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ON A CERTAIN MODEL FOR CALCULATION OF THE EFFECTIVE CROSS SECTIONS FOR EXCITATION OF ATOMS

L. VAĬNSHTEĬN, L. PRESNYAKOV, and I. SOBEL'MAN

P. N. Lebedev Physics Institute, Academy of Sciences, U.S.S.R.

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A new method for calculation of the effective cross sections for excitation of atoms by electrons is proposed, based on a model in which the atom + electron system can be described by a comparatively simple wave function with unseparated variables. The method yields for the 1s—2p and 1s—2s transitions in the hydrogen atom results that are in good agreement with the experiments.

1. INTRODUCTION

As is well known, the simplest method of calculating the effective cross section for the excitation and ionization of atoms by electrons—the Born method—gives good results at high electron velocities. But the Born method is strictly speaking not valid in the very region where the cross sections usually reach their maxima. Nonetheless, it is extensively used, since it gives qualitatively sensible results, although the maximum of the cross section is as a rule exaggerated by a factor of 2 or 3 and is shifted towards the lower energies. It must be emphasized that this statement is based on the experimental data which concern only a few transitions from the ground state. There are no reliable experimental data at present for transitions between strongly excited states. Relatively simple corrections to the Born approximation, such as distortion of the incident and scattered waves, account of exchange, etc., cannot improve the results appreciably. Moreover, in some cases (for example in the approximation of distorted waves without exchange) the results become worse.

It is possible to get better results in principle by taking into account the effect of the polarization of the electron shell of the atom. Here, however, difficulties arise in connection with the need of taking into account a large number of intermediate states. Calculations [1,2] show that an account of one or two intermediate states is patently insufficient.

A general shortcoming of all the methods based on expansion of the wave function of a system in terms of the unperturbed atomic functions (second Born approximation, method of distorted waves, etc.) is that what comes to the forefront is actually an account of the attraction of the electron by the screened nucleus, and no account is taken (in the wave functions) of the repulsion of the atomic electron by the incident electron. Yet, it is just this effect which is of primary significance for inelastic collisions. It therefore becomes necessary to search for such methods of solving the problem, in which the repulsion of the electrons is taken into account even in the first approximation, that is, in the wave functions.

In the present paper we investigate the possibility of one model, which makes possible description of the atom-plus-electron system by means of relatively simple wave functions with non-separated variables. The method proposed has some common features with the impulse approximation [3], as will be indicated in detail below.

2. CALCULATION OF THE EXCITATION CROSS SECTIONS WITHOUT ACCOUNT OF EXCHANGE

Let us consider the simplest case of excitation of the hydrogen atom. The exact expression for the effective cross section of the transition between two arbitrary states, denoted below by the indices 0 and 1, can be written in the form 1)

$$\sigma_{01} = \frac{k_1}{4\pi^2 k_0} \int \left| \langle \varphi_1^* (\mathbf{r}_1)\, e^{-i\mathbf{k}_1\mathbf{r}_2} | V | \Psi_0 (\mathbf{r}_1, \mathbf{r}_2) \rangle \right|^2 dO, \qquad (1)$$

$$V = \frac{1}{|\mathbf{r}_2 - \mathbf{r}_1|} - \frac{1}{r_2}, \qquad (2)$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the coordinates of the atomic and incident electrons, $\mathbf{k}_0$ and $\mathbf{k}_1$ are the wave vectors of the incident and scattered electrons, and $\Psi_0(\mathbf{r}_1, \mathbf{r}_2)$ is the solution of the Schrödinger equation

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1) We use everywhere atomic units with the Rydberg unit for the energy, $\mathrm{Ry} = me^4/2\hbar^2$.

$$\left\{\frac{1}{2}\Delta_1 + \frac{1}{2}\Delta_2 + \frac{1}{r_1} + \frac{1}{r_2} - \frac{1}{|\mathbf{r}_2 - \mathbf{r}_1|} + E\right\}\Psi_0(\mathbf{r}_1, \mathbf{r}_2) = 0, \tag{3}$$

satisfying the boundary condition

$$\Psi_0(\mathbf{r}_1, \mathbf{r}_2) \underset{r_2\to\infty}{\sim} \varphi_0(\mathbf{r}_1)\, e^{i\mathbf{k}_0\mathbf{r}_2} + \sum_n f_n(\theta, \Phi)\,\varphi_n(\mathbf{r}_1)\frac{e^{ik_nr_2}}{r_2}, \tag{4}$$

with φ_n the unperturbed atomic functions.

