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Study of the Discrepancy between "Prior" and "Post" Approximations in Quantum Calculations of the e -H Excitation Cross Sections by the Correlations Method

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In the calculation of excited-state cross sections for electron impact on hydrogen atoms, the hypothesis $A = \vec{\nabla}_1 \ln \phi_j(\vec{r}_1) \cdot (\vec{\nabla}_R \ln g_j^* - \vec{\nabla}_0 \ln g_j^*) = 0$ is used to solve the Schrödinger equation of the system. The purpose of this work is to take into account this term assuming that $\vec{\nabla}_1 \ln \phi_j(\vec{r}_1)$ is equal to a constant vector \vec{C}_j dependent on the atomic state under consideration. Taking into account the justification and the consequences of this hypothesis, the equation of the system is solved when one puts the term A into this form. The transition amplitudes T_{0n} are calculated by "prior" and "post" approximations and compared, and the cross sections are obtained and discussed for four transitions. These various results show that the introduction of the term A favors the prior approximation because it is expressed by a constant modification of the incident electron energy, which is not the case for the post approximation.

I. INTRODUCTION

The excitation cross section for electron impact on a hydrogen atom from its initial state (0) to an excited state (n) is described (in the atomic unit system), the exchange being neglected, by the relation

$$\sigma_{0n} = \frac{k_n}{4\pi^2 k_0} \int |T_{0n}|^2 d\Omega, \quad (1)$$

where \vec{k}_0 and \vec{k}_n are the wave vectors of the incident and scattered electrons, and $d\Omega$ is an element of

solid angle.

There are two equivalent relationships to express the transition amplitude:

$$T_{0n}^{\text{prior}} = \langle \phi_n(\vec{r}_1) e^{i\vec{k}_n \cdot \vec{r}_2} | \hat{V} | \psi_0^+(\vec{r}_1, \vec{r}_2) \rangle \quad (2)$$

or

$$T_{0n}^{\text{post}} = \langle \psi_n^-(\vec{r}_1, \vec{r}_2) | \hat{V} | \phi_0(\vec{r}_1) e^{i\vec{k}_0 \cdot \vec{r}_2} \rangle. \quad (3)$$

The interaction potential V has the value

$$V = \frac{1}{|\vec{r}_2 - \vec{r}_1|} - \frac{1}{r_2}. \quad (4)$$

The indices 1 and 2 characterize, respectively,

the atomic and scattered electrons, and $\phi_0(\vec{r}_1)$ and $\phi_n(\vec{r}_1)$ represent the initial and final states of the hydrogen atom. The functions $\psi_0^+(\vec{r}_1, \vec{r}_2)$ and $\psi_n^-(\vec{r}_1, \vec{r}_2)$ are two solutions of the equation of stationary states:

$$\left(\frac{1}{2} \nabla_1^2 + \frac{1}{2} \nabla_2^2 + \frac{1}{r_1} + \frac{1}{r_2} - \frac{1}{|\vec{r}_2 - \vec{r}_1|} + E_j \right) \psi_j^*(\vec{r}_1, \vec{r}_2) = 0 \quad (5)$$

with the following asymptotic behavior:

$$\psi_0^*(\vec{r}_1, \vec{r}_2) \xrightarrow[r_2 \rightarrow \infty]{} \phi_0(\vec{r}_1) e^{i\vec{k}_0 \cdot \vec{r}_2} + \sum_j \phi_j(\vec{r}_1) f_{0j}^*(\vec{\Omega}) \times e^{ik_j r_2 / r_2} \quad (6)$$

and

$$\psi_n^-(\vec{r}_1, \vec{r}_2) \xrightarrow[r_2 \rightarrow \infty]{} \phi_n(\vec{r}_1) e^{i\vec{k}_n \cdot \vec{r}_2} + \sum_j \phi_j(\vec{r}_1) f_{nj}^-(\vec{\Omega}) \times e^{-ik_j r_2 / r_2} \quad (7)$$

In the method used by Vainshtein, Presnyakov, and Sobelman (VPS),² the total wave function is represented by

$$\psi_j^*(\vec{r}_1, \vec{r}_2) = \phi_j(\vec{r}_1) g_j^*(\vec{r}_1, \vec{r}_2) \quad (8)$$

If j indicates the initial state, the wave function $\psi_0^*(\vec{r}_1, \vec{r}_2)$ corresponds to the "prior" approximation" whereas if j indicates the final state, the wave function $\psi_n^-(\vec{r}_1, \vec{r}_2)$ corresponds to the "post" approximation.³

By substituting the wave function given by relation (8) into Eq. (5), we deduce the exact equation which must obey $g_j^*(\vec{r}_1, \vec{r}_2)$:

$$\left(\frac{1}{2} \nabla_1^2 + \frac{1}{2} \nabla_2^2 + \frac{1}{r_2} - \frac{1}{|\vec{r}_2 - \vec{r}_1|} + \frac{1}{2} k_j^2 + \vec{\nabla}_1 \ln \phi_j(\vec{r}_1) \cdot \vec{\nabla}_1 \right) \times g_j^*(\vec{r}_1, \vec{r}_2) = 0 \quad (9)$$

Introducing the new variables \vec{R} and $\vec{\rho}$ defined by

$$\vec{R} = \frac{1}{2}(\vec{r}_1 + \vec{r}_2), \quad \vec{\rho} = \frac{1}{2}(\vec{r}_2 - \vec{r}_1), \quad (10)$$

Eq. (9) then becomes

$$\left(\frac{1}{2} \nabla_R^2 + \frac{1}{2} \nabla_\rho^2 + \frac{2}{|\vec{R} + \vec{\rho}|} - \frac{1}{\rho} + k_j^2 + \vec{\nabla}_1 \ln \phi_j(\vec{r}_1) \cdot (\vec{\nabla}_R \ln g_j^* - \vec{\nabla}_\rho \ln g_j^*) \right) g_j^*(\vec{R}, \vec{\rho}) = 0 \quad (11)$$

In their previous work,^{2,3} VPS tried to find a solution to the approximate equation

$$\left(\frac{1}{2} \nabla_R^2 + \frac{1}{2} \nabla_\rho^2 + 1/R - 1/\rho + k_j^2 \right) g_{aj}^*(\vec{R}, \vec{\rho}) = 0, \quad (12)$$

which led to the following two hypotheses: (a) The term

$$A = \vec{\nabla}_1 \ln \phi_j(\vec{r}_1) \cdot (\vec{\nabla}_R \ln g_j^* - \vec{\nabla}_\rho \ln g_j^*) \quad (13)$$

is neglected, and (b) it is supposed that $\vec{R} \approx \vec{\rho}$ and

it follows that

$$|\vec{R} + \vec{\rho}| = 2R. \quad (14)$$

We wish to modify the first hypothesis and deduce its consequences in its modified form.

II. INFLUENCE OF TERM A IN DETERMINING CROSS SECTIONS BY "PRIOR" AND "POST" APPROXIMATIONS

A. Modified "Prior" and "Post" Wave Functions

To neglect the term A means that a solution $g_{aj}^*(\vec{R}, \vec{\rho})$ should be found which no longer depends upon the state of the hydrogen atom this state being different in each approximation. It is therefore evident *a priori* that the relative results of both these approximations cannot converge.

In order to take account of this term and, at the same time, of the atomic states, we let

$$\vec{\nabla}_1 \ln \phi_j(\vec{r}_1) = \vec{C}_j. \quad (15)$$

In this equation we assume that \vec{C}_j is a constant vector different for different atomic states. Thus the solution $g_{aj}^*(\vec{R}, \vec{\rho})$ will depend on the state through this vector.

According to this modification, the exact equation (11) becomes

$$\left[\frac{1}{2} \nabla_R^2 + \frac{1}{2} \nabla_\rho^2 + 1/R - 1/\rho + k_j^2 + \vec{C}_j \cdot (\vec{\nabla}_R \ln g_j^* - \vec{\nabla}_\rho \ln g_j^*) \right] g_j^* = 0. \quad (16)$$

If we put the solution of Eq. (16) in the form

$$g_j^*(\vec{R}, \vec{\rho}) = \Theta_j^*(\vec{R}) \eta_j^*(\vec{\rho}), \quad (17)$$

we get

$$(\nabla_R^2 + 2\vec{C}_j \cdot \vec{\nabla}_R + 2/R + k_j^2) \Theta_j^*(\vec{R}) = 0, \quad (18a)$$

$$(\nabla_\rho^2 - 2\vec{C}_j \cdot \vec{\nabla}_\rho - 2/\rho + k_j^2) \eta_j^*(\vec{\rho}) = 0. \quad (18b)$$

Let us try to find a solution of the form

$$\psi(\vec{r}) = \phi_r(\vec{r}) e^{\sum \lambda_i x_i}, \quad (19)$$

and let us determine the value of the parameter λ_i such that the terms in $\vec{\nabla}$ cancel out in these equations. We get

$$\Theta_j^*(\vec{R}) = \Phi_{Rj}^*(\vec{R}) e^{-\sum \lambda_i C_j x_i} \quad \text{with } \vec{R} = \{X_i\}, \quad (20a)$$

$$\eta_j^*(\vec{\rho}) = \Phi_{\rho j}^*(\vec{\rho}) e^{\sum \lambda_i C_j x_i} \quad \text{with } \vec{\rho} = \{x_i\}. \quad (20b)$$

Assuming $\vec{R} \approx \vec{\rho}$, we get

$$g_j^*(\vec{R}, \vec{\rho}) = \Phi_{Rj}^*(\vec{R}) \Phi_{\rho j}^*(\vec{\rho}). \quad (21)$$

These wave functions must then obey both of the equations

$$(\nabla_R^2 + 2/R + K_j^2) \Phi_{Rj}^*(\vec{R}) = 0, \quad (22a)$$

$$(\nabla_\rho^2 - 2/\rho + K_j^2) \Phi_{\rho j}^*(\vec{\rho}) = 0, \quad (22b)$$

with

$$K_j^2 = k_j^2 - \sum_i C_{ji}^2. \quad (23)$$

We state that introducing in the differential equation the neglected term in the form suggested here, in the "prior" case, is equivalent to replacing, in the differential equations, the real energy of the incident electron by a virtual and smaller energy depending on the initial state considered. The wave function relating to the "prior" approximation can then be expressed as

$$g_0^+(\vec{R}, \vec{\rho}) = N_0 e^{i\vec{K}_0 \cdot (\vec{R} + \vec{\rho})} F(i/K_0, 1, iK_0 R - i\vec{K}_0 \cdot \vec{R}) \\ \times F(-i/K_0, 1, iK_0 \rho - i\vec{K}_0 \cdot \vec{\rho}), \quad (24)$$

where $F(a, b, z)$ is the confluent hypergeometric function, the vector \vec{K}_0 having the direction of the incident wave vector \vec{k}_0 and its modulus being given by Eq. (23).

In the "post" approximation, taking into account the previously neglected term, we see that the energy of the scattered electron is smaller than that given by energy conservation.

The wave function in this approximation is given by

$$g_n^-(\vec{R}, \vec{\rho}) = N_n e^{i\vec{K}_n \cdot (\vec{R} + \vec{\rho})} F(-i/K_n, 1, -iK_n R - i\vec{K}_n \cdot \vec{R}) \\ \times F(i/K_n, 1, -iK_n \rho - i\vec{K}_n \cdot \vec{\rho}), \quad (25)$$

with K_n given by Eq. (23). The normalization coefficients are then

$$N_j = \Gamma(1 - i/K_j) \Gamma(1 + i/K_j). \quad (26)$$

Let us note, before proceeding, that the wave functions given by Eqs. (24) and (25) do not have the asymptotic behavior required since the unperturbed wave is not obtained when $V \rightarrow 0$.

By this theoretical hypothesis, we therefore cannot hope to obtain a real physical representation of the collision phenomenon. However, as we shall see, this study allows us, on the one hand, to know the importance of neglected terms and, on the other hand, to choose between the two approximations, a choice not possible with the formal theory.

In fact, if we consider that the hydrogen atom is initially in its ground state, the calculation of \vec{C}_j gives us for the "prior" approximation

$$\sum_i C_{0i}^2 = 1. \quad (27)$$

The virtual energy is therefore independent with regard to the position of the electron in the atom. This is no longer the case with the "post" approximation since $\sum_i C_{ji}^2$ depends on the position r_1 for the spherically symmetric excited states and also on the orientation for the nonspherical states. These considerations show that the neglected terms in the "prior" approximation can be estimated, and

therefore compensation can be made for them, whereas this is not the case in the "post" approximation.

B. Modified "Prior" and "Post" Transition Amplitudes

The transition amplitude in the "prior" approximation is obtained by replacing the wave function given by Eqs. (8) (with $j=0$) and (24) in expression (2). Then we obtain

$$T_{0n}^{\text{prior}} = \frac{8N_0}{(2\pi)^3} \int g_{0n}(\vec{q} - \vec{s}) d\vec{s} \\ \times \int e^{i\vec{s} \cdot \vec{R}} V F(i/K_0, 1, iK_0 R - i\vec{K}_0 \cdot \vec{R}) \\ \times F(-i/K_0, 1, iK_0 \rho - i\vec{K}_0 \cdot \vec{\rho}) e^{i(\vec{q} - \vec{s}) \cdot \vec{\rho}} d\vec{R} d\vec{\rho}, \quad (28)$$

where

$$\vec{q} = \vec{K}_0 - \vec{K}_n, \quad (29)$$

$$g_n(\vec{\alpha}) = \int \phi_0(\vec{r}_1) \phi_n^*(\vec{r}_1) e^{i\vec{\alpha} \cdot \vec{r}_1} d\tau_1. \quad (30)$$

Since in the Born approximation the transition amplitude relative to the attractive term $1/r_2$ is zero, it can be considered² (the VPS method being a modification of the Born approximation) that this term is negligible compared to the contribution of the term $1/|\vec{r}_2 - \vec{r}_1|$, and this hypothesis is justified by Omidvar.⁴ Moreover, the integral over \vec{R} approaches infinity when $|\vec{s}| \rightarrow 0$ and, as in Ref. 2, we suppose that the main contribution to T_{0n} comes from the region $s=0$ since, in this region, $g_{0n}(\vec{q} - \vec{s})$ is a slowly varying function. From this it follows that $g_{0n}(\vec{q} - \vec{s}) \sim g_n(\vec{q})$ (called the "peaking approximation"), and thus Eq. (28), after integration over s , is reduced to

$$T_{0n}^{\text{prior}} = 4N_0 g_n(\vec{q}) \int (e^{2i\vec{q} \cdot \vec{r}}/r) F(i/K_0, 1, iK_0 r - i\vec{K}_0 \cdot \vec{r}) \\ \times F(-i/K_0, 1, iK_0 \rho - i\vec{K}_0 \cdot \vec{r}) d\vec{r}. \quad (31)$$

Using Nordsieck's method⁵ to calculate this integral, we get

$$T_{0n}^{\text{prior}} = 4N_0 g_n(\vec{q}) (\pi/q^2) F(-i/K_0, i/K_0, 1, z), \quad (32)$$

with

$$z = \left(\frac{K_0^2 - k_n^2 + q^2}{K_0^2 - k_n^2 - q^2} \right)^2. \quad (33)$$

This last relation is always such that

$$|z| < 1, \quad (34)$$

whatever may be the excited state under consideration.

