

Born Series in the Theory of Electron Impact Ionization of an Atom

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Abstract—In this review, a generalization of few-body quantum scattering theory is given for the case of Coulomb interaction. Since in this specific case the scattering amplitude, which is a solution to a resolvent-type equation, possesses a singularity when the complex parameter z tends to the energy shell, a definition of the physical amplitude is provided. A recipe for regularizing integrals (eliminating divergences), which describe the terms of a perturbation theory series for different perturbing potentials, is formulated. As an example, the general theory is applied to the calculations of differential cross sections for a quasi-elastic electron impact ionization reaction on atomic hydrogen.

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INTRODUCTION

As is known, the various integral equations satisfied by the wave functions or T -matrix [1, 2, 3, 4] can be used for determining the wave functions and transition amplitudes in multiparticle systems with short-range pair potentials. Since solving these equations completely is a very complicated task, approximate methods are frequently used, that with the expansion of wave functions and amplitudes in a Born series being a very widespread one. Here, the following aspect is crucial: if an entrance reaction channel corresponds to a collision of two fragments, then the terms of a Born series for the transition amplitudes have definite values close to (on) the energy shell. On the other hand, the case of particle systems with Coulomb interaction is much more intricate: a Born series, constructed according to the same scheme as in the case of short-range potentials, diverges upon taking the z parameter—a complex system energy—on the energy shell [5, 6]. As a result, the transition amplitudes also diverge on the energy shell (that is, there is no compensation of singularities coming from different order terms).

The reason for this phenomenon is well known: the standard formalism of the multichannel scattering theory, based on either integral Lippmann–Schwinger (LS) equations or resolvent-type integral equations (Faddeev, Weinberg–van Winter, and others), is not applicable to systems of charged particles. This is because of the so-called Coulomb singularities not being isolated in these equations (with the exception of the Veselova equations [1, 7] determining three-particle amplitude for the energies below the breakup threshold in which the two-particle Coulomb singularities are explicitly isolated). The existence of such singularities is predicted by the standard Coulomb scattering theory [3, 6, 8, 9] and, in fact,

follows from the general theory of infrared divergences in QED [10, 11]. However, isolation of Coulomb singularities related to the breakup of a system into three or more fragments in the resolvent-type equations has not been successful so far. The attempt to isolate a three-particle Coulomb singularity in the Faddeev equations undertaken in [12, 13] led to a homogeneous equation for the coefficient factor in front of the singularity. Establishing a relationship between the Faddeev components of the breakup amplitude was the only success of those studies.

To avoid the above-mentioned problems, systems of differential equations for the wave function components in the coordinate representation (Mercuriev equations) were formulated in order to describe the dynamics of systems of charged particles, whereas, for calculating the scattering amplitudes, various approximations based on either the distorted wave method in pair subsystems (e.g., Peterkop’s method of effective charges [14]) or the approximate expressions for the Coulomb wave function of three-particle systems as a whole (the Redmond–Mercuriev method [1, 15], Bencze approach [16], and others) were developed. Since the coordinate asymptotics of the multiparticle Coulomb wave function are quite complicated, especially in the so-called singular domains [1, 17], Mercuriev equations were not widespread in the study of dynamics of specific quantum systems. As for the approximate methods mentioned above, their main shortcoming is the problem of evaluating further approximations, behind which there emerges once again a question as to the properties of the solutions to the resolvent-type integral equations.

The history of the development of the multiparticle Coulomb scattering theory was several decades long,

with a substantial number of scientists and scientific schools participating in the process. Among the most famous Russian (Soviet) schools, the following should be mentioned. Petersburg (Leningrad) (L.D. Faddeev, S.P. Merkuriev, A.M. Veselova, Yu.A. Kuperin, A.A. Kvitsinskii, S.L. Yakovlev, et al.), Tashkent (A.M. Mukhamedzhanov, D.M. Latypov, A.S. Kadyrov, et al.), and Riga (R.K. Peterkop, M.K. Gailitis, et al.), Kyiv (V.F. Kharchenko, S.A. Shadchin, et al.). Of the numerous foreign scientists, one should mention the names of J. Dollard, D. Muhlerin, I.I. Zinnes, C. Chandler, A.G. Gibson, E. Prugovečki, J. Zorbas, E.O. Alt, L.P. Kok, H. van Haeringen, M.R.H. Rudje, M.J. Seaton, and many others. The seminal papers by V.A. Fock and J. Schwinger had a large influence on the development of the ideas. It is virtually impossible to cite every paper in the field we review; therefore, in what follows only citations required by the context will be referred to, and we will mainly follow our principal works in the course of review.

In this review, the problem of constructing the Born series for the amplitudes of multiple ionization processes is considered in the framework of the consistent Coulomb scattering quantum theory. