

Taking the Coulomb effects into account in the reactions of one-electron charge exchange

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Abstract. Within the framework of a single mathematical approach based on the first iteration of the Dodd–Greider equations, direct and two-step mechanisms of electron capture have been described, and their correlation with angular distributions of reaction products have been ascertained. The purpose of this modification of the Dodd–Greider integral equations for the quantum mechanical operator of three-particle scattering with rearrangement is taking into account the Coulomb asymptotic behavior of wave functions in the problem of inelastic scattering with redistribution. On this basis, the theory of the reaction of single-electron charge exchange was constructed when collision of the hydrogen-like atom with a positively charged ion is performed with taking into account the effects of the multiple Coulomb scattering of electron by ion target residue. In particular, the amplitude of the reaction is distinguished as the first iterative term for solving the Dodd–Greider equations for the operator of three bodies, and the short-acting interaction that causes the electron transitions is taken into account in the distorting potential. It has shown that in the one-fold scattering approximation, this method leads to the so-called first Coulomb–Born approximation, where asymptotic behavior of particles in the input and output channels of the reaction is described by two-particle Coulomb wave functions. A more detailed study of the reaction of the resonance charge transfer between proton and hydrogen atom showed that without a correct inclusion of the Coulomb interaction into the wave function of the final state, to recreate Thomas’ peak in the angular distributions of the products of this reaction cannot be. The proposed method provides a good agreement with the experimental data of both complete and differential cross-sections due to advantages of this method, in particular, rather full consideration of the interaction after the collision and rapid convergence of the series of the Dodd–Greider perturbation theory.

Keywords: Coulomb interaction, operator of three-particle scattering with rearrangement, Thomas’ mechanism of charge exchange.

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1. Introduction

The details of the elementary processes in atomic collisions are necessary for solving many problems of nuclear physics and astrophysics, physics and chemistry of plasma and controlled thermonuclear synthesis, upper atmosphere physics, quantum electronics, and so on. Appearance of modern powerful ion accelerators [1] in many laboratories in the world allowed to get unique experimental material, especially on high-charged ions and multielectron ion-atomic processes, which in totality did stimulating influence on the theory of atomic collisions.

Experimental studies of charge exchange between protons and hydrogen or helium atoms [2, 3] confirmed the important role of the two-step electron capture mechanism, which was first considered on the basis of the classical mechanics by Thomas [4] and is called the Thomas mechanism of charge exchange. According to the model [4], the electron capture takes place as if in two stages: first, the flying particle is scattered by electron of target atom at the angle determined by kinematics of collision of two free particles which is called Thomas’ angle. In so doing, this flying particle causes the ionization of the target with the flight of electron at the angle 60° to the direction of the initial

beam, and then the emitted electron rescatters by ion-residue in the direction of motion of the fast particle and is captured by it in a bound state. Quantum-mechanical analogue of this mechanism of charge exchange is electron transitions through a continuous spectrum from a target atom into the states related with the fast particle.

With sufficiently large energies of particles, the two-step mechanism of electron capture is manifested in differential cross-sections at Thomas' angle in the form of maximum – Thomas' peak that is experimentally detected and is theoretically reproducible when the interaction is included in the final state, which is equivalent to taking into account many-time electron charge exchange by the residual ion. If, however, the charge exchange cross-sections are calculated without taking into account the interaction in the final state or in the one-time scattering approximation [5], the Thomas peak does not appear, but between theoretical and experimental cross-sections the qualitative differences arise.

The problem of describing the angular and energy dependences of the cross-sections of single-electron charge exchange between $A^{Z_\alpha^+}$ ions and B atoms:



became recently the object of not only experimental [2, 3], but also theoretical [5, 6, 7, 8] study. According to the multiparticle scattering theory, we consider a system consisting of a flying particle, active electrons, and residual ion. Since the interaction of particles that take part in the reactions is the Coulomb one, the basis for the theoretical description can be taken as the modified integral equations by Fadeev–Yakubovsky for systems of several charged particles [9]. However, the practical realization of the theoretical apparatus of integral equations is associated with considerable computational difficulties. In the transition to the systems with a large number of particles, the theoretical apparatus is sharply complicated and, accordingly, the ability to carry out a rigorous quantitative calculation of such systems reduces. The possibility of analytical solution of the system of integral equations with potentials close to interatomic interactions is rather an exception, but not rule.

Well-developed asymptotic (by large interatomic distances) methods of the theory of ion-atom collisions in our case do not work, because here, on the contrary, small interatomic distances are important [10, 11].

Along with the rigorous formulations of the problem of three bodies in the literature on the theory of scattering, there are some examples of approximate dynamical equations that are suitable for a number of cases and do not need the sophisticated technique to their solving necessary for finding solutions of exact equations. In the role of such equations, we give preference to the Dodd–Greider equations [12] for the scattering operator with the rearrangement in the system of three particles. The known difficulties of the

nonrelativistic quantum-mechanical problem of three-particle scattering with rearrangement (mathematical fundamentals of the multiparticle scattering theory [9]) are solved in the Dodd–Greider theory by introducing into consideration two complementary three-particle potentials that exclude the appearance of disconnected diagrams in the nucleus of the obtaining equation for the transition operator. Therefore, the iterative series obtained on the basis of this equation are manifested as the rapidly convergence ones in this problem, which allows us to carry out not only evaluation, but even exact direct calculations.

2. Application of the Dodd–Greider integral equations

The complex problem of the interaction of atom and ion in the reaction (1) considered here is an idealized problem of nonrelativistic interaction of three spinless particles: α (projectile A^{Z_α}), γ (active electron e^-) and β (target ion B^+) with the masses m_α , m_γ and m_β , respectively. The motion of the center of mass is assumed to be separated. According to the possibility of splitting the three-particle system into the fragments $(\beta, \gamma) + \alpha$, $(\alpha, \gamma) + \beta$, $(\alpha, \beta) + \gamma$, we introduce the channel Hamiltonians $H_j = H_0 + V_j$ ($j = \alpha, \beta, \gamma$) along with the full Hamiltonian $H = H_0 + V$, where H_0 is the operator of the kinetic energy of the system of three particles in the system of their center of mass, $V = \sum_{j=\alpha, \beta, \gamma} V_j$ being the full interaction. The lower index j in V_j defines a particle that does not take part in this interaction (for example, V_α is the operator of the pair interaction of the particles β and γ). We shall also define the channel “interaction” v_j . Let's assume that it can be represented in the form of a sum of the Coulomb and rapidly descending short-acting parts. Coordinates used to describe the relative position of particles are related by the following relationships (the above masses are denoted by a and b):

$$\vec{s} = (a/m_\gamma)\vec{x} - \vec{r}_\alpha, \quad \vec{x} = (b/m_\gamma)\vec{s} + \vec{r}_\beta, \quad \vec{R} = \vec{x} - \vec{s}. \quad (2)$$