In the same way, the "post" transition amplitude is expressed by

$$T_{0n}^{\text{post}} = 4N_n^* g_n(\vec{q}) (\pi/q^2) F(-i/K_n, i/K_n, 1, z), \quad (35)$$

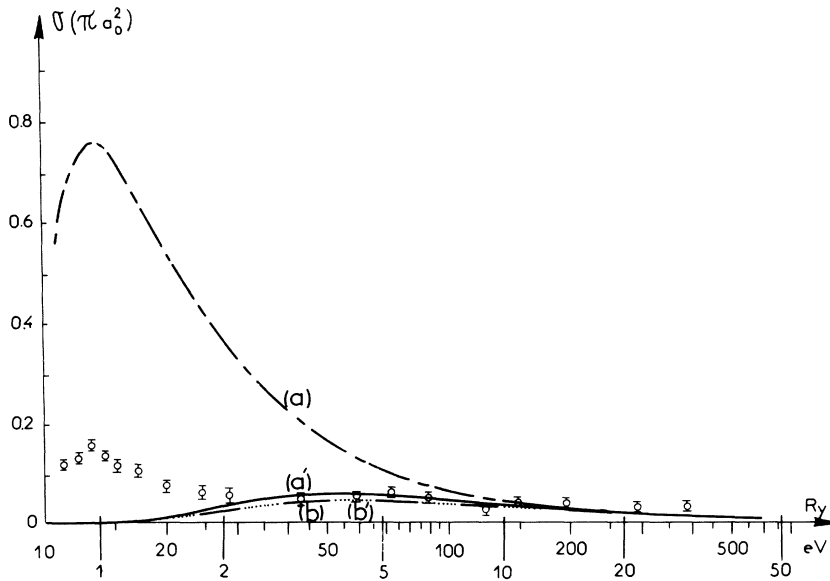


FIG. 1. Cross-section calculations for the $1s \rightarrow 2s$ excitation of atomic hydrogen by electron impact. Curves (a) (---) and (b) (---): VPS "prior" and "post" approximations without term A . Curves (a') (—) and (b') (·····): "prior" and "post" approximations including term A . Φ : experimental results (Ref. 6).

with

$$z = \left(\frac{k_0^2 - K_n^2 - q^2}{q^2 + k_0^2 - K_n^2} \right)^2, \quad (36)$$

$$\vec{q} = \vec{k}_0 - \vec{K}_n. \quad (37)$$

Here \vec{K}_n is the wave vector having the same direction as \vec{k}_n but with its modulus given by Eq. (23); the $\sum_i C_{ni}^2$, which here are dependent upon the position of the atomic electron, are calculated using for the distances r_1 the maximum probability position of the atomic electron under consideration in the excited state ns or np . Moreover, in the case of the np excitation, the azimuthal angle Θ is taken to be zero.

C. Excitation Cross Sections: Numerical Results and Discussion

The "prior" and "post" cross sections are obtained by replacing the transition amplitudes given by Eqs. (32) and (35) in relation (1). The numerical calculations are plotted in Figs. 1–4 which, respectively, represent the excitation cross sections relative to transitions $1s \rightarrow 2s$, $1s \rightarrow 3s$, $1s \rightarrow 4s$, and $1s \rightarrow 2p$. The curves corresponding to the "prior" approximation without term A are indicated by (a) and those corresponding to the "prior" approximation with term A are identified by (a'); the same notation applies to the curves (b) and (b') which are related to the "post" approximation without and

