X-641-66-245

NASA TM X-55501

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BY

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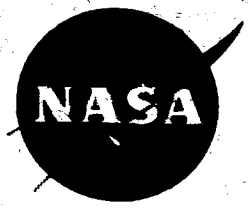
JUNE 1966



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Preprint for Publication

ON VAINSHTEIN'S METHOD APPLIED TO THE ELECTRON IMPACT EXCITATION AND IONIZATION OF ATOMS

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ABSTRACT

In previous papers Vainshtein and collaborators have introduced a method of calculation which in some respects gives better agreement with observation than do other methods. In their derivation the integral for the excitation and ionization amplitudes is treated approximately. In this paper this integral is derived exactly, and it is shown that an overall improvement in agreement with observation is obtained. The theory has some features in common with the close-coupling approximation. In particular, at the threshold of excitation and ionization the cross section has oscillatory behavior. A feature of the theory not presently understood is that the exchange amplitude is indeterminate.

I. FORMULATION OF THE THEORY

In problems of excitation and ionization effects of collisions of electrons with atoms, Vainshtein, Presnyakov, and Sobelman[1] have introduced a method of approximation which to some extent reduces the discrepancy between theories and observations. Their approach may be summarized as follows:

For the case of the electron-hydrogen system, let $\mathbf{r}_1$, $\mathbf{r}_2$ represent the position vectors of the atomic and the incident electrons, $\mathbf{k}_1$, $\mathbf{k}_2$ the momentum

vectors before and after collision of the incident electron, and $\mathbf{q} = \mathbf{k}_1 - \mathbf{k}_2$. If we designate the initial and final states by the indices 1 and 2, and use atomic units, the transition amplitude will be given by

$$T(1, 2) = \left\langle \phi_2 (\mathbf{r}_1) e^{i\mathbf{k}_2 \cdot \mathbf{r}_2} \left| \frac{1}{|\mathbf{r}_2 - \mathbf{r}_1|} - \frac{1}{r_2} \right| \psi(\mathbf{r}_1, \mathbf{r}_2) \right\rangle , \qquad (1)$$

where $\phi_2 (\mathbf{r}_1)$ is the wave function of the atomic electron after collision, and $\psi(\mathbf{r}_1, \mathbf{r}_2)$ is the total wave function of the system with a specified asymptotic form. The excitation or the ionization cross section is then given by

$$Q(1, 2) = \frac{1}{2\pi a_0^2 k_1^2} \int_{k_1 - k_2}^{k_1 + k_2} |T(1, 2)|^2 \, q \, dq , \qquad (2)$$

as being the Bohr radius.

With some plausible approximations Vainshtein et al. have shown that (1) reduces to

$$T(1, 2) = \frac{4\pi}{q^2} A \langle 2 | e^{i\mathbf{q} \cdot \mathbf{r}} | 1 \rangle , \qquad (3)$$

where 1 and 2 refer to the initial and final states of the atomic electron. In this expression A is a dimensionless quantity given by

$$A = \frac{Nq^2}{\pi} \int d\mathbf{r} \, \frac{e^{2i\mathbf{q} \cdot \mathbf{r}}}{r} F(i\nu, 1, ik_1 r - i\mathbf{k}_1 \cdot \mathbf{r}) \times F(-i\nu, 1, ik_1 r - i\mathbf{k}_1 \cdot \mathbf{r}) , \qquad (4)$$

where

$$N = \Gamma(1 - i\nu)\Gamma(1 + i\nu) , \qquad \nu = \frac{1}{k_1 + \sqrt{\epsilon_0}} , \tag{5}$$

ϵ_0 being the ionization energy of the atom. It should be noticed that by putting $A = 1$, the Born approximation results.

To facilitate the integration in (4), Vainshtein et al. make a further approximation by replacing $2i\,\mathbf{q}\cdot\mathbf{r}$ with $-2i\,\mathbf{q}\cdot\mathbf{r}$. Since the effect of this approximation is not known, it is interesting to carry out the integration in (4) exactly and compare the resulting calculated cross sections with observation. This will now be done and it will be shown that an overall improvement in this comparison is obtained. The method thus allows for further investigations.

Choosing the Z-axis along $\mathbf{k}_1$ and introducing the spherical coordinates q, θ_1, ϕ_1 for $\mathbf{q}$, and parabolic coordinates ξ, η, ϕ for $\mathbf{r}$, with $\xi = r - z$, and $\eta = r + z$, the integration in (4) with respect to ϕ and η can easily be carried out. The expression for A becomes

$$A = N\left(\frac{iq}{\cos\theta_1}\right)\int_0^\infty \exp\left[\frac{-iq\xi}{\cos\theta_1}\right] F\left(i\nu,\ 1,\ ik_1\xi\right) \times F\left(-i\nu,\ 1,\ ik_1\xi\right) d\xi . \tag{6}$$

The integration over ξ is performed by using an expression for an integral over two confluent hypergeometric functions.[2] In this way we obtain

$$A = N F(i\nu, -i\nu, 1, x) , \qquad x = \left(\frac{k_1^2 - k_2^2 + q^2}{k_1^2 - k_2^2 - q^2}\right)^2 . \tag{7}$$