In the terms of the corresponding Jacobian coordinates of the input and output channels of the reaction (1), the operator of the kinetic energy H_0 can be represented in two equivalent forms:

$$H_0 = -\frac{\Delta_{\vec{r}_\alpha}}{2\mu_\alpha} - \frac{\Delta_{\vec{x}}}{2a} = -\frac{\Delta_{\vec{r}_\beta}}{2\mu_\beta} - \frac{\Delta_{\vec{s}}}{2b}, \quad (3)$$

where $\Delta_{\vec{r}_\alpha}$, $\Delta_{\vec{x}}$, $\Delta_{\vec{r}_\beta}$, $\Delta_{\vec{s}}$ are the Laplace operators for the variables \vec{r}_α , \vec{x} , \vec{r}_β , and \vec{s} , respectively. The values μ_α and μ_β denote the reduced masses of the corresponding groups of particles:

$$\mu_\alpha = \frac{m_\alpha(m_\beta + m_\gamma)}{m_\alpha + m_\beta + m_\gamma}, \quad \mu_\beta = \frac{m_\beta(m_\alpha + m_\gamma)}{m_\beta + m_\alpha + m_\gamma}. \quad (4)$$

Let us separate the channel potentials v_j ($j = \alpha, \beta$) into two parts:

$$v_j = V - V_j = U_j + W_j, \quad (5)$$

one of which W_j (it is usually called the ‘‘distorting’’ potential) reveals small by the magnitude of the far-acting Coulomb background that defines the asymptotic behavior of wave functions of the scattering problem at long distances, and another $-U_j$ – gives the remainder generated by a purely short-acting part of the potential v_j that causes transitions of electron and is considered as perturbation.

From the definition of channel Hamiltonian $H_\alpha(H_\beta)$, it follows that it describes the asymptotic situation, when the particle $\alpha(\beta)$ does not interact with anything, and the other two particles are in the bound state in the potential $V_\alpha(V_\beta)$. Thus, the proper states $|\Phi_i^\alpha\rangle(|\Phi_f^\beta\rangle)$ of the Hamiltonian $H_\alpha(H_\beta)$ have the form of the products:

$$\begin{aligned} |\Phi_i^\alpha\rangle &= |\varphi_i(\bar{x})\exp(i\bar{k}_\alpha\bar{r}_\alpha)\rangle, \\ |\Phi_f^\beta\rangle &= |\varphi_f(\bar{s})\exp(i\bar{k}_\beta\bar{r}_\beta)\rangle, \end{aligned} \quad (6)$$

where $\varphi_i(\varphi_f)$ is the wave function of the bound state of the pair (β, γ) $((\alpha, \gamma))$, $\exp(i\bar{k}_\alpha\bar{r}_\alpha)$ ($\exp(i\bar{k}_\beta\bar{r}_\beta)$) is the plane wave describing the relative motion of free particles $\alpha(\beta)$ and (β, γ) $((\alpha, \gamma))$ in the initial (final) state with the relative momentum \bar{k}_α (\bar{k}_β). Strictly speaking, in the case of charged particles in (6) plane waves in the initial and final states should be distorted by phase factors, logarithmically dependent on the distance between particles [9]. This distortion is caused by the physical fact that the asymptotic motion of particles in the Coulomb field is never free, and the particles weakly interact at infinitely large distances between them. It follows that in the case of long-range action, the above definitions of channel Hamiltonians require modification.

With taking into account the comments made above, let us introduce for consideration the modified channel asymptotic states $|\Phi_i^{\alpha+}\rangle$ and $|\Phi_f^{\beta-}\rangle$, that, in distinct from $|\Phi_i^\alpha\rangle$ and $|\Phi_f^\beta\rangle$, correctly describe effects of the far-acting Coulomb field in the processes of charge exchange. Let's describe their structure. Let $\xi_\alpha = r_\alpha - \hat{k}_\alpha\bar{r}_\alpha$ ($\xi_\beta = r_\beta - \hat{k}_\beta\bar{r}_\beta$) are the parabolic coordinates of the particle $\alpha(\beta)$ before (after) collision;

\hat{k}_j ($j = \alpha, \beta$) are the unit vector in the direction of the vector \bar{k}_j : $\hat{k}_j = \bar{k}_j/k_j$. The functions $\Phi_i^{\alpha+}(\Phi_f^{\beta-})$ are the products of the wave functions by the bound state of pair (β, γ) $((\alpha, \gamma))$ and distorted plane wave $f_\alpha^+(f_\beta^-)$ with the unit amplitude:

$$\Phi_i^{\alpha+} = \varphi_i(\bar{x})f_\alpha^+(\bar{r}_\alpha) \equiv \varphi_i(\bar{x})\exp(i\bar{k}_\alpha\bar{r}_\alpha + i\sigma_\alpha), \quad (7)$$

$$\Phi_f^{\beta-} = \varphi_f(\bar{s})f_\beta^-(\bar{r}_\beta) \equiv \varphi_f(\bar{s})\exp(i\bar{k}_\beta\bar{r}_\beta - i\sigma_\beta). \quad (8)$$

The Coulomb phases σ_α and σ_β , distorting the plane waves, are defined by the equations:

$$\begin{aligned} \sigma_\alpha &= v_\alpha \ln(k_\alpha \xi_\alpha), \quad v_\alpha = n_\alpha/v, \quad \bar{v} = \bar{k}_\alpha/\mu_\alpha, \\ \sigma_\beta &= v_\beta \ln(k_\beta \xi_\beta), \quad v_\beta = n_\beta/v, \quad \bar{v} = \bar{k}_\beta/\mu_\beta. \end{aligned} \quad (9)$$

The parameter $n_\alpha(n_\beta)$ that characterizes the value of the effective Coulomb interaction is equal to the product of the total charge of the pair (β, γ) $((\alpha, \gamma))$ on the charge of the third particle $\alpha(\beta)$.

