

AN EFFECTIVE-CHARGE MODEL FOR THE PROBLEM OF PHOTODETACHMENT OF NEGATIVELY CHARGED HYDROGEN IONS

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Abstract: In this work we take into consideration the calculation of the photodetachment cross section of negatively charged hydrogen ions through the use of an effective-charge model and the two-electron Green's function for summation over final states of the system. The analytical form of this function is obtained by the convolution of the one-particle Coulomb Green's functions in the framework of the regular perturbation theory and the operator method. In order to obtain results, we have approximated the value of the Green function via the numerical method with the support of the Mathematica software. In contrast to former *ab initio* calculations, our approach leads to a greater theoretical value than the experimental one.

Key words: effective-charge model; transition matrix elements; photodetachment cross section; Coulomb Green's function; regular perturbation theory.

1. Introduction

The problem of photodetachment cross section of the negatively hydrogen ion (H^-) is of great interest to astrophysicists because the process mainly determines the absorption of infrared and visible light in the photosphere of stars over a wide temperature range (Aller, 1963; Motz, 1970). A detailed overview of the theoretical and experimental result obtained in the study of this process was already presented (Vandevraye, Babilotte, Blondel, 2014) [3]. The high precision measurements of the photodetachment cross section were described in this article and a substantial difference between experimental and theoretical results have been found. As noted in a study (Vandevraye,

fields. It is important to emphasize that the energy and the wave functions of the initial (ground) state H^- were found via a variational method with a very high accuracy (Frolov, 2003; Frolov, 2015). Possibly, a major source of discrepancy between the theory and the experiment was defined by correlative effects in the calculation of a sum over the final states of the system that consists of hydrogen atom and electron.

It is known that in the case of the interaction of a hydrogen atom with external fields, the summation over the final states can be performed by a presentation of this sum through the one-particle Green's function of an electron in the Coulomb field (Dalgarno, Lewis, 1955; Shakeshaft, 2004). With this approach, the calculation of matrix elements and the summation over the final state reduce to integration of the well-known analytical expression together with the wave function of the initial state.

In the case of H^- there are two electrons in the final state and the analogous approach leads to the two-particle Green's function. Recently, in our work (Feranchuk, Triguk, 2011) an analytical representation for the Green's function of the two-electron system in the Coulomb field was obtained. It allowed us to develop a regular perturbation theory (RPT) for

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Babilotte, Blondel, 2014), H^- ion is one of the simplest quantum systems and the treatment of this difference is crucial to clarify the role of electron correlations in the description of the interaction of atoms with external

calculating the energy and wave functions of the ground and excited states of the helium atom. Already in the second order, RPT ensures the accuracy of the approximation about 0.1%. The important features of RPT are the ability to calculate the corrections to zero order approximation without introducing an additional variational parameter and the possibility to generalize this method for many-electron systems.

In the present article we approbate RPT for the analysis of the transition probabilities in quantum systems in the example of the calculation of the total cross section for the H ion photodetachment. With this purpose the considered cross-section is represented via the Green's function of an atomic system with the energy corresponding to the initial state. In order to illustrate the effectiveness of this method, the photoionization cross section (photoelectric effect) for the hydrogen atom is calculated and this result is compared with the well-known value obtained by direct summation over the final states (Barestetskii, Lifshitz, Pitaevskii, 1980). For the two-electron system being H⁻ ion, the wave functions of the ground state and the Green's function of the final state of the system are calculated on the basis in the zero approximation of RPT. The theoretical value proves to be greater than the experimental one in contrast to other *ab initio* calculations (Vandevraye, Babilotte, Blondel, 2014). General formulas for calculation of the next order corrections are also deduced.

2.Green's function of an atomic system and the total photodetachment cross section

Let us consider the N electron atomic system which is described by Hamiltonian H with the set of eigenvectors $|\Psi_\nu(\xi)\rangle$ and eigenvalues E_ν

$$H|\Psi_\nu(\xi)\rangle = E_\nu|\Psi_\nu(\xi)\rangle, \quad (1)$$

where the quantum numbers ν include both continuous and discrete spectrum, and the set of variables ξ is defined by the coordinates and spins of all electrons.

We also introduce the Green's function of the system:

$$(H - E)G_E(\xi, \xi') = \delta(\xi, \xi');$$

$$G_E(\xi, \xi') = -\sum_\nu \frac{|\Psi_\nu(\xi)\rangle\langle\Psi_\nu(\xi')|}{E - E_\nu}. \quad (2)$$

Interaction between the atom and the electromagnetic field for nonrelativistic approximation is defined by the operator (Barestetskii, Lifshitz, Pitaevskii, 1980) ($\hbar = c = 1$)

$$V_e = \frac{-e_0\sqrt{4\pi}}{\sqrt{2\omega}} \sum_{l=1}^N \frac{(e_s p_l)}{m} \left(e^{ikr} a_{k,s}^{rr} + e^{-ikr} a_{k,s}^{r+} \right), \quad (3)$$

where $e_0(e_0^2 = \alpha = 1/137)$ is the electron charge, m is its mass; p_l is the momentum operator of the atomic electron; $a_{k,s}^r, a_{k,s}^{r+}$ are the operators of annihilation and creation of the photon with polarization e_s , wave vector \hat{k} and frequency $\omega = |\hat{k}|$.

We use below the atomic units with $m = 1$; the length and the energy are measured in the Bohr radius a_0 and the atomic unit of energy ε_0 , correspondingly.

$$a_0 = 0.529 \cdot 10^{-8} \text{ cm}; \varepsilon_0 = 27.21 \text{ eV}; \omega \rightarrow \frac{\hbar\omega[\text{eV}]}{\varepsilon_0}. \quad (4)$$

For the photon frequency range, which is of interest in the considered problem, one can use the dipole approximation omitting exponent in the operator (3). Then, in the first-order perturbation theory on the operator V_e , the total photon absorption cross section with the transition of an atom from the initial state $|\Psi_i\rangle$ to all possible final states $|\Psi_f\rangle$ is given by the following formula (Barestetskii, Lifshitz, Pitaevskii, 1980).

$$\sigma = \frac{4\pi^2\alpha}{\omega} \sum_f \left| \langle\Psi_f| (e_s \sum_{l=1}^N \nabla_l) |\Psi_i\rangle \right|^2 \delta(E_i + \omega - E_f). \quad (5)$$

When the photon frequency $(\omega + E_i) > 0$, i.e $E_f > 0$, this expression describes the cross section of the photoelectric effect, when the atomic system goes into the states of the continuous spectrum. Let us now use the identity

$$\delta(E_i + \omega - E_f) = \frac{1}{\pi} \text{Im} \frac{1}{E_i + \omega - E_f - i\delta}. \quad (6)$$

The square of the matrix element is a real value and based on the definition (5) the formula (5) can be transformed as:

$$\begin{aligned} \sigma &= \frac{4\pi\alpha}{\omega} \text{Im} \sum_f \frac{\langle \Psi_i(\xi) | (e_s \sum_{l=1}^N \nabla_l) | \Psi_f(\xi) \rangle^2}{E_i + \omega - E_f - i\delta} = \\ &= \frac{4\pi\alpha}{\omega} \text{Im} \int d\xi d\xi' G_{E_i + \omega - i\delta}(\xi, \xi') \times \\ &\quad \times (e_s \sum_{l=1}^N \nabla_l \Psi_i^*(\xi)) (e_s \sum_{l=1}^N \nabla_l \Psi_i(\xi')). \end{aligned} \quad (7)$$

Thus, the calculation of the matrix elements and summation over the final states of the system are reduced to the integration of the Green's function with the initial wave functions.

In order to evaluate effectiveness of the considered approach, let us calculate the cross section of the photoelectric effect for the hydrogen atom with the nucleus charge Z . In this case the summation in (5) can be done analytically (Barestetskii, Lifshitz, Pitaevskii, 1980). In this case, the wave function of the ground state has the simple form:

$$\Psi_i^{\mathbf{r}}(r) = R_{10}(r) Y_{00}(\Omega) = \frac{2Z^{3/2} e^{-Zr}}{\sqrt{4\pi}}; E_i \equiv E_0 = -\frac{Z^2}{2}. \quad (8)$$

Without loss of the generality, the quantization axis when integrating over the angular variables of the atom can be directed along the photon polarization vector $e_s \parallel Oz$, so that

$$(e_s \nabla) \Psi_i^{\mathbf{r}}(r) = -Z \cos \theta \Psi_i^{\mathbf{r}}(r) = -Z \sqrt{\frac{4\pi}{3}} Y_{10}(\Omega) \Psi_i^{\mathbf{r}}(r).$$

For a one-electron atom, the analytical solution of the equation (2) is well known and defines the so-called Coulomb Green's function (CGF). It is written, for example, in (Veselov, Labzovskii, 1986). Using its expansion on spherical harmonics

$$G_E^{\mathbf{r} \mathbf{r}'} = \sum_{l, m_l} \frac{1}{rr'} G_E(r, r') Y_{l, m_l}^*(\Omega) Y_{l, m_l}(\Omega'), \quad (9)$$

and integrating over the angular variables, one can find

$$\begin{aligned} \sigma &= \frac{16\pi\alpha Z^5}{-3\omega} \text{Im} \int d\Omega d\Omega' dr dr' r^2 r'^2 \sum_{l, m_l} G_{\omega + E_0 - i\delta, l}^{(1)}(r, r') \\ &\quad \times Y_{l, m_l}^*(\Omega) Y_{l, m_l}(\Omega') Y_{10}(\Omega) Y_{10}(\Omega') e^{-Z(r+r')} = \\ &= -\frac{16\pi\alpha Z^5}{3\omega} \text{Im} \int dr dr' rr' G_{\omega + E_0 - i\delta, 1}^{(1)}(r, r') e^{-Z(r+r')}. \end{aligned}$$

The radial part of CGF can be written as the product of the Whittaker functions (Gradshteyn, Ryzhik, 1963).

$$\begin{aligned} G_{\omega + E_0 - i\delta, 1}^{(1)}(r, r') &= \frac{\nu \Gamma(2 - \nu)}{Z \Gamma(4)} M_{\nu, 3/2}(\frac{2Z}{\nu} r_<) W_{\nu, 3/2}(\frac{2Z}{\nu} r_>), \\ \nu &= \frac{Z}{\sqrt{-2(\omega + E_0 - i\delta)}}; r_< = \min(r, r'), r_> = \max(r, r'). \end{aligned} \quad (10)$$

Then one can obtain

$$\begin{aligned} \sigma &= -\frac{8\pi\alpha Z^4}{9\omega} \text{Im} \left\{ \left[\nu \Gamma(2 - \nu) \times \right. \right. \\ &\quad \times \left. \int_0^\infty dr \int_0^r dr' M_{\nu, 3/2}(\frac{2Z}{\nu} r') W_{\nu, 3/2}(\frac{2Z}{\nu} r) e^{-Z(r+r')} rr' + \right. \\ &\quad \left. \left. + \int_r^\infty dr \int_r^\infty dr' M_{\nu, 3/2}(\frac{2Z}{\nu} r) W_{\nu, 3/2}(\frac{2Z}{\nu} r') e^{-Z(r+r')} rr' \right] \right\}. \end{aligned} \quad (11)$$

Note that the parameter $\delta \rightarrow 0$ defines the correct branch of the complex valued parameter ν , which should correspond to a positive sign of σ in (11).

The integral in the equation (11) can be calculated numerically with the Mathematica package with any required accuracy. The obtained results coincide exactly with the results of the calculation of the photoelectric effect cross section for the hydrogen atom when the direct summation over the final states can be fulfilled analytically (Barestetskii, Lifshitz, Pitaevskii, 1980) in order to pass to the conventional units, the result should be multiplied by $a_0^2 \approx 2.8 \times 10^{-17} \text{ cm}^2$

$$\sigma = -\frac{2^9 \pi \alpha}{3Z^2} \left(\frac{|E_0|}{\omega} \right)^4 \frac{e^{-4u \text{arctg} u}}{1 - e^{-2\pi u}}; u = \sqrt{\frac{|E_0|}{\omega + E_0}}. \quad (12)$$

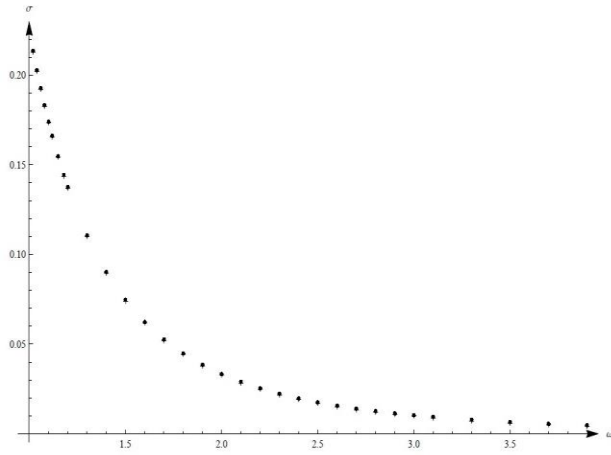


Figure 1. The dependence of σ on ω : (*) – numerical results, (+) – the results of calculations using formula (12)

3. Photodetachment cross section for a two-electron system

Let us consider now the problem of the ion H⁻ photodetachment. In this case the analytical solution of equations (1) and (2) are not found. Therefore one should use approximate methods for calculating both the wave function of the initial state and the Green's function of the final states. In this article we use the approach based on the regular perturbation theory (RPT) described in Refs. (Feranchuk, Triguk, 2011; Feranchuk, Ivanov, VH Le, Ulyanekov, 2015).

In order to solve the Schrodinger equation (1) for the initial state vector in the framework of RPT, the Hamiltonian of zero approximation and the perturbation operator are chosen as follows:

$$\begin{aligned}
 H|\Psi_0(1,2)\rangle &= E_0|\Psi_0(1,2)\rangle; H = H_0(1,2) + V; \\
 H_0(1,2) &= \frac{1}{2}(p_1^2 + p_2^2) - Z^*\left(\frac{1}{r_1} + \frac{1}{r_2}\right); \\
 V(1,2) &= -(Z - Z^*)\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + \frac{1}{|r_1 - r_2|}.
 \end{aligned} \tag{13}$$

Here the effective charge Z^* is the only variational parameter. With this choice the perturbation theory on the operator $V(1;2)$ leads in the second order of RPT to the following analytical results:

$$\begin{aligned}
 E_0 &\approx -Z^2 + \frac{5}{8}Z - 0.15759; \\
 \Psi_0^{(0)}(r_1, r_2) &= 4Z^{*3}e^{-Z^*(r_1+r_2)}Y_{00}(\Omega_1)Y_{00}(\Omega_2); \\
 \Psi_0(r_1, r_2) &\approx \Psi_0^{(0)}(r_1, r_2) - \\
 &\int dr_1' dr_2' G_E^{(2)}(Z^*, r_1, r_2, r_1', r_2')V(1,2)\Psi_0^{(0)}(r_1', r_2').
 \end{aligned} \tag{14}$$

The summation over the intermediate states when calculating the second order corrections in the framework of RPT was fulfilled by means of the analytical representation for the two-particle CGF $G_E^{(2)}(E, r_1, r_2; r_1', r_2')$ (Feranchuk, Triguk, 2011; Feranchuk, Ivanov, VH Le, Ulyanekov, 2015). It was also shown that the optimal value $Z^* = Z - 5/16$ for the variational parameter is calculated from the condition $E_0^{(1)} = 0$.