We write the function Ψ_0 in the form

$$\Psi_0(\mathbf{r}_1, \mathbf{r}_2) = \varphi_0(\mathbf{r}_1)\, g(\mathbf{r}_1, \mathbf{r}_2). \tag{5}$$

In the Born approximation $g(\mathbf{r}_1, \mathbf{r}_2) = \exp(i\mathbf{k}_0 \cdot \mathbf{r}_2)$. In the general case the function g satisfies an equation which can be conveniently written, for the sake of what follows, in the form

$$\begin{aligned}\{\Delta_1 + \Delta_2 + 2/|\mathbf{r}_2 + \mathbf{r}_1| - 2/|\mathbf{r}_2 - \mathbf{r}_1| + k_0^2\}g \\ = \{2/|\mathbf{r}_2 + \mathbf{r}_1| - 2/r_2 - 2(\nabla_1 \ln\varphi_0)\nabla_1\}g.\end{aligned} \tag{6}$$

We change over to new variables $\boldsymbol{\rho} = (\mathbf{r}_2 - \mathbf{r}_1)/2$ and $\mathbf{R} = (\mathbf{r}_2 + \mathbf{r}_1)/2$, which describe respectively the relative motion of the atomic and incident electrons and the motion of their center of inertia

$$\begin{aligned}&\{{}^1/_2\Delta_R + {}^1/_2\Delta_\rho + 1/R - 1/\rho + k_0^2\}\, g(\mathbf{R}, \boldsymbol{\rho}) = Qg(\mathbf{R}, \boldsymbol{\rho});\\ &Q = \{1/R - 2/|\mathbf{R} + \boldsymbol{\rho}| - (\nabla_1 \ln\varphi_0)(\nabla_R \ln g - \nabla_\rho \ln g)\}.\end{aligned} \tag{7}$$

Equation (7) is exact. We now introduce the principal assumption of our method, taking for the function g the solution of (7) without the right half. The function g will then describe the scattering of free electrons by each other and the motion of their center of inertia in the field of the nucleus. This, properly speaking, is the model which we are using. Some refinement of the model (introduction of an effective charge and allowance for exchange) will be considered in later sections.

The variables $\mathbf{R}$ and ρ can be separated in (7) without the right half, and a solution satisfying the necessary boundary conditions is of the form[4]

$$\begin{aligned}g(\mathbf{R}, \boldsymbol{\rho}) = Ne^{i\mathbf{k}_0(\mathbf{R}+\boldsymbol{\rho})} F(i\nu, 1, ik_0R - i\mathbf{k}_0\mathbf{R})\\ \times F(-i\nu, 1, ik_0\rho - i\mathbf{k}_0\boldsymbol{\rho}),\end{aligned} \tag{8}$$

where F stands for the confluent hypergeometric function,

$$\nu = k_0^{-1}, \qquad N = \Gamma(1 - i\nu)\,\Gamma(1 + i\nu).$$

We proceed to calculate the matrix element in (1) with the aid of (5) and (8). In the Born approximation a nonvanishing contribution is made only by the first term in (2). We confine ourselves in this case also to only this term. Representing $\varphi_1^*(\mathbf{r}_1)\,\varphi_0(\mathbf{r}_1)$ in the form of a Fourier integral

$$\varphi_1^*(\mathbf{r}_1)\,\varphi_0(\mathbf{r}_1) = \int\tilde{\varphi}(\boldsymbol{\varkappa})\, e^{-i\boldsymbol{\varkappa}\mathbf{r}_1} d\boldsymbol{\varkappa},$$

we obtain for the matrix element in (1)

$$\begin{aligned}J = 4N\int ds\,\tilde{\varphi}(\mathbf{q} - \mathbf{s})\int d\mathbf{R}\, e^{i\mathbf{s}\mathbf{R}} F(i\nu, 1, ik_0R - i\mathbf{k}_0\mathbf{R})\\ \times\int d\boldsymbol{\rho}\,\frac{e^{i(2\mathbf{q}-\mathbf{s})\boldsymbol{\rho}}}{\boldsymbol{\rho}} F(-i\nu, 1, ik_0\rho - i\mathbf{k}_0\boldsymbol{\rho}),\end{aligned} \tag{9}$$

where $\mathbf{q} = \mathbf{k}_0 - \mathbf{k}_1$.