Since in this expression x is larger than unity, F cannot be expressed as an expansion in ascending powers in x; but by using the analytic continuation of F this expansion can be accomplished. Using the analytic continuation of F we obtain[3]

$$A = 2N R_e \left\{ \frac{\Gamma(-2i\nu)(-x)^{-i\nu}}{\Gamma(-i\nu)\Gamma(1-i\nu)} F\left(i\nu, i\nu, 2i\nu+1, \frac{1}{x}\right) \right\} . \tag{8}$$

The ambiguity in the double valuedness of $(-)^{-i\nu}$ in the above expression can be removed by requiring A to be equal to its analytic continuation at $x = 1$. We find that we must have

$$(-)^{-i\nu} = \cosh \pi\nu , \tag{9}$$

and (8) reduces to

$$A = (\pi\nu \coth \pi\nu)^{1/2} R_e \left[e^{i(\phi - \nu \ln 4x)} F\left(i\nu, i\nu, 2i\nu+1, \frac{1}{x}\right) \right] , \tag{10}$$

with

$$\phi = \arg\Gamma(1+i\nu) - \arg\Gamma\left(\frac{1}{2}+i\nu\right) . \tag{11}$$

This completes the evaluation of A.

By evaluating the matrix element in (3) for $1s \rightarrow 2s$ and $1s \rightarrow 2p$ transitions, and substitution of the results into (2), we find that

$$Q(1s, 2s) = \frac{256}{k_1^2} \int A^2 D^2 \, q \, dq \, , \tag{12}$$

$$Q(1s, 2p\,m = 0) = \frac{9 \times 64}{k_1^2} \int A^2 D^2 \cos^2 \chi \, \frac{dq}{q} \, , \tag{13}$$

$$Q(1s, 2p\,m = \pm 1) = \frac{9 \times 32}{k_1^2} \int A^2 D^2 \sin^2 \chi \, \frac{dq}{q} \, , \tag{14}$$

$$D = \left(\frac{9}{4} + q^2\right)^{-3} \, , \qquad \cos \chi = \hat{k}_1 \cdot \hat{q} \, , \tag{15}$$

where in (13) and (14) the quantization axis is chosen along the incident beam (cf. Ref. 4).

For ionization we find similarly

$$Q(1s, \mathbf{k}) = \frac{512}{\pi k_1^2} \int A^2 \left| \frac{\left[(1+ik)^2 + q^2\right]^{i/k-1} \left[(1 - i/k)\, \mathbf{q} \cdot \mathbf{k} - q^2\right]}{\left[1 + (\mathbf{q}-\mathbf{k})^2\right]^{2+i/k}} \right|^2 \times \frac{dq}{k\, q^3 \left(1 - e^{-2\pi/k}\right)} \, , \tag{16}$$

with $\mathbf{k}$ the momentum vector of the ejected electron. Eq. (16) gives the cross section per unit momentum range of the ejected electron in the direction of $\mathbf{k}$. The total ionization cross section is obtained by integrating the above expression

with respect to **k**:

$$Q(1s, c) = \int Q(1s, \mathbf{k})\, d\mathbf{k} \ . \tag{17}$$

In Eqs. (12), (13), (14), and (16) Q is exposed in units of πa_0^2 and we have set $a_0 = 1$.

II. THE EXCHANGE AMPLITUDE

In treatment of the exchange amplitude there is an error in the paper by Vainshtein et al.: Their Equation (16) for the exchange amplitude should be replaced by

$$T^{ex}_{(1,2)} = \frac{4\pi}{q^2} B \langle 2 | e^{i\mathbf{q}\cdot\mathbf{r}} | 1 \rangle \ , \tag{18}$$

with

$$B = \frac{Nq^2}{\pi} \int d\mathbf{r}\, \frac{e^{2i\mathbf{k}_1\cdot\mathbf{r}}}{r}\, F\left(i\nu, 1, ik_1 r - i\mathbf{k}_1\cdot\mathbf{r}\right) \times F\left(-i\nu, 1, ik_1 r - i\mathbf{k}_1\cdot\mathbf{r}\right) . \tag{19}$$

By evaluating this integral similarly to the evaluation of the integral for A, we find that

$$B = \left(\frac{q}{k_1}\right)^2 (\pi\nu \coth \pi\nu)^{1/2} \cos\left(\phi + \nu \ln \frac{\delta}{4}\right)^2 . \tag{20}$$

$$\delta \to 0$$

As δ tends to zero the cosine factor oscillates with increasing frequency between -1 and +1, and B becomes indeterminate. We conclude that the exchange amplitude is not defined in this approximation.

