## Contour of K-electron Compton line

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An expression for the contour of the Compton line in the region of the maximum, and the angular distribution, is obtained with relative accuracy of the order of  $(\alpha Z)^2$  for photon scattering by K electrons.

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In preceding papers<sup>1,2</sup> we obtained the differential cross section of relativistic Compton scattering by Kelectrons in the zeroth order in  $\alpha Z$  at large momentum transfers to the nucleus,  $q \gg \eta$ , and obtained the correction of order  $\alpha Z$  for small  $q \sim \eta$ , where  $\eta = m\alpha Z$  is the average momentum of the electron on the K shell. The result led to an expression for the contour of the Compton line (the distribution in the energy and in the emission angle of the final photon) with a relative accuracy of order  $\alpha Z$  in the region of the Compton maximum. Upon integration over energies of the final photons, the terms linear in  $\alpha Z$  drop out and the previously obtained<sup>1</sup> distribution with respect to the emission angle of the final photon coincides with the Klein-Nishina formula<sup>3</sup>. To find the corrections to the Klein-Nishina formula it suffices to find the corrections of order  $(\alpha Z)^2$  for the contour of the Compton line in the region of the maximum, inasmuch as the region outside the peak makes a contribution of the order of  $(\alpha Z)^4$  to the angular distribution.<sup>1</sup> This is done in the present paper for final-photon emission angles  $\vartheta \gg \eta/\omega_1$  and at initial photon energies  $\omega_1$  much larger than the binding energy  $\eta^2/2m$ . In the region of small angles  $\vartheta \leq \eta/\omega$  the contour of the Compton line and the angular distribution are described by the Schnaidt formula<sup>1,4</sup> and differ by 100% from the Klein-Nishina formula.

The corrections to the contour of the Compton line in the region of the Compton peak, up to terms of orders  $(\alpha Z)^3$ , are determined by the small momenta  $q \leq \eta$ transferred to the nucleus. To calculate the corrections of order  $\alpha Z$  and  $(\alpha Z)^2$  to the contour of the Compton line in the region of the peak, it suffices to use the wave functions of the initial and final electrons in the Furry-Sommerfeld-Maue (FSM) approximation<sup>5</sup> and the Green's function of the intermediate electron with one Coulomb correction. This is equivalent to calculating corrections of the order of  $(\alpha Z)^2$  for zero-spin parts<sup>5</sup> ( $\varphi_0$ ) of the wave functions of the electrons in addition to the results obtained previously.<sup>1</sup>

To prove the foregoing we examine the diagrams<sup>1</sup> of Fig. 1a with three intermediate and final electrons, Fig. 1b with the Coulomb correction to the final elec-

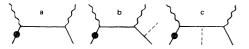


FIG. 1. Feynman diagrams of the process. The shaded block denotes the wave function of the bound electron.

tron, and Fig. 1c with the Coulomb correction to the Green's function of the intermediate electron. The cross diagrams are of the same order of magnitude. The diagram 1a contains terms of order of unity. In view of the small momentum  $q = p - \kappa$  transferred to the nucleus, where  $\varkappa = k_1 - k_2$  and p,  $k_1$ , and  $k_2$  are the momenta of the initial and final photons, the small angles  $\vartheta \leq \eta/\omega_1$  correspond to small  $\varkappa$  and to small momenta  $p(\varkappa \sim p \leq \eta)$ . At  $p \gg \eta$  the diagram 1b contains terms of order  $\alpha Z$  of the first correction  $\varphi_0^{(1)}$  to the spinless particle of the wave function  $\varphi_0$  of the final electron<sup>3</sup> and terms of order  $(\alpha Z)^2$  of the spin correction  $\varphi_1^{(0)} \sim q \varphi_0^{(1)} / m$ , containing the principal term in  $\alpha Z$  of the function  $\varphi_1$  (Ref. 5). In the diagram with two Coulomb corrections to the wave function of the final electron, which is not shown here, it is necessary to take into account only the second correction  $\varphi_0^{(2)}$  to the zero-spin part of the wave function of the final electron, which makes a contribution of the order of  $(\alpha Z)^2$ . The corrections  $\varphi_1^{(1)}$  and  $\varphi_2^{(0)}$  in the expansions of the functions  $\varphi_1$  and  $\varphi_2$  in terms of  $\alpha Z$  (Ref. 5) need not be taken into account, since they make a contribution of the order of  $(\alpha Z)^3$ . Thus, it suffices to use a wave function in the form  $\varphi_0 + \varphi_1$  (the FSM approximation), and take into account in  $\varphi_1$  only the first nonvanishing term in the expansion in  $\alpha Z$ . Similar statements can be made also for the wave function of the initial state. However, this function is known in closed form and its expansion up to terms of order  $(\alpha Z)^2$  can be carried out directly.6