We will realize the further construction on the basis of separating the distorting potentials W_α and W_β into two parts:

$$W_\alpha = w_\alpha + W_{\alpha d}, \quad W_\beta = w_\beta + W_{\beta d}, \quad (10)$$

where w_α and w_β are arbitrary short-acting potentials, which depend on the relative coordinates \bar{r}_α and \bar{r}_β , respectively; it is assumed that these potentials descend enough rapidly at $r_j \rightarrow \infty$. We also assume that, for sufficiently large r_j , the potentials W_{jd} coincide with the purely Coulomb ones:

$$W_{\alpha d} \xrightarrow{r_\alpha \rightarrow \infty} W_{\alpha d}^c \equiv \frac{n_\alpha}{r_\alpha}, \quad W_{\beta d} \xrightarrow{r_\beta \rightarrow \infty} W_{\beta d}^c \equiv \frac{n_\beta}{r_\beta}, \quad (11)$$

where $W_{\alpha d}^c(W_{\beta d}^c)$ is the effective Coulomb potential acting between the particle $\alpha(\beta)$ and the center of mass of the system (β, γ) $((\alpha, \gamma))$. Denote with $H_{\alpha d}(H_{\beta d})$ the modulated channel Hamiltonian generated by the potential $W_{\alpha d}(W_{\beta d})$:

$$H_{\alpha d} = H_\alpha + W_{\alpha d}, \quad H_{\beta d} = H_\beta + W_{\beta d} \quad (12)$$

and will construct $W_{\alpha d}(W_{\beta d})$ in such calculation in order to satisfy the Schrödinger equations:

$$(H_{\alpha d} - E)\Phi_i^{\alpha+} = 0, \quad E = E_i + k_\alpha^2/2\mu_\alpha, \quad (13)$$

$$(H_{\beta d} - E)\Phi_f^{\beta-} = 0, \quad E = E_f + k_{\beta}^2/2\mu_{\beta}. \quad (14)$$

Here, $E_i(E_f)$ is the energy of the bound state of the pair (β, γ) $((\alpha, \gamma))$, E – total energy of the three-particle system. Introduction of the Hamiltonian $H_{\alpha d}(H_{\beta d})$ has deep physical reasons. Electron at any point in the space undergoes the influence of the Coulomb field of each center – a fact well known from the general quantum-mechanical problem of scattering by the Coulomb potential that distorts the phase of the scattered particle over the whole area of motion. So, perturbations $W_{\alpha d}, W_{\beta d}$, approximating the potential of a distant Coulomb center, must be taken into account in the channel (*i.e.*, zero) Hamiltonian [13].

Let us now define the full Green function (resolvent) of the system of three particles:

$$G^{\pm}(E) = (E - H \pm i\varepsilon)^{-1}. \quad (15)$$

Let's denote by $G_{\alpha d}^+(G_{\beta d}^-)$ Green's function of the model channel Hamiltonian $H_{\alpha d}(H_{\beta d})$:

$$\begin{aligned} G_{\alpha d}^+ &= (E - H_{\alpha d} \pm i\varepsilon)^{-1}, \\ G_{\beta d}^- &= (E - H_{\beta d} \pm i\varepsilon)^{-1}, \end{aligned} \quad (16)$$

where ε is the infinitely small positive number. Let us introduce in the consideration the wave operator by Möller $\omega_{\alpha}^+(\omega_{\beta}^-)$ [14], which transforms the channel eigenfunction $\Phi_i^{\alpha+}(\Phi_f^{\beta-})$ into a distorted wave $\chi_i^{\alpha+}(\chi_f^{\beta-})$ in the input (output) reaction channel (1):

$$|\chi_i^{\alpha+}\rangle = \omega_{\alpha}^+|\Phi_i^{\alpha+}\rangle, \quad |\chi_f^{\beta-}\rangle = \omega_{\beta}^-|\Phi_f^{\beta-}\rangle. \quad (17)$$

Now we introduce the $U_{\alpha\beta}^{\pm}$ [15], which possess such a property that their matrix elements between the Coulomb asymptotic states $|\Phi_i^{\alpha+}\rangle$ and $|\Phi_f^{\beta-}\rangle$ on the mass surface are the physical amplitudes of the transition $T_{\alpha\beta}^{\pm}$ from the channel α to the channel β in the “post” and “prior” formalisms according to:

$$T_{\alpha\beta}^{\pm} = \langle \Phi_f^{\beta-} | U_{\alpha\beta}^{\pm} | \Phi_i^{\alpha+} \rangle. \quad (18)$$

For the transition operators $U_{\alpha\beta}^{\pm}$, we may write the integral equations obtained and considered for the first time by Dodd and Greider [15]. Taking into account the further qualitative analysis, for an illustration we will write the equation for $U_{\alpha\beta}^-$:

$$\begin{aligned} U_{\alpha\beta}^- &= \omega_{\beta}^{-*}(\nu_{\alpha} - W_{\alpha})\omega_{\alpha}^+ + \\ &+ \omega_{\beta}^{-*}(\nu_{\beta} - W_{\beta})G_{\beta d}^-U_{\alpha\beta}^-. \end{aligned} \quad (19)$$

In the prior-formalism of this theory, the potential W_{β} is arbitrary, and the potential W_{α} should not lead to rearrangement in the channel β . The first term in the right side of the equation (19) leads to an amplitude in the Born approximation with distorted waves

$$\begin{aligned} T_{\alpha\beta}^-(DWB) &= \langle \Phi_f^{\beta-} | \omega_{\beta}^{-*}(\nu_{\alpha} - W_{\alpha})\omega_{\alpha}^+ | \Phi_i^{\alpha+} \rangle \equiv \\ &\equiv \langle \chi_f^{\beta-} | (\nu_{\alpha} - W_{\alpha}) | \chi_i^{\alpha+} \rangle. \end{aligned} \quad (20)$$