III. THE THRESHOLD BEHAVIOR

Let ϵ represent the excess energy above threshold of the excitation or ionization of the incident electron. Then for sufficiently small ϵ the integrations in (12), (13), (14), (16) and (17) can be carried out analytically. Without the algebraic details, the following results are obtained:

$$Q(1s, 2s) = \frac{1}{3} C \epsilon^{1/2} , \tag{12A}$$

$$Q(1s, 2p\,m = 0) = C \epsilon^{1/2} , \tag{13A}$$

$$Q(1s, 2p\,m = \pm 1) = 0 , \tag{14A}$$

where ϵ is measured in rydberg and C is given by

$$C = \frac{2^9}{3^5 \sqrt{3}} (\pi\nu \coth \pi\nu) \left[1 + R_e \frac{e^{2i\nu \ln(3\epsilon)}}{1 + 4i\nu} \right] , \tag{21}$$

ν being defined by (5). For ionization we find similarly

$$Q(1s, c) = \frac{1}{2} \left(\frac{16}{3e} \right)^2 (\pi\nu \coth \pi\nu) \left[1 + 3 R_e \frac{e^{2i\nu \ln(4\epsilon)}}{(1 + 4i\nu)(3 + 4i\nu)} \right] \epsilon^{3/2} , \tag{17A}$$

with e the base of natural logarithms. It should be noticed that by letting $\nu \to 0$, the Born approximation results.

IV. DISCUSSION OF RESULTS

Eqs. (12), (13), (14), (16), and (17) were integrated numerically. The results are given in Table I. In Fig. 1 the result of calculation for 1s - 2s transition is plotted along with the Born and the 1s - 2s - 2p close-coupling approximations. The circles with the indicated probable errors are the experimental points due to Stebbings, Fite, Hummer, and Brackmann.[5] It is seen that the present calculation gives a narrow maximum close to the threshold with a peak comparable to the peak of the broad maximum which appears at higher energies. A similar secondary maximum is found in the theory of the close-coupling calculation by the author [6], although this is not shown in the figure.

Crothers and McCarroll[7] have developed a theory which parallels the method of Vainshtein and collaborators except that the alternative form for the transition amplitude has been used and an effective charge with real and imaginary part has been placed on the electrons. Their results also indicate a secondary maximum close to the threshold.

Figure 2 similarly compares the results of the three theories with experiment for the 1s - 2p excitation cross section. The experimental curve is obtained by drawing a line through the mean values of the measured cross sections by Fite and Brackmann.[8] The present theory shows a secondary maximum close to the threshold. Similarly, the close-coupling theory and the theory of Crothers and McCarroll[7] show a secondary maximum. The maximum for the close coupling is not shown in the figure. In the measurement of Fite et al. there is an indication that a secondary maximum might exist. In two other experiments which will be described shortly this maximum has been found.

Experimentally it is convenient to introduce a cross section $Q_\perp$ which is proportional to the number of Lyman alpha photons emitted perpendicular to the direction of the incident electron in a 1s - 2p electron excitation experiment. This cross section, using the theory of Percival and Seaton,[4] is given by

$$Q_\perp = 0.918\, Q(1s, 2p) + 0.246\, Q(1s, 2p\, m = 0) \quad . \tag{22}$$

In Fig. 3 the three theoretical curves are plotted together with the experimental curve of Fite and Brackmann. The results of 1s - 2s - 2p coupling near the threshold are due to Damburg and Gailitis,[9] while at higher energies the values of Burke and Smith[10] have been used. It is seen that both the 1s - 2s - 2p coupling and the present theory show secondary maximum near the threshold while in the experimental curve there is an indication that such a maximum might exist. Recently there have been two new measurements on 1s - 2p excitation functions by Chamberlain, Smith, and Heddle,[11] and by Smith[12] in which the observed position and the magnitude of this maximum is given. The position approximately coincides with the indicated theoretical position.

In Fig. 4 the results of the Born approximation and the present theory are compared with the results of two experiments on ionization. To save space we will not discuss other theoretical models. Experiment I is due to Fite and Brackmann[13] while experiment II belongs to Rothe, Marino, Neynaber, and Trujillo.[14] It is seen that the agreement between the present theory and experiment I at low and intermediate energies is satisfactory and better than the agreement found for the case of excitation. The theoretical curve crosses the experimental curve at two points. However, at higher energy the agreement between the two

curves is not satisfactory. At high energy the present calculation agrees better with experiment II. The reason for the discrepancy between the two experimental measurements is not known, since in both of them the same technique has been used.

It should be mentioned that Presnyakov[15] has applied the formulation of Vainshtein et al. with the approximate integral to the ionization of H atom. His curve is similarly in good agreement but consistently smaller than the experimental curve I.

Finally we should discuss the threshold behavior. From (12A), (13A), and (14A) it is seen that, the excitation cross section is proportional to $\epsilon^{1/2}$ times an oscillating factor which oscillates with increasing frequency as ϵ tends to zero. Gailitis and Damburg[16] have shown that similar oscillations are exhibited by the 1s - 2s - 2p close-coupling theory. These oscillations in the close coupling approximation are due to the formation of the bound states of the composite system, due to the $1/r^2$ potential of the atom induced by the incident electron. This potential in the close coupling theory is due to the superposition of the degenerate states of the atom in the total wave function of the system. The present method, however, which is a two channel approximation, lacks the superposition of more than two states, but as the coordinates used to express the final state wave function are different from the coordinates of the initial state, the final state wave function is not an eigenfunction of the unperturbed Hamiltonian of the initial state, it therefore must contain in itself many eigenfunctions of the initial state. In this way effects similar to close coupling are exhibited. However, in the close coupling theory the 1s - 2s and the 1s - 2p cross sections

are finite at the threshold, and their ratio approaches 1.393, while in the present theory these cross sections become zero, and their ratio approaches 1/3.