Inasmuch as the integral with respect to $\mathbf{R}$ increases without limit as $\mathbf{s} \to 0$, we replace the slowly varying function $\tilde{\varphi}(\mathbf{q} - \mathbf{s})$ by $\tilde{\varphi}(\mathbf{q})$. In this case, generally speaking, we make an incorrect estimate of the contribution made to (9) by the region $\mathbf{s} \sim \mathbf{q}$, since $\tilde{\varphi}(0) = 0$. We can show, however, that the resultant error is cancelled to some degree by replacement of $\exp[i(2\mathbf{q} - \mathbf{s}) \cdot \rho]$ by $\exp[i(-2\mathbf{q} - \mathbf{s}) \cdot \rho]$. After this replacement, using the known convolution theorem of Fourier transform theory, we obtain

$$\begin{aligned}J = 4N\tilde{\varphi}(\mathbf{q})\int d\mathbf{r}\,\frac{e^{-i2\mathbf{q}\mathbf{r}}}{r} F(i\nu, 1, ik_0r - i\mathbf{k}_0\mathbf{r})\\ \times\Big| F(-i\nu, 1, ik_0r - i\mathbf{k}_0\mathbf{r}).\end{aligned}$$

This integral can be calculated exactly by the method proposed in Nordsieck's paper[5]. We present the final result

$$J = \frac{4N\pi}{q^2}\tilde{\varphi}(\mathbf{q})\, F(-i\nu, i\nu, 1, x);$$

$$\sigma_{01} = \frac{8\pi}{k_0^2}\int\limits_{k_0-k_1}^{k_0+k_1}\frac{dq}{q^3}\,|\langle 1\,|\,e^{i\mathbf{q}\mathbf{r}}\,|\,0\rangle|^2\,[f(\nu, x)]^2; \tag{10}$$

$$f(\nu, x) = \pi\nu\,[\operatorname{sh}\pi\nu]^{-1} F(-i\nu, i\nu, 1, x);$$

$$x = \left[\frac{\mathbf{q}\mathbf{k}_0}{q^2 + \mathbf{q}\mathbf{k}_0}\right]^2 = \left[\frac{\Delta\varepsilon + q^2}{\Delta\varepsilon + 3q^2}\right]^2, \tag{11}^*$$

where F is the hypergeometric function and $\Delta\epsilon = k_0^2 - k_1^2$ is the excitation energy.

Expression (10) differs from Born's formula in the presence of the additional factor $[f(\nu, s)]^2$ under the integral sign. When $k_0 \gg 1$, the function $f(\nu, x) \approx 1$ and (10) coincides with the Born approximation. When $k_0 \lesssim 1$, the function $f(\nu, x)$ can differ appreciably from unity. It is important that for all values of the parameters we have $f(\nu, x) \le 1$, so that the cross sections are always smaller than the Born cross sections. For fixed k_0 and $q \to 0$ we have $f(\nu, x) \to 1$.

The appearance of the factor $[f(\nu, x)]^2$ in (10) is connected with the fact that we used in the calculations not the plane wave $\exp(i\mathbf{k}_0 \cdot \mathbf{r}_2)$, but the function g, which has an explicit dependence on the interelectron distance $\mathbf{r}_2 - \mathbf{r}_1 = 2\rho$. Therefore expression (10) takes into account, to some degree of

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*sh = sinh.

approximation, both the distortion of the incident wave and the polarization of the electron shell of the atom.

Inasmuch as $f(\nu, x) \leq 1$, the repulsion of the electrons prevails over the attraction of the incident electron by the nucleus within the framework of the given model. In the usual method of distorted waves, the situation is reversed, and the cross sections exceed the Born cross sections, in direct contradiction with experiment. If account is taken of polarization effects by perturbation theory methods or by solving the system of equations and accounting for the strong coupling, it is always necessary to confine oneself to a consideration of a small number of perturbing levels and as a rule these correspond to open scattering channels. An account of the closed channels increases the computational difficulties enormously. Within the framework of the present method, on the other hand, the contribution made to the polarization of an infinite number of perturbing levels is taken into account in a certain approximation. This is seen from the fact that the function $\Psi_0(\mathbf{r}_1, \mathbf{r}_2)$, defined by (5) and (8), is generally speaking not orthogonal to any of the unperturbed atomic functions.

3. INTRODUCTION OF THE EFFECTIVE CHARGE

We now consider one of the possible ways of refining g. We take it upon ourselves to reduce as much as possible the magnitude of the discarded right half of the equation, and to introduce a dependence on the characteristics of the atomic state into the function g. This can be done by introducing into the equation a suitably selected effective charge ζ.

We rewrite (7) in the form

$$\begin{aligned}\{{}^1\!/_2\, \Delta_R + {}^1\!/_2\, \Delta_\rho + \zeta/R - \zeta/\rho + k_0^2\}\, g \\ = \{\zeta/\mathrm{R} - 2/|\mathbf{R} + \boldsymbol{\rho}| + (1 - \zeta)/\rho \\ - (\nabla_1 \ln \varphi_0)(\nabla_R \ln \chi - \nabla_\rho \ln \chi)\}\, g; \\ \chi = e^{-i\mathbf{k}_0(\mathbf{R}+\boldsymbol{\rho})} g. \end{aligned} \tag{12}$$

The solution of this equation without the right half is given by (8) with $\nu = \zeta/k_0$. Substituting the so defined function g in the right half of (12), we can show that for large R and ρ we have

$$\begin{aligned}|(\nabla_1 \ln \varphi_0)\, \nabla_R \ln \chi| \sim \sqrt{\varepsilon_0}\,\zeta/k_0 R + O(R^{-2}), \\ |(\nabla_1 \ln \varphi_0)\, \nabla_\rho \ln \chi| \sim \sqrt{\varepsilon_0}\, \zeta/k_0 \rho + O(\rho^{-2}),\end{aligned} \tag{13}$$

where ϵ_0 is the ionization energy of the state 0.

The first terms of the expansion in (13), with ζ = const and $k_0 \to 0$, increase without limit. We choose ζ in such a way as to eliminate this divergence and simultaneously ensure the same order of magnitude of all the discarded terms of the equation; to this end we stipulate

$$(1 - \zeta)/\rho = \sqrt{\varepsilon_0}\,\zeta/k_0\rho.$$

Hence

$$\zeta = k_0/(k_0 + \sqrt{\varepsilon_0}), \qquad \nu = (k_0 + \sqrt{\varepsilon_0})^{-1}. \tag{14}$$

With such a definition of ζ, the order of magnitude of ν^{-1} is that of the relative velocity of the electrons for arbitrary values of k_0, corresponding to the physical meaning of this quantity.

4. ACCOUNT OF EXCHANGE

We now take the exchange effect into consideration. The function $g(\mathbf{R}, \boldsymbol{\rho})$ in the approximation (8) is symmetrical with respect to the coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$, so that a rearrangement of the coordinates of the electrons in (5) leads to a replacement of $\varphi_0(\mathbf{r}_1)$ and $\boldsymbol{\rho}$ by $\varphi_0(\mathbf{r}_2)$ and $\boldsymbol{\rho}' = -\boldsymbol{\rho}$. As a result, the exchange integral takes the form

$$\begin{aligned} J^{\mathrm{exch}} = 4\iint d\mathbf{R}\, d\boldsymbol{\rho}'\, \varphi_1^*(\mathbf{r}_1)\, e^{-i\mathbf{k}_1\mathbf{r}_2} \frac{1}{\rho'} \varphi_0(\mathbf{r}_2)\, g(\mathbf{R}, \boldsymbol{\rho}') \\ = 4N \iint d\mathbf{s}_1\, d\mathbf{s}\, \tilde{\varphi}_1^*(\mathbf{s}_1)\, \tilde{\varphi}_0(\mathbf{s} - \mathbf{q} - \mathbf{s}_1) \\ \times \int d\mathbf{R}\, e^{i\mathbf{s}\mathbf{R}} F(i\nu, 1, ik_0 R - i\mathbf{k}_0\mathbf{R}) \\ \times \int d\boldsymbol{\rho}' \frac{e^{i(2\mathbf{k}_0 - \mathbf{s} - 2\mathbf{s}_1)\boldsymbol{\rho}'}}{\rho'} F(-i\nu, 1, ik_0\rho' - i\mathbf{k}_0\boldsymbol{\rho}'), \end{aligned} \tag{15}$$

where $\tilde{\varphi}_1^*$ and $\tilde{\varphi}_0$ are the Fourier transforms of the corresponding atomic functions.

