mathbf{r}} + w(\mathbf{r}) \tag{32}$$

where

$$w(\mathbf{r}) = -\frac{1}{2\pi} \int V(\mathbf{r}') \frac{e^{i\mathbf{k}_1 \cdot \mathbf{r}' + ik_1 |\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' \tag{33}$$

The condition for the validity of the first Born approximation is that $|w(\mathbf{r})| \ll 1$ for all values of $\mathbf{r}$.

In the problem under consideration, besides the short range forces, an important contribution arises from the long range force due to the $1/r^2$ potential. The following case considers a bound-to-bound transition, and derives a general expression for $V(r)$ when r is small or large. Then, by making use of (33), the validity of the Born approximation is established in terms of the energy of the incident particle. The results obtained can also be extended to the case of ionization.

. In spherical coordinates, the discrete hydrogenic-wave function is given by

$$\phi\,(nlm, \mathbf{r}) = r^{-1}\; P\;(nl, r)\; Y_{lm}\,(\hat{r})\,, \tag{34}$$

where $Y_{l_m}\,(\hat{r})$ is the spherical harmonics, and $r^{-1}\,P\,(nl, r)$ the radial function given by (Landau and Lifshitz 1958)

$$P\;(nl, r) = b_{nl}\; e^{-\frac{1}{2}\rho}\;\rho^{l+1}\,F\,(-n+l+1,\; 2l+2,\; \rho)\,,$$

$$b_{nl} = \frac{1}{(2\,l+1)\,!}\;\left[\frac{\alpha\;(n+l)\,!}{2\,n\,(n-l-1)\,!}\right]^{\frac{1}{2}}\;,\;\; \alpha = \frac{2\,Z}{na_0}\,,\;\; \rho = \alpha\,r\;. \tag{35}$$

For evaluation of (31) we make use of the standard expansion

$$|\,\mathbf{r}_1 - \mathbf{r}_2\,|^{-1} = \sum_{\lambda=0}^{\infty}\;\sum_{\mu=-\lambda}^{\lambda}\;\frac{4\pi}{2\lambda+1}\;\frac{r_<^{\lambda}}{r_>^{\lambda+1}}\;Y_{\lambda\mu}\,(\hat{r}_1)\;Y^*_{\lambda\mu}\,(\hat{r}_2)\;, \tag{36}$$

with $r_<$ the smaller, and $r_>$ the larger, of r_1 and r_2. Substitution of (34) and (36) into (31), and an integration with respect to $\hat{r}_1$, leads to

$$V\,(nlmn'\,l'm', \mathbf{r}_2) = \sum_{\lambda}\left[\frac{4\pi\;(2\,l'+1)}{(2\,l+1)\,(2\,\lambda+1)}\right]^{\frac{1}{2}}\cdot\;\; C\,(l'\lambda l,\; m'\mu m)$$

$$\times\; C\,(l'\lambda l,\; 000)\; Y_{\lambda\mu}\,(\hat{r}_2)\;\mathcal{Y}_{\lambda}\,(nln'l',\; r_2)\;, \tag{37}$$

where $\mu = m - m'$, and λ takes on values for which the C coefficients do not vanish. Also

$$\mathcal{Y}_\lambda(nln'l', r_2) = r_1^{-(\lambda+1)} \int_0^{r_1} P(nl, r_2)\, P(n'l', r_2)\, r_2^{\lambda}\, dr_2$$

$$+ \; r_1^{\lambda} \int_{r_1}^{\infty} P(nl, r_2)\, P(n'l', r_2)\, r_2^{-(\lambda+1)}\, dr_2 \; . \qquad (38)$$

First we consider the case $r \ll 1$. Since in this case $P(nl, r)$ varies as r^{l+1}, and always $\lambda \leq l + l'$, (38) leads to

$$\mathcal{Y}_\lambda(nln'l', r \ll 1) \sim r^{\lambda} \int_0^{\infty} P(nl, r')\, P(n'l', r')\, r'^{-(\lambda+1)}\, dr' \, . \qquad (39)$$

The definite integral on the right-hand side can be evaluated for specific cases. Since the smallest value of λ is $|l - l'|$, we conclude that for a bound-to-bound transistion the potential is finite at the origin with the proportionality relation

$$V(nln'l', \mathbf{r}) \propto r^{|l-l'|}, \quad r \to 0 \; . \qquad (40)$$

In contrast to the case of elastic scattering where the potential is a screened Coulomb potential, the inelastic collision potential is finite at the origin.

For the opposite case of $r \gg 1$ we obtain

$$\mathcal{Y}_\lambda(nln'l', r \gg 1) \sim r^{-(\lambda+1)} \int_0^{\infty} P(nl, r')\, P(n'l', r')\, r'^{\lambda}\, dr' \, . \qquad (41)$$

Since the definite integral is a constant, and the smallest value of λ is $|l - l'|$ through (37) we find

$$V(nln'l', \mathbf{r}) \propto r^{-|l-l'|-1}, \quad r \to \infty . \qquad (42)$$

An exception is the $l = l'$ transition in which case the integral in (41) vanishes on account of orthogonality of the radical function, and the potential vanishes exponentially. The potential in this case is then similar to a square well potential.

From (42) we conclude that when l and l' differ by unity, the incident particle, in addition to short range forces, is also moving in a $1/r^2$ potential. An expression is drived below for the validity of the Born approximation for a dipole potential σ/r^2, with σ being the dipole moment. But first σ is evaluated for transition between the ground and any excited state with $l=1$ (primes are dropped for the final states for convenience). Evaluation of σ follows from substitution of $P(10, r)$ and $P(n1, r)$ from equation (35) into the integral in (41), and a straight forward integration. By taking $Z = 1$ we find that

$$V(100n\,1m, |\mathbf{r}| \gg 1) \sim \sqrt{\frac{4\pi}{3}}\, Y^*_{1m}(\hat{r})\, \frac{\sigma}{r^2} ,$$

$$\sigma = \frac{16\, n^{7/2}}{\sqrt{3}\,(n^2 - 1)^{5/2}} \left(\frac{n-1}{n+1}\right)^n . \tag{43}$$

Values of σ in units of $e^2 a_0$ for $n = 2$ to 10 are given in Table 1. From (43) it is seen that as n increases, σ diminishes as $n^{-3/2}$.

Considering the case of ionization the dipole moment depends on the velocity of the ejected electron. To treat this case, first a partial wave expansion of $\psi^+(\mathbf{r})$, (4), with the same normalization and phase, is made. With the z-axis along the momentum of the ejected electron, this is given by (Schiff 1955)

$$\psi^{+}(kl, \mathbf{r}) = r^{-1} \sum_{l=0}^{\infty} P(kl, r)\ Y_{l0}(\hat{r}) \ , \tag{44}$$

where

$$P(kl, r) = c_{kl}\, e^{-\frac{1}{2}\rho}\, \rho^{\,l+1}\ F(-i\beta + l + 1,\ 2l + 2,\ \rho),$$

$$c_{kl} = \frac{N_c \sqrt{4\pi\,(2l+1)}}{\alpha\ (2l+1)\,!} \prod_{\lambda=1}^{l} (i\beta - \lambda), \quad \alpha = -2ik, \quad \beta = \frac{Z}{a_0 k}, \rho = \alpha r, \tag{45}$$

with N_c given by (4). It should be noted that by letting $i\beta \to n$, α will become the same as that given by (35).

To evaluate the dipole moment for the case of ionization, $P(nl, r)$ in (41) is replaced by $P(10, r)$ given by (35), and $P(n'l', r)$ is replaced by $P(kl, r)$ given by (45). Then for $\lambda = 1$ the integration is carried out by the standard methods. In this way by combining (37) and (41) it can be seen that*

$$V(100k10, |\mathbf{r}| \gg 1) = \sigma \cos(\hat{r}.\hat{k}) / r^2 \ ,$$

$$\sigma = \frac{8\sqrt{2}}{2\pi} \left(\frac{2\pi/k}{1 - \exp\,[-2\pi/k]} \right)^{\frac{1}{2}} \frac{(1 + ik) \quad \exp\,[-2\varphi/k]}{(1 + k^2)^{\,3}}, \quad \varphi = \tan^{-1} k. \tag{46}$$

For $k \ll 1$, $\sigma = 8e^{-2} \Big/ \sqrt{\pi k}$, and for $k \ll 1$, $\sigma = i4\sqrt{2}/\pi k^5$.

*When an electron is scattered by a potential which has imaginary parts, conservation of the current for the ingoing and outgoing wave functions is not satisfied. The lack of this conservation law also holds for a real potential in the Born approximation.

To summarize, in an inelastic collision of a charged particle with an atomic system, the effective potential in which the particle moves is always finite at the origin. Except for $l = l'$ transistions, the potential has long ranges, the most important being $1/r^2$ for $l' = l \pm 1$ transitions.

Since the potential is finite at the origin for small distances from the nucleus, it can be approximated by a square well potential. The criterion for the validity of the Born approximation for this potential is that $k_1 a \gg 1$, with k_1 the momentum of the incident particle, and a the potential range (Schiff 1955). It will be shown below that the criterion for the validity of the Born approximation for a potential

$$V(r) = \begin{cases} -\sigma/r^2 & , \quad r \geqslant a \\ 0 & , \quad r \leqslant a \end{cases} \tag{47}$$

is similarly $k_1 a \gg 1$.

To find the criterion for the validity of the Born approximation for the scattering of a particle in a $\frac{1}{r^2}$ potential, we replace $V(r)$ in (33) by its dipole form given by (41). By introducing $\mathbf{x} = \mathbf{r} - \mathbf{r}'$, this leads to

$$w(\mathbf{r}) = \frac{\sigma e^{i\mathbf{k}_1 \cdot \mathbf{r}}}{2\pi} \int x dx d\hat{x} \, \frac{e^{ik_1 x - i\mathbf{k}_1 \cdot \mathbf{x}}}{|\mathbf{r} - \mathbf{x}|^2} \quad . \tag{48}$$

For the purpose of angular integration in (48) we take the z-axis along $\mathbf{k}_1$. Then making use of expansion (36) and the expansion

$$e^{i\mathbf{k}_1 \cdot \mathbf{x}} = \sum_{\lambda=0}^{\infty} i^{\lambda} \sqrt{4\pi (2\lambda+1)}\; j_{\lambda}(k_1 x)\, Y_{\lambda 0}(\hat{x}) , \tag{49}$$

in (48) it can be found that

$$w(\mathbf{r}) = 8\pi\, \sigma e^{i\mathbf{k}\cdot\mathbf{r}} \sum_{ll'\lambda} \frac{(-i)^{\lambda}(2\lambda+1)\, I(r)}{(2l+1)^{1/2}(2l'+1)^{3/2}}$$

$$\times \sum_{m} C(\lambda\, ll', omm)\, C(\lambda ll', ooo)\, Y^{*}_{lm}(\hat{r})\, Y_{l'm}(\hat{r}) , \tag{50}$$

where $ll'\lambda m$ takes on values for which $C(\lambda\, ll', omm)$ does not vanish, and

$$I(r) = \frac{1}{r^{l+l'+2}} \int_a^r x^{l+l'+1}\, j_{\lambda}(kx)\, e^{ikx}\, dx$$

$$+ r^{l+l'} \int_r^{\infty} \frac{1}{x^{l+l'+1}}\, j_{\lambda}(kx)\, e^{ikx}\, dx . \tag{51}$$

In (49) $j_{\lambda}(k_1 x)$ is the spherical Bessel's function.

Assuming that $k_1 a \gg 1$, and using the asymphatic form of $j_{\lambda}(k_1 x)$, it can be found that

$$I(r) \sim i^{\lambda+1} (l+l'+1)^{-1} \left[1 - \tfrac{1}{2} (a/r)^{l+l'+1}\right] (k_1 r)^{-1} , \; k_1 a \gg 1. \tag{52}$$

Combining (50) and (52) shows that $|w(\mathbf{r})| \ll 1$ when $k_1 a \gg 1$.

When th kinetic energy of a particle is comparable to σ/r^2 at a distance on the order of a from the center of force, bound states can be formed (Landau

and Lifshitz 1958). This will give rise to resonances not predicted in the Born approximation. The condition $k_1 a \gg 1$ also insures that this resonance will not happen.

For potentials falling faster than $1/r^2$, the criterion $k_1 a \gg 1$ is naturally sufficient. Then by taking the effective potential as the sum of the long and short range forces, with the neglect of the other modes of excitations, the Born approximation is valid when $k_1 a \gg 1$.

The range a for different transistions can be taken to be the distance beyond which the product $P(nl, r)\, P(n'l', r)$ falls off exponentially. With reference to (35) we may take

$$a = 2(\alpha + \alpha')^{-1} . \tag{53}$$

For excitation this condition reads $a = (n + n')^{-1}\, nn'(a_0/Z)$. Then for excitation of the ground state it is found that $a \cong a_0/Z$, while for excitation of the highly excited states, when $n' \cong n$, it is found that $a \cong n\,(a_0/Z)$. In the latter case the ranges expands. The condition $k_1 \gg 1/a$ then implies that for a fixed incident energy, the Born approximation is more valid for excitation of the excited states. In the excitation of the excited states it should also be noted that the threshold energy is smaller and the peak in the cross section appears at smaller incident energy. If we measure the wave number of the incident electron in units of the wave number of the bound electron in the state n, and express it

by k_T, then $k_T = nk_1$, and the criterion becomes $k_T \gg Z/a_0$, which is the same as the criterion for excitation of the ground state.

For ionization of the nth state $a = na_0/Z$ is obtained. The validity criterion is then $k_T \gg Z/a_0$.

A connection exists between the Born and Bethe approximations. The Bethe approximation (Bethe 1930, Landau and Lifshitz 1958) consists of the assumption that $\Delta E \ll k_1^2$, where ΔE is the energy transfer by the incident electron. With this assumption, the cross section can be written

$$Q \sim k_1^{-2} \; [A \ln k_1^2 + B], \tag{54}$$

with A and B being constants dependent upon the atomic parameters and excitation energy for a given process. For $n \to n'$ excitation, $\Delta E = (1/n^2 - 1/n'^2) Z^2/a_0^2$, and for ionization $\Delta E = Z^2/n^2 a_0^2 + \epsilon$ (cf. 11). Since in ionization $dQ/d\epsilon$ has appreciable value only when ϵ is much smaller or comparable to $Z^2/n^2 a_0^2$, the assumption $\Delta E \ll k_1^2$ is equivalent to $k_1 \gg Z/na_0$, which is the same as the criterion for the validity of the Born approximation in ionization. This means that in the energy region where Q, as calculated by the Born approximation, agrees with Q as given by (54), the agreement can be taken as a test for the validity of the Born approximation. In the next section, it will be shown that for ionization of a level with the principal quantum number n, the value of k_1 at which the Born approximation can be approximated by (54) is indeed inversely proportional to n, as expected.

4. RESULTS AND DISCUSSION

To calculate the ionization cross section, the explicit form of $T\ (nlm, \mathbf{k})$ given by (21) and (28) is substituted into (8) and integration with respect to q and the polar angle of $\hat{k}$ is carried out numerically. No integration with respect to the angle of azimuth of $\hat{k}$ is necessary. With $dQ/d\epsilon$ determined, a final numerical integration is performed according to (10) to determine the total cross section Q.

A quantity of interest is the average energy of an ejected electron for a given incident energy. This is given by

$$\overline{\epsilon} = \int_0^{\epsilon_{max}} \epsilon \left(\frac{dQ}{d\epsilon}\right) d\epsilon / Q . \tag{55}$$

In the following figures and Tables 2 through 6, $dQ/d\epsilon$, Q, and $\overline{\epsilon}$ are given.

In Figures 1 through 4 the total ionization cross section for $n = 2$ through 5 and all possible l values is plotted as a function of the incident energy. In Figure 5, the total cross section is given as a function of energy for $n = 1$ through 5, each case being averaged with respect to the azimuthal quantum numbers. Figures 6 through 10 are similar to Figures 1 through 5 except that $(E/I)\ Q$ is plotted as a function of log (E/I), with E/I the incident energy in threshold units, and the abscissa extended to much higher incident energies. If,

as the incident energy increases, Q, as given by the Born approximation, approaches the Q given by (54), then the curves given by Figures 6 through 10 should approach straight lines with slopes given by A and with intersections with the ordinates given by B. This is noted to be the case. As indicated in Section 3, the agreement between the two Q values can be taken as a measure of the validity of the plane wave assumption for the incident electron in the Born approximation. Some deviation from the straight lines noted in the figures is due to the inaccuracy in the numerical integration for the cross section at high incident energies.

Estimates of A and B for different cases are useful for practical plasma and astrophysical calculations. Kingston (1965) gives accurate numerical values for A for n = 1 through 5 and all possible l values. Calculation of B is much more difficult, and should be estimated from the graphs.

Studies of the Figures 1 through 10 show that for a given n and incident energy, the total cross section tends to increase with increasing l for low and intermediate energies, but the trend is reversed at the higher energies. The latter situation has been predicted by Bethe (1930).

These figures also show that similar situations exist with respect to n, namely that for low an intermediate energies, for a fixed energy, the cross section increases with an increase in n; but at high energies, this quantity decreases with an increase in n. The latter situation is consistent with the correspondence principle according to which as n increases, the quantal and

classical results should agree with each other. Classically, at high incident energies, the cross section is inversely proportional to the incident energy, and as n increases, A [in (54)] must tend to zero in order to bring Q [as given in (54)] into agreement with the classical cross section. The decrease in A as n increases is clearly seen in Figure 10. There exist a wealth of experimental and theoretical results for the ground state ionization. The subject has been recently reviewed by Rudge (1968). In contrast, no measurement is available for the excited state ionization, and, with few exceptions, the only available calculation other than the Born approximation is the classical calculation.

Mentioned here is the classical impulse approximation which is valid at high incident energies. The original calculation in this method was done by Thomson (1912), and recently the method has been revived by Gryzinski (1958). Among many calculations by this method, the one with the least number of approximations is discussed here. Gerjoy (1966) has formulated the problem of energy transfer between two moving charged particles. Garcia (1969) has applied this formulation to the ionization of hydrogenic atoms, where quantum mechanical momentum distribution is assumed for the bound electron. He finds the differential cross section for a given n, averaged with respect l, to be given by

$$\frac{dQ_c}{d\epsilon} = \frac{8e^4}{3\beta_1 I^3 J^3}\left\{(3J + 4)\left(\tan^{-1} y + \frac{y}{1 + y^2}\right) + \frac{2y(J-4)}{(1 + y^2)^2}\right\} ,$$

$$J = 1 + \epsilon/I \ , \quad \beta_1 = E/I \ , \quad y = (\beta_1 - J)^{1/2}, \tag{56}$$

with e being the electronic charge, and E and ϵ being the incident and the ejected electron energies in rydbergs. $I = Z^2 e^2/n^2 a_0$ is the ionization potential in Ry of the level n concerned. The total cross section as in (10) is given by

$$Q_c = \int_0^{\epsilon_{max}} \frac{dQ_c}{d\epsilon} \, d\epsilon \ . \tag{57}$$

In Figure 10 $(E/I)\, Q_c$ is plotted as a function of log (E/I) for comparison with the quantal cross sections. It is seen that as n increases the quantal calculation approaches the classical one. Since both the Born and impulse approximation are valid at high energies, this constitutes a verification of the correspondence principle.

As the incident energy E increases, the classical cross section varies as E^{1}. This is seen by noticing that

$$\frac{dQ_c}{d\epsilon} \sim \frac{4\pi e^4}{\beta_1 I^3 J^2} \left(1 + \frac{4}{3J}\right), \qquad \beta_1 \gg 1, \ J \ll \beta_1 . \tag{58}$$

Thus it follows that

$$Q_c \sim \int_1^{\beta_1} \frac{dQ_c}{dJ} dJ \sim \frac{20\pi e^4}{3 I^3 \beta_1} = \frac{20 n^4 \pi a_0^2}{3 Z^4 E}, \tag{59}$$

where only the leading term in the inverse powers of β_1 is retained.

Equation (59) is in agreement with the asymptotic form of the other classical impulse approximation formulas.

Kingston (1968) has made a classical calculation equivalent to the classical calculation contained in (56) and (57). He has made a comparison between his results and the privately communicated Born calculation of this author. His views are consistent with those given here. However, his calculation is not extended beyond $k_T = 5$.

In Figure 11 the differential cross section for the ground state ionization and incident energy of 25 threshold units is plotted as a function of the energy of the ejected electron. The classical expression given by (56) is also plotted for comparison. For $E/I \gg 1$ agreement is noted between the quantal and classical calculations. The reason is that formulas for both theories have the same asymptotic forms. This can be seen in the following. From (58) it can be seen that for $\beta_1 \gg \epsilon/I \gg 1$,

$$dQ/d\epsilon \sim (4\pi e^4/E\epsilon^2)\ (1 - 2\,I/3\epsilon)\,,\ E \gg \epsilon \gg I\,. \tag{60}$$

Omidvar (1969) has similarly shown that the first two leading terms in the expansion of $dQ/d\epsilon$ as inverse powers of ϵ/I calculated by the Born approximation are identical to (60).

Inokuti and Vriens in their classical binary encounter theory find the same expression as (60) (private communication, 1968).

The main disagreement between $dQ/d\epsilon$ and $dQ_c/d\epsilon$ is for $\epsilon/I \ll 1$ where the two quantities have different functional forms. Obviously the classical expression is not valid in this case. The importance of the region $\epsilon \ll I$ is the fact that most electrons in a high energy collision are ejected with small energies. The large contribution to the total cross section from the region $\epsilon \ll I$ accounts for the difference between the quantal and classical total cross sections. Position of the average energy, $\bar{\epsilon}$, is shown in Figure 11 by means of a vertical line. This position also indicates that large numbers of ejected electrons have small energies.

At this point it is also convenient to discuss the exchange effect. This effect is important when ϵ is comparable to E. Contribution of this effect to $dQ/d\epsilon$ is of the order of $1/E\epsilon^2$ (Landau and Lifshitz 1958). Integration of $1/E\epsilon^2$ with respect to ϵ in the region that ϵ is comparable to E shows that the ratio of the contribution of the exchange effect to the total cross section is of the order of $1/E$, and in the region of the validity of the Born approximation can be neglected.

In Figures 12 through 14, the differential cross section for the 2s and the 2p ionization for the incident energies of 4, 25, and 100 threshold units are plotted versus energy of the ejected electrons. The positions of the average energy of the ejected electrons, $\bar{\epsilon}$, [cf. (55)], are indicated by vertical lines.

Concerning the accuracy of the numerical results presented here, two checks have been made to rule out a systematic error in the calculations. One is the comparison between the present and previous results (Omidvar 1965) for a given n and n_1. In the present calculation, the z-axis is along $\mathbf{k}$, while in the old calculation this axis is along the momentum transfer. When the two results have been summed with respect to m, agreement between them is found. The next check has shown agreement between two sets of results where, in one set, summation has been performed with respect to n_1, and in the second set with respect to l.

Gaussian quadratures have been used as a method of integration, and for each Q as a function of the parameters k_T, n, and l, the number of intervals of the integrations has been increased until successive values of the Q have fallen within 1% of each other. An exception to this rule is made for $n = 5$ where the differences are 2 to 3%.

Since the range of integration increases as k_T^2 increases, numerical values at low k_T^2 are more accurate than those for large k_T^2.

5. SPECTRUM OF THE SECONDARY ELECTRONS IN THE PASSAGE OF AN ENERGETIC ELECTRON IN AN ATOMIC HYDROGEN GAS

In this section are considered the number of ejected electrons per unit of their energy range, and the total number of ejected electrons, when an energetic electron enters an atomic hydrogen gas and is brought to rest through ionization.

We assume that the atoms are in their ground state. The results obtained can be applied to the case of hydrogen gas if the few electron volts binding energy of the hydrogen molecules can be neglected compared to the energy of the primary.

If ΔE is defined as the energy lost by the primary during the course of a single collision due to all inelastic processes, in anology to (55) it can be calculated by the expression

$$\Delta E = \left[\sum_{n=2}^{\infty} (E_n - E_o)\, Q_n + \int_0^{\epsilon_{max}} (I + \epsilon) \frac{dQ}{d\epsilon}\, d\epsilon \right] \Big/ Q_{in}, \tag{61}$$

where Q_n is the cross section for excitation of the nth level, E_o and E_n are energies of the ground and n^{th} levels, I is the ionization potential, and Q_{in} the total inelastic cross section. If dN is the number of ions produced when a primary of energy E loses an amount of energy dE, we must have $dN = (dE/\Delta E)\ (Q/Q_{in})$ with Q, as before, being the total ionization cross section. The number of ejected electrons having energies between ϵ and $\epsilon + d\epsilon$ is a fraction $(dQ/d\epsilon)\, d\epsilon/Q$ of dN. This number can then be written

$$\frac{\partial^2 N}{\partial \epsilon \partial E}\, d\epsilon dE = \frac{dQ/d\epsilon}{Q}\ \frac{Q}{Q_{in}\Delta E}\, d\epsilon\, dE = \frac{dQ/d\epsilon}{Q_{in}\,\Delta E}\, d\epsilon dE\,. \tag{62}$$

If the initial energy of the primary is E_{max}, the number of electrons with energies between ϵ and $\epsilon + d\epsilon$ is given by

$$\frac{\partial N}{\partial \epsilon} = \int_{1+\epsilon}^{E_{max}} \frac{dQ}{d\epsilon} \times \frac{dE}{Q_{in}\Delta E} \quad . \tag{63}$$

For evaluation of (63), a knowledge of $Q_{in}\Delta E$ is necessary. Accurate evaluation of this quantity is difficult. However, at high incident energy and within the approximation applied to the derivation of (54), it can be written (bethe 1930, Landau and Lifshitz 1958)

$$Q_{in}\Delta E \sim (8Z/E) \ ln \ (2E/\bar{I}) \ , \tag{64}$$

with Q_{in} in units of πa_0^2 and E in rydberg. In (64) Z is the number of atomic electrons, and $\bar{I}$ is the average excitation energy in rydberg. For the ground state atomic hydrogen $\bar{I} = 1.105$ Ry.

Although the Born approximation is inaccurate at low incident energies, it is likely that the ratio of two quantities calculated according to the Born approximation will be more accurate than the quantities by themselves. The ratio in question is $Q/Q_{in}\Delta E$ given by (62). Making use of (54) and (64), we can write

$$\frac{\partial N}{\partial \epsilon} = \frac{1}{8Z} \int_{I+\epsilon}^{E_{max}} \frac{dQ/d\epsilon}{Q} \times \frac{(A \ ln \ E + B) \ dE}{ln \ (2E/\bar{I})} \quad , \tag{65}$$

with I the ionization potential of the bound electron. Using (65), $\partial N/\partial \epsilon$ for the ground state atomic hydrogen has been evaluated numerically. Figure 15 is a plot of $\partial N/\partial \epsilon$ versus ϵ for various initial primary energy E_{max}.

The total number of secondary electrons for a given E_{max} is obtained by integrating (65) with respect to ϵ . This is given by

$$N = \frac{1}{8Z}\int_{I}^{E_{max}} \frac{A \ln E + B}{\ln(2E/\bar{I})}\, dE$$

$$= \frac{A}{8Z}\left\{E_{max} - I + \frac{\bar{I}}{2}\left[\frac{B}{A} - \ln\left(\frac{2}{\bar{I}}\right)\right]\left[E_i\left(\ln\left(\frac{2E_{max}}{\bar{I}}\right)\right) - E_i\left(\ln\left(\frac{2I}{\bar{I}}\right)\right)\right]\right\} , \qquad (66)$$

where $E_i(x)$ is the exponential integral.

Using (66), a plot of N for the ground state of atomic hydrogen is given in Figure 16. Dalgarno and Griffing (1958) have calculated N due to ionization by the primary and all higher generation electrons. This result is also shown in Figure 16. As the incident energy increases, the value of N given by Dalgarno and Griffing increases more rapidly than the value of N given by (66), mainly due to the ionization produced by the higher generation electrons.

The energy spectrum given here can also be used to deduce the energy spectrum of the tertiary electrons due to energetic secondary electrons, etc.

It is of interest to know that when ϵ is several threshold units, for any target atom or molecule $dQ/d\epsilon$ to a good approximation is given by the Rutherford formula which is given by the leading term of (60) multiplied by Z. Making use of (54) and the leading term of (60) in (65) results in the following analytic formula:

$$\frac{\partial N}{\partial \epsilon} \approx \frac{1}{2\epsilon^2}\int_{I+\epsilon}^{E_{max}} \frac{dE}{\ln(2E/\bar{I})}$$

$$= \frac{\bar{I}}{4\epsilon^2}\left[E_i\left(\ln \frac{2E_{max}}{\bar{I}}\right) - E_i\left(\ln \frac{2(I+\epsilon)}{\bar{I}}\right)\right], \epsilon \gg I . \qquad (67)$$

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Table 1

Atomic dipole moments in units of $e^2 a_0$ for 1s $\rightarrow np$ transistions.

n	2	3	4	5	6	7	8	9	10
β	0.7449	0.2983	0.1759	0.1205	0.0896	0.0701	0.0569	0.0474	0.0403

Table 2.

Ionization of the $n=2$ levels. k_T is the ratio of the speed of the incident electron to the speed of the bound electron. k_T^2 gives the incident energy in threshold units. Q is the total cross section in units of πa_0^2, and $\bar{\epsilon}$ is the average energy of the ejected electron in Ry. l is the azimuthal quantum number. For each l the relevant quantities have been averaged with respect to the magnetic quantum number m.

	$l=0$		$l=1$	
k_T	$n^{-4}Q$	$n^2\bar{\epsilon}$	$n^{-4}Q$	$n^2\bar{\epsilon}$
1.2	0.668	0.163	0.643	0.155
1.4	1.017	0.321	1.083	0.303
1.6	1.103	0.465	1.234	0.443
1.8	1.074	0.596	1.227	0.572
2.0	1.001	0.714	1.152	0.689
2.5	0.792	0.965	0.902	0.936
3.0	0.620	1.165	0.692	1.130
3.5	0.493	1.328	0.541	1.285
4.0	0.399	1.462	0.431	1.414
4.5	0.329	1.572	0.352	1.523
5.0	0.276	1.663	0.292	1.619
6.0	0.202	1.814	0.210	1.783
7.0	0.155	1.911	0.159	1.923
8.0	0.122	1.969	0.124	2.043
9.0	0.099	1.999	0.100	2.145
10.0	0.082	2.009	0.082	2.229
15.0	0.040	2.142	0.039	2.496
20.0	0.023	2.120	0.022	2.575
25.0	0.015	2.117	0.014	2.59
30.0	0.011	2.125	0.010	2.59

Table 3

Ionization of the $n = 3$ levels.
Notations and explanations are the same as in Table 2.

k_T	$l = 0$		$l = 1$		$l = 2$	
	$n^{-4}Q$	$n^2\bar{\epsilon}$	$n^{-4}Q$	$n^2\bar{\epsilon}$	$n^{-4}Q$	$n^2\bar{\epsilon}$
1.2	0.708	0.167	0.701	0.161	0.665	0.150
1.4	1.034	0.327	1.072	0.317	1.149	0.297
1.6	1.101	0.473	1.161	0.462	1.307	0.437
1.8	1.059	0.607	1.127	0.594	1.290	0.569
2.0	0.978	0.729	1.046	0.714	1.199	0.689
2.5	0.760	0.990	0.816	0.971	0.917	0.944
3.0	0.587	1.200	0.630	1.178	0.692	1.146
3.5	0.463	1.372	0.494	1.349	0.533	1.311
4.0	0.373	1.514	0.396	1.495	0.421	1.449
4.5	0.306	1.628	0.324	1.625	0.340	1.569
5.0	0.255	1.717	0.270	1.743	0.281	1.674
6.0	0.185	1.752	0.195	1.937	0.200	1.853
7.0	0.140	1.792	0.148	2.064	0.150	2.019
8.0	0.110	1.833	0.116	2.162	0.116	2.145
9.0	0.089	1.883	0.093	2.202	0.093	2.270
10.0	0.074	1.974	0.077	2.239	0.076	2.389
15.0	0.035	2.218	0.036	2.361	0.035	2.771
20.0	0.021	2.365	0.021	2.510	0.020	2.963
25.0	0.014	2.382	0.014	2.609	0.013	3.045
30.0	0.010	2.388	0.010	2.614	0.009	3.139

Table 4

Ionization of the $n = 4$ levels.
Notations and explanations are the same as in Table 2.

k_T	$l = 0$		$l = 1$		$l = 2$		$l = 3$	
	$n^{-4}Q$	$n^2\bar{\epsilon}$	$n^{-4}Q$	$n^2\bar{\epsilon}$	$n^{-4}Q$	$n^2\bar{\epsilon}$	$n^{-4}Q$	$n^2\bar{\epsilon}$
1.2	0.726	0.168	0.724	0.164	0.709	0.157	0.661	0.144
1.4	1.048	0.328	1.070	0.323	1.116	0.311	1.186	0.290
1.6	1.108	0.476	1.143	0.469	1.219	0.454	1.358	0.431
1.8	1.059	0.611	1.099	0.603	1.185	0.585	1.335	0.564
2.0	0.973	0.735	1.013	0.726	1.098	0.706	1.233	0.686
2.5	0.749	1.001	0.783	0.989	0.849	0.965	0.930	0.946
3.0	0.575	1.216	0.602	1.203	0.649	1.174	0.694	1.154
3.5	0.450	1.387	0.472	1.383	0.504	1.344	0.530	1.325
4.0	0.360	1.515	0.378	1.543	0.401	1.484	0.416	1.470
4.5	0.294	1.602	0.309	1.690	0.326	1.608	0.335	1.595
5.0	0.244	1.660	0.258	1.820	0.270	1.725	0.274	1.705
6.0	0.175	1.707	0.186	1.966	0.194	1.956	0.194	1.898
7.0	0.133	1.844	0.141	2.015	0.146	2.166	0.144	2.078
8.0	0.105	1.954	0.110	2.044	0.113	2.274	0.112	2.214
9.0	0.085	2.056	0.089	2.099	0.091	2.351	0.089	2.360
10.0	0.070	2.118	0.073	2.189	0.074	2.417	0.072	2.496
15.0	0.034	2.422	0.034	2.481	0.035	2.615	0.033	2.977

Table 5

Ionization of the $n = 5$ levels.
Notations and explanations are the same as in Table 2.

k_T	$l = 0$		$l = 1$		$l = 2$		$l = 3$		$l = 4$	
	$n^{-4}Q$	$n^2\bar{\epsilon}$	$n^{-4}Q$	$n^2\bar{\epsilon}$	$n^{-4}Q$	$n^2\bar{\epsilon}$	$n^{-4}Q$	$n^2\bar{\epsilon}$	$n^{-4}Q$	$n^2\bar{\epsilon}$
1.2	0.603	0.170	0.648	0.165	0.695	0.162	0.704	0.152	0.648	0.140
1.4	1.058	0.328	1.073	0.325	1.101	0.317	1.143	0.304	1.208	0.284
1.6	1.114	0.476	1.137	0.472	1.185	0.462	1.262	0.447	1.393	0.427
1.8	1.062	0.612	1.089	0.607	1.143	0.595	1.230	0.578	1.367	0.561
2.0	0.974	0.737	1.001	0.732	1.056	0.717	1.140	0.699	1.257	0.685
2.5	0.744	1.003	0.769	1.001	0.814	0.979	0.876	0.960	0.937	0.948
3.0	0.566	1.193	0.590	1.236	0.623	1.191	0.664	1.173	0.694	1.159
3.5	0.438	1.312	0.463	1.445	0.485	1.366	0.512	1.346	0.528	1.325
4.0	0.349	1.403	0.370	1.609	0.387	1.518	0.405	1.486	0.413	1.435
4.5	0.284	1.503	0.301	1.713	0.315	1.662	0.327	1.603	0.331	1.616
5.0	0.236	1.615	0.250	1.773	0.261	1.798	0.269	1.710	0.271	1.729
6.0	0.171	1.812	0.180	1.859	0.188	2.038	0.192	1.951	0.190	1.928
7.0	0.130	1.951	0.136	1.976	0.142	2.128	0.144	2.171	0.141	2.103
8.0	0.102	2.035	0.106	2.098	0.110	2.250	0.112	2.342	0.109	2.254
9.0	0.082	2.171	0.086	2.215	0.089	2.293	0.089	2.468	0.087	2.415
10.0	0.068	2.228	0.070	2.301	0.073	2.374	0.073	2.569	0.070	2.547

Table 6

Ionization of the $n = 1$, 2, 3, 4, and 5 levels.
For each n the relevant quantities have been averaged with respect to l.
Notations and explanations are the same as in Table 2.

k_T	n = 1		n = 2		n = 3		n = 4		n = 5	
	$n^{-4}Q$	$n^{2}\bar{\epsilon}$	$n^{-4}Q$	$n^{2}\bar{\epsilon}$	$n^{-4}Q$	$n^{2}\bar{\epsilon}$	$n^{-4}Q$	$n^{2}\bar{\epsilon}$	$n^{-4}Q$	$n^{2}\bar{\epsilon}$
1.2	0.575	0.156	0.649	0.157	0.682	0.156	0.692	0.153	0.671	0.152
1.4	0.998	0.302	1.067	0.308	1.110	0.307	1.134	0.305	1.146	0.303
1.6	1.169	0.438	1.201	0.449	1.236	0.449	1.258	0.448	1.273	0.447
1.8	1.193	0.561	1.189	0.578	1.210	0.581	1.226	0.581	1.238	0.580
2.0	1.145	0.672	1.114	0.696	1.123	0.702	1.133	0.703	1.142	0.703
2.5	0.937	0.901	0.874	0.944	0.866	0.958	0.866	0.964	0.867	0.966
3.0	0.743	1.074	0.674	1.139	0.660	1.163	0.655	1.173	0.654	1.180
3.5	0.594	1.208	0.529	1.296	0.513	1.330	0.506	1.346	0.504	1.357
4.0	0.483	1.314	0.423	1.426	0.408	1.472	0.401	1.491	0.397	1.504
4.5	0.400	1.402	0.346	1.535	0.331	1.594	0.326	1.617	0.321	1.628
5.0	0.336	1.475	0.288	1.630	0.274	1.702	0.268	1.730	0.264	1.738
6.0	0.247	1.591	0.208	1.791	0.197	1.870	0.191	1.917	0.188	1.944
7.0	0.190	1.680	0.158	1.920	0.148	2.008	0.143	2.079	0.141	2.106
8.0	0.151	1.750	0.124	2.024	0.115	2.116	0.111	2.185	0.109	2.250
9.0	0.123	1.804	0.100	2.108	0.093	2.204	0.089	2.289	0.087	2.371
10.0	0.102	1.866	0.082	2.174	0.076	2.293	0.073	2.390	0.071	2.476
15.0	0.050	2.026	0.039	2.408	0.035	2.573	0.034	2.736		
20.0	0.029	2.092	0.023	2.462	0.020	2.746				
25.0	0.020	2.114	0.015	2.474	0.013	2.826				
30.0	0.014	2.119	0.010	2.477	0.009	2.881				

FIGURE CAPTIONS

Figure 1. Total cross section for the ionization of the $n = 2$ level of atomic hydrogen. Cross sections, in units of $n^{-4}\pi a_0^2$, are averaged with respect to the magnetic quantum number m for each azimuthal quantum number l. For low and intermediate incident energies Q for $l = 1$ is larger than Q for $l = 0$ for a fixed energy, but at high energies it falls below $l = 0$ values (cf, Figure 6).

Figure 2. Total cross section for the ionization of the $n = 3$ level. Similar to the $n = 2$ case, for low and intermediate energies Q increases as l increases. The situation is reversed at high energies.

Figure 3. Total cross section for the ionization of the $n = 4$ level.

Figure 4. Total cross section for the ionization of the $n = 5$ level.

Figure 5. Total cross section for the ionization of the $n = 1$, 2, 3, 4, and 5. For each n, the cross section has been averaged with respect to the azimuthal quantum number l. E is the energy of the incident electron, and I is the ionization potential for the level concerned. With the scaling shown in the Figure, and for a given low energy, the cross section increases with the increasing order of n. The situation reverses for energies higher than a few threshold units.

Figure 6. A plot of $(E/I)\,Q$ versus $log_{10}(E/I)$ for ionization of the $n = 2$ and $l = 0$, 1 states. At high energy the graphs approach straight lines. Slopes

and intersections of these lines with the ordinate give the two parameters necessary for the high-energy calculation of Q.

Figure 7. A plot of $(E/I)\,Q$ versus $log_{10}(E/I)$ for ionization of the $n = 3$, $l = 0, 1, 2$ states. Notations are the same as in Figure 6.