In Figure 5 the ionization at threshold is shown for three theoretical models and two experiments. The theoretical curves are the Born, the present calculation, and the two-Coulomb-S-wave theory of Geltman[17] and Peterkop.[18] In the latter theory a system with total angular momentum $L = 0$ is considered where the two electrons in the final states move in two different Coulomb fields. The Born cross section is proportional to $\epsilon^{3/2}$, the two Coulomb wave theory to ϵ, and the present theory does not obey a definite power law. The oscillating term in (17A) makes the cross section curve to appear more linear than the Born approximation curve.

The curve in experiment I is due to Fite and Brackmann, and has a slope of $1.06\ \pi a_0^2/\text{ryd}$. The curve in experiment III is due to McGowan, and Fineman,[19] and has a slope of $0.87\ \pi a_0^2/\text{ryd}$, although it has been maintained by McGowan and Fineman that they have not established the true linearity of their ionization yield curve.

Further study on ionization threshold has been done by Wannier,[20] Rudge and Seaton,[21] and Temkin.[22] It has been maintained by Rudge and Seaton that quantum mechanically the cross section should be linear with respect to the excess energy above threshold. Nevertheless based on the argument that the long range $1/r^2$ potential is a common feature of both excitation and ionization processes, and the threshold of excitation is not given by a power law, the threshold of ionization may not similarly be given by a power law.

ACKNOWLEDGMENT

I wish to thank B. Baxter for assistance in programming of the numerical integration.

REFERENCES

1. L. Vainshtein, L. Presnyakov, and I. Sobelman, Soviet Physics, JETP 18, 1383 (1964).

2. L. D. Landau, and E. M. Lifshitz, Quantum Mechanics (Addison Wesley Publishing Co. Inc., Reading, Mass., 1958), P. 505.

3. P. M. Morse, and H. Feshbach, Methods of Theoretical Physics (McGraw-Hill Book Co. Inc., 1953), P. 670.

4. I. C. Percival and M. J. Seaton, Phil. Trans. Roy. Soc. A, 251, 113 (1958).

5. R. F. Stebbings, W. L. Fite, D. G. Hummer, and R. T. Brackmann, Phys. Rev. 119, 1939 (1960).

6. K. Omidvar, Phys. Rev. 113, A970 (1964).

7. D. Crothers, and R. McCarroll, Proc. Phys. Soc. 86, 753 (1965).

8. W. L. Fite, and R. T. Brackmann, Phys. Rev. 112, 1141 (1958).

9. R. Damburg and M. Gailitis, Proc. Phys. Soc. (London) 82, 1068 (1963).

10. P. G. Burke, and K. Smith, Rev. Mod. Phys. 34, 458 (1962).

11. G. E. Chamberlain, S. J. Smith, and D. W. O. Heddle, Phys. Rev. Letters, 12, 647 (1964).

12. S. J. Smith, Proc. 4th Int. Conf. on Atomic Collisions, Quebec, Canada (1965).

13. W. L. Fite, and R. T. Brackmann, Phys. Rev. 112, 1141 (1958).

14. E. W. Rothe, L. L. Marino, R. H. Neynaber, and S. M. Trujillo, Phys. Rev. 125, 582 (1962).

15. L. Presnyakov, Soviet Physics, JETP 20, 760 (1965).

16. M. Gailitis and R. Damburg, Proc. Phys. Soc. (London) 82, 192 (1963).

17. S. Geltman, Phys. Rev. 102, 171 (1956).

18. R. K. Peterkop, Izv. Akad. Latv. SSR, 9, 79 (1960); Izv. Akad. Nauk SSR, 24, 947 (1960).

19. J. W. McGowan and M. A. Fineman, Proc. 4th Int. Conf. on Atomic Collisions, Quebec, Canada (1965).

20. G. H. Wannier, see Ref. 2, P. 456.

21. M. R. H. Rudge and M. J. Seaton, Proc. Roy. Soc. (London) A283, 262 (1965).

22. A. Temkin, Phys. Rev. Letters 16, 835 (1966).

TABLE I. The excitation cross section of hydrogen from the ground state to the 2s, 2p, m = 0, ±1, and the continuum in units of πa_0^2. The energy of the incident electron, k_1^2, is given in ryd. k_2^2 is the excess energy in ryd of the incident electron after the excitation of the n = 2 level. Q(1s, 2p) is the cross section for excitation to all the 2p levels. All excitation cross sections show two maxima.

k_1^2	k_2^2	Q(1s, 2s)	Q(1s, 2p 0)	Q(1s, 2p ± 1)	Q(1s, 2p)	Q(1s, c)
	0.01	0.101	0.307	0.001	0.309	
	0.03	0.132	0.400	0.006	0.412	
	0.05	0.130	0.386	0.011	0.407	
0.81		0.128	0.374	0.013	0.399	
1.00		0.124	0.399	0.041	0.481	0.000
1.44		0.137	0.707	0.116	0.939	0.270
1.96		0.122	0.753	0.187	1.128	0.556
2.56		0.104	0.684	0.231	1.146	0.743
3.24		0.087	0.590	0.251	1.093	0.821
4.00		0.074	0.502	0.256	1.015	0.828
6.25		0.051	0.339	0.239	0.818	0.724
9.00		0.038	0.240	0.210	0.660	0.600
12.25		0.029	0.178	0.181	0.541	0.494
16.00		0.023	0.137	0.157	0.451	0.411
20.25		0.018	0.108	0.137	0.382	0.348
25.00		0.015	0.088	0.120	0.328	0.298

