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TWO-PHOTON TRANSITIONS IN HYDROGEN-LIKE ATOMS

MLADEN MARTINIS and MARKO STOJIĆ

R. Bošković Institute, P. O. Box 1016, HR-10001 Zagreb, Croatia

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Different methods for evaluating two-photon transition amplitudes in hydrogen-like atoms are compared with the improved method of direct summation. Three separate contributions to the two-photon transition probabilities in hydrogen-like atoms are calculated. The first one coming from the summation over discrete intermediate states is performed up to $n_c(max) = 35$. The second contribution from the integration over the continuum states is performed numerically. The third contribution coming from the summation from $n_c(max)$ to infinity is calculated in an approximate way using the mean level energy for this region. It is found that the choice of $n_c(max)$ controls the numerical error in the calculations and can be used to increase the accuracy of the results much more efficiently than in other methods.

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1. *Introduction*

The very idea of studying two-photon transitions between discrete stationary states of an atom goes back to the work of Marie Göppert-Mayer [1], who considered the scattering of photons by the bound-state electrons in the atom. A method for calculating these transition probabilities requires the use of the second-order perturbation theory

$$W^{(2)}_{mm'} = (\frac{2\pi}{\hbar}) \mid {\sum_n}' \frac{< m'|H'|n >< n|H'|m >}{E^{(0)}_m - E^{(0)}_n} \mid^2 \delta({E'_m}^{(0)} - E^{(0)}_m) \,, \tag{1}$$

where $H = H_0 + H'$ contains a zero-order part H_0 and the perturbation H', and $|n >$ is a complete set of eigenstates of H_0

$$H_0|m >= E^{(0)}_m|m > \ . \tag{2}$$

A characteristic of the second-order perturbation theory is the summation of matrix elements over all intermediate states with discrete eigenvalues and the integration over intermediate states in the continuum. This problem is so complicated that one can seldom evaluate it without making some gross approximation. There exist several different methods which avoid the difficult problem of explicit summation, in particular when a large number of intermediate states becomes important and has to be taken into account.

In this paper, we compare the results of three different methods for calculating the transition probabilities in hydrogen-like atoms by improving the method of direct summation (MDS) [2,3]. The following methods are compared: the method of implicit summation [4–6], the method of Green functions [7–13] and the method of Kelsey and Macek [14]. The paper is organized as follows. Sections 2, 3 and 4 contain short descriptions of the above-mentioned methods. Section 5 gives our improvements of the method of direct summation, together with the results of comparison with other methods. The conclusion summarizes our investigation.

2. *Method of implicit summation*

In the non-relativistic approximation, the actual evaluation of a two-photon transition amplitude involves the matrix elements of the dipole operator between complete sets of states of the target atom. Such sets usually contain both a denumerable set of discrete states and a non-denumerable set of continuum states. It is the integration over the continuum that poses the main difficulty in numerical calculations. One of the powerful methods of by-passing this problem is to use an indirect numerical approach of inhomogeneous differential equations [5,15,16].

The idea is to write down the complete Schröedinger equation, order by order, in the perturbation H'

$$H_0\Psi_m^{(0)} = E_m^{(0)}\Psi_m^{(0)}, \tag{3}$$

$$(H' - E_m^{(1)})\Psi_m^{(0)} = (E_m^{(0)} - H_0)\Psi_m^{(1)}, \tag{4}$$

$$E_m^{(1)} = \int \Psi_m^{(0)*} H' \Psi_m^{(1)}\,\mathrm{d}\tau. \tag{5}$$

$$E_m^{(2)} = \int \Psi_m^{(0)*}(H' - E_m^{(1)})\Psi_m^{(1)}\,\mathrm{d}\tau. \tag{6}$$

The form of $E_m^{(2)}$ as given by (6) is equivalent to the more usual form

$$E_m^{(2)} = \sum_n{}' \frac{< n|H'|n >< n|H'|n >}{E_m^{(0)} - E_n^{(0)}}. \tag{7}$$

Finding $E_m^{(2)}$ is thus reduced to solving the differential equation (4) for $\Psi_m^{(1)}$ [4–6]. One of the ways of solving [4] in the case of non-relativistic hydrogen atom is to use the Laplace transformed wave function

$$S(p,\nu_i) = \int_0^\infty U(r,\nu_i) e^{-pr}\,\mathrm{d}r, \tag{8}$$

where in the dipole approximation

$$U(r,\nu_i) = \sum_{n_c,l_c} r|n_c l_c> \frac{<n_c l_c|r|n_f l_f>}{E_n - E_{n_f} + E_{\nu_i}}. \tag{9}$$

In fact, we seek a closed form expression for

$$P_f g(\nu_i) = \sum_{n_c,l_c} \frac{<n_g l_g|r|n_c l_c><n_c l_c|r|n_f l_f>}{E_{n_c} - E_{n_f} + E_{\nu_i}} \tag{10}$$

which we first transform into the form

$$P_f g(\nu_i) = <n_g l_g|rF|n_f l_f> \tag{11}$$

by introducing the F operator defined by

$$F = \sum_{n_c,l_c} \frac{|n_c l_c><n_c l_c|r}{E_{n_c} - E_{n_f} + E_{\nu_i}}. \tag{12}$$

The Schrödinger equation for $F|n_f l_f>$ now becomes

$$(H_0 - E_{n_f} + E_{\nu_i})F|n_f l_f> = r|n_f l_f>, \tag{13}$$

which we write in the form

$$\left[E_{\nu_i} - E_{n_f} - \frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \left(\frac{Ze^2}{r} - \frac{\hbar^2}{2m}\frac{l_c(l_c+1)}{r^2}\right)\right] U(r,\nu_i) = r^2|n_f l_f>, \tag{14}$$

where $U(r,\nu_i)$ is given by (9). The Laplace transformed wave function $S(p,\nu_i)$ satisfies the differential equation

$$\left(E_{\nu_i} - E_{n_f} - \frac{\hbar^2}{2m}p^2\right)\frac{\mathrm{d}^2 S(p,\nu_i)}{\mathrm{d}p^2} - \left(\frac{2\hbar^2}{m}p - Ze^2\right)\frac{\mathrm{d}S(p,\nu_i)}{\mathrm{d}p}$$

$$+ \frac{\hbar^2}{2m}[l_c(l_c+1) - 2]S(p,\nu_i) = \int_0^\infty r^4 R_{n_f l_f}(r) e^{-pr}\,\mathrm{d}r, \tag{15}$$

which can be solved using the standard mathematical methods. Knowledge of $S(p,\nu_i)$ can be used to find $U(r,\nu_i)$, and then

$$P_f g(\nu_i) = \int\limits_0^\infty R_{n_g l_g}(r) U(r,\nu_i) r^2 \,\mathrm{d}r, \tag{16}$$

where $R_{n_g l_g}(r)$ is the radial part of the Coulomb wave function. This method is often used to calculate cross-sections in multi-photon ionization processes, as well as to evaluate the transition probabilities from higher exicited states of the hydrogen atom to the ground state.

3. Method of Green functions

This method is often used for solving inhomogeneous differential equations.For a two-photon transition [7], we write equation (13) of the preceding section in the form

$$(H_0 - E)F|n_f l_f >= r|n_f l_f >, \tag{17}$$

where

$$E = E_{n_f} - E_{\nu_i}, (i = 1, 2). \tag{18}$$

To find

$$P_f g(\nu_i) =< n_g l_g | rF | n_f l_f >, \tag{19}$$

we have to solve (17) for $F|n_f l_f >$. The Green function is defined as a solution of the equation

$$(H_0 - E) g_l(E, r, r') = -\frac{1}{r^2}\delta(r - r'), \tag{20}$$

which, in the case of the Coulomb potential, is of the form

$$\left[-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{dr}}\left(r^2\frac{\mathrm{d}}{\mathrm{dr}}\right) - \frac{l(l+1)}{r^2}\right) - \frac{Ze^2}{r} - E\right] g_l(E, r, r') = -\frac{1}{r^2}\delta(r - r'). \tag{21}$$

The solutions of (21) are given in terms of the well-known Whittaker functions

$$g_l(E, r, r') = -\frac{m a_0}{\hbar^2}\frac{\Gamma(l+1-n)}{\Gamma(2l+2)}\frac{\nu}{Zrr'} M_{n,l+1/2}\left(\frac{2Zr<}{n a_0}\right) W_{n,l+1/2}\left(\frac{2Zr>}{n a_0}\right), \tag{22}$$

where a_0 is the Bohr radius. The solution of the Schrödinger equation (17) is now given by

$$F R_{n_f l_f}(r) = -\int\limits_0^\infty g_l(E, r, r') r' R_{n_f l_f}(r') r'^2 \,\mathrm{d}r'. \tag{23}$$

Because of its accuracy, the method of Green functions has been succesfully used in many multi-photon processes [8-12] and in higher-order processes [7,13] of perturbation theory.

4. *Method of Kelsey and Macek*

This method [14] represents a reformulation of the method of implicit summation treated in Sect. 2. The perturbation wave function is found by solving the corresponding inhomogeneous Schrödinger equation by means of the parametric differentitation using the generating function for Laguerre polynomials. Let us consider the case of two-photon spontaneous emission given by

$$P_f g(\nu) = \sum_c \frac{< g|\boldsymbol{r}\boldsymbol{\epsilon}_1|c >< c|\boldsymbol{r}\boldsymbol{\epsilon}_2|f >}{E_c - E}, \tag{24}$$

where $E = E_f - E_\nu$.
Using differential operators, this expression can be written in the form

$$P_f g(\nu) = \left| \left(\boldsymbol{\epsilon}_1 \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{k}_g}\right) \left(\boldsymbol{\epsilon}_2 \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{k}_f}\right) \sum_c \frac{< g|\mathrm{e}^{\mathrm{i}\boldsymbol{k}_g\boldsymbol{r}}|c >< c|\mathrm{e}^{\mathrm{i}\boldsymbol{k}_f\boldsymbol{r}}|f >}{E - E_c} \right|_{\boldsymbol{k}_g = \mathbf{o}, \boldsymbol{k}_f = \mathbf{o}} . \tag{25}$$