In the approximation in which we calculated the integral (9), we can leave out $\mathbf{s}$ from the argument of the function $\tilde{\varphi}_0$. In addition, we leave out the term $i2\mathbf{s}_1$ from the argument of the exponential in the integral with respect to ρ'. At large values of k_0, the validity of such a simplification is obvious. In the region of small k_0, the role of this term increases, generally speaking, but the order of magnitude of the integral (15) is determined in this case by a small normalization factor N.

Using again the convolution theorem and the method of Nordsieck[5], we obtain

$$\begin{aligned} J^{\mathrm{exch}} = 4N\tilde{\varphi}(\mathbf{q}) \int d\mathbf{r} \frac{e^{-i2\mathbf{k}_0\mathbf{r}}}{r} F(i\nu, 1, ik_0 r - i\mathbf{k}_0\mathbf{r}) \\ \times F(-i\nu, 1, ik_0 r - i\mathbf{k}_0\mathbf{r}) \\ = \frac{4N\pi}{k_0^2} \tilde{\varphi}(\mathbf{q})\, F\left(-i\nu, i\nu, 1, \frac{1}{4}\right). \end{aligned} \tag{16}$$

Recently Ochkur[6] proposed a method which makes it possible, without going outside the framework of the plane-wave approximation, to eliminate certain shortcomings of the Born-Oppenheimer method. In an analogous approximation ($g = \exp[i\mathbf{k}_0 \cdot \mathbf{r}_1]$), the method used above to calculate the integral (15) leads, although in a way different than that of Ochkur, to the same results. This circumstance seems to us of extreme importance. We note, however, that the difference between the exact value of the integral (15) and the approximate expression (16) is much smaller than the difference between the Born-Oppenheimer and the Ochkur formulas.

Taking exchange into account, the formula for the effective cross section assumes the form

$$\sigma_{01} = \sigma_{01}^{+} + \sigma_{01}^{-}, \tag{17}$$

$$\sigma_{01}^{\pm} = c^{\pm} \frac{8\pi}{k_0^2} \int\limits_{k_0-k_1}^{k_0+k_1} \frac{dq}{q^3} \left| \langle 1 | e^{i\mathbf{qr}} | 0 \rangle \right|^2 \left\{ f(\nu, x) \pm \left(\frac{q}{k_0} \right)^2 f\left(\nu, \frac{1}{4} \right) \right\}^2, \tag{18}$$

$$x = \left[\frac{\Delta\varepsilon + q^2}{\Delta\varepsilon + 3q^2} \right]^2. \tag{19}$$

The function $f(\nu, x)$ is determined by (11). In the case of the hydrogen atom $c^{+} = 1/4$ and $c^{-} = 3/4$.

5. DISCUSSION OF THE RESULTS

With the aid of the formulas obtained we have made numerical calculations of the cross sections of the transitions 1s—2p, 1s—2s, and 4s—5p. The calculations were made with an electronic computer. We note that the function $f(\nu, x)$ is real and can be calculated with the aid of the ordinary series for the hypergeometrical functions (see [7]). Consequently, the presence of a correction multiplier in the integrand of (18) does not lead to any appreciable complications of the numerical calculations.

In Fig. 1 are compared the results of the calculations for $\nu = (k_0 + \sqrt{\epsilon_0})^{-1}$ with and without account of the exchange and for $\nu = k_0^{-1}$ without account of exchange. In Fig. 2 the results of the calculations with the aid of (18) ($\nu = (k_0 + \sqrt{\epsilon_0})^{-1}$) of the cross sections of the transitions 1s—2p and 1s—2s are compared with the experimental data [8,9] and with the results of calculations by other methods [1]. As can be seen, the proposed model gives in these cases very good agreement with experiment. As regards the transitions between the excited states, it is seen from the 4s—5p transition as an example (Fig. 1c) that this method leads to a considerably stronger decrease in the cross section compared with the Born method. In addition, the similarity between the sections in threshold energy units, which is typical for the Born method, is violated. Unfortunately, for transitions of this type there are no experimental data. It is therefore