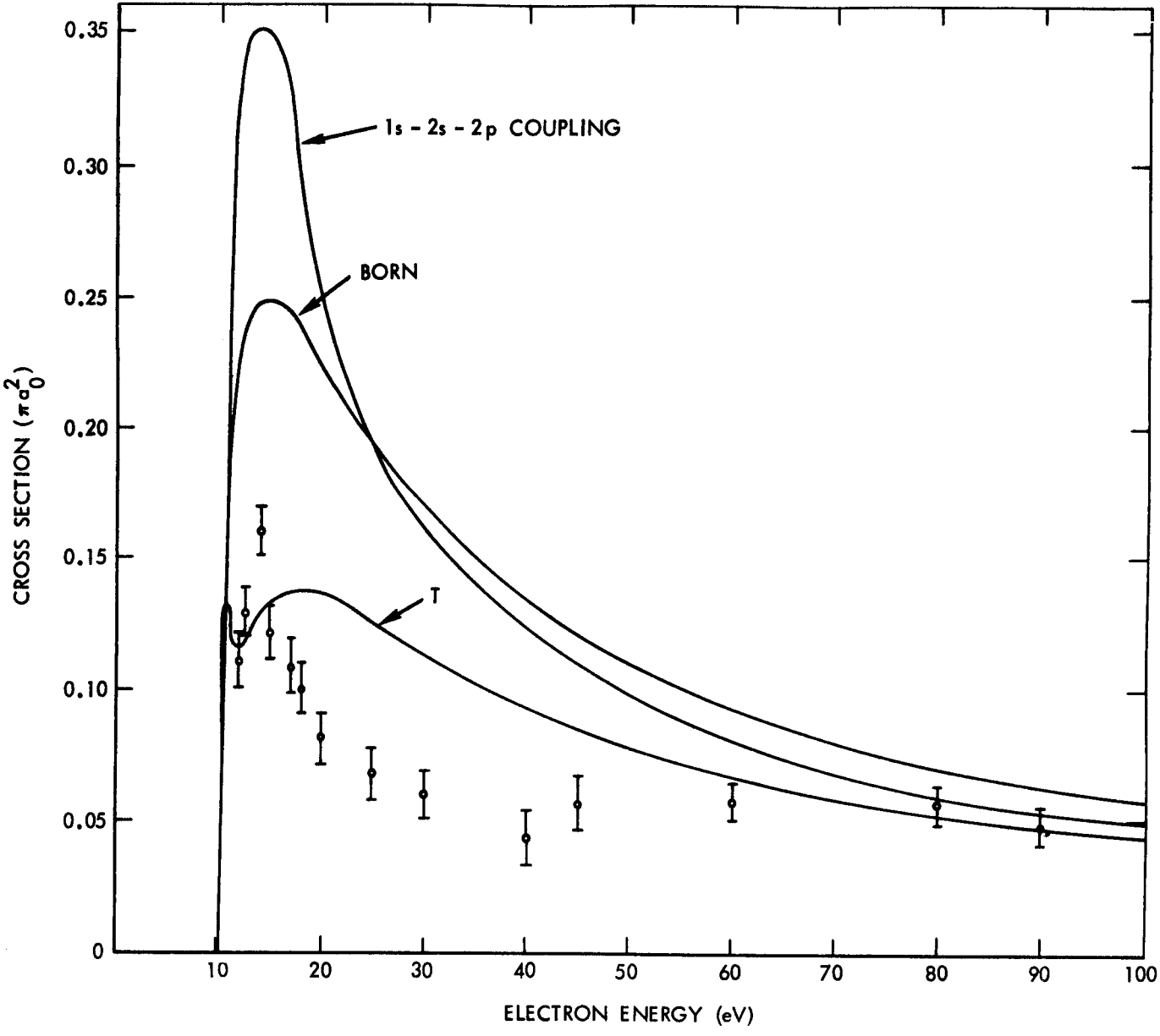

Figure 1—The 1s-2s excitation. T is the present theory. The circles with the indicated errors are the measurements of Stebbings, Fite, Hummer and Brackmann.

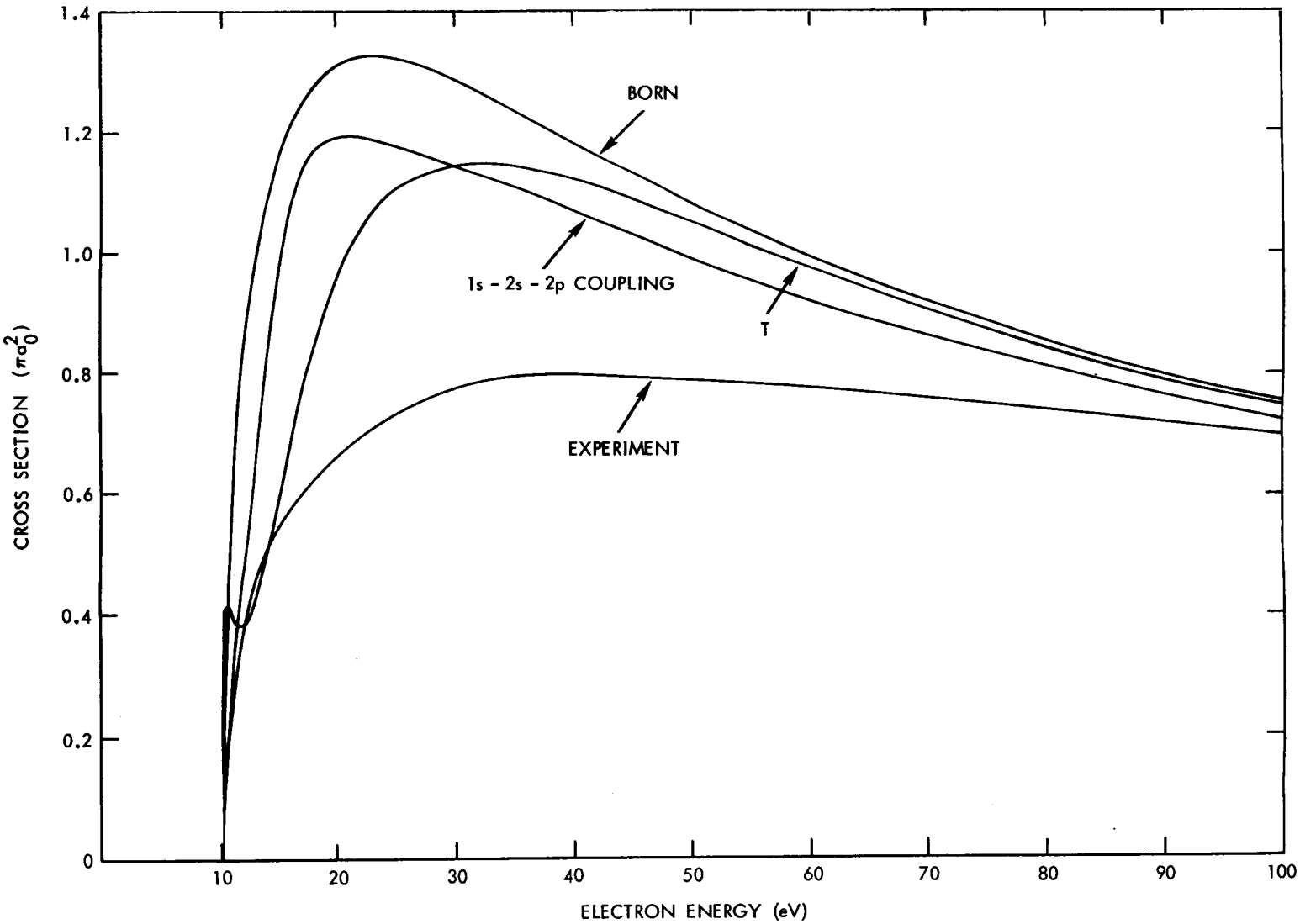

Figure 2–The 1s-2p excitation. T is the present theory. The experimental curve is due to Fite and Brackmann.