Figure 8. A plot of $(E/I)\,Q$ versus $log_{10}(E/I)$ for ionization of the $n = 4$ states. Notations are the same as in Figure 6.

Figure 9. A plot of $(E/I)\,Q$ versus $log_{10}(E/I)$ for ionization of the $n = 5$ states. Notations are the same as in Figure 6.

Figure 10. A plot of $(E/I)\,Q$ versus $log_{10}(E/I)$ for $n = 1, 2, 3, 4$, and 5 levels. For each n, Q has been averaged with respect to the different l. The classical formulais that of the impulse approximation with quantum mechanical momentum distribution assumed for the bound electron. As n increases the quantum mechanical results approach those given classically in accordance with the correspondence principle.

Figure 11. A comparison of the results of the Born, the asymptatic Born, and the classical theories for the differential cross section with ground state ionization of hydrogen. The asymptatic Born is valid for $\epsilon \gg 1$. The incident energy is 25 rydbergs. The average ejected electron energy $\bar{\epsilon}$ is shown by a vertical line.

Figure 12. Differential cross section for the $n = 2$ level ionization for an incident energy of 4 threshold units. Positions of $\bar{\epsilon}(2s)$ and $\bar{\epsilon}(2p)$ are shown by vertical lines.

Figure 13. Differential cross section for $n = 2$ and an incident energy of 25 threshold units. Notations are the same as in Figure 12.

Figure 14. Differential cross section for $n = 2$ and an incident energy of 100 threshold units. Notations are the same as in Figure 12.

Figure 15. Number of the secondary electrons per unit range of their energy, $\partial N/\partial\epsilon$, versus ϵ for different primary energies. The primary energies E_1 through E_7 are 10, 20, 30, 40, 60, 80, and 100 units of the ionization potential, respectively.

Figure 16. Total number of the ejected electrons versus the primary energy. Curve 1 is the result of the present calculation. Curve 2 is due to Dalgarno and Griffing (1958).

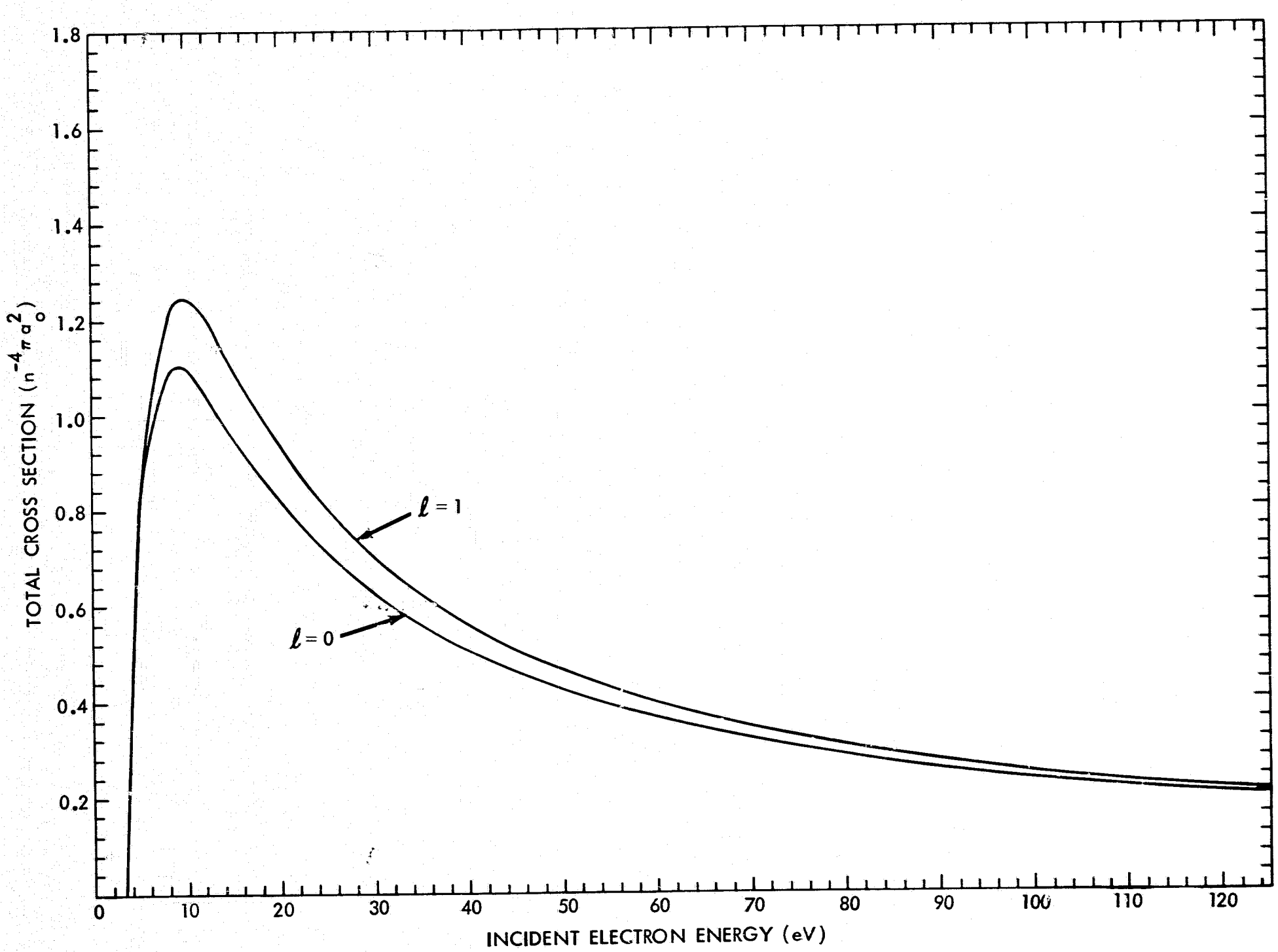
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
TOTAL CROSS SECTION ($n^{-4}\pi a_o^2$)
$\ell = 1$
$\ell = 0$
0
10
20
30
40
50
60
70
80
90
100
110
120
INCIDENT ELECTRON ENERGY (eV)

Figure 1

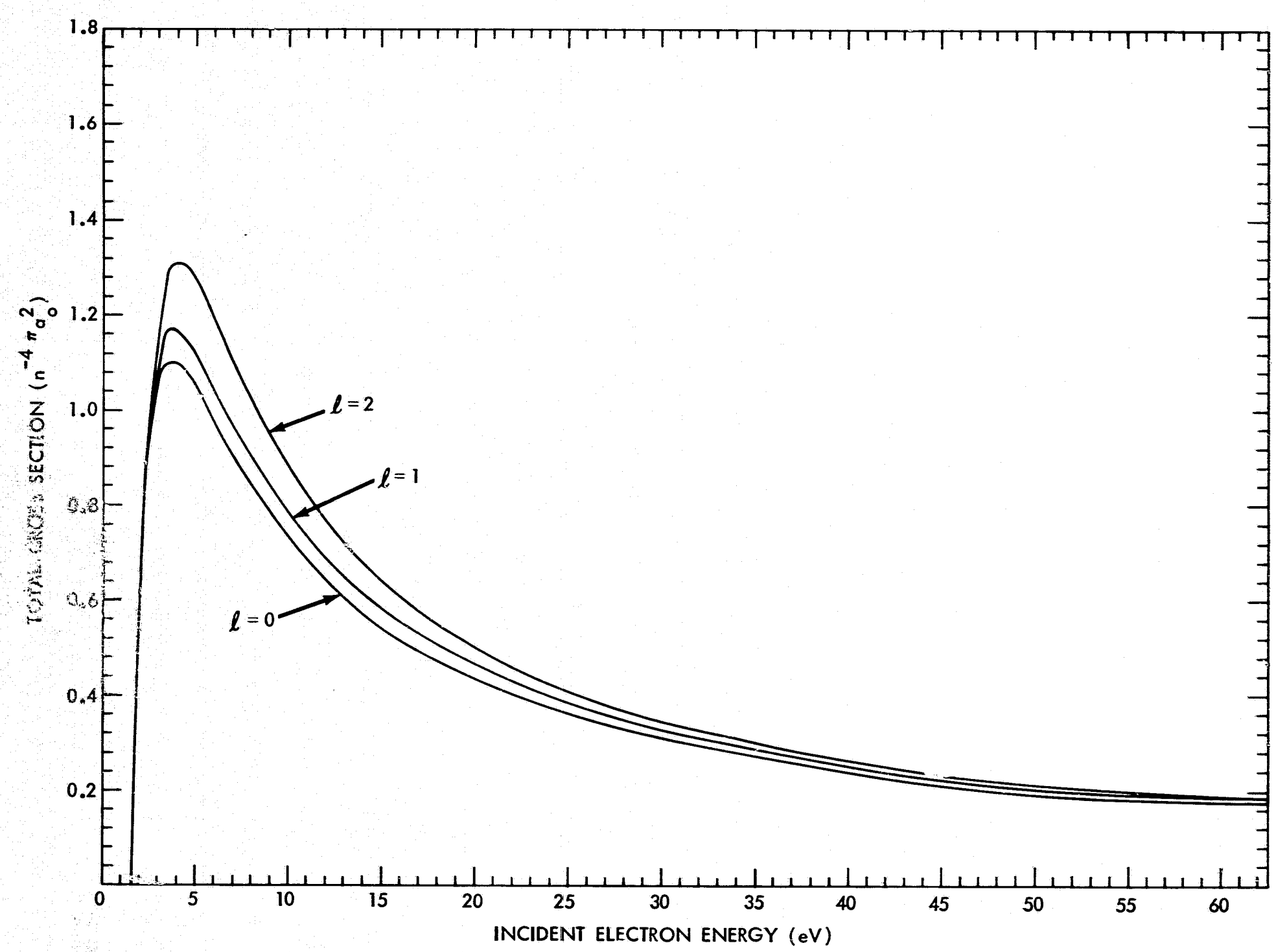
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
TOTAL CROSS SECTION ($n^{-4} \pi a_o^2$)
$\ell = 2$
$\ell = 1$
$\ell = 0$
0
5
10
15
20
25
30
35
40
45
50
55
60
INCIDENT ELECTRON ENERGY (eV)

Figure 2

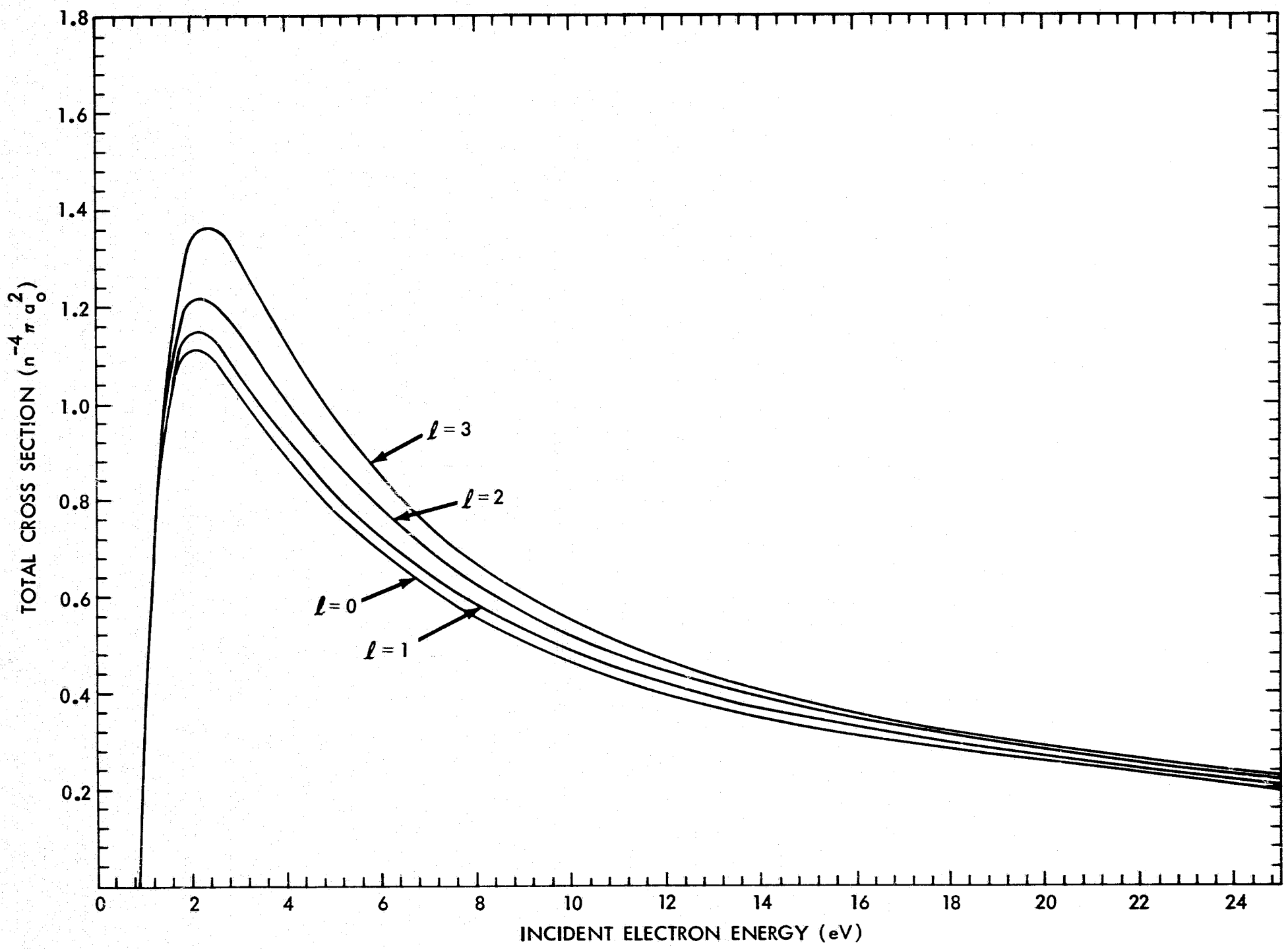
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
TOTAL CROSS SECTION ($n^{-4} \pi a_o^2$)
$\ell = 3$
$\ell = 2$
$\ell = 0$
$\ell = 1$
0
2
4
6
8
10
12
14
16
18
20
22
24
INCIDENT ELECTRON ENERGY (eV)