If the wave functions of the initial $|g>$ and final $|f>$ state of the hydrogen atom are also written in terms of suitably defined differential operators

$$\begin{aligned} |f >&= Df(\mu_f, \boldsymbol{a}_f) e^{-\mu_f r + i\boldsymbol{a}_f\boldsymbol{r}}|_{\mu_f=1/n_f, \boldsymbol{a}_f=0} \, , \\ |g >&= Dg(\mu_g, \boldsymbol{a}_g) e^{-\mu_g r + i\boldsymbol{a}_g\boldsymbol{r}}|_{\mu_g=1/n_g, \boldsymbol{a}_g=0} \, , \end{aligned} \tag{26}$$

then the expression for $P_{fg}(\nu)$ reduces to

$$P_f g(\nu) = \tag{27}$$

$$\left| \left(\boldsymbol{\epsilon}_1 \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{k}_g}\right) \left(\boldsymbol{\epsilon}_2 \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{k}_g}\right) Df(\boldsymbol{\mu}_f, \boldsymbol{a}_f) Dg(\boldsymbol{\mu}_g, \boldsymbol{a}_g) M_f g \right|_{\mu_f=\frac{1}{n_f}, \mu_g=\frac{1}{n_g}, \boldsymbol{a}_f=\boldsymbol{a}_g=\boldsymbol{k}_g=\boldsymbol{k}_f=0} ,$$

where

$$M_f g = \sum_c \frac{< \mathrm{e}^{-\mu_g r}|\mathrm{e}^{i\boldsymbol{p}_g\boldsymbol{r}}|c >< c|\mathrm{e}^{i\boldsymbol{p}_f\boldsymbol{r}}|\mathrm{e}^{-\mu_f r} >}{E - E_c} \tag{28}$$

and

$$\begin{aligned} \boldsymbol{p}_f &= \boldsymbol{k}_f + \boldsymbol{a}_f \, , \\ \boldsymbol{p}_g &= \boldsymbol{k}_g - \boldsymbol{a}_g . \end{aligned} \tag{29}$$

The sum over c goes over all hydrogen wave functions corresponding to continuum states as well as to bound states. By constructing an integral expression for the auxiliary function

$$|\Psi(\boldsymbol{p}_f, \boldsymbol{r}) >= \sum_c \frac{|c >< c|\mathrm{e}^{\mathrm{i}\boldsymbol{p}_f\boldsymbol{r}}|\, \mathrm{e}^{-\mu_f r} >}{E - E_c} \, , \tag{30}$$

we can rewrite M_{fg} in the form

$$M_{fg} =< \mathrm{e}^{-\mu_g r}|\mathrm{e}^{\mathrm{i}\boldsymbol{p}_g\boldsymbol{r}}|\Psi(\boldsymbol{p}_f,\boldsymbol{r}) > \ . \tag{31}$$

The problem of finding M_{fg} is thus reduced to finding the solution of the inhomogeneous equation

$$(H_0 - E)|\Psi(\boldsymbol{p}_f,\boldsymbol{r}) >= -\mathrm{e}^{\mathrm{i}\boldsymbol{p}_f\boldsymbol{r}}\,|\mathrm{e}^{-\mu_f r} > . \tag{32}$$

Since the inhomogeneous term in (32) singles out a particular direction of $\boldsymbol{p}_f$ in space, we can use parabolic coordinates to reduce the problem to the differential equation for Laguerre polynomials. This method can be extended also to higher-order matrix elements [17].

5. Method of direct summation

In this section we show how the method of direct summation [2,3] over intermediate states can be improved to give the same level of accuracy as obtained using other more frequently applied methods. The usual approach in this method for calculating the effects of second-order pertubation theory is to retain only one or a few dominant states in the summation over all intermediate states. The remaining states are estimated by introducing the notion of mean level energy [18]. Our modified method of direct summation consists in retaining the maximal number of discrete intermediate states allowed by the available computer time. This approach is illustrated on an example of a two-photon transition amplitude between two bound states of the electron. The starting equation is again (10):

$$P_f g(\nu_i) = \sum_{n_c,l_c} \frac{< n_g l_g|r|n_c l_c >< n_c l_c|r|n_f l_f >}{E_{n_c} - E_{n_f} + E_{\nu_i}}, \tag{33}$$

which we split into three separate contributions: the first coming from the summation over discrete intermediate states up to $n_c(max) = 35$; the second coming from the integration over the continuum states; and the third coming from the summation from $n_c(max)$ to infinity. We write

$$P_f g(\nu_i) = P_f g^{(1)}(\nu_i) + P_f g^{(2)}(\nu_i) + P_f g^{(3)}(\nu_i), \tag{34}$$

where

$$P_f g^{(1)}(\nu_i) = \sum_{l_c} \sum_{n_c}^{n_c(max)} \frac{< n_g l_g|r|n_c l_c >< n_c l_c|r|n_f l_f >}{E_{n_c} - E_{n_f} + E_{\nu_i}}, \tag{35}$$

$$P_f g^{(2)}(\nu_i) = \sum_{l_c} \frac{2}{\pi} \int_0^{\infty} \frac{< n_g l_g|r|k l_c >< k l_c|r|n_f l_f >}{E_I + \frac{1}{2}k^2 + E_{\nu_i}} k^2 \,\mathrm{d}k, \tag{36}$$

with

$$E_I = E_\infty - E_{n_f} \tag{37}$$

and

$$\begin{gathered} P_fg^{(3)}(\nu_i) = (\bar{E} - E_{n_f} + E_{\nu_i})^{-1}[< n_g l_g | r^2 | n_f l_f > \\ - \textstyle\sum_{l_c} (\sum_{n_c}^{n_c(max)} < n_g l_g | r | n_c l_c >< n_c l_c | r | n_f l_f > \\ + \frac{2}{\pi} \int\limits_0^\infty < n_g l_g | r | k l_c >< k l_c | r | n_f l_f > k^2 \, \mathrm{d}k)], \end{gathered} \tag{38}$$

where

$$\bar{E} = \frac{1}{2}[E_{n_c(max)} + E_\infty]\,. \tag{39}$$

The spectral distribution of the two-photon transition probability is given by

$$A(\nu_1) = \frac{2^{10}\pi^6}{c^6} e^4 \nu_1^3 \nu_2^3 |P^{(2)}|^2, \tag{40}$$

where c is the velocity of light, e the charge of the electron and

$$|P^{(2)}|^2 = \frac{1}{(2l_g+1)(2l_f+1)} \sum_{m_g,m_f} |(P_fg(\nu_1) + P_fg(\nu_2))A_{l_f l_g}|^2_{\mathrm{av}}. \tag{41}$$

Here, $\nu_1 + \nu_2 = (E_f - E_g)/h$, and $A_{l_f l_g}$ is the angular part of the transition amplitude given by

$$A_{l_f l_g} = \sum_{m_c} < Y_{l_g m_g}(\Omega) | \hat{r} \boldsymbol{\epsilon}_1 | Y_{l_c m_c}(\Omega) >< Y_{l_c m_c}(\Omega) | \hat{r} \boldsymbol{\epsilon}_2 | Y_{l_f m_f}(\Omega) > . \tag{42}$$

The subscript "av" in (41) denotes averaging over the angle between the two photon polarization vectors $\boldsymbol{\epsilon}_1$ and $\boldsymbol{\epsilon}_2$. Introducing a new dimensionless variable

$$x = \frac{\nu_1}{\nu_1 + \nu_2}\,, \tag{43}$$

we can write the spectral distribution of the two-photon transition probability in the form

$$A(x) = \frac{1}{4} \left(\frac{\alpha}{a_0}\right)^6 \left(\frac{n_f^2 - n_g^2}{n_f^2 n_g^2}\right)^6 x^3 (1-x)^3 |P^{(2)}(x)|^2, \tag{44}$$

where α is the fine-structure constant, and

$$|P^{(2)}(x)|^2 = \frac{1}{(2l_g+1)(2l_f+1)} \sum_{m_g,m_f} |(P_fg(x) + P_fg(1-x))A_{l_f l_g}|^2_{\mathrm{av}}, \tag{45}$$

with

$$P_f g(x) = \sum_{n_c l_c} \frac{< n_g l_g|r|n_c l_c >< n_c l_c|r|n_f l_f >}{E_{n_c} - E_{n_f} + x(E_{n_f} - E_{n_g})} \,. \tag{46}$$

Using (34), we split the summations over intermediate states in Eqs.(45) and (46) into three separate parts

$$P_f g^{(1)}(x) = \sum_{l_c} \sum_{n_c}^{n_c(max)} \frac{< n_g l_g|r|n_c l_c >< n_c l_c|r|n_f l_f >}{E_{n_c} - E_{n_f} + x(E_{n_f} - E_{n_g})}, \tag{47}$$

$$P_f g^{(2)}(x) = \sum_{l_c} \frac{2}{\pi} \int\limits_0^\infty \frac{< n_g l_g|r|k l_c >< k l_c|r|n_f l_f >}{E_I + \frac{1}{2}k^2 + x(E_{n_f} - E_{n_g})} k^2 \,\mathrm{d}k, \tag{48}$$

and

$$\begin{aligned} P_f g^{(3)}(x) = (\bar{E} - E_{n_f} + x(E_{n_f} - E_{n_g})^{-1}[< n_g l_g|r^2|n_f l_f > \\ - \textstyle\sum_{l_c}(\sum_{n_c}^{n_c(max)} < n_g l_g|r|n_c l_c >< n_c l_c|r|n_f l_f > \\ + \frac{2}{\pi}\int\limits_0^\infty < n_g l_g|r|k l_c >< k l_c|r|n_f l_f > k^2 \,\mathrm{d}k)]. \end{aligned} \tag{49}$$

The expression (46) is now

$$P_f g(x) = P_f g^{(1)}(x) + P_f g^{(2)}(x) + P_f g^{(3)}(x). \tag{50}$$

We observe that $A(x) = A(1-x)$, so that numerical calculations should be performed only from $x = 0$ to $x = 0.5$

The results of our calculations for $n_c(max) = 35$ are presented in Table 1. The comparison with other methods is given in Tables 2 to 7.

6. Conclusion

In this paper we have analysed computational difficulties appearing in two-photon transition probabilities in hydrogen-like atoms by studying

$$P_f g(\nu_i) = \sum_{n_c, l_c} \frac{< n_g l_g|r|n_c l_c >< n_c l_c|r|n_f l_f >}{E_{n_c} - E_{n_f} + E_{\nu_i}}. \tag{51}$$

Table 1. Transition amplitudes $A(x)$ of two-photon transition probabilities calculated by the method of direct summation (in units of 10^{10} s^{-1}*).*