For the ion H⁻, $Z = 1$, $E_0 \approx -0.5326$, so that the oneparameter function (14) ensures accuracy ~1% in comparison with the variational energy calculation based on the trial wave function of the ground state with a large number of parameters ($E_0 \approx -0.5278$) (Frolov, 2015). It seems to us that such accuracy is sufficient for the considered problem, for the discrepancy between the experimental and theoretical values being found in Ref. (Vandevraye, Babilotte, Blondel, 2014) is about 20%.

In the final state of the system, a single electron is at a bound state, and the other goes into a continuous spectrum. Therefore the correlation between electrons is rather small and the zero order Hamiltonian should be selected as follows:

$$\begin{aligned}
 H|\Psi_f(1,2)\rangle &= E_f|\Psi_f(1,2)\rangle; H = H_f^0(1,2) + V_f; \\
 H_0(1,2) &= \frac{1}{2}(P_1^2 + P_2^2) - Z\left(\frac{1}{r_1} + \frac{1}{r_2}\right); V_f(1,2) = \frac{1}{|r_1 - r_2|}.
 \end{aligned} \tag{15}$$

The operator of the ion interaction with the electromagnetic field does not depend on the spin of electrons, so the initial and final states of the ion H⁻ corresponds to the total spin $S = 0$ and the symmetric wave function of the coordinates. Therefore the RPT expansion for $|\Psi_f(1,2)\rangle$ is different from (14):

$$\Psi_f^{(0)}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}} \left[\psi_v(\mathbf{r}_1) \psi_p(\mathbf{r}_2) + \psi_v(\mathbf{r}_2) \psi_p(\mathbf{r}_1) \right];$$

$$\Psi_f(\mathbf{r}_1, \mathbf{r}_2) \approx \Psi_f^{(0)}(\mathbf{r}_1, \mathbf{r}_2) - \int d\mathbf{r}_1' d\mathbf{r}_2' G_E^{(2)}(\mathbf{Z}, \mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_1', \mathbf{r}_2') V(1, 2) \Psi_f^{(0)}(\mathbf{r}_1', \mathbf{r}_2'). \tag{16}$$

Here ψ_v, ψ_p are the well-known electron wave functions in the Coulomb field of the nucleus corresponding to discrete and continuous spectra correspondingly.

Taking into account the symmetry of the wave functions of the electron coordinates, the expression (7) for the H⁻ photodetachment cross section can be written in the following form:

$$\sigma \approx \frac{16\pi\alpha}{\omega} \text{Im} \sum_f \frac{\left| \langle \Psi_f(\mathbf{r}_1, \mathbf{r}_2) | (e_s \nabla_1) | \Psi_i(\mathbf{r}_1, \mathbf{r}_2) \rangle \right|^2}{\omega - I - E_f - i\delta}. \tag{17}$$

Here I = 0.5278 is the H⁻ ionization potential calculated, for example, in Ref. (Frolov, 2015). In the experiment (Vandevraye, Babilotte, Blondel, 2014) the cross section was measured with a photon wavelength of 1064 nm which corresponds to the frequency value $\omega = 0.04282$ in the atomic units.