Figure 3

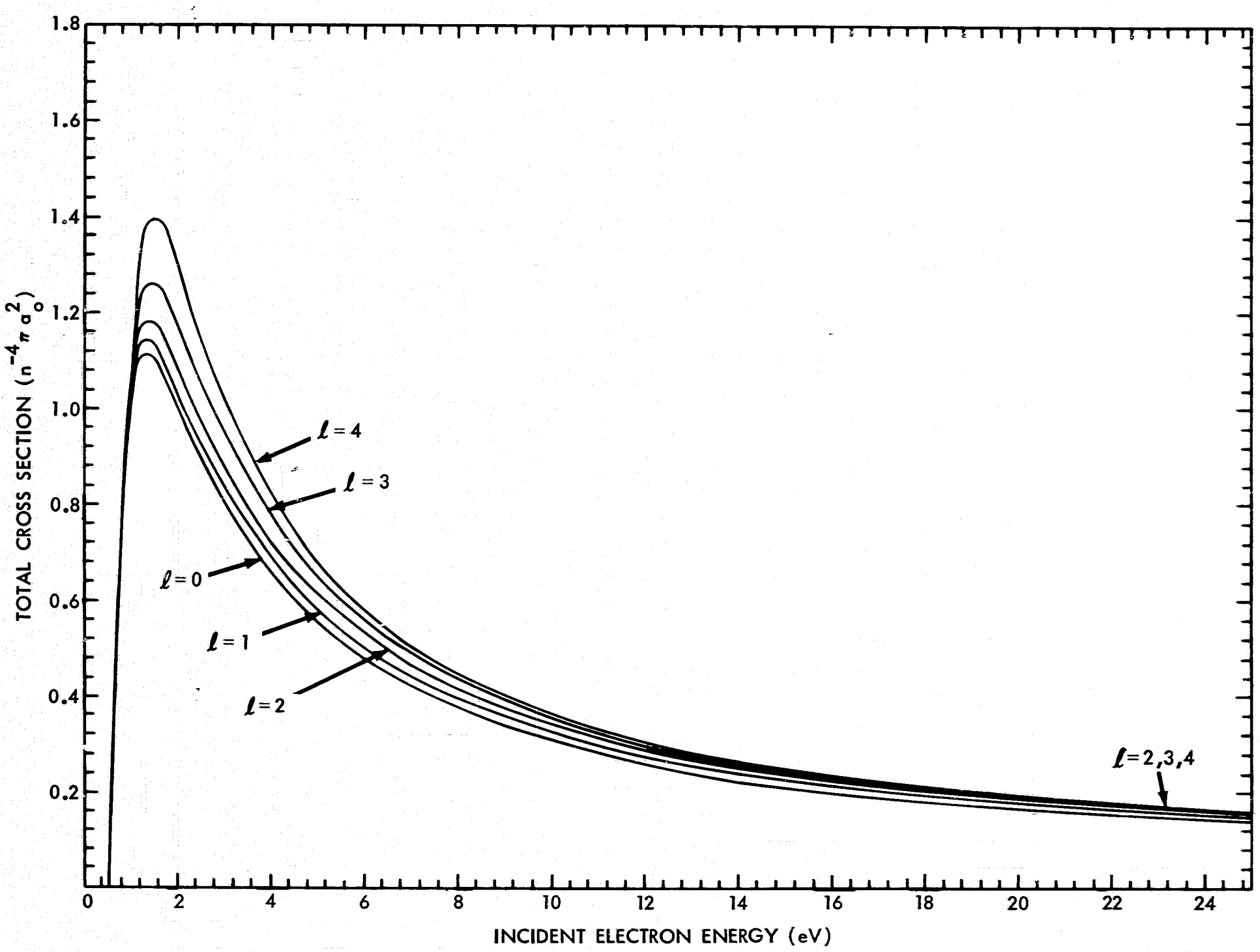
TOTAL CROSS SECTION ($n^{-4}\pi a_o^2$)
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0
2
4
6
8
10
12
14
16
18
20
22
24
INCIDENT ELECTRON ENERGY (eV)
$\ell = 4$
$\ell = 3$
$\ell = 0$
$\ell = 1$
$\ell = 2$
$\ell = 2,3,4$

Figure 4

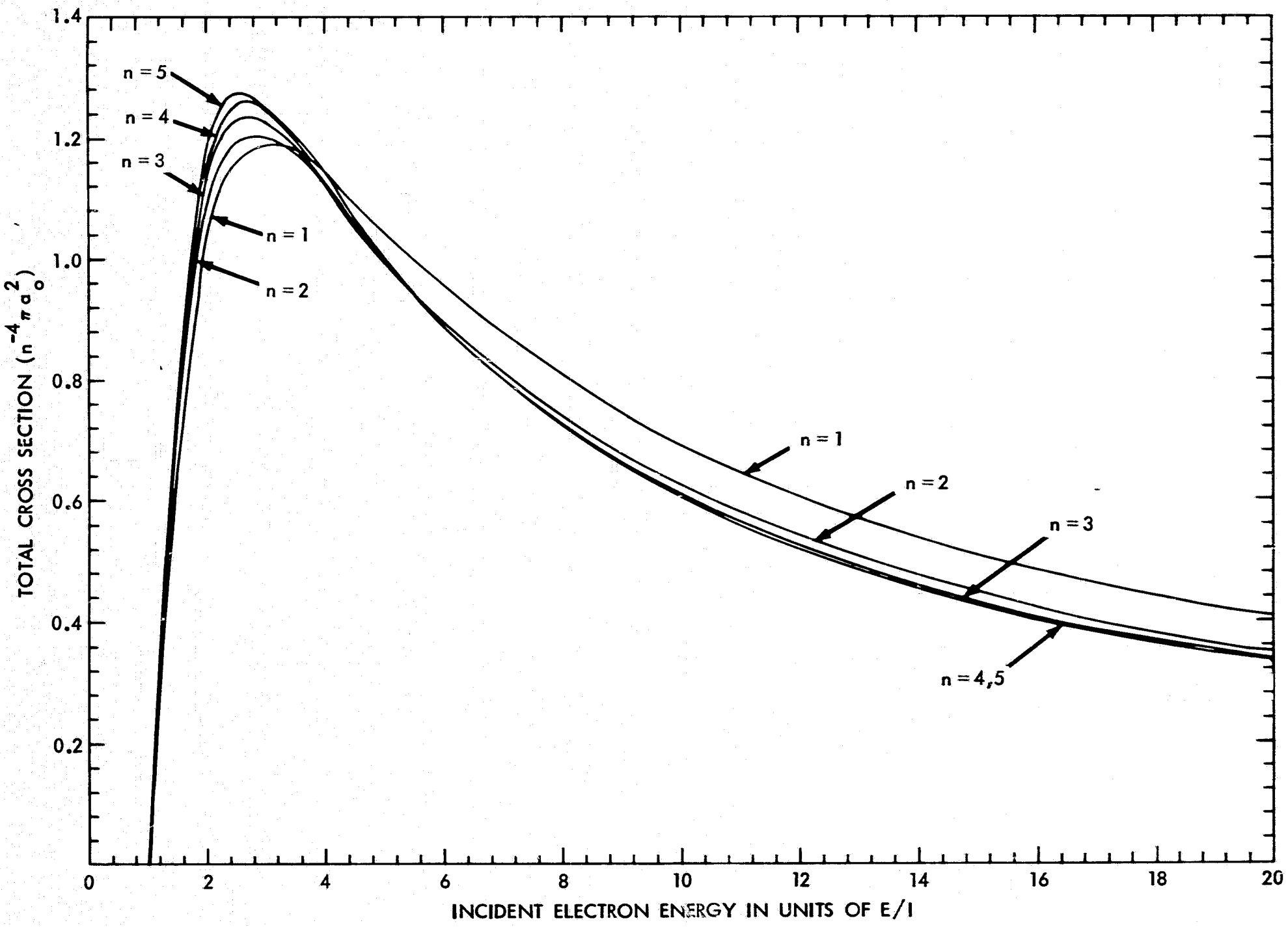
1.4
1.2
1.0
0.8
0.6
0.4
0.2
TOTAL CROSS SECTION ($n^{-4}\pi a_o^2$)
n = 5
n = 4
n = 3
n = 1
n = 2
n = 1
n = 2
n = 3
n = 4,5
0
2
4
6
8
10
12
14
16
18
20
INCIDENT ELECTRON ENERGY IN UNITS OF E/I

Figure 5

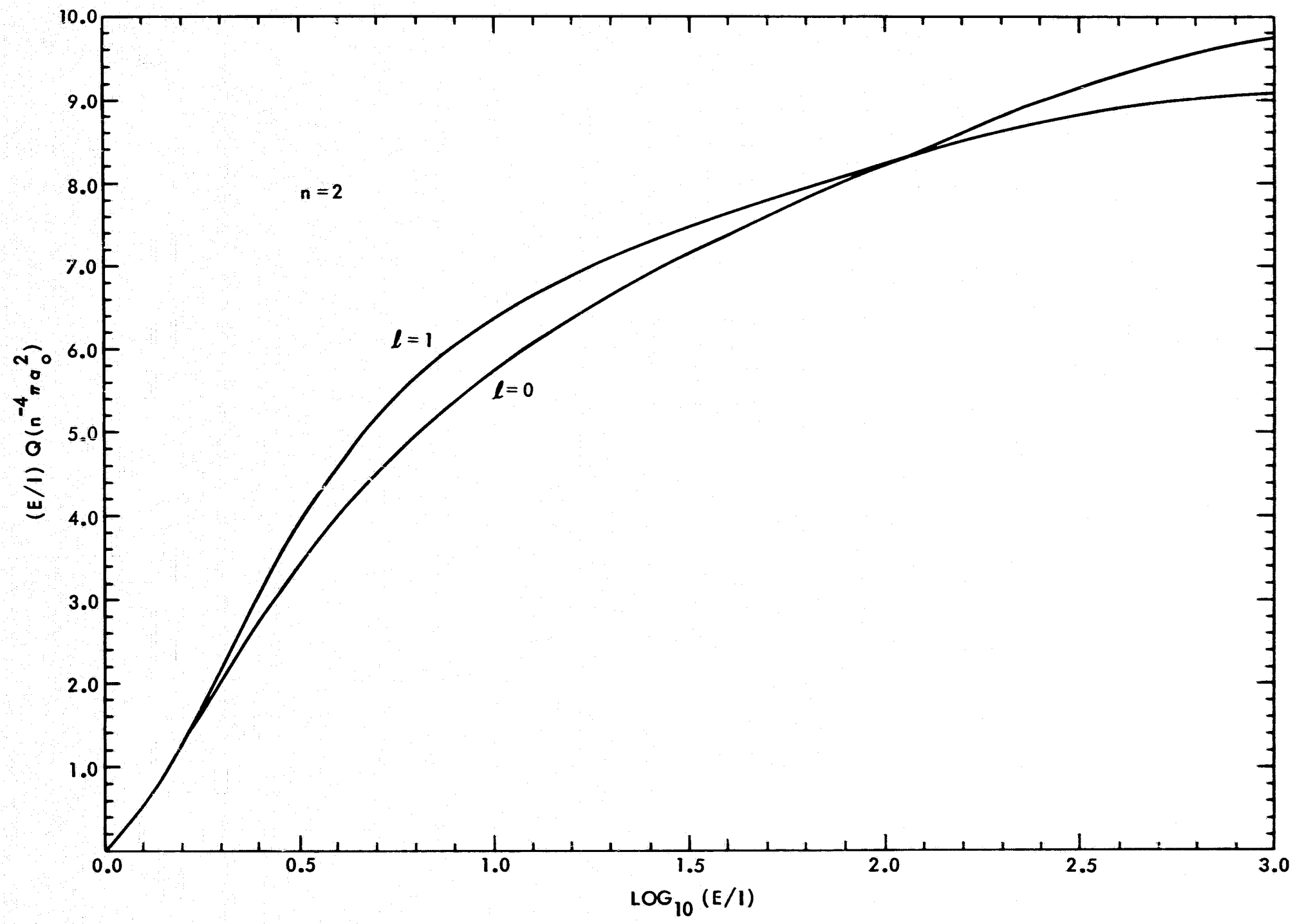
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
0.5
1.0
1.5
2.0
2.5
3.0
n = 2
ℓ = 1
ℓ = 0
(E/I) Q(n^-4 π a_o^2)
LOG10 (E/I)

Figure 6

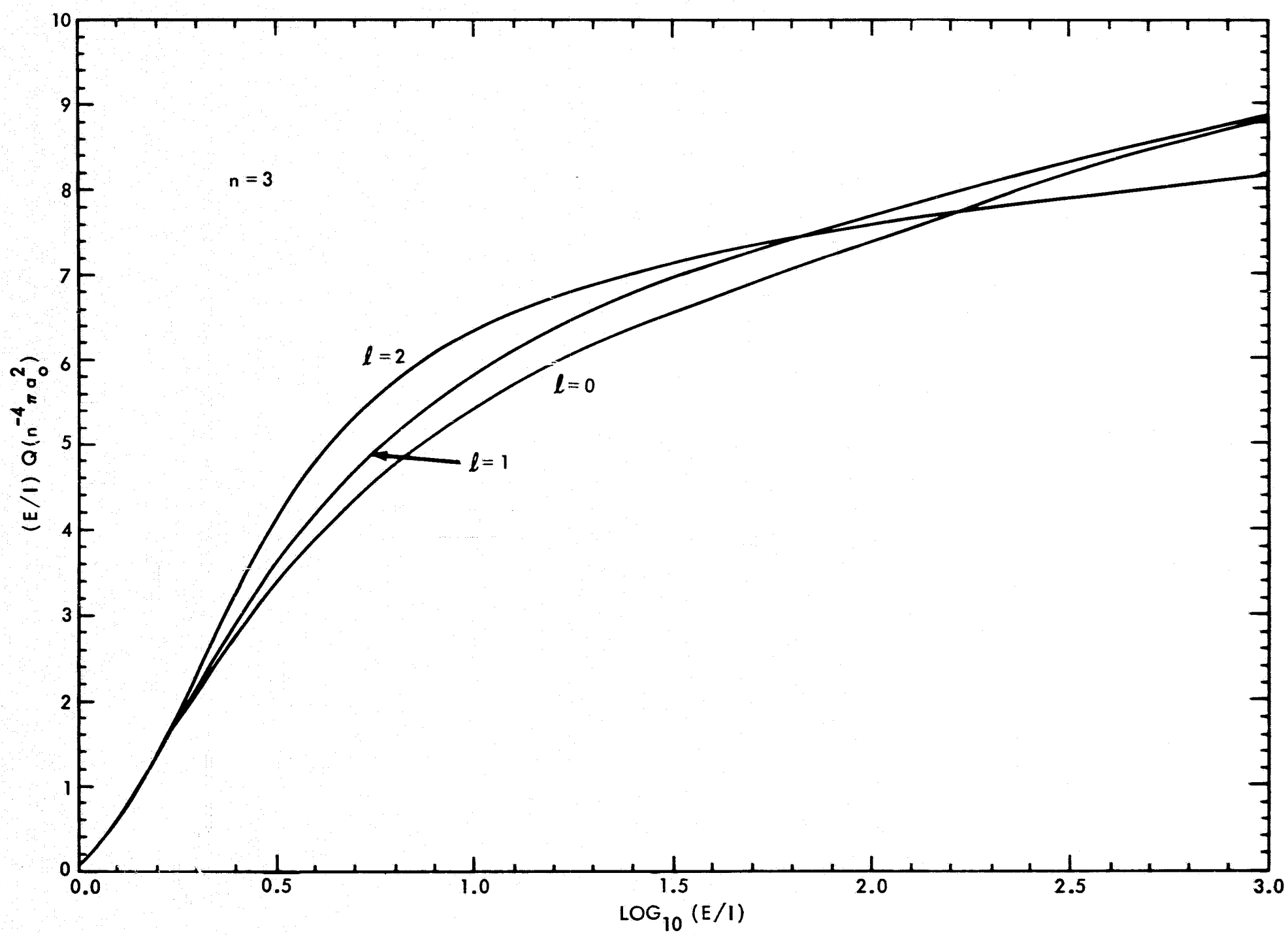
n = 3
ℓ = 2
ℓ = 0
ℓ = 1
(E/I) Q($n^{-4}\pi a_o^2$)
LOG$_{10}$ (E/I)
0
1
2
3
4
5
6
7
8
9
10
0.0
0.5
1.0
1.5
2.0
2.5
3.0

Figure 7

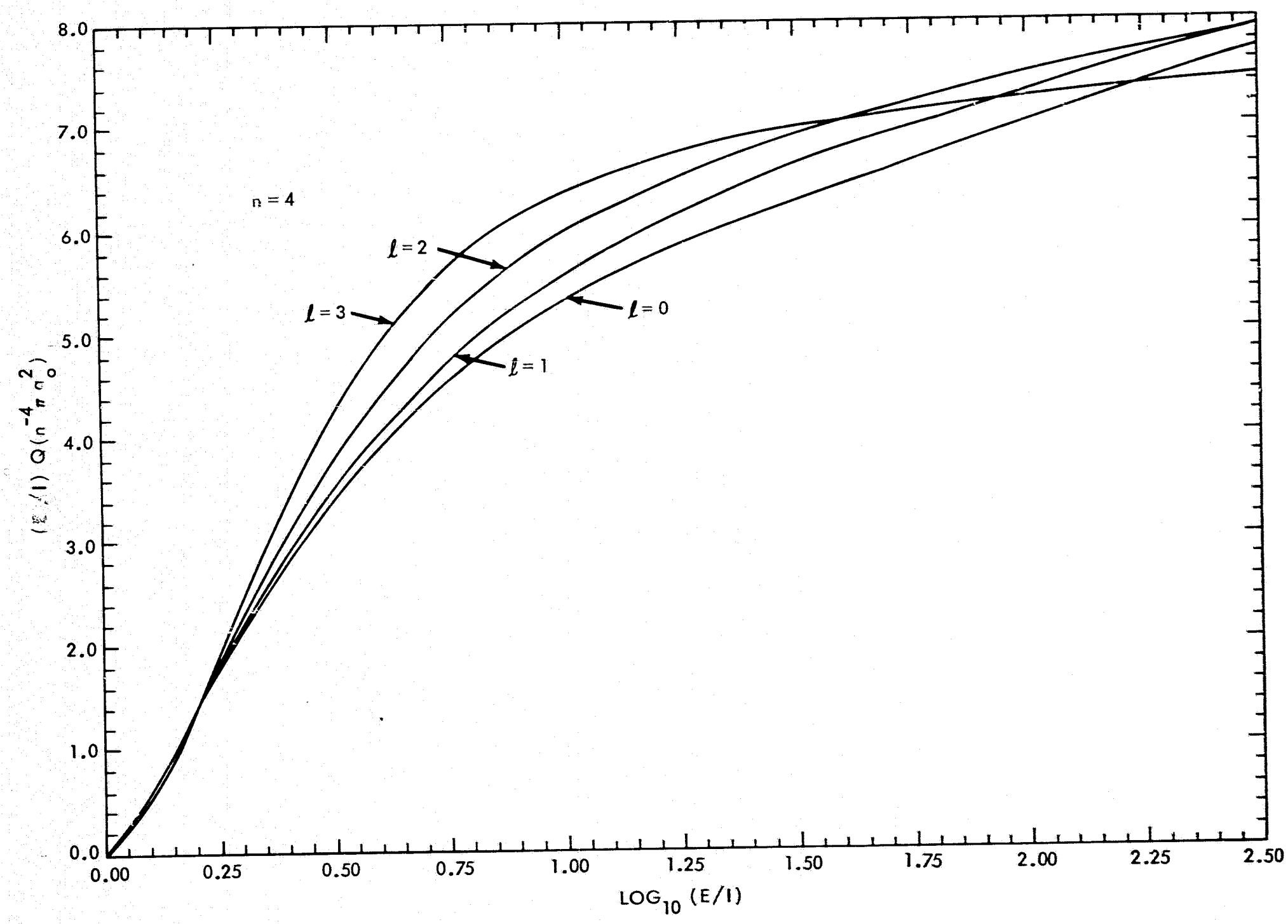
n = 4
ℓ = 2
ℓ = 3
ℓ = 0
ℓ = 1
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
2.00
2.25
2.50
LOG10 (E/I)
(E/I) Q(n^-4 π n_o^2)

Figure 8

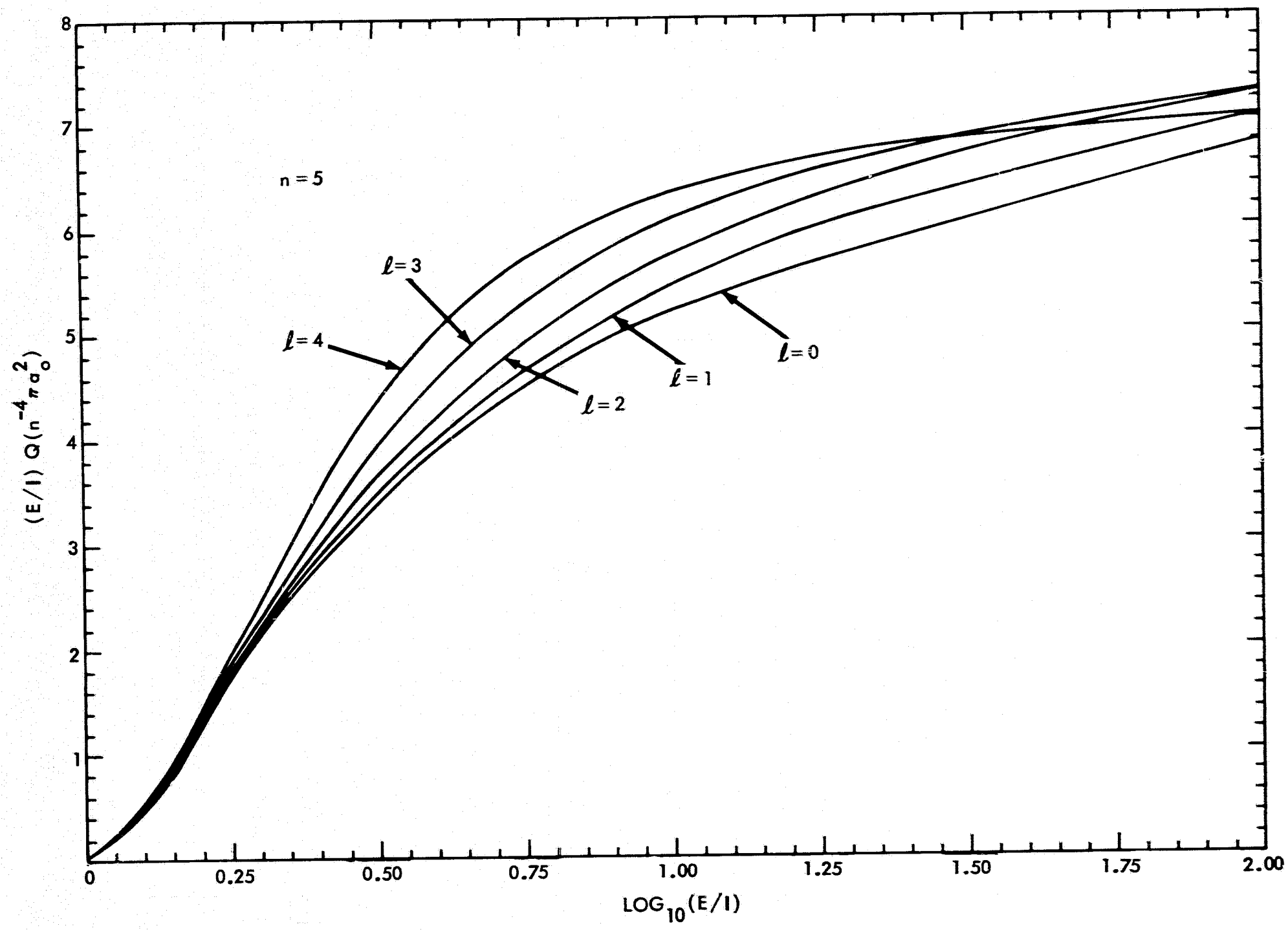
n = 5
ℓ = 3
ℓ = 4
ℓ = 2
ℓ = 1
ℓ = 0
(E/I) Q(n^-4 π a_o^2)
LOG10(E/I)
0
0.25
0.50
0.75
1.00
1.25
1.50
1.75
2.00
1
2
3
4
5
6
7
8

Figure 9

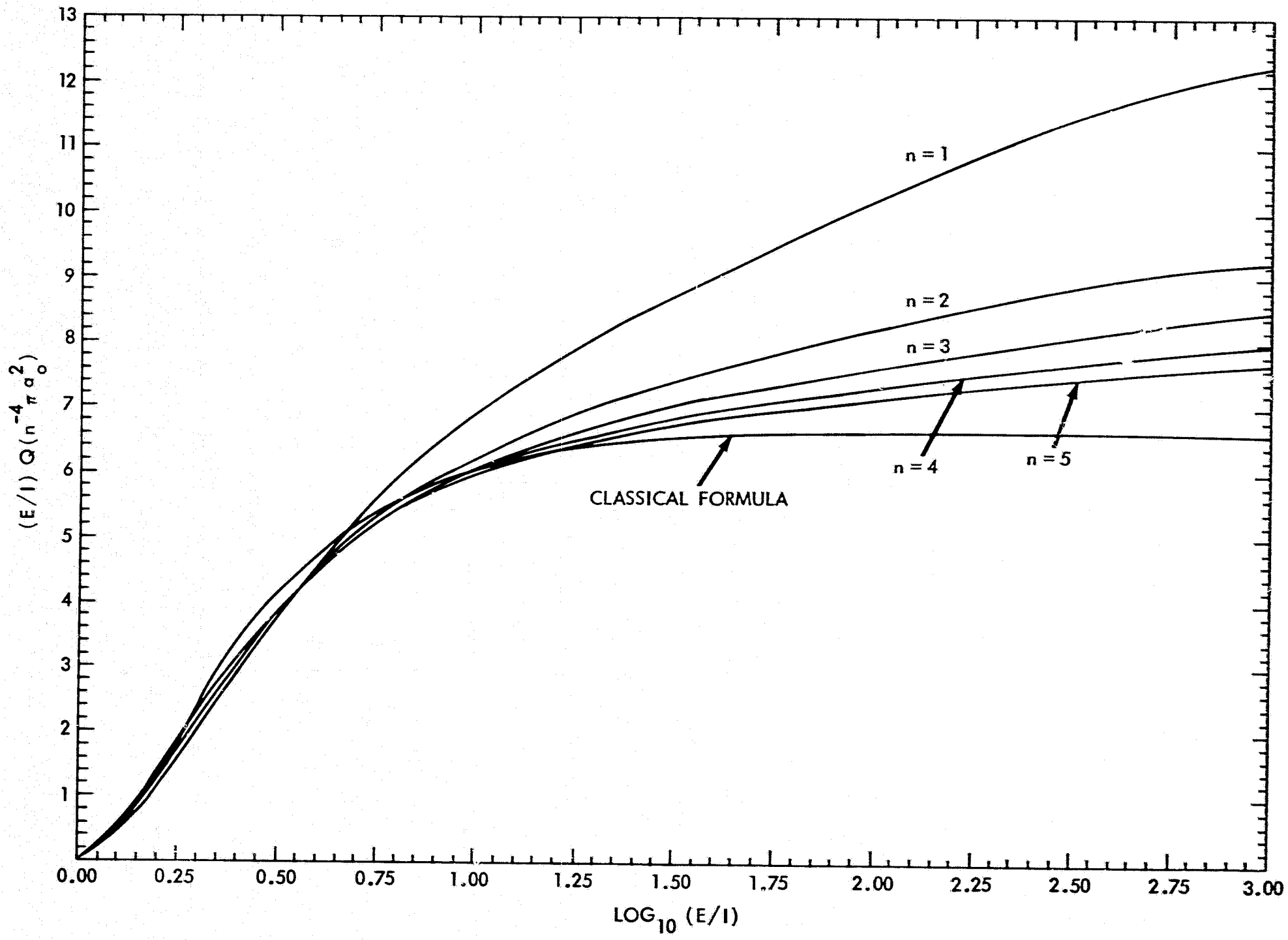
13
12
11
10
9
8
7
6
5
4
3
2
1
(E/I) Q($n^{-4}\pi a_o^2$)
n = 1
n = 2
n = 3
n = 4
n = 5
CLASSICAL FORMULA
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
2.00
2.25
2.50
2.75
3.00
LOG_{10} (E/I)

Figure 10

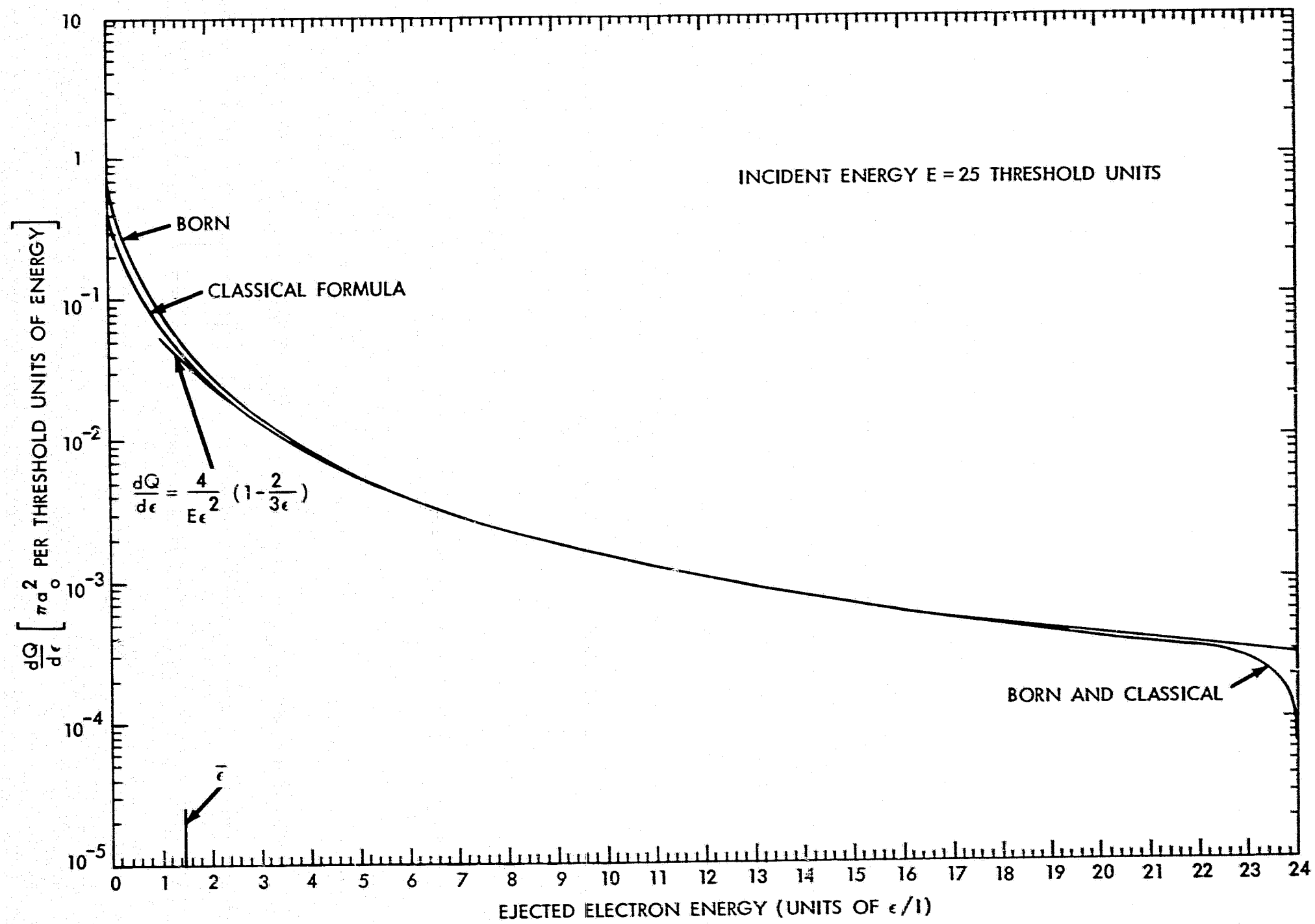
INCIDENT ENERGY E = 25 THRESHOLD UNITS
BORN
CLASSICAL FORMULA
$\frac{dQ}{d\epsilon} = \frac{4}{E\epsilon^2}\left(1-\frac{2}{3\epsilon}\right)$
BORN AND CLASSICAL
$\bar{\epsilon}$
$\frac{dQ}{d\epsilon}\left[\pi a_o^2 \text{ PER THRESHOLD UNITS OF ENERGY}\right]$
10
1
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
EJECTED ELECTRON ENERGY (UNITS OF ϵ/I)

Figure 11

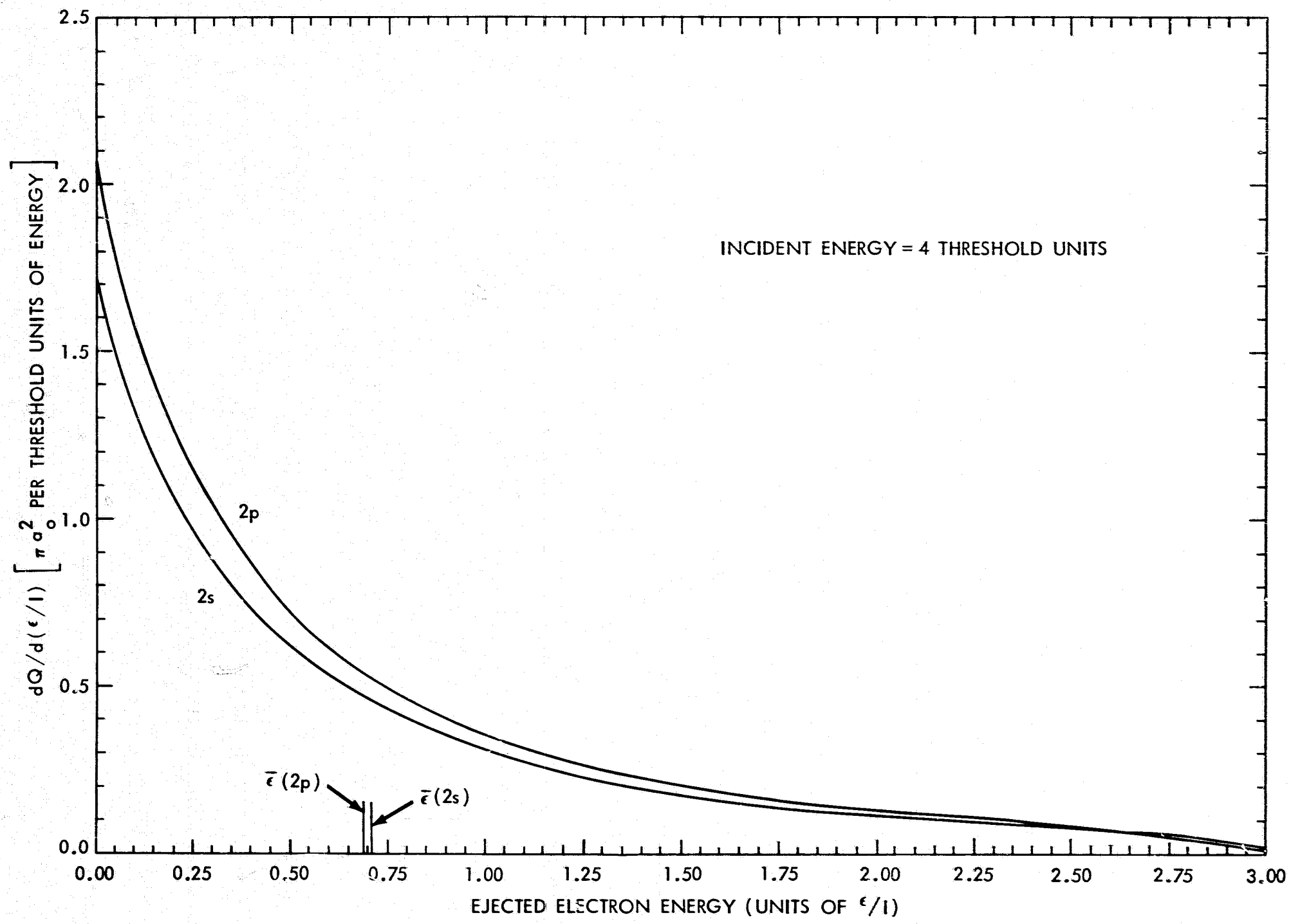
INCIDENT ENERGY = 4 THRESHOLD UNITS
2p
2s
$\bar{\epsilon}$ (2p)
$\bar{\epsilon}$ (2s)
$dQ/d(\epsilon/I)$ $[\pi a_o^2$ PER THRESHOLD UNITS OF ENERGY$]$
EJECTED ELECTRON ENERGY (UNITS OF ϵ/I)
0.0
0.5
1.0
1.5
2.0
2.5
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
2.00
2.25
2.50
2.75
3.00

Figure 12

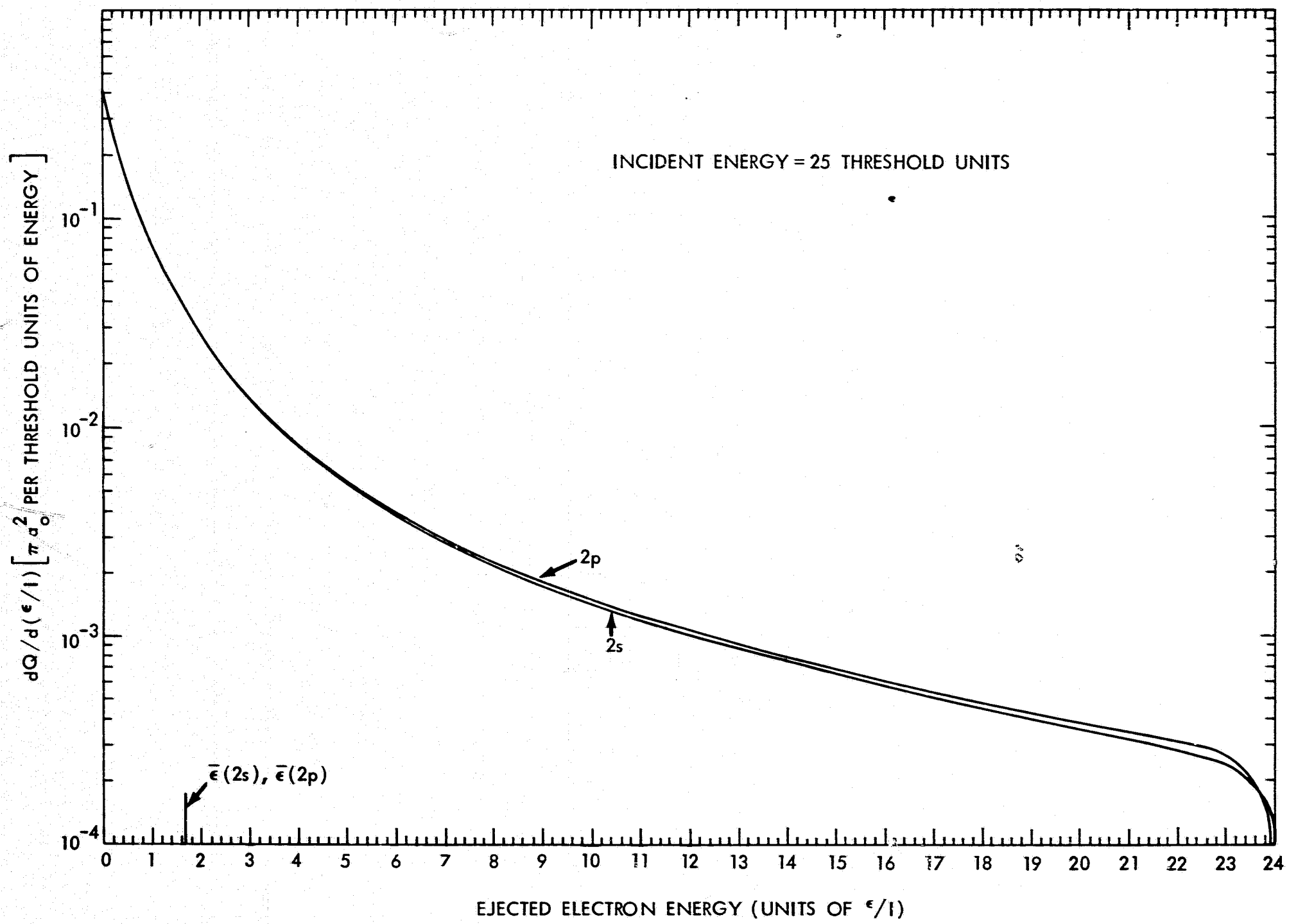
INCIDENT ENERGY = 25 THRESHOLD UNITS
dQ/d(ε/I) [π a₀² PER THRESHOLD UNITS OF ENERGY]
10⁻¹
10⁻²
10⁻³
10⁻⁴
2p
2s
ε̄(2s), ε̄(2p)
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
EJECTED ELECTRON ENERGY (UNITS OF ε/I)