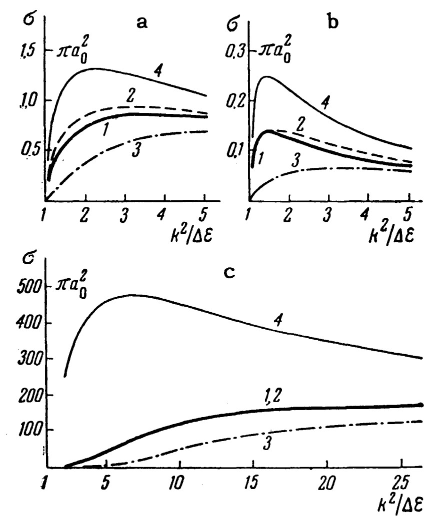

FIG. 1. Effective cross sections of the transitions 1s–2p (a), 1s–2s (b), and 4s–5p (c) in the hydrogen atom, calculated in the following approximations (see the curve): 1 – formulas (18) and (14); 2 – formulas (10) and (14); 3 – formula (10); 4 – Born approximation with $\nu = k_0^{-1}$.

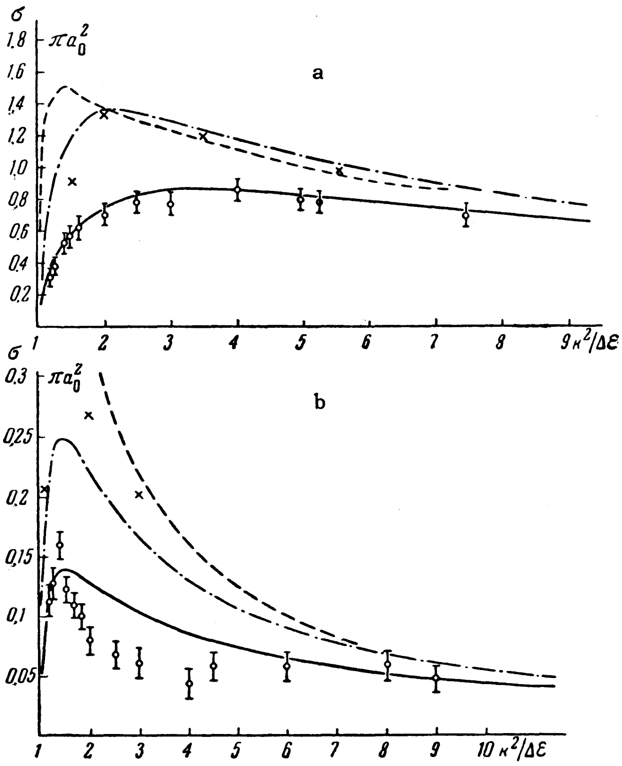

FIG. 2. Comparison of the calculations of the effective cross sections of the transitions 1s–2p (a) and 1s–2s (b) with the experimental data: dash-dot curve – Born approximation, dashed curve – method of distorted waves, solid curve – formulas (18) and (14) of the present paper; the symbol × – method of strong coupling of three levels 1s–2s–2p.[1]

not clear to what degree this result corresponds to the true state of the matter.

As can be seen from Fig. 1, an account of exchange hardly influences the results. The introduction of the effective charge (14), as expected, exerts a stronger influence, particularly near the excitation threshold.

As noted earlier, the proposed method has some similarity to the impulse approximation. This approximation is, however, mathematically more complicated, owing to the presence of additional integration in the momentum space. Finally, Akerib and Borowitz [3] describe the motion of the electron c.m.s. by means of a plane wave, which leads to an incorrect asymptotic wave function (the appearance of a Coulomb phase shift in the incident wave). In principle, this shortcoming can be eliminated by replacing the plane wave with a Coulomb function, similar to that contained in (8). However, even without this complication the matrix element of the transition cannot be calculated exactly.

The calculation of this matrix element is carried out in [3] in an approximation which is hard to justify. As a result of these approximations, the final formula in [3] reduces to a formula which can be obtained exactly in the simplified variant of our model, corresponding to a description of the motion of the c.m.s. of the electron by a plane wave. It must be noted that there is an appreciable discrepancy between the final formulas of Akerib and Borowitz [3] and the presented plots, making it essentially difficult to discuss the results of that work 2) .

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2) The final formulas in [3] contain several misprints, the elimination of which leads to no agreement between the results of the plots and the formulas.

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