x	2s — 1s	3s — 1s	4s — 1s	5s — 1s	6s — 1s	3s — 2s
0.01	0.75027(5)	1.32210(5)	1.79346(5)	2.51679(5)	7.61870(5)	2.34869(3)
0.03	2.01947(5)	3.30610(5)	6.01079(5)	9.69951(3)	4.10253(5)	6.62749(3)
0.05	3.04865(5)	5.00530(5)	2.82699(7)	2.00304(5)	2.60965(4)	1.04191(4)
0.08	4.26571(5)	8.10480(5)	3.39893(4)	5.58558(5)	9.96978(5)	1.53428(4)
0.10	4.91461(5)	1.18066(6)	1.34452(5)	1.02353(4)	7.40505(3)	1.81949(4)
0.12	5.46430(5)	2.07796(6)	2.33462(5)	5.95720(4)	1.74200(4)	2.07528(4)
0.15	6.14277(5)	3.59520(7)	4.73769(5)	1.39491(5)	6.01413(4)	2.41129(4)
0.18	6.68520(5)	8.33323(5)	1.78873(6)	3.19402(5)	1.29093(5)	2.69824(4)
0.20	6.98722(5)	6.13569(4)	3.02986(18)	9.44409(5)	2.75486(5)	2.86594(4)
0.22	7.24985(5)	5.43062(0)	5.15081(5)	1.26444(8)	1.97533(6)	3.01683(4)
0.25	7.58174(5)	3.19350(4)	7.48626(3)	5.42995(4)	1.09816(5)	3.21484(4)
0.28	7.85166(5)	7.27128(4)	5.55102(3)	8.38264(0)	1.25839(3)	3.38246(4)
0.30	8.00256(5)	9.53651(4)	1.65531(4)	3.26212(3)	6.21301(2)	3.47896(4)
0.32	8.13318(5)	1.14185(5)	2.71180(4)	8.75731(3)	3.50191(3)	3.56419(4)
0.35	8.29542(5)	1.36306(5)	4.00279(4)	1.61673(4)	7.97130(3)	3.67239(4)
0.38	8.42189(5)	1.52534(5)	4.95243(4)	2.17384(4)	1.14242(4)	3.75863(4)
0.40	8.48834(5)	1.60706(5)	5.42722(4)	2.45258(4)	1.31567(4)	3.80464(4)
0.42	8.54157(5)	1.67008(5)	5.79521(4)	2.66816(4)	1.44960(4)	3.84185(4)
0.45	8.59813(5)	1.73689(5)	6.17411(4)	2.88945(4)	1.58689(4)	3.88173(4)
0.48	8.62811(5)	1.77123(5)	6.36997(4)	3.00359(4)	1.65761(4)	3.90303(4)
0.50	8.63378(5)	1.77768(5)	6.40665(4)	3.02492(4)	1.67082(4)	3.90707(4)

Table 1 (continued)

x	4s — 2s	5s — 2s	6s — 2s	4s — 3s	5s — 3s	6s — 3s
0.01	5.04088(5)	7.41813(5)	9.67945(5)	2.80480(4)	6.85830(4)	1.08233(5)
0.03	1.37568(6)	2.07039(6)	3.43332(6)	8.00361(4)	1.92104(5)	3.05367(5)
0.05	2.14248(6)	3.67557(6)	3.71953(7)	1.27089(5)	3.03840(5)	5.11369(5)
0.08	3.24356(6)	1.04546(7)	1.37759(5)	1.89614(5)	4.62692(5)	9.66030(5)
0.10	4.03489(6)	8.59497(7)	1.14783(6)	2.26587(5)	5.70865(5)	1.61890(6)
0.12	4.96327(6)	1.00970(7)	2.86891(6)	2.60232(5)	6.88081(5)	3.70822(6)
0.15	6.92189(6)	6.39544(3)	5.26010(7)	3.05136(5)	9.00013(5)	1.21426(8)
0.18	1.06127(7)	5.87544(5)	6.55559(5)	3.44138(5)	1.20106(6)	3.46245(5)
0.20	1.59099(7)	1.08826(6)	2.19973(3)	3.67215(5)	1.50243(6)	1.65086(4)
0.22	2.95105(7)	1.65529(6)	1.71918(5)	3.88163(5)	1.96690(6)	9.43451(3)
0.25	3.65807(8)	2.86663(6)	5.65696(5)	4.15918(5)	3.44120(6)	9.02563(4)
0.28	4.55734(7)	5.55791(6)	1.10250(6)	4.39651(5)	9.24841(6)	2.05707(5)
0.30	7.99842(6)	1.09007(7)	1.69220(6)	4.53415(5)	3.89609(7)	3.09980(5)
0.32	2.22705(6)	3.85158(7)	2.84325(6)	4.65636(5)	6.89166(8)	4.61999(5)
0.35	3.63419(5)	7.21356(7)	1.09671(7)	4.81234(5)	6.06485(6)	9.36828(5)
0.38	2.91083(4)	3.53334(6)	2.05260(8)	4.93733(5)	1.29988(6)	2.89210(6)
0.40	2.16464(1)	1.15720(6)	6.64158(6)	5.00427(5)	6.37871(5)	1.34827(7)
0.42	1.60208(4)	4.64652(5)	1.66320(6)	5.05853(5)	3.60412(5)	3.33766(8)
0.45	5.83221(4)	1.50103(5)	4.68889(5)	5.11682(5)	1.90480(5)	3.65578(6)
0.48	8.83377(4)	7.01370(4)	2.35154(5)	5.14801(5)	1.32359(5)	1.38008(6)
0.50	9.44907(4)	5.93553(4)	2.05003(5)	5.15392(5)	1.23189(5)	1.17630(6)

Table 1 (continued)

x	5s — 4s	6s — 4s	6s — 5s	3d — 1s	4d — 1s	5d — 1s
0.01	5.94609(7)	1.59343(8)	1.74526(7)	4.09579(4)	8.39785(4)	1.62265(5)
0.03	1.70442(8)	4.51327(8)	5.01303(7)	1.54102(5)	6.20636(5)	3.33482(5)
0.05	2.71690(8)	7.19090(8)	8.00771(7)	3.48320(5)	9.25566(7)	7.97317(4)
0.08	4.07492(8)	1.10023(9)	1.20420(8)	1.04958(6)	2.02711(5)	4.28931(6)
0.10	4.88463(8)	1.35606(9)	1.44574(8)	2.39326(6)	6.53331(3)	1.84140(5)
0.12	5.62576(8)	1.62661(9)	1.66746(8)	6.91625(6)	3.27254(4)	2.01471(4)
0.15	6.62131(8)	2.09283(9)	1.96627(8)	2.94083(8)	5.00058(5)	2.26173(4)
0.18	7.49191(8)	2.70129(9)	2.22848(8)	2.49702(7)	6.31733(6)	4.12068(5)
0.20	8.00966(8)	3.25362(9)	2.38481(8)	8.33483(6)	2.42388(19)	2.99593(6)
0.22	8.48130(8)	4.01480(9)	2.52747(8)	4.41721(6)	1.10356(7)	9.80713(8)
0.25	9.10864(8)	5.94024(9)	2.71761(8)	2.41611(6)	2.39326(6)	2.38100(6)
0.28	9.64733(8)	1.03889(10)	2.88121(8)	1.62792(6)	1.20663(6)	8.56882(5)
0.30	9.96066(8)	1.80949(10)	2.97651(8)	1.33887(6)	8.99922(5)	5.86327(5)
0.32	1.02394(9)	4.33978(10)	3.06140(8)	1.14343(6)	7.21456(5)	4.47388(5)
0.35	1.05960(9)	9.69916(12)	3.17010(8)	9.51518(5)	5.65751(5)	3.36375(5)
0.38	1.08824(9)	4.41470(10)	3.25750(8)	8.31169(5)	4.76917(5)	2.77053(5)
0.40	1.10360(9)	1.42925(10)	3.30441(8)	7.76059(5)	4.38323(5)	2.52150(5)
0.42	1.11607(9)	6.99029(10)	3.34250(8)	7.35372(5)	4.10629(5)	2.34596(5)
0.45	1.12947(9)	3.55891(9)	3.38347(8)	6.95189(5)	3.83921(5)	2.17913(5)
0.48	1.13664(9)	2.53353(9)	3.40540(8)	6.75058(5)	3.70777(5)	2.09789(5)
0.50	1.13801(9)	2.37747(9)	3.40957(8)	6.71333(5)	3.68362(5)	2.08303(5)

Table 1 (continued)

x	6d — 1s	3d — 2s	4d — 2s	5d — 2s	6d — 2s	4d — 3s
0.01	7.70385(5)	3.05266(1)	8.95400(2)	2.14071(3)	3.56437(3)	3.63344(0)
0.03	4.02993(5)	8.53441(1)	2.90400(3)	8.06912(3)	2.05869(4)	1.01163(1)
0.05	1.29638(4)	1.33019(2)	5.41044(3)	1.99523(4)	4.65362(5)	1.56932(1)
0.08	2.06279(6)	1.93585(2)	1.08844(4)	1.04769(5)	4.20002(3)	2.26603(1)
0.10	4.30057(5)	2.27932(2)	1.65691(4)	1.52059(6)	7.47540(2)	2.65337(1)
0.12	5.39192(4)	2.58256(2)	2.52351(4)	4.36586(5)	1.34697(4)	2.98940(1)
0.15	5.57788(1)	2.97358(2)	4.97599(4)	2.89986(4)	9.45003(5)	3.41281(1)
0.18	8.12663(4)	3.30065(2)	1.12038(5)	4.49415(3)	7.94067(4)	3.75663(1)
0.20	5.09668(5)	3.48873(2)	2.22711(5)	5.74516(2)	2.24477(4)	3.94931(1)
0.22	9.22575(6)	3.65596(2)	5.61839(5)	2.48333(2)	8.62316(3)	4.11715(1)
0.25	2.44661(6)	3.87247(2)	1.17289(7)	7.50646(3)	1.51147(3)	4.32898(1)
0.28	6.16524(5)	4.05301(2)	2.71353(6)	4.40137(4)	1.45461(2)	4.50046(1)
0.30	3.93359(5)	4.15580(2)	7.77762(5)	1.51931(5)	3.28933(3)	4.59572(1)
0.32	2.89343(5)	4.24588(2)	3.87740(5)	9.02204(5)	1.66864(4)	4.67772(1)
0.35	2.11291(5)	4.35922(2)	2.03771(5)	3.60589(6)	1.93002(5)	4.77880(1)
0.38	1.71398(5)	4.44875(2)	1.36171(5)	3.84940(5)	8.74112(6)	4.85691(1)
0.40	1.55023(5)	4.49622(2)	1.12806(5)	2.16965(5)	4.85259(5)	4.89765(1)
0.42	1.43609(5)	4.53445(2)	9.79235(4)	1.52336(5)	2.02139(5)	4.93013(1)
0.45	1.32862(5)	4.57528(2)	8.49227(4)	1.11676(5)	1.11528(5)	4.96443(1)
0.48	1.27662(5)	4.59702(2)	7.89775(4)	9.66493(4)	8.75550(4)	4.98255(1)
0.50	1.26713(5)	4.60114(2)	7.79167(4)	9.41645(4)	8.39740(4)	4.98598(1)