Although formally the equation (19) is accurate, its solution cannot be obtained as based on the approach associated with the use of standard methods of finding solutions of integral equations. The fact is that the core of the integral equation (19) contains disconnected diagrams that correspond to processes in which one of the particles does not interact with two other ones. Therefore, the arguments given in [15] raise doubts concerning the convergence of the Born series of the method of distorted waves, that is, iterative decomposition of the equation (19). This circumstance dictates the necessity of a certain rearrangement of the equation (19), which is similar to that performed when the equations of the multiple scattering theory and Faddeev's equations are derived [16]. The integral equations obtained as a result of the rearrangement, in contrast to (19), do not contain disconnected diagrams in their nuclei and can be solved by the standard methods. We will not describe here the bulky constructions that correspond to such a rearrangement of the equation (19), because they were considered in detail in the paper [12]. Let's bring only the final result. For this, we introduce the auxiliary potential ν_{κ} that corresponds to the virtual intermediate channel “ κ ”, as well as the corresponding to it Green's operator $g_{\kappa}^+ = (E - H + \nu_{\kappa} + i\varepsilon)^{-1}$. In these notations, the modified (with taking account the long-range nature of the Coulomb interactions) Dodd–Greider equation for quantum mechanical operator $U_{\alpha\beta}^-$ of a three-particle scattering with rearrangement results in the final form:

$$U_{\alpha\beta}^- = I + KU_{\alpha\beta}^-, \quad (21)$$

where

$$\begin{aligned} I &= \omega_{\beta}^{-*} [1 + (\nu_{\beta} - W_{\beta})g_{\kappa}^+] (\nu_{\alpha} - W_{\alpha})\omega_{\alpha}^+, \\ K &= \omega_{\beta}^{-*} (\nu_{\beta} - W_{\beta})g_{\kappa}^+ \nu_{\kappa} G_{\beta d}^+. \end{aligned} \quad (22)$$

The main advantage of Eq. (21) before Eq. (19) is that the arbitrariness in the choice of the potentials ν_{κ} and W_{β} can be used in order to obtain the equations with

predefined properties. Using (21), the amplitude of the transition $T_{\alpha\beta}^-$ (18) can be represented as follows:

$$T_{\alpha\beta}^- = \langle \Phi_f^{\beta-} | U_{\alpha\beta}^- | \Phi_i^{\alpha+} \rangle = \langle \Phi_f^{\beta-} | I | \Phi_i^{\alpha+} \rangle + \langle \Phi_f^{\beta-} | KU_{\alpha\beta}^- | \Phi_i^{\alpha+} \rangle = \langle \Phi_f^{\beta-} | I | \Phi_i^{\alpha+} \rangle + MS, \quad (23)$$

where MS are the terms that take into account the multiple rescattering. If assuming that the processes with multiple scattering do not affect the shape of the angular distribution, then the second term in (23) can be omitted. In this case, the amplitude of the reaction (1) in the prior-formalism is given by the expression:

$$T_{\alpha\beta}^- = \langle \Phi_f^{\beta-} | \omega_{\beta}^{-*} [1 + g_{\kappa}^+ (\nu_{\beta} - W_{\beta})] \times \langle \nu_{\alpha} - W_{\alpha} | \omega_{\alpha}^+ | \Phi_i^{\alpha+} \rangle = T_{\alpha\beta}^-(DWB) + \langle \Phi_f^{\beta-} | \omega_{\beta}^{-*} [g_{\kappa}^+ (\nu_{\beta} - W_{\beta})] (\nu_{\alpha} - W_{\alpha}) \omega_{\alpha}^+ | \Phi_i^{\alpha+} \rangle. \quad (24)$$

The comparison of the equations (20) and (24) shows that the first term $T_{\alpha\beta}^-$ in the right side of (24) indicates the amplitude of the direct one-step charge exchange mechanism within the Born approach with the distorted waves. The second term in (24) directly describes the two-step mechanism of electron capture through an intermediate state that is located in discrete or continuous spectrum. An analogous result takes place also for the amplitude of the transition $T_{\alpha\beta}^+$ in the post-formalism:

$$T_{\alpha\beta}^+ = \langle \Phi_f^{\beta-} | \omega_{\beta}^{-*} (\nu_{\beta} - W_{\beta}) \times \langle [1 + g_{\kappa}^+ (\nu_{\alpha} - W_{\alpha})] \omega_{\alpha}^+ | \Phi_i^{\alpha+} \rangle. \quad (25)$$

In conclusion, let us consider again the fundamental properties of the equation (21). From the formal point of view, it is difficult to be solved like to the Faddeev-type equations [9]. However, the equation (21) need not be precisely solved. The essence of this method is that there is only an iterative approximation for the operator that describes its system rearrangement. The Dodd–Greider theory [12] gives good results in the study of single- and double-electron processes with redistribution of particles [6, 8], since the second and higher orders of the series of perturbation theory, which are obtained when iterating the integral equation (21) for the transition operator $U_{\alpha\beta}^-$, do not contain in disconnected diagrams their nuclei, in contrast to the usual series of perturbation theory. Thus, transformation of the equation (19) to (21) of the type of the distorted waves method allows to obtain the iterative series (they are usually called quasi-Born or Coulomb–Born series) for the transition operator that, as shown in [6, 17, 18], converge rapidly, that is, the first iterations of the corresponding integral equations allows one to obtain a result that practically coincides with the exact solution.

3. Amplitude of the charge exchange

Let us transform the initial expression (24) for the amplitude of the reaction $T_{\alpha\beta}^-$. For this purpose, we introduce into consideration the scattering state vector $|\Psi_f^{\beta-}\rangle$ in such a manner:

$$|\Psi_f^{\beta-}\rangle = [1 + g_{\kappa}^{+*} (\nu_{\beta} - W_{\beta})] |\chi_f^{\beta-}\rangle. \quad (26)$$

We substitute (17) and (26) into (24), as a result we obtain the following representation for the amplitude of the reaction $T_{\alpha\beta}^-$ with taking into account the direct and two-step mechanisms:

$$T_{\alpha\beta}^- = \langle \Psi_f^{\beta-} | (\nu_{\alpha} - W_{\alpha}) | \chi_i^{\alpha+} \rangle. \quad (27)$$

To derive a differential equation for the wave function $\Psi_f^{\beta-}$, we multiply both parts of the equation (26) left by $(E - H + \nu_{\kappa}^* - i\varepsilon)$ and go to the boundary $\varepsilon \rightarrow +0$. As a result, we obtain the equation:

$$(E - H + \nu_{\kappa}^*) |\Psi_f^{\beta-}\rangle = \nu_{\kappa}^* |\chi_f^{\beta-}\rangle. \quad (28)$$

Since the search for solutions of the nonhomogeneous equation (28) with the real local potential ν_{κ} is related with great mathematical difficulties, then it is worthwhile to try replacing this potential with the operator. It is also necessary that the solution of the corresponding homogeneous equation permits the representation in the form:

$$|\Psi_f^{\beta-}\rangle = |\varphi_f(\bar{s}) h_{\beta}^- \rangle. \quad (29)$$