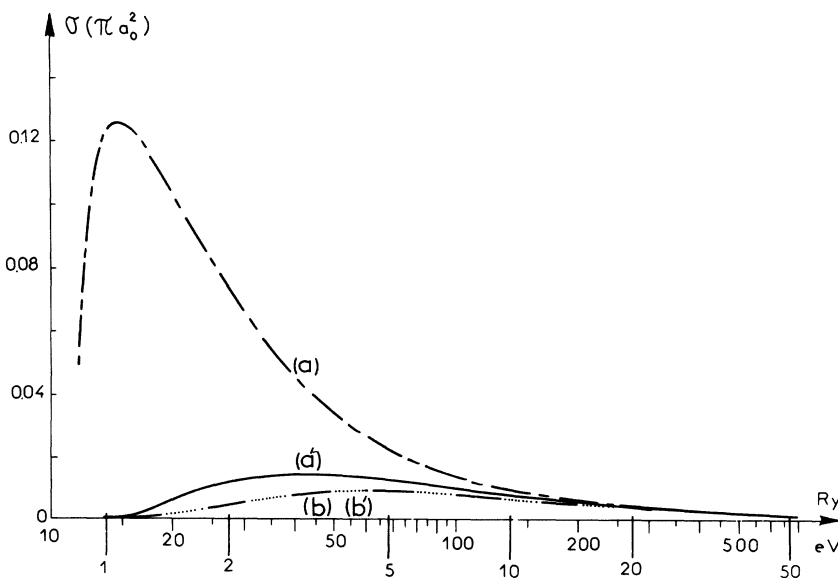


FIG. 2. Cross-section calculations for $1s \rightarrow 3s$ excitation of atomic hydrogen by electron impact (curves are labeled as in Fig. 1).

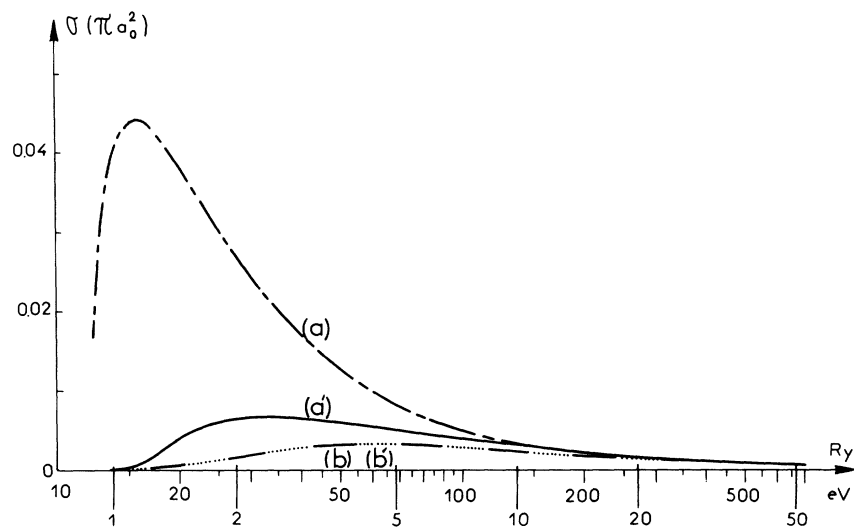


FIG. 3. Cross-section calculations for $1s \rightarrow 4s$ excitation of atomic hydrogen by electron impact (curves are labeled as in Fig. 1).

with term A . The curves (b') almost coincide with the curves (b) as we have $K_n \approx k_n$ for the chosen values of r_1 and Θ .

In the studies previously obtained with "prior" and "post" approximations, either by neglecting the term^{2,3} A or by taking into account the neglected terms by introducing an effective charge^{3,8}, the divergence, in the case of small energies, between the results of each approximation remains appreciable even though, in our modification, we note a good convergence for the transitions under consideration—especially in the excited states of spherical symmetry. For the $2p$ excited state, the convergence is not as good, but this result can be explained by studying the term $\sum_i C_{ni}^2$. Indeed for the

ns excited states the variations of this term depend only very slightly upon the variations of r_1 for an electron position with a finite probability, making the present hypothesis, which takes A into account, valid. On the contrary, for the $2p$ state we get

$$\sum_i C_{ni}^2 = \frac{1}{4} + \frac{1}{r_1^2 \cos^2 \Theta_1} - \frac{1}{r_1},$$

a relation which greatly depends upon the possible variations of Θ .