Figure 13

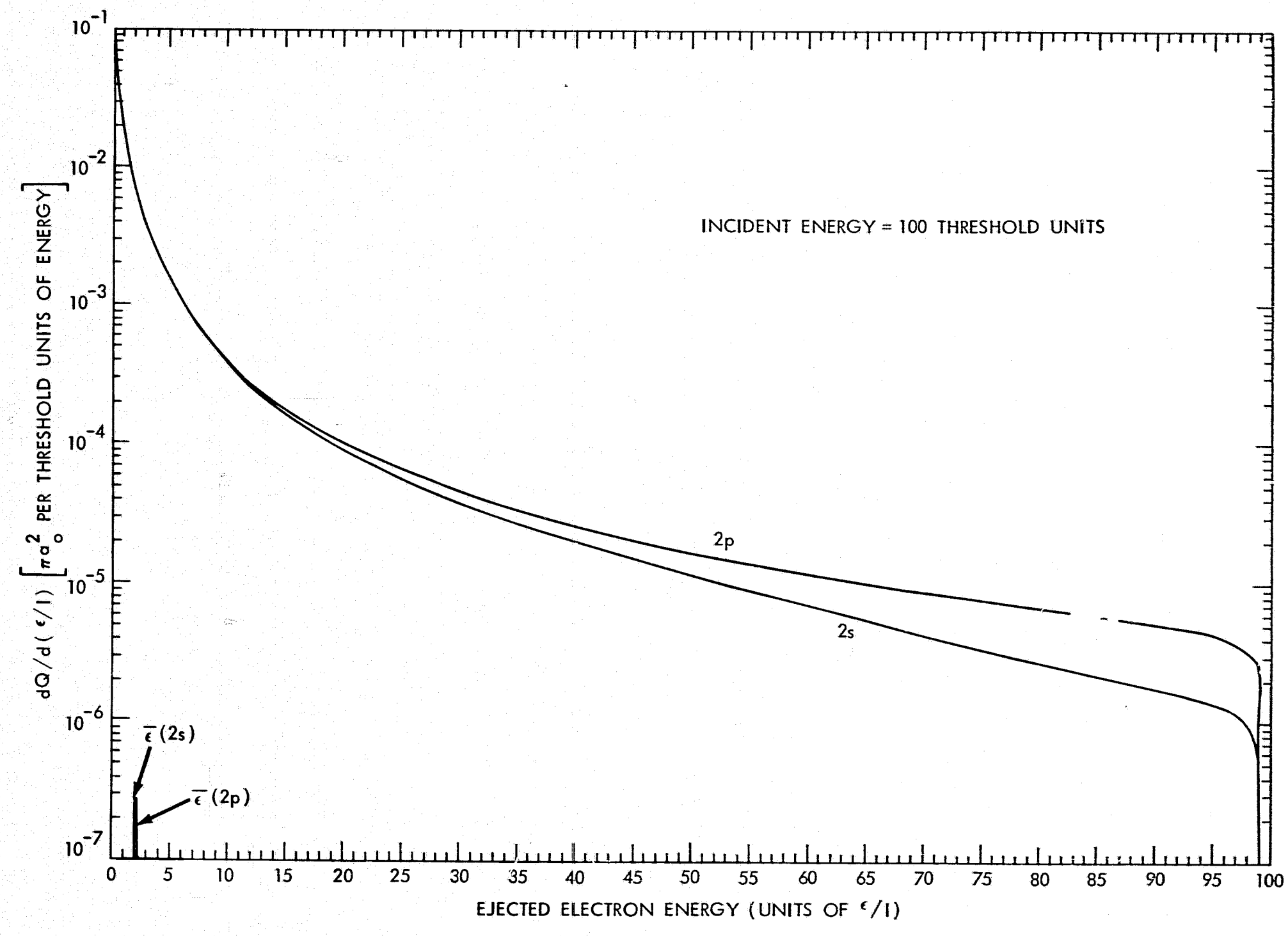
INCIDENT ENERGY = 100 THRESHOLD UNITS
2p
2s
$\bar{\epsilon}$ (2s)
$\bar{\epsilon}$ (2p)
$dQ/d(\epsilon/I)$ $[\pi a_o^2$ PER THRESHOLD UNITS OF ENERGY$]$
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
0 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100
EJECTED ELECTRON ENERGY (UNITS OF ϵ/I)

Figure 14

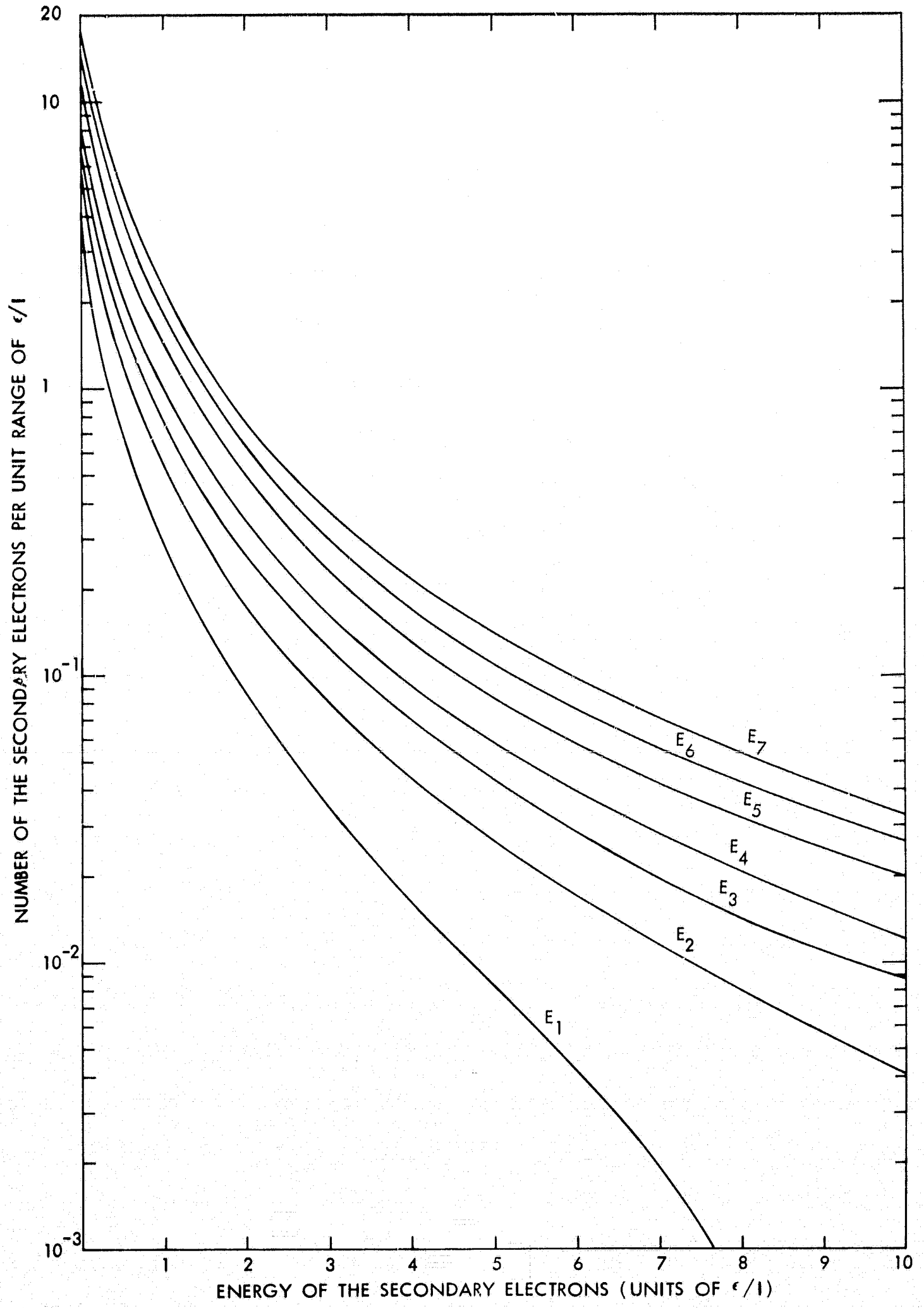
20
10
1
10^{-1}
10^{-2}
10^{-3}
NUMBER OF THE SECONDARY ELECTRONS PER UNIT RANGE OF ϵ/I
E_1
E_2
E_3
E_4
E_5
E_6
E_7
1
2
3
4
5
6
7
8
9
10
ENERGY OF THE SECONDARY ELECTRONS (UNITS OF ϵ/I)

Figure 15

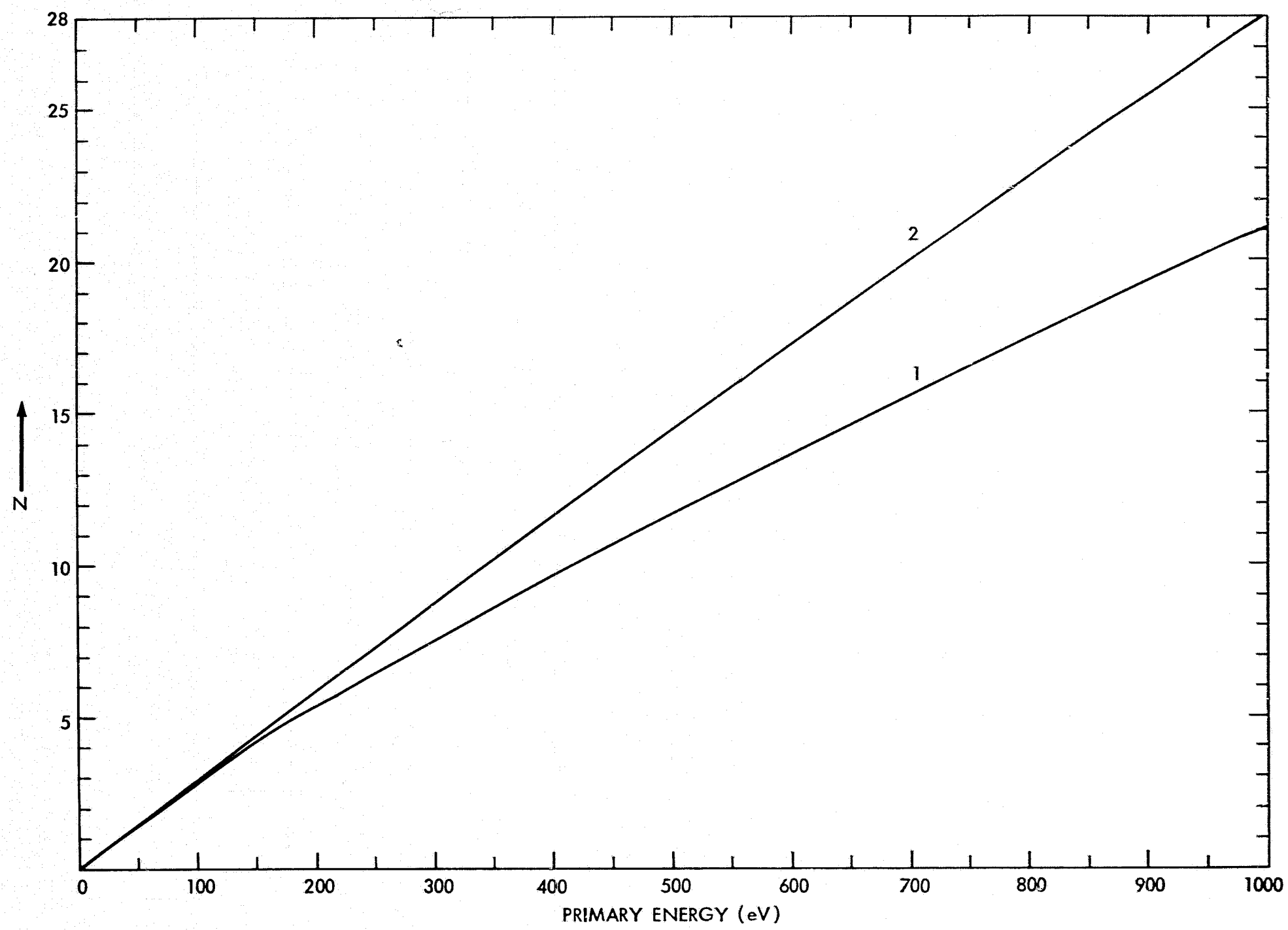
28
25
20
15
10
5
N
2
1
0
100
200
300
400
500
600
700
800
900
1000
PRIMARY ENERGY (eV)

Figure 16