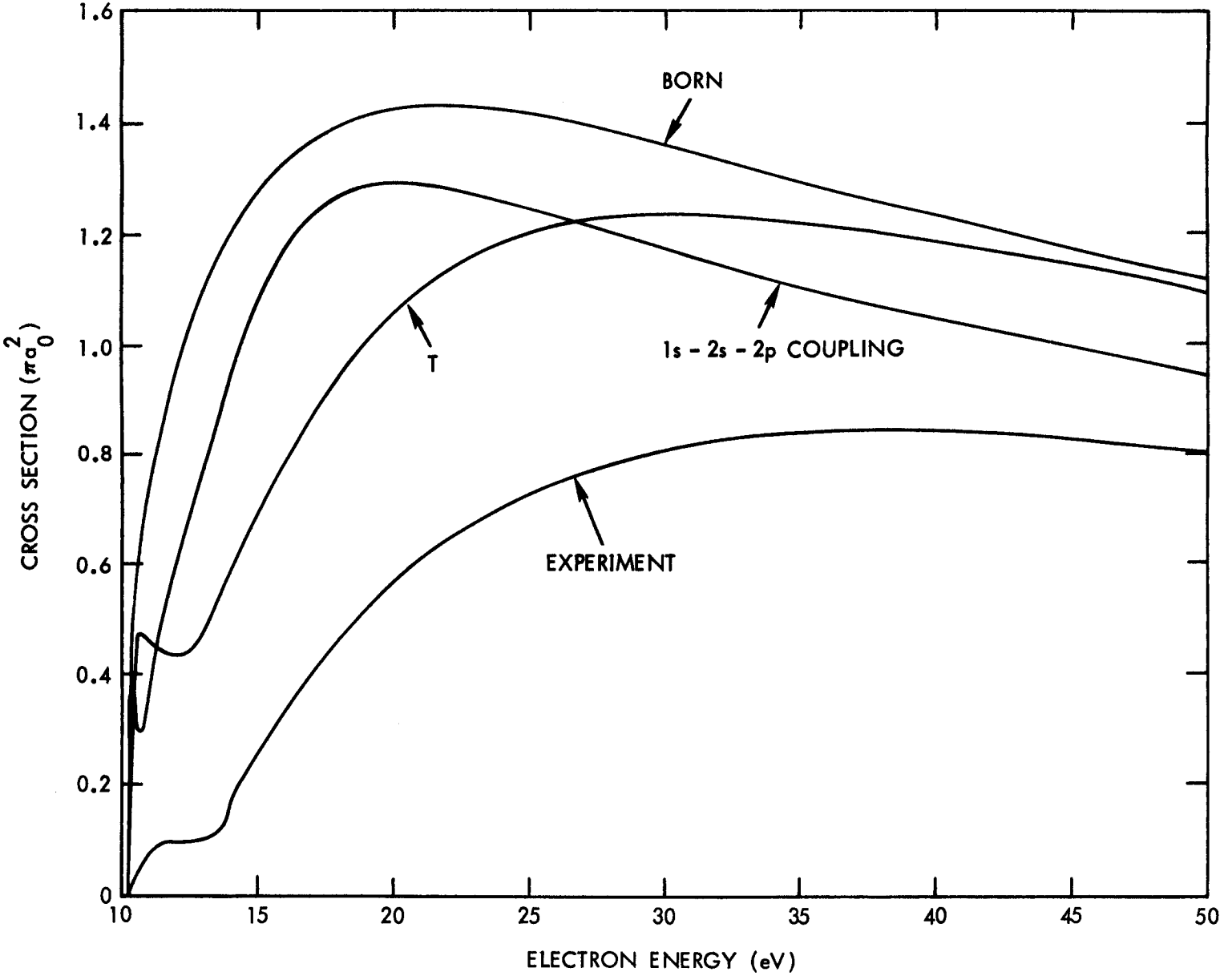

Figure 3–The cross section $Q_{\perp}(1s, 2p)$. The notation is the same as in Figure 2. The experimental curve is due to Fite and Brackmann.