III. CONCLUSION

From this study, one can conclude the following

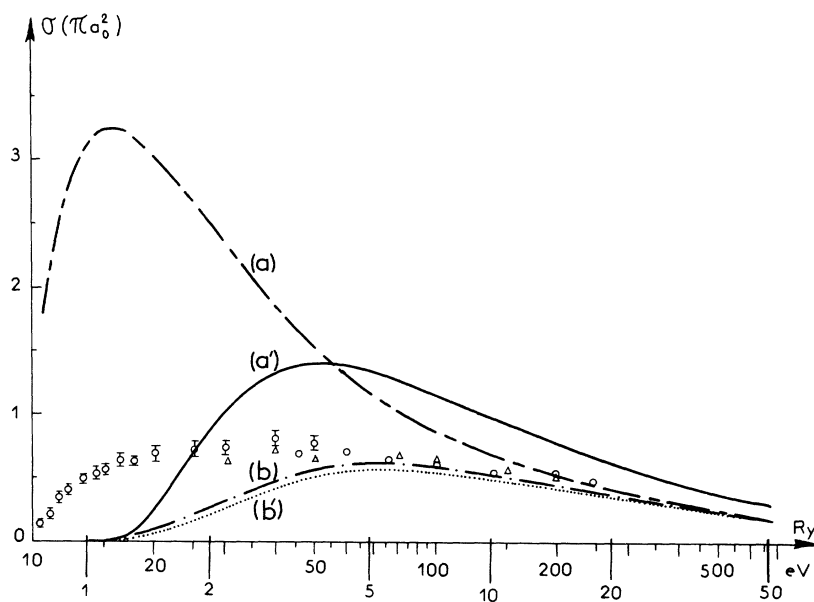


FIG. 4. Cross-section calculations for $1s \rightarrow 2p$ excitation of atomic hydrogen by electron impact (curves are labeled as in Fig. 1). Experimental results are from Ref. 7.

important points.

(i) The numerical results show that the important divergence at small energies of the cross sections calculated by "prior" and "post" is due to the neglected term A which does not play the same role in the two cases.

(ii) Furthermore, this study enables us to deduce that in the "post" approximation for excited states ns , the neglected term is small, but for other non-spherical excited states, it is impossible to know its importance. On the other hand, in the "prior" approximation the term A plays an appreciable role at small energies and, in order to take it into account, one can modify the energy of the incident electron by a constant value. If compensation can be made for this modification, the "prior" approximation then offers a decided advantage since this correction must remain the same whatever the final state. However in the "post" approximation it would seem difficult to introduce a correction which takes into account the neglected terms.

(iii) An examination of Eqs. (22a) and (22b) shows us that to neglect the term A is equivalent to over-

estimating the attractive potential and therefore underestimating the repulsive potential. Thus, as we show elsewhere, a compensation of the neglected term can be obtained by modifying these potentials.

(iv) Finally, the sign change $+i$ to $-i$ arbitrarily introduced by VPS,² a device by which the modulus of z passes from a greater value than 1 to a lesser value, was apparently intended not for the purpose of compensating the overestimation of the "peaking" approximation, as recognized by these authors, but to take into account the neglected term A ; in this case the effective charge would no longer play the role attributed to it by these authors, and in particular its physical meaning would not be significant.

In conclusion, the wave functions (24) and (25) chosen to represent the state of the system do not have satisfactory asymptotic behavior and therefore do not represent the physical problem considered here. As a result one cannot expect a convergence between these results and experimental values at small energies.

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