Table 1 (continued)

x	5d — 3s	6d — 3s	5d — 4s	6d — 4s	6d — 5s
0.01	9.20069(5)	2.47132(6)	7.23226(3)	1.78595(5)	2.00096(3)
0.03	2.87927(6)	8.42636(6)	2.00795(4)	5.49902(5)	5.54420(3)
0.05	5.13290(6)	1.74027(7)	3.10534(4)	9.61465(5)	8.55595(3)
0.08	9.51370(6)	4.73347(7)	4.46200(4)	1.72121(6)	1.22525(4)
0.10	1.35388(7)	1.05907(8)	5.20695(4)	2.38352(6)	1.42653(4)
0.12	1.90078(7)	3.42009(8)	5.84618(4)	3.24299(6)	1.59794(4)
0.15	3.18637(7)	2.23137(10)	6.63980(4)	5.13208(6)	1.80889(4)
0.18	5.58562(7)	2.10929(8)	7.27172(4)	8.32738(6)	1.97403(4)
0.20	8.50378(7)	7.49050(7)	7.61976(4)	1.18264(7)	2.06400(4)
0.22	1.37177(8)	3.35316(7)	7.91853(4)	1.73746(7)	2.14042(4)
0.25	3.36380(8)	1.01612(7)	8.28882(4)	3.39968(7)	2.23383(4)
0.28	1.30658(9)	1.32754(6)	8.58179(4)	8.02166(7)	2.30646(4)
0.30	7.15960(9)	8.11470(4)	8.74154(4)	1.72245(8)	2.34546(4)
0.32	1.66737(11)	4.24888(6)	8.87705(4)	5.12319(8)	2.37814(4)
0.35	2.27543(9)	4.07185(7)	9.04123(4)	1.59046(11)	2.41718(4)
0.38	7.68430(8)	3.11092(8)	9.16558(4)	1.00092(9)	2.44626(4)
0.40	5.10144(8)	2.31973(9)	9.22957(4)	3.97446(8)	2.46103(4)
0.42	3.84745(8)	8.54209(10)	9.28009(4)	2.34126(8)	2.47259(4)
0.45	2.94751(8)	1.48630(9)	9.33296(4)	1.49330(8)	2.48459(4)
0.48	2.58816(8)	7.36531(8)	9.36068(4)	1.21521(8)	2.49082(4)
0.50	2.52720(8)	6.62774(8)	9.36589(4)	1.17110(8)	2.49199(4)

Table 2. Comparison of the results of the method of implicit summation (MIS) [19] and our method of direct summation (MDS).

		MIS [19]	MDS
Transition	ν (10^{15}Hz)	$A(\nu)$ (10^{-15})	$A(\nu)$ (10^{-15})
2s — 1s	1.233	8.638	8.6338
3s — 1s	1.4614	1.779	1.7777
4s — 1s	1.5413	0.6410	0.64066
5s — 1s	1.5783	0.3026	0.30249
6s — 1s	1.5984	0.1672	0.16708
3d — 1s	1.4614	6.717	6.7133
4d — 1s	1.5413	3.685	3.6836
5d — 1s	1.5783	2.084	2.0830
6d — 1s	1.5984	1.268	1.2671

Table 3. Comparison of our MDS results for 2s – 1s *transitions and the MDS results [20,21] obtained using the reduced base of pseudostate solutions of the Dirac equation.*

	MDS	MDS	MDS
	[20]	[21]	
x	$A(x)$	$A(x)$	$A(x)$
0.0625	2.032	2.03239	2.032614
0.1250	3.158	3.15792	3.158095
0.1875	3.844	3.84452	3.844661
0.250	4.284	4.28435	4.284451
0.3125	4.570	4.56958	4.569656
0.3750	4.748	4.74855	4.748615
0.4375	4.847	4.84732	4.847368
0.500	4.879	4.87892	4.878965

We considered three separate contributions to (51). The first one coming from the summation over discrete intermediate states was performed up to $n_c(max) = 35$. The second contribution from the integration over the continuum states was performed numerically. The third contribution coming from the summation from $n_c(max)$ to infinity was calculated in an approximate way using the mean energy level for this region. This improved method of direct summation shows (see Table 1) that by choosing a sufficiently large $n_c(max)$ (in our case $n_c(max) = 35$), we can obtain a good agreement with other more frequently used methods, as shown in Tables 2 to 7. The accuracy of our final results depends on the choice of $n_c(max)$. However, the control of the numerical error in the calculations is much easier in

Table 4. Comparison of MDS results [22], results of the Method of Green functions (MGF) [23] and our results (last column) for 2s – 1s *transitions.*

x	$A(x)$[22]	$A(x)$[23]	$A(x)$
0.00	0.00	0.00	0.00
0.05	1.725	1.723	1.7228
0.10	2.783	2.777	2.7772
0.15	3.481	3.471	3.4713
0.20	3.961	3.949	3.9485
0.25	4.306	4.284	4.2844
0.30	4.546	4.522	4.5222
0.35	4.711	4.688	4.6877
0.40	4.824	4.797	4.7967
0.45	4.889	4.859	4.8588
0.50	4.907	4.879	4.8789

Table 5. Comparison of the results of the method of Kesley and Macek (MKM) [24] and our results (last column) in the case of 2s – 3s *transitions.*

	MKM [24]	MDS
x	$A(x)$	$A(x)$
0.05	0.02683	0.026827
0.10	0.04685	0.046847
0.15	0.06209	0.062085
0.20	0.07379	0.073791
0.25	0.08278	0.082773
0.30	0.08958	0.089574
0.35	0.09456	0.094554
0.40	0.09796	0.097959
0.45	0.09995	0.099945
0.50	0.1006	0.100597