In accordance with (7) one can represent the value (17) as the following integral:

$$\sigma \approx -\frac{16\pi\alpha}{\omega} \text{Im} \int d\xi G_{\omega-I-i\delta}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_1', \mathbf{r}_2') \times \left(e_s \nabla_1 \Psi_i(\mathbf{r}_1, \mathbf{r}_2) \right) \left(e_s \nabla_1' \Psi_i(\mathbf{r}_1', \mathbf{r}_2') \right), \tag{18}$$

where $d\xi = d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_1' d\mathbf{r}_2'$ and $G_{\omega-I-i\delta}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_1', \mathbf{r}_2')$ is the two-electron Green's function that should be found from Eq.(2) with Hamiltonian (15).

In the present article we restrict ourselves to the RPT zero approximation for the calculation of the integral (18). It means that the wave function of the system ground state is chosen in the following form:

$$\Psi_i \approx \Psi_0^{(0)} = \psi_0^{(0)}(\mathbf{r}_1) \psi_0^{(0)}(\mathbf{r}_2) = 4Z^{*3} e^{-Z*(r_1+r_2)}. \tag{19}$$

In the same approximation the symmetrized two-particle Green's function is defined by the following equation with Hamiltonian $H_f(1; 2)$ from Eq.(15):

$$(\hat{H}_f - \omega + I + i\delta) G_{\omega-I-i\delta}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_1', \mathbf{r}_2') = \delta(\mathbf{r}_1 - \mathbf{r}_1') \delta(\mathbf{r}_2 - \mathbf{r}_2');$$

$$G_{\omega-I-i\delta}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_1', \mathbf{r}_2') = \sum_{f_1, f_2} \frac{|\psi_{f_1}^{(0)}(\mathbf{r}_1) \psi_{f_2}^{(0)}(\mathbf{r}_2)\rangle \langle \psi_{f_1}^{(0)}(\mathbf{r}_1') \psi_{f_2}^{(0)}(\mathbf{r}_2')|}{2(I - \omega + i\delta + E_{f_1} + E_{f_2})} + \sum_{f_1, f_2} \frac{|\psi_{f_1}^{(0)}(\mathbf{r}_2) \psi_{f_2}^{(0)}(\mathbf{r}_1)\rangle \langle \psi_{f_1}^{(0)}(\mathbf{r}_2') \psi_{f_2}^{(0)}(\mathbf{r}_1')|}{2(I - \omega + i\delta + E_{f_1} + E_{f_2})} \tag{20}$$

One can find the function (20) as the convolution of the analytical one-particle CGF by means of the trick considered in Refs. (Feranchuk, Triguk, 2011; Feranchuk, Ivanov, VH Le, Ulyanenko, 2015) for He atom. Let us use the following identity:

$$\int_{-\infty}^{\infty} \frac{dt}{(t+a-i\delta/2)(t-b+i\delta/2)} = -\frac{2\pi i}{a+b-i\delta}, \tag{21}$$

with real values a and b and a small parameter $\delta \rightarrow 0$.

Then one can apply this identity to the expression

$$\frac{1}{\omega - I - (E_{f_1} + E_{f_2}) - i\delta} = \frac{-1}{2\pi i} \int_{-\infty}^{\infty} \frac{dt}{(t + \frac{\omega - I}{2} - E_{f_1} - i\frac{\delta}{2})(t - \frac{\omega - I}{2} + E_{f_2} + i\frac{\delta}{2})}. \tag{22}$$

This allows one to transform the two-particle Green's function as follows:

$$G_{\omega-I-i\delta}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_1', \mathbf{r}_2') = \frac{1}{4\pi i} \int_{-\infty}^{\infty} dt [G_{\frac{\omega-I}{2}+t-i\frac{\delta}{2}}(\mathbf{r}_1, \mathbf{r}_1') G_{\frac{\omega-I}{2}-t-i\frac{\delta}{2}}(\mathbf{r}_2, \mathbf{r}_2') + G_{\frac{\omega-I}{2}+t-i\frac{\delta}{2}}(\mathbf{r}_2, \mathbf{r}_2') G_{\frac{\omega-I}{2}-t-i\frac{\delta}{2}}(\mathbf{r}_1, \mathbf{r}_1')]. \tag{23}$$