To separate the only solution from the set of solutions of the differential equation (28), we must supplement this equation with the boundary conditions:

$$\begin{aligned} \Psi_f^{\beta-} &\xrightarrow{r_{\beta} \rightarrow \infty} \Phi_f^{\beta-} = \varphi_f(\bar{s}) f_{\beta}^-(\bar{r}_{\beta}) = \\ &= \varphi_f(\bar{s}) \exp [ik_{\beta}^- \bar{r}_{\beta} - i\nu_{\beta} \ln(k_{\beta} \xi_{\beta})]. \end{aligned} \quad (30)$$

Substituting the function (29) into the equation (28), we obtain the equation with respect to h_{β}^- :

$$\begin{aligned} \varphi_f(\bar{s}) (E - E_f - H_0 - \nu_{\beta}) h_{\beta}^- + \\ + (1/b) \nabla_{\bar{s}} \varphi_f(\bar{s}) \nabla_{\bar{s}} h_{\beta}^- + \nu_{\kappa}^* (\varphi_f(\bar{s}) h_{\beta}^-) = 0. \end{aligned} \quad (31)$$

To eliminate the disconnected diagrams from the nucleus K (22), the operator ν_{κ} must be chosen so that it acts only on a variable \bar{s} , which is related to a pair subsystem

(α, γ) . This operator \mathfrak{v}_κ is derived, for example, from the formula:

$$\mathfrak{v}_\kappa \Psi = -(1/b) \nabla_{\vec{s}} \varphi_f(\vec{s}) \nabla_{\vec{s}} (\Psi / \varphi_f(\vec{s})) \quad (32)$$

on the set of elements $\Psi \in H$, where H is a subspace of states that corresponds to a continuous spectrum of the energy operator H [6]. Consequently, with the choice of the operator \mathfrak{v}_κ in the form (32), the nucleus K of the integral equation (21) is determined only by the terms to which fully disconnected diagrams correspond. This means that the iterative series of the equation (21) must converge faster in the broader energy region than the initial Born series in the three-body problem.

With taking into account the explicit form (32) of the operator \mathfrak{v}_κ and expression (3) for the operator of the kinetic energy H_0 , the equation (31) takes the form:

$$\left(E - E_f + \frac{\Delta_{\vec{r}_\alpha}}{2\mu_\alpha} + \frac{\Delta_{\vec{x}}}{2a} + \frac{Z_\beta}{x} - \frac{Z_\alpha Z_\beta}{R} \right) h_\beta^- = 0. \quad (33)$$

According to the formulas (29) and (30), the asymptotic behavior of the function h_β^- for $r_\beta \rightarrow \infty$ has the form of a distorted plane wave with the unit amplitude:

$$\begin{aligned} h_\beta^- \xrightarrow{r_\beta \rightarrow \infty} f_\beta^-(\vec{r}_\beta) = \\ = \exp \left[ik_\beta^- \vec{r}_\beta - \frac{iZ_\beta(Z_\alpha - 1)}{v'} \ln(k_\beta^- r_\beta + \vec{k}_\beta^- \vec{r}_\beta) \right]. \end{aligned} \quad (34)$$

In the case of the change $R \rightarrow r_\alpha$, the variables in the equation (33) are separated, and the corresponding wave functions are explicitly expressed in two-part terms:

$$h_\beta^- = C^{(-)} \mathfrak{R}^{(-)}(\vec{x}) \mathfrak{Z}^{(-)}(\vec{r}_\alpha). \quad (35)$$

The two-particle Coulomb wave functions of scattering $\mathfrak{R}^{(-)}(\vec{x})$ and $\mathfrak{Z}^{(-)}(\vec{r}_\alpha)$ are determined through a confluent hypergeometric function by equalities:

$$\begin{aligned} \mathfrak{R}^{(-)}(\vec{x}) = \Gamma \left(1 + \frac{iaZ_\beta}{q} \right) \exp \left(\frac{\pi a Z_\beta}{2q} \right) \times \\ \times \exp(i\vec{q}\vec{x}) F(-iaZ_\beta/q, 1, i\vec{q}\vec{x} - i\vec{q}\vec{x}), \end{aligned} \quad (36)$$

$$\begin{aligned} \mathfrak{Z}^{(-)}(\vec{x}) = \Gamma \left(1 - \frac{i\mu_\alpha Z_\alpha Z_\beta}{q_\alpha} \right) \exp \left(-\frac{\pi \mu_\alpha Z_\alpha Z_\beta}{2q} \right) \times \\ \times \exp(i\vec{q}_\alpha \vec{x}_\alpha) F(-i\mu_\alpha Z_\alpha Z_\beta/q, 1, i\vec{q}_\alpha \vec{x}_\alpha - i\vec{q}_\alpha \vec{x}_\alpha). \end{aligned} \quad (37)$$

The coefficient $C^{(-)}$ and variables \vec{q} and \vec{q}_α , which appear when separating the variables, can be determined by stitching h_β^- with the eikonal asymptotic limit (34) at $r_\beta \rightarrow \infty$.

Summing up, let us write the wave function of the finite state $\Psi_f^{\beta-}$ that describes the scattering the charged particle β by a hydrogen-like system (α, γ) in our problem:

$$\Psi_f^{\beta-} = \mu_\beta^{i\vec{v}'} \varphi_f(\vec{s}) \exp(i\vec{k}_\beta^- \vec{r}_\beta) \mathfrak{R}^{(-)}(\vec{x}) \mathfrak{Z}^{(-)}(\vec{r}_\alpha), \quad (38)$$

where

$$\mathfrak{R}^{(-)}(\vec{x}) = N^{(+)}(v'_i) F(-iv'_i, 1, -iv'_i x - i\vec{v}' \vec{x}),$$

$$v'_i = Z_\beta / v', \quad \vec{v} = \vec{k}_\beta^- / \mu_\beta,$$

$$\mathfrak{Z}^{(-)}(\vec{r}_\alpha) = N^{(-)}(v') F(iv', 1, -ik_\beta^- r_\alpha - i\vec{k}_\beta^- \vec{r}_\alpha),$$

$$N^{(+)}(v'_i) = \Gamma(1 + v'_i) \exp(\pi v'_i / 2),$$

$$N^{(-)}(v') = \Gamma(1 - v') \exp(\pi v' / 2).$$

The function $\Psi_f^{\beta-}$ takes into account interaction of the bound electron γ with the residual target ion β and interaction of heavy particles α and β between themselves. The wave function of the initial state $\chi_i^{\alpha+}$ is determined from [19]. Using these expressions for wave functions and transition operator [14], as well as the relations (27) and (38), we can obtain the following representation for the amplitude of the charge-transfer reaction with account of Coulomb interaction in the final state:

$$\begin{aligned} T_{\alpha\beta}^- = N(v, v_\alpha) \iint d\vec{r}_\alpha d\vec{x} \exp(i\vec{k}_\alpha \vec{r}_\alpha - i\vec{k}_\beta^- \vec{r}_\beta) \varphi_f^*(\vec{s}) \times \\ \times [Z_\alpha / r_\alpha - Z_\alpha / s] \varphi_i(\vec{x}) F(iv'_i, 1, iv'_i x + i\vec{v}' \vec{x}) \times \\ \times F(-iv_\alpha, 1, ik_\alpha r_\alpha - i\vec{k}_\alpha \vec{r}_\alpha) \times \\ \times F(-iv', 1, ik_\beta^- r_\alpha - i\vec{k}_\beta^- \vec{r}_\alpha), \end{aligned} \quad (39)$$

where

$$\begin{aligned} N(v, v_\alpha) = \mu_\beta^{-v'_i} \Gamma(1 + iv_\alpha) \Gamma(1 - iv'_i) (1 + iv') \times \\ \times \exp[-\pi(v_\alpha + v' - v'_i) / 2]. \end{aligned} \quad (40)$$

Calculation of the amplitude (39) in the general case, when $Z_\beta \neq 1$, is complicated by the presence of three confluent hypergeometric functions under the integral sign. However, there is an important special case when calculating the matrix element in (39) can be reduced to one-dimensional numerical integration. The above is related to the charge exchange reaction at the collision of proton (or some other charged particle: positron, nucleus *etc.*) with hydrogen atom ($Z_\beta = 1$). In this case, the

Coulomb parameter $\nu_\alpha = 0$ and the confluent hypergeometric function $F(-i\nu_\alpha, 1, ik_\alpha r_\alpha - i\bar{k}_\alpha \bar{r}_\alpha)$ in the formula (39) is equal to unity. We note that in our consideration the effects of multiple Coulomb rescattering of captured electron by the ion-residue of the target are already approximately summed up in the distorting factor $\mathfrak{R}^{(-)}(\bar{x})$.

For further calculations, we will use the expressions for wave functions of bound states [6, 14] and the integral representation for the confluent hypergeometric function [20]:

$$F(a, c, z) = \frac{1}{B(a, c-a)} \times \int_0^1 dt t^{(a-1)} (1-t)^{c-a-1} \exp(zt), \quad (41)$$

where $B(x, y)$ is the Euler beta-function [20] that simply expresses through the Γ -function ($B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$), and the integration must be carried out in the complex plane z , choosing the correct contour (dependent on a) that bypasses the points 0 and 1. Changing the order of integration for integrals included in (40) (the integral function possesses properties sufficient for such a transposition of integrals), we obtain the representation for $T_{\alpha\beta}^-$:

$$T_{\alpha\beta}^- = \frac{N(\nu, \nu_\alpha = 0)N_2}{B(iv'_t, 1 - iv'_t)B(-iv', 1 + iv')} \times \int_0^1 dt_1 t_1^{iv'_t-1} \int_0^1 dt_2 (1-t_2)^{iv'} I(t_1, t_2), \quad (42)$$

$$I(t_1, t_2) = \lim_{\varepsilon \rightarrow 0} Z_\alpha \left[\frac{\partial^2}{\partial \lambda_\alpha \partial \lambda_\beta} - \frac{\partial^2}{\partial \lambda_\beta \partial \varepsilon} \right] J, \quad (43)$$

$$J = \iint d\bar{x} d\bar{r}_\alpha \exp(-\bar{k}_\beta \bar{r}) \frac{\exp(-\lambda_\alpha s)}{s} \times \exp(i\bar{k}_\alpha \bar{r}_\alpha + i\bar{k}_\beta t_2) \frac{\exp(-\delta_1 r_\alpha)}{r_\alpha} \frac{\exp(-\delta_2 x)}{x} \exp(it_1 \bar{v} \bar{x}) \quad (44)$$

with $\delta_1 = \varepsilon - ik_\beta t_2$, $\delta_2 = \lambda_\beta - iv'_t$, $\lambda_\alpha = Z_\alpha$, $\lambda_\beta = Z_\beta$.

Using the results of our previous works [6, 14] for the matrix element J , we obtain:

$$J = \frac{16\pi^2 m_\gamma}{a^2} \int_0^\infty \frac{dx}{c_{11}x^2 + 2c_{12}x + c_{22}}, \quad (45)$$

where

$$c_{11} = |\bar{q}_1 - \bar{q}_2|^2 + (\rho_1 + \rho_2)^2, \\ c_{22} = [q_1^2 + (\rho_1 + \lambda_\alpha)^2][q_2^2 + (\rho_2 + \lambda_\alpha)^2], \\ c_{12} = \lambda_\alpha [|\bar{q}_1 - \bar{q}_2|^2 + (\rho_1 + \rho_2)^2] + \rho_2 [\lambda_\alpha^2 + q_1^2 + \rho_2^2] + \rho_1 [\lambda_\alpha^2 + q_1^2 + q_2^2].$$

Let us transform the formula (45) by separating the dependence of t_1 and t_2 in the explicit form in the denominator of the subintegral expression. After completing this transformation, the obtained expressions can be combined in the following representation for the amplitude of charge exchange

$$T_{\alpha\beta}^- = \frac{16\pi^2}{a^2} N(\nu, \nu_\alpha = 0) N_2 Z_\alpha \times \lim_{\varepsilon \rightarrow 0} \left(\frac{\partial^2}{\partial \lambda_\alpha \partial \lambda_\beta} - \frac{\partial^2}{\partial \lambda_\beta \partial \varepsilon} \right) \int_0^\infty \Pi(x) dx, \quad (46)$$

where

$$\Pi(x) = (B(iv'_t, 1 - iv'_t)B(-iv', 1 + iv'))^{-1} \times \int_0^1 dt_1 t_1^{iv'_t-1} \int_0^1 dt_2 \frac{(1-t_2)^{iv'}}{t_2^{iv'+1} (A + Bt_1 + Dt_2 + Ct_1 t_2)}. \quad (47)$$

Explicit expressions for the coefficients A , B , C , and D are given in Appendix. After integrating by t_1 and t_2 [20], the final expression for $\Pi(x)$ has the form:

$$\Pi(x) = A^{-1} (1 + D/A)^{-iv'} (1 + B/A)^{iv'} \times F\left(iv'_t, -iv, 1; \frac{BD - AC}{(A + D)(A + B)}\right). \quad (48)$$

We compare the proposed approach with the method of continuum distorted wave (CDW) approximation. For the first time, the CDW approach was used by Cheshire [21] for calculations of the cross-sections of resonance charge exchange of fast protons on hydrogen atoms. Later in his work [22] Gayet showed that the amplitude of the transition in the CDW approach can be obtained as the first quasi-Born term of series of the perturbation theory by Dodd-Greider [15] for the operator of three-particle scattering with rearrangement. It is worthwhile to emphasize that, in the standard CDW approximation, only the interaction before and after collisions of active electron with far removed core is taken into account. At large scattering angles, as it follows from the calculations of differential cross-sections of charge exchange in the eikonal approximation, an important role is played by interaction of the heavy particles α and β between themselves, which, however, is not taken into account in the CDW approximation.