Table 6 (below-left). Same as the Table 4, but for 3s – 1s *transitions.*

	MGF [25]	MDS
x	$A(x)$ (10^{-15})	$A(x)$ (10^{-15})
0.01125	1.4662	1.46615
0.0225	2.6254	2.62535
0.03375	3.6308	3.63085
0.05625	5.5534	5.55349
0.1125	1.6208(1)	1.62083(1)
0.12375	2.4132(1)	2.41328(1)
0.135	4.4913(1)	4.49133(1)
0.14625	1.5516(2)	1.55166(2)
0.1575	7.2245(3)	7.22364(3)
0.16875	4.9055(1)	4.90546(1)
0.180	8.3333	8.33323
0.19125	1.9874	1.98741
0.2025	4.1926	4.19256
0.21375	3.2841(-2)	3.28448(-2)
0.2250	1.7903(-2)	1.79047(-2)
0.28125	7.4246(-1)	7.42465(-1)
0.3375	1.2789	1.27891
0.39375	1.5836	1.58357
0.450	1.7369	1.73689

Table 7 (below-right). Same as the Table 6, but for 3d – 1s *transitions.*

	MGF [25]	MDS
x	$A(x)$ (10^{-15})	$A(x)$ (10^{-15})
0.01125	0.4624	0.46624
0.0225	1.0512	1.05195
0.03375	1.8246	1.82454
0.05625	4.3849	4.38494
0.1125	4.4478(1)	4.44777(1)
0.12375	8.8797(1)	8.87977(1)
0.135	2.2736(2)	2.27355(2)
0.14625	1.1178(3)	1.11779(3)
0.1575	7.7546(4)	7.75368(4)
0.16875	8.3739(2)	8.37376(2)
0.180	2.4971(2)	2.49702(2)
0.19125	1.2344(2)	1.23436(2)
0.2025	7.5715(1)	7.57141(1)
0.21375	5.2362(1)	5.23622(1)
0.2250	3.9085(1)	3.90852(1)
0.28125	1.6060(1)	1.60603(1)
0.3375	1.0204(1)	1.02036(1)
0.39375	7.9156	7.91556
0.450	6.9518	6.95189

in our approach then in other models discussed in this paper. The change of the values of the fundamental constants over last twenty years influence our results only by about 0.01%.

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References

[1] M. Göppert-Mayer, Ann. Phys. (Leipzig) **9** (1931) 273.

[2] H. B. Bebb and A. Gold, Phys. Rev. **143** (1966) 1.

[3] H. B.Bebb, J. Math. Phys. **7** (1966) 955.

[4] J. E. Lenard-Jones, Proc. Roy. Soc. A **129** (1930) 598.

[5] C. Schwartz, Annals of Physics **6** (1959) 156. C. Schwartz and J. J Tiemann, Annals of Physics **6** (1959) 178.

[6] G. E. Brown, R. E. Peierls and J. B. Woodward, Proc. Roy. Soc. Ser. A **227** (1954) 51.

[7] B. A. Zon and L. P. Rapaport, Zh. Eksp. Teor. Fiz. (pismo) **7** (1968) 70.

[8] S. Klarsfeld, Phys. Lett. A **30** (1969) 382.

[9] B. A. Zon and N. L. Manakov, Zh. Eksp. Teor. Fiz. **60** (1971) 1264.

[10] L. P. Rapaport, B. A. Zon and L. P. Manakov, Zh. Eksp. Teor. Fiz. **56** (1969) 400.

[11] S. Klarsfeld, Nuovo Cimento Lett. **3** (1979) 395.

[12] B. A. Zon and N. L. Manakov, Zh. Eksp. Teor. Fiz. **61** (1971) 968.

[13] V. A. Davidkin, B. A. Zon, N. L. Manakov and L. P. Rapaport, Zh. Eksp. Teor. Fiz. **60** (1971) 124.

[14] E. J. Kelsey and J. Macek, J. Math. Phys. **17** (1976) 1182.

[15] R. M. Sternheimer, Phys. Rev. **84** (1951) 244.

[16] A. Dalgarno and J. T. Lewis, Proc. Roy. Soc. A **233** (1956) 70.

[17] C. K. Au, Phys. Lett. A **51** (1975) 442;**58** (1976) 493.

[18] H. A. Bethe and E. E. Salpeter, Handbuch der Physik, Band XXXV, Springer-Verlag **88** (1957).

[19] J. H. Tung, X. M. Ye, G. J. Salamo and F. T. Chan, Phys. Rev. A **30** (1984) 1175.

[20] W. R. Johnson, Phys. Rev. Lett. **29** (1972) 1123.

[21] S. P. Goldman and G. W. F. Drake, Phys. Rev. A **24** (1981) 183.

[22] L. Spitzer and J. L. Greenstein, Astrophys. J. **114** (1951) 407.

[23] S. Klarsfeld, Phys. Lett. A **30** (1969) 382.

[24] V. Florescu, Phys. Rev. A **30** (1984) 2441.

DVOFOTONSKI PRIJELAZI U SUSTAVIMA SLIČNIM VODIKU

Uspoređujemo niz metoda za računanje dvofotonskih prijelaza u sustavima sličnim vodiku s poboljšanom metodom izravnog zbrajanja. Računaju se tri odvojena doprinosa dvofotonskim prijelaznim vjerojatnostima. Prvi je zbrajanje preko diskretnih međustanja do $n_c(max) = 35$. Drugi je doprinos od integracije preko stanja u kontinuumu i provodi se numerički. Treći je doprinos od stanja $n_c(max)$ do neizmjernosti i računa se aproksimativno rabeći srednju vrijednost energije za to područje. Nalazimo da je odabirom n_c nadzor nad numeričkom pogreškom u računima mnogo učinkovitiji nego u drugim metodama.