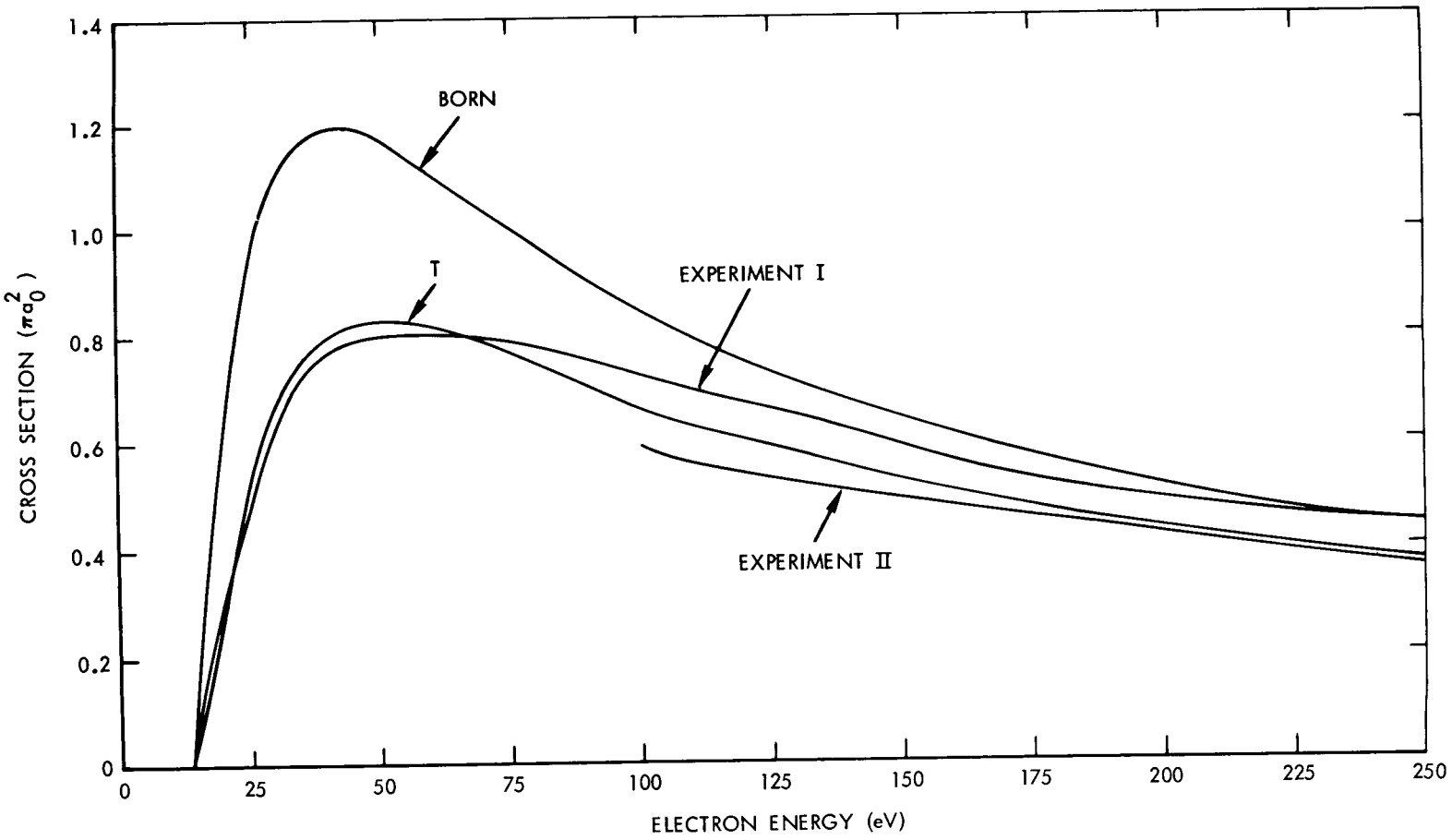

Figure 4—Ionization of the ground state. T is the present theory. Experiment I is due to Fite and Brackmann. Experiment II belongs to Rothe, Marino, Neynaber, and Trujillo.

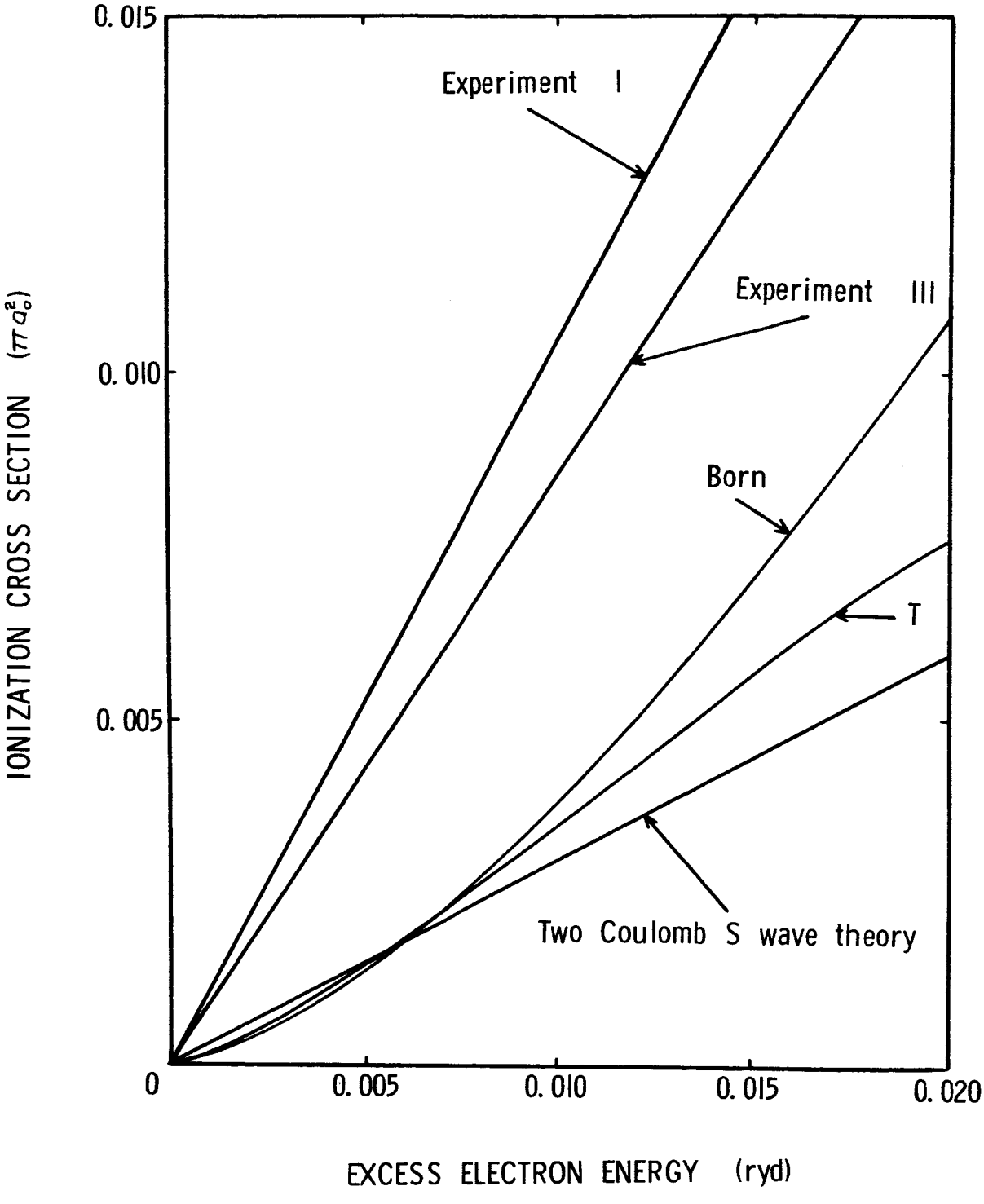

Figure 5—Ionization at threshold. T is the present theory. Experiment I is the same as in Figure 4. Experiment III is due to McGowan and Fineman.