4. Results of calculations

We consider the application of the foregoing formalism to the calculation of angular and energy dependences of the cross-sections of the reaction of charge exchange of proton on hydrogen atom:



This reaction represents a special interest and serves as a standard for checking different theories of processes with rearrangement, since in this case potentials of interaction in the channels and the wave functions of bound states are precisely known.

First, before proceeding to discuss the results of the investigating the reaction (49), let us note the following things. For the process (1), the scattering amplitude $T_{\alpha\beta}^-$ has a distinct maximum (in fact, there are two ones) within the region of small angles $\Theta \leq m_\gamma/\mu \ll 1$, $\mu = m_\alpha m_\beta / (m_\alpha + m_\beta)$. It is this area of the angles of scattering that is considered below. In the case of the reaction (49), when the particles α and β are protons, the exchange part of the scattering amplitude is negligibly small.

Results of calculations of total cross-sections with amplitudes from [19] (dashed curve) and equation (46) (solid curve) in comparison with the results of the CDW method (dashed-point curve) and the smoothed results of experiments [17] (dots) are presented in Fig. 1. With decreasing the velocity of colliding particles, the CDW approximation becomes incorrect [17] and, as seen from Fig. 1, leads to overestimated values of the cross-sections, but the proposed in this work model of approximation of distorted waves with accounting the Coulomb interaction in the final state is better agreed (Fig. 1, solid curve) with the experimental data.

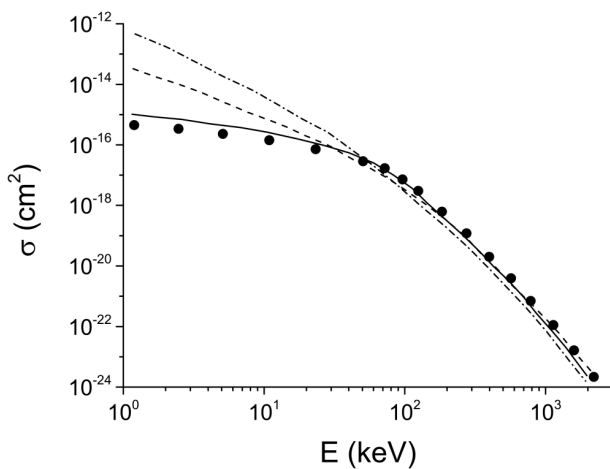


Fig. 1. Total cross-sections of the charge exchange process at the collision of proton with hydrogen atom.

The demands for the improvement of theoretical representations have led to the fact that main emphasis of theoretical and experimental works shifted from the study of integral values, which characterize different processes, to the study of the differential values that give more detailed information about the role of different mechanisms of the reaction and is more rigid test for theoretical models. In differential cross-sections of charge exchange, the two-step mechanism of electron capture is manifested in the form of a characteristic sharp maximum at the angle of scattering by Thomas Θ_T – Thomas' peak. Experimentally, the Thomas peak was first observed in the angular distributions of hydrogen atoms formed during the charge exchange of protons on helium [23] at an energy of several Mega-electron-Volts at the angle 0.5 milliradian.

The results of calculating the differential cross-sections of electron capture by protons in hydrogen with the amplitudes from the work [13] and equation (46) for two energy values are compared with the experimental

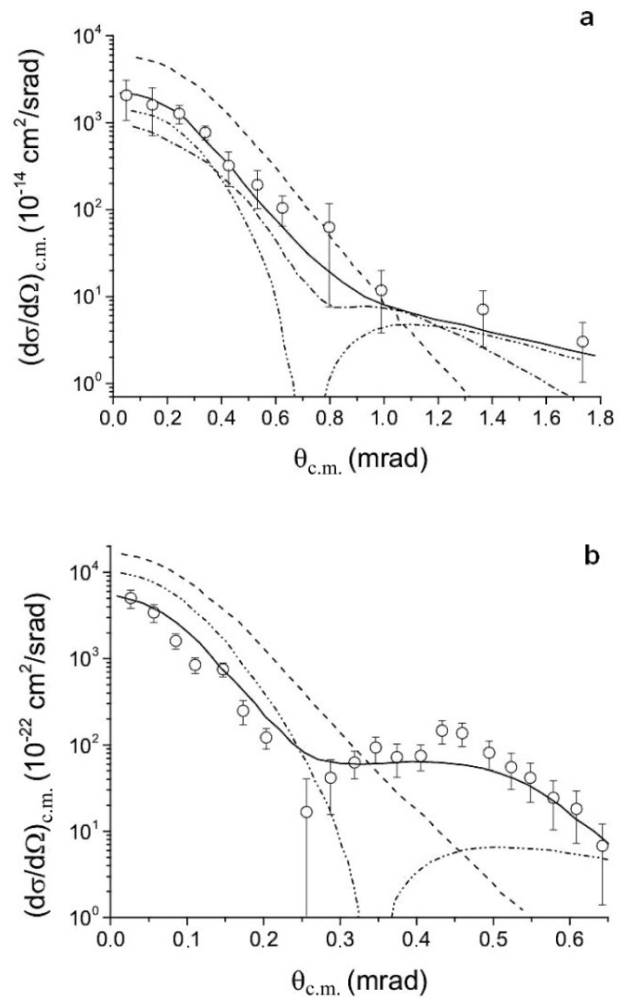


Fig. 2. Differential cross-sections of charge exchange of protons on hydrogen in dependence on the scattering angle in the coordinates of the center of mass system. The energy of protons is 125 keV (a) and 500 keV (b).

data [24], the results of the CDW method [17] and Oppenheimer–Brinkman–Kramer (OBK) approximation in Fig. 2. The greatest interest for methodical comparisons is calculations of angular distributions with the amplitude of simple one-step charge exchange mechanism [19] and calculations by formula (46), when into the analysis of the reaction (49), except for the one-step one, the two-step (Thomas’) electron capture mechanism is also included. It is seen that taking into account two-step effects leads to appearance of the pronounced maximum (Thomas’ peak) at the site of the Jackson–Schiff “laydown”, which is obtained within the framework of the simple one-step mechanism.

At large scattering angles, the interaction of heavy particles plays an important role, which, however, is not accounted in the CDW approximation. In our consideration, accounting of this interaction in the wave function of the finite state $\Psi_f^{\beta-}$ (multiplier $\mathfrak{S}^{(-)}(\vec{r}_\alpha)$ in the formula (39)) leads to a more smooth decrease of the cross-sections with the growth of the scattering angle, which corresponds to the observed experimental behavior of the cross-sections.

In conclusion, it should be emphasized that, when using the Coulomb–Born approximation, we neglect the effects of rescattering, that is, we do not take into account the possible multi-step mechanisms of the reaction. With increasing incident particles energy, we observe increase of the role of two-step transitions through the intermediate state that is located in a discrete or continuous spectrum. Quantitative description of these transitions becomes possible only with the total inclusion of the interaction after collision into the wave function of the final state, which is equivalent to accounting the effects of the multiple rescattering of electron by the ion-residue of target.

Appendix

Here are the expressions for the coefficients A , B , C , and D from (47):

$$\begin{aligned}
 A &= - \left(\frac{4bx}{m_\gamma} - \frac{2m_\gamma x^2}{a} - \frac{2b}{m_\gamma} (m_\gamma/a - b/m_\gamma)^2 k_\alpha^2 - \frac{2b}{m_\gamma} (\lambda_\alpha + m_\gamma \lambda_\beta/a)^2 \right) (\vec{k}_\alpha \vec{k}_\beta) + \\
 &+ 2 \left(k_\alpha^2 + \varepsilon^2 + \lambda_\alpha^2 + (b/m_\gamma)^2 k_\alpha^2 \right) x + \left(k_\alpha^2 + \varepsilon^2 + 2m_\gamma \varepsilon \lambda_\beta/a + (m_\gamma/a)^2 (k_\beta^2 + \lambda_\beta^2) \right) x^2 + \\
 &+ \left(k_\alpha^2 + (b/m_\gamma)^2 k_\beta^2 + (\varepsilon + \lambda_\alpha)^2 \right) \left((b/m_\gamma - m_\gamma/a)^2 k_\beta^2 + (\lambda_\alpha + m_\gamma \lambda_\beta/a)^2 \right). \\
 B &= 2 \left[(b/a - (m_\gamma/a)^2) (k_\alpha^2 + (b/m_\gamma)^2 k_\beta^2 - 2b(\vec{k}_\alpha \vec{k}_\beta)/m_\gamma + (\varepsilon + \lambda_\alpha)^2) - (m_\gamma/a)^2 x^2 \right] (\vec{k}_\beta \vec{v}') + \frac{m_\gamma}{a} \times \\
 &\times \left[(\vec{k}_\alpha \vec{v}') - i(\varepsilon + m_\gamma \lambda_\beta/a) v' \right] x^2 - i(b/a)^2 (k_\beta^2 - 2m_\gamma(\vec{k}_\alpha \vec{k}_\beta)/b + (m_\gamma/b)^2 (k_\alpha^2 + (\varepsilon + \lambda_\alpha)^2)) (a\lambda_\alpha/m_\gamma + \lambda_\beta) v' \Big]. \\
 C &= 2m_\gamma/a \left[\left(x^2 + 2(b/m_\gamma - m_\gamma/a) (\vec{k}_\alpha \vec{k}_\beta) - i(\varepsilon + \lambda_\alpha) k_\beta - bk_\beta^2/m_\gamma \right) (\vec{k}_\alpha \vec{v}') - (x^2 k_\beta + 2(\lambda_\alpha + m_\gamma \lambda_\beta/a) \times \right. \\
 &\left. \times ((\varepsilon + \lambda_\alpha) k_\beta + i((\vec{k}_\alpha \vec{k}_\beta) - bk_\beta^2/m_\gamma)) v' \right]. \\
 D &= 2 \left[\left(2x + x^2 + ((b/m_\gamma - m_\gamma/a)^2 k_\beta^2 + (\lambda_\alpha + m_\gamma \lambda_\beta/a)^2) \right) (\vec{k}_\alpha \vec{k}_\beta) - i(2\varepsilon x + (\varepsilon + m_\gamma \lambda_\beta/a) x^2 + (\varepsilon + \lambda_\alpha) \times \right. \\
 &\left. \times (\lambda_\alpha + m_\gamma \lambda_\beta/a)^2) k_\beta^2 - i(\varepsilon + \lambda_\alpha) (b/m_\gamma - m_\gamma/a)^2 k_\beta^3 - (b/m_\gamma) (b/m_\gamma - m_\gamma/a)^2 k_\beta^4 \right].
 \end{aligned}$$

5. Conclusion

As can be seen from the above discussion, the universal mathematical basis for construction of approximated charge exchange theory can be based on equations of the quantum scattering theory in systems of several particles, and the iterations of these equations form representation for the amplitudes in the form of the series (23), and the number of terms taken into account defines the order of rescattering.

Summing up the results of the theoretical studies of Thomas’ peak in differential cross-sections, first of all, it should be noted that the Coulomb rescattering of electron by the ion-residue of the target in the final state affects stronger than all the others on the form of the angular distributions, which is equivalent to rather total accounting the interaction after the collision. If so charge exchange cross-sections are calculated without accounting the Coulomb interaction in the final state or in the one-step approximation, then the Thomas peak does not occur in the angular distributions, and there are qualitative differences between the theoretical and experimental cross-sections. Fig. 2 shows the example of such a “direct” analysis of the experimental cross-section for the reaction (49) on the base of the formulae of the OBK approximation, which leads to increasing the cross-sections at small scattering angles and very fast their descending at large scattering angles.

In general, the obtained correlations of theoretical and experimental data allows one to conclude about the adequacy of the method of calculating differential cross-sections of charge exchange in the wide area of energies and proton scattering angles, which is based on the use in calculations of the amplitude of the first quasi-Born term of the iterative series the Dodd–Greider equation, modified for the Coulomb interaction.

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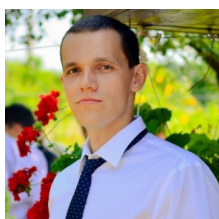
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