Taking into account the spherical harmonics orthogonality conditions when integrating over the angles, the following result can be obtained after summation over the photon polarizations:

$$\begin{aligned} \sigma &= -\frac{64Z^{*8}\alpha}{3\omega} \operatorname{Re} \int_{-\infty}^{\infty} dt \int_0^{\infty} r_1 r_1' r_2 r_2' dr_1 dr_1' dr_2 dr_2' e^{-Z^*(r_1+r_1'+r_2+r_2')} \times \\ &\quad \times [G_{\frac{\omega-I}{2}+t-i\frac{\delta}{2},1}(r_1, r_1') G_{\frac{\omega-I}{2}-t-i\frac{\delta}{2},0}(r_2, r_2')] = \\ &+ G_{\frac{\omega-I}{2}+t-i\frac{\delta}{2},0}(r_1, r_1') G_{\frac{\omega-I}{2}-t-i\frac{\delta}{2},1}(r_2, r_2')] = \\ &= -\frac{128Z^{*8}\alpha}{3\omega} \operatorname{Re} \int_{-\infty}^{\infty} dt \int_0^{\infty} r_1 r_1' r_2 r_2' dr_1 dr_1' dr_2 dr_2' e^{-Z^*(r_1+r_1'+r_2+r_2')} \times \\ &[G_{\frac{\omega-I}{2}+t-i\frac{\delta}{2},1}(r_1, r_1') G_{\frac{\omega-I}{2}-t-i\frac{\delta}{2},0}(r_2, r_2')]. \end{aligned} \quad (26)$$

Expression (26) includes a five-dimensional integral which was calculated numerically using the package Mathematics and the interpolation of the results for intermediate integrals. It should be noted that the special numerical procedure was used for taking into account the contributions of the first order poles of the integrand on the parameter t .

The results for $Z = 1$ and $\omega = 0.04282$ were calculated and the corresponding photodetachment cross section is approximately equal to 3.86 in comparison with the experimental result 3.48 ± 0.15 obtained in (G'en'evriez, Urban, 2015).

4. Conclusion

The results show that the zero order calculation of RPT transition matrix elements for the atomic system delivers the same accuracy as that of stationary energy states. A closed expression is firstly obtained for the two-particle Coulomb Green's function, being useful to calculate cross sections for many-body systems. At the same time RPT allows us to calculate the correlative corrections to the observed characteristics of the system without introducing additional variation parameters.

MÔ HÌNH ĐIỆN TÍCH HIỆU DỤNG ĐỐI VỚI BÀI TOÁN TIẾT DIỆN HIỆU DỤNG CỦA HYDROGEN TÍCH ĐIỆN ÂM

Tóm tắt: Một phương pháp tiếp cận mới để tính tiết diện hiệu dụng của ion hydro tích điện âm được nghiên cứu và đề xuất. Phương pháp giải dựa trên việc sử dụng mô hình điện tích hiệu dụng và hàm Green hai điện tử đối với trường hợp tính tổng các trạng thái cuối cùng của hệ. Dạng giải tích của hàm này thu được bằng cách tích hợp các hàm Green một hạt trong khuôn khổ của lý thuyết nhiễu điều chỉnh và phương pháp toán tử. Để thu được giá trị so sánh với kết quả thực nghiệm, chúng tôi đã giải gần đúng giá trị hàm Green bằng phương pháp số với sự hỗ trợ của phần mềm Mathematica. Trái ngược với các phương pháp ban đầu (ab initio), cách tiếp cận của chúng tôi dẫn đến giá trị lý thuyết lớn hơn so với giá trị thực nghiệm.

Từ khóa: mô hình điện tích hiệu dụng; các phần tử ma trận chuyển tiếp; tiết diện quang hóa; hàm Coulomb Green; lý thuyết nhiễu loạn điều chỉnh, phương pháp toán tử.

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