At small  $p \leq \eta$ , all the terms of the expansion in  $\alpha Z$  of the functions  $\varphi_0$ ,  $\varphi_1$ , and  $\varphi_2$  the Coulomb parameter  $\xi = \alpha Z E / p \approx \eta / p$ , must be taken into account. In this case, to obtain the result accurate to terms of order  $(\alpha Z)^2$ , it is necessary to take the functions  $\varphi_0$ ,  $\varphi_1$ , and  $\varphi_2$  fully into account. Therefore our results at  $p \leq \eta$ are valid accurate to terms of order  $\alpha Z$ , but not  $(\alpha Z)^2$ .

The diagram 1c differs in an additional integration with respect to the intermediate momentum f. The phase volume and the quantity f is determined by the behavior of the wave function of the initial state:  $f \sim \eta$ and  $d^3f \sim \eta^3$ . The integrand acquires in addition to the diagram of Fig. 1a a factor  $\sim \alpha Z/\omega_1(\mathbf{q} - \mathbf{f})^2$ . As a result, at  $q \sim \eta$ , after integration, the diagram of Fig. 1c turns out to be of the order of  $d^3f \alpha Z/\omega_1(\mathbf{q} - \mathbf{f})^2 \sim (\alpha Z)^2$  relative to the diagram 1a. In the diagram 1c the wave functions of the electron can be taken into account in the first nonvanishing approximation in  $\alpha Z$  (the functions  $\varphi_0^{(0)}$ ). Similar arguments lead to the conclusion that the diagram with two Coulomb corrections to the Green's function of the electron is of the order of  $(\alpha Z)^4$  relative to the diagram of Fig. 1a and its calculation is unnecessary in our approximation.<sup>1)</sup>

The results of the calculations with the Coulomb wave functions and the Green's function are valid, strictly speaking, for single-electron ions. However, by virtue of the smallness of the screening for K electrons, the obtained results remain valid for neutral atoms.

The differential cross section, summed over the polarizations of the photons and electrons take at small  $q \sim \eta$  with allowance for the correction terms of order  $(q/m)^2$  and  $(\alpha Z)^2$  [no expansion in the parameter  $\xi$  is carried out at  $p \leq \eta$ , and the terms of order  $(q/m)^2$  and  $(\alpha Z)^2$  should be discarded], the form

$$d\sigma = \frac{r_0^2}{\pi^2} \frac{\eta^5}{a^4} |N_p|^2 e^{-2\xi\varphi} \frac{\varepsilon + m}{\omega_4} S d\Gamma, \qquad (1)$$

$$d\Gamma = \frac{d^3p \ d^3k_2}{\varepsilon\omega_2} \delta(\varepsilon + \omega_2 - \varepsilon_0 - \omega_1),$$

$$\varphi = \operatorname{arc} \operatorname{ctg} \frac{\eta^2 + \varkappa^2 - p^2}{2p\eta}, \quad \varkappa = \mathbf{k}_1 - \mathbf{k}_2.$$
(3)

Here  $r_0 = \alpha/m$  is the classical radius of the electron,  $a = q^2 + \eta^2$ ,  $\xi = \alpha Z \varepsilon/p$ ,  $N_p = e^{-/2} \Gamma(1 + i\xi)$ ,  $|N_p|^2 = 2\pi\xi/(1 - e^{-2\pi\xi})$ ,  $\Gamma(x)$  is the Euler gamma function,  $\varepsilon(\varepsilon_0)$  is the energy of the final (initial) electron,  $\omega_2(\omega_1)$  is the energy of the scattered (incident) photon

$$S = \left(2T_{2}L_{1} - (1-t)(1+t+v_{1}+v_{2})(L_{1}+\gamma q_{1}+\lambda x_{1}) + \frac{1}{4}(1-t^{2})(1-v^{2})q^{2}+\gamma F_{21}(\mathbf{q})+\lambda F_{21}(\mathbf{x}) + A\Phi_{1}(\mathbf{q})-\lambda(\epsilon+1)\Phi_{1}(\mathbf{v}) + \frac{2}{\omega_{1}}\left\{2v_{2}[(\gamma-q_{2})(tq_{1}-q_{2})+\lambda(tx_{1}-x_{2})] + (q^{2}-q_{1}^{2})T_{2}-q_{2}M_{12}(\mathbf{q})\right\} + \frac{2}{\omega_{2}}\left\{q_{1}(\mathbf{vq}-v_{2}q_{2}+q_{1}-tq_{2})-2\gamma M_{21}(\mathbf{q})-2\lambda M_{21}(\mathbf{x})\right\} + \frac{4v^{2}}{\omega_{1}^{2}}(q^{2}-q_{1}^{2}) - \frac{2v^{2}}{\omega_{2}\omega_{1}}(q^{2}-q_{1}^{2}-q_{2}^{2}+tq_{2}q_{1})\right) + (1\leftrightarrow 2,\omega_{1}\leftrightarrow -\omega_{2}).$$

In formula (4) we have put m = 1 and introduced the notation

$$\begin{split} \mathbf{v} &= \frac{\mathbf{p}}{e+1}, \quad v_i = \mathbf{vn}_i, \quad q_i = \mathbf{qn}_i, \quad \varkappa_i = \mathbf{xn}_i; \\ \mathbf{n}_i = \mathbf{k}_i / \omega_i \ (i=1, 2), \ t = \mathbf{n}_2 \mathbf{n}_i, \\ T_i = 1 + v^2 - 2tv_i, \ L_i = L + \gamma q_i + \lambda \varkappa_i, \\ L &= (1+A)^2 + \xi^2 (B-1)^2 + \frac{\alpha^2 Z^2}{2} \Big( \frac{1}{2} + \ln \frac{a}{\eta^2} + \frac{q^2 - \eta^2}{q\eta} \operatorname{arctg} \frac{q}{\eta} \Big) - \frac{3}{4} \ q^2 - q_2 q_i, \\ A &= \frac{a(\varkappa^2 - p^2 - \eta^2)}{|b|^2}, \quad B = \frac{a(\varkappa^2 + p^2 + \eta^2)}{|b|^2}, \quad \lambda = \frac{2\eta^2 a}{|b|^2}, \\ \gamma = 1 + A + q_1 + q_2, \ b = \varkappa^2 - (p + i\eta)^2, \\ |b|^2 = bb^* = [(\varkappa - p)^2 + \eta^2] \ [(\varkappa + p)^2 + \eta^2], \\ F_{ij}(\mathbf{q}) = (1 - t)^2 \mathbf{vq} + (1 - t) \ (1 + v^2 + 2v_i) q_j, \\ M_{ij}(\mathbf{q}) = \mathbf{vq} - v_i q_i + v^2 (q_j - tq_i), \\ \Phi_i(\mathbf{q}) = (1 + t) \ v^2 q_i - (3 + t^2) \ \mathbf{vq}. \end{split}$$

The terms linear in q (with account taken of the corrections made in Refs. 1 and 7) coincide with our earlier results.<sup>2</sup>

The distribution in energy and photon emission angle (the contour of the Compton line) is obtained from (1) by integrating with respect to q and  $\varphi$ :

$$\frac{d\sigma}{d\omega_{2} dt} = \frac{\omega_{1}\omega_{2}\varepsilon}{\varkappa p} \frac{d\sigma}{d\varkappa dp};$$
(5)
$$\frac{\omega_{1}+\varepsilon_{0}=\omega_{2}+\varepsilon, \ \varepsilon_{0}=m(1-\alpha^{2}Z^{2})^{\frac{1}{4}}, \ \varepsilon=(m^{2}+p^{2})^{\frac{1}{4}};$$

$$\frac{d\sigma}{d\varkappa dp} = \frac{16}{3} \frac{d\sigma_{0}(p)}{dp} - \frac{\eta^{5}}{(x^{2}+\eta^{2})^{3}} \left\{ 1+2\xi \operatorname{arctg} \frac{x^{2}+\eta^{2}+2px}{2p\eta} + \gamma_{1} \frac{x}{m} + \gamma_{2} \frac{x^{2}}{m^{2}} + \gamma_{3}\alpha^{2}Z^{2} \right\};$$
(6)
$$\gamma_{1} = \frac{3}{2} \frac{\varepsilon}{p} + \frac{f_{1}(\mathbf{n},\varkappa) + f_{2}(\mathbf{n}_{2}\varkappa)}{\varkappa f_{0}}, \quad x=\varkappa - p,$$

$$f_0 = \frac{r_0^2}{2} \left\{ \frac{\omega_1}{\omega_2} + \frac{\omega_2}{\omega_1} + \left( \frac{m}{\omega_1} - \frac{m}{\omega_2} \right)^2 + 2 \left( \frac{m}{\omega_1} - \frac{m}{\omega_2} \right) \right\}, \quad f_i = \omega_i \frac{\partial f_0}{\partial \omega_i}$$

Here  $d\sigma_0(p)/dp$  is the cross section for scattering by the free electron.

The expressions for  $\gamma_2$  and  $\gamma_3$  are unwieldy, although they can be obtained analytically from (1). We therefore do not present them here and obtain these coefficients in formula (6) by numerical integration.

Formula (6) is valid accurate to terms of order  $(\alpha Z)^2$  near the Compton maximum  $x \leq \eta$ . Far from the maximum, the principal term in  $\alpha Z$  can be obtained from formula (19) of Ref. 2. At small  $p \leq \eta$  the principal term of the distribution coincides with the formula from Ref. 4 [see also formula (35b) in Ref. 1].

The term linear in x in (6), which drops out on going to the angular distribution (after integration with respect to the photon energy  $\omega_2$  or with respect to p), leads to a shift of the maximum of the Compton line<sup>8,9</sup> by an amount  $\Delta x \sim \eta^2/m$  relative to x = 0 (or by  $\Delta \omega_2$  $\sim \eta^2/m$  relative to  $\omega_2 = \omega_{20}$ ). Terms of order  $x^2/m^2$  and  $(\alpha Z)^2$  in (6) lead to a shift of the maximum by an amount  $\sim \eta^4/m^3$ . To calculate the shift of the maximum  $\Delta \omega_2$  it is necessary to take into account the dependence of  $d\sigma_0/dp$  and  $\varkappa$  on  $\omega_2$ .<sup>1</sup> As a result we obtain for the principal term of the shift of the Compton line

$$\Delta\omega_{2} = \frac{\eta^{2}}{12m} \frac{\varepsilon\omega_{20}}{m\omega_{1}} \left\{ 1 + 2 \frac{\varepsilon - m}{\varepsilon} \left[ \left( 1 + \frac{m}{\omega_{1}} \right) \left( 1 + \frac{f_{1}}{f_{0}} \right) + \left( t + \frac{\varepsilon}{\omega_{1}} \right) \frac{f_{2}}{f_{0}} \right] + O\left(\alpha^{2}Z^{2}\right) \right\}.$$
(7)

Here  $\Delta \omega_2 = \omega_2^{\text{max}} - \omega_{20}$ ,  $\omega_{20} = m\omega_1/(m + \omega_1(1 - t))$  is the frequency of the photons scattered through an angle  $\vartheta$  by the free electrons,  $\omega_2^{\text{max}}$  is the frequency corresponding to the maximum intensity of the photons scattered from the K shell through an angle  $\vartheta$ , and the quantities  $f_0$ ,  $f_1$ , and  $f_2$  are defined in (6), where we must put  $\omega_2 = \omega_{20}$ .

In the nonrelativistic case  $\eta \ll \omega_1 \ll m$  and  $p \gg \eta$ , formula (7) simplifies to

$$\Delta\omega_2 = \frac{\eta^2}{12m} \left\{ 1 + \frac{\omega_1}{m} (1-t) + O\left(\frac{\omega_1^2}{m^2}\right) \right\}.$$
(8)

At  $\omega_2 \gg \varepsilon$  and  $p \gg \eta$  we have

$$\Delta\omega_{z} = \frac{\eta^{2}}{12m} \frac{3\varepsilon - 2m}{m} \left\{ 1 - \frac{\varepsilon - m}{\omega_{1}} \frac{3\varepsilon - 4m}{3\varepsilon - 2m} + O\left(\frac{\varepsilon^{2}}{\omega_{1}^{2}}\right) \right\}.$$
 (9)

The next term  $\sim \eta^4/m^3$  of the shift of the maximum can be obtained from (1) and (6) by numerical integration.

The width of the Compton peak is determined from (6) by the condition  $\Delta x \sim \eta$ . In terms of the variable  $\omega_2$  and at a fixed angle  $\vartheta$ , this condition takes the form

 $\Delta \omega_2 \sim \eta p \omega_{20} / (m \omega_1)$ ,

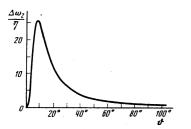


FIG. 2. Dependence of the width of the Compton line  $\Delta \omega_2$  on the scattering angle at  $\omega_1 = 100$ .

where we must put  $\omega_2 = \omega_{20}$  in the calculation of p. The width  $\Delta \omega_2$  of the Compton contour changes when the scattering angle changes in the following manner: 1)  $\Delta \omega_2 \sim \eta^2/m$  at  $\vartheta \sim \eta/\omega_1$  ( $p \le \eta$ ), 2)  $\Delta \omega_2 \sim \eta$  at  $\vartheta \sim m/\omega_1$ , 3)  $\Delta \omega_2 \sim \eta \omega_1/m$  at  $\vartheta \sim (m/\omega_1)^{1/2}$ , 4)  $\Delta \omega_2 \sim \eta$  at  $\vartheta \sim 1$ . The dependence of  $\Delta \omega_2$  on the angle  $\vartheta$  at  $\omega_1 = 100m$  is shown in Fig. 2. In the nonrelativistic case, the question of the width of the Compton line was considered by Sommerfeld<sup>8</sup> and by Dymond.<sup>10</sup>

Figure 3 shows the Compton-line contours calculated by formula (6). The region beyond the maximum of the contour was calculated by means of our general formula<sup>1, 2</sup> which takes into account only the principal terms of the expansion in  $\alpha Z$ . At small angles  $\vartheta$ , in accordance with the Schnaidt formula, the Compton maximum is decreased because of the factor  $\frac{1}{3}2^6e^{-4}$  $\approx 0.4$ , and the width of the Compton line is shortened in terms of the variable  $\omega_2(\Delta \omega_2 \sim \eta^2/m)$ . In addition, an appreciable part of the contour goes outside the physical region at small angles  $\vartheta$ . In the limit of small  $\alpha Z$  the boundary of the physical region ( $\vartheta = 0$ ) at  $p \to 0$ is  $x = \eta^2/2m$ , i.e., by virtue of  $\Delta x \sim \eta$  half of the maximum goes outside the limits of the physical region. With increasing Z, the fraction of the contour that goes

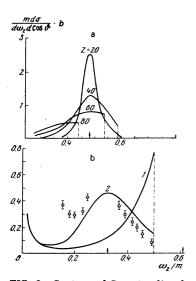


FIG. 3. Contour of Compton line for  $\omega_1 = 320$  keV. The arrow notes the position of the free Compton line, the dashed line shows the limit of the physical region. a) Form of the contour for different Z for a scattering angle 60°. b) Contour for scattering by holmium (Z = 67) for scattering angles 20° (curve 1) and 140° (curve 2). The experimental points for the angle 140° were taken from Ref. 11.

out of the physical region increases because of the positive shift of the maximum (7). This explains the apparent decrease of the width of the contour of the Compton line with increasing Z, which was observed by Spitale and Bloom,<sup>11</sup> wherein  $\omega_1 \sim \eta$ , and therefore the region of small angles  $\vartheta \leq \eta/\omega_1 \sim 1$ . The infrared growth of the cross section as  $\omega_2 \neq 0$  should, according to theoretical calculations, start at smaller  $\omega_2$  than given in experiment.<sup>11</sup>

Integrating formula (5) with respect to the energies of the secondary photons we obtain the distribution with respect to the angles of the final photons:

$$\frac{d\sigma}{dt} = \frac{d\sigma_0}{dt} [1 + (\alpha Z)^2 f(\omega_1, \vartheta)], \quad \vartheta \gg \frac{\eta}{\omega_1};$$
(10)

The function  $f(\omega_1, \vartheta)$  for arbitrary  $\omega_1$  and  $\vartheta$  was obtained by numerically integrating formula (5). At small  $\vartheta \leq \eta/\omega_1$  the angular distribution is determined by integrating the Schnaidt formula<sup>4</sup> over the photon energies  $\omega_2$ . Plots of the angular distribution against the angle  $\vartheta$  and the experimental data of Refs. 12–17 are shown in Fig. 4. We note that allowance for terms of order  $(\alpha Z)^2$  at  $Z \geq 50$  changes significantly the values for the angular and energy distributions of the photons obtained by us in Refs. 1 and 2 in the principal approximation in  $\alpha Z$  (the difference for Z = 70 is approximately by a factor of two), thus greatly improving the agreement between the formulas obtained in the present paper and the experimental data.

Integration of formula (10) with respect to the emission angles  $\vartheta$  leads to a total cross section for the Compton scattering with relative accuracy of the order of  $(\alpha Z)^2$ . The region of small angles  $\vartheta \leq \eta / \omega_1$ , for which (10) is not valid, makes a contribution of the

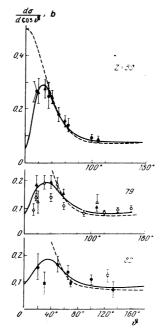


FIG. 4. Angular distribution of the photons in scattering of a beam of quanta of energy 662 keV by K electrons of tin, gold, and lead. Experimental points:  $\blacktriangle$ -from Ref. 12,  $\blacksquare$ -13,  $\Box$ -14,  $\bullet$ -15,  $\bigcirc$ -16,  $\triangle$ -17.

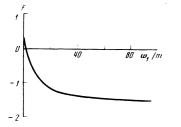


FIG. 5. The function  $F(\omega_1)$  in expression (11), which determines the correction to the total cross section.

order of  $(\alpha Z)^4$  to the cross section:

 $\sigma(\omega_i) = \sigma_0(\omega_i) \left[ 1 + (\alpha Z)^2 F(\omega_i) \right].$ 

(11)

A plot of the function  $F(\omega_1)$ , obtained by numerical integration, is shown in Fig. 5. At very large  $\omega_1 \gg m$  the function F tends to the limit

 $F(\omega_1) \rightarrow \ln 2 - \frac{s}{2} + O(1/\ln (2\omega_1/m)).$ 

We note that the correction of order  $(\alpha Z)^2$  in the angular distribution (10) and in the total cross section (11) does not vanish with increasing  $\omega_1$ .

<sup>1)</sup>By virtue of the influence of the wave functions of the initial and final electrons, the Coulomb parameter  $\xi = \alpha ZE/p$  in the expansion of the Green's function of the intermediate electron appears in the amplitude of the Compton effect on a bound atomic electron only starting with diagrams that include three Coulomb lines.

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## The adiabatic approximation in the problem of the collision of a particle with a bound two-particle system in the case of a separable interaction

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The Faddeev equations are solved in the adiabatic approximation, using separable potentials. The cross sections for dissociative attachment of electrons to diatomic molecules are computed on the basis of the obtained solutions, and a comparison with the experimental data is carried out.

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## INTRODUCTION

In this paper we consider the collision of a light particle of mass  $m_1$  with a bound system of two heavy particles (reduced mass  $m_{23} \gg m_1$ ) on the basis of the Faddeev equations.<sup>1</sup> The adiabatic approximation in this problem consists in the use of the solutions of the Faddeev equations for  $m_{23} \rightarrow \infty$  to compute the cross sections. If we represent the interaction of the particle  $m_1$  with each of the heavy particles in accordance with the model of zero-range potentials (ZRP), then for  $m_{23}$ 

 $\rightarrow \infty$  the Faddeev equations for the problem in question admit of an exact analytical solution, which has been found by Drukarev.<sup>2</sup>

In the present paper we show that the Faddeev equations in the adiabatic approximation also possess an exact analytical solution in the case when the interaction of the particle  $m_1$  with each of the heavy particles is represented by a separable potential.

As a specific example, we consider the reaction involving the dissociative attachment (DA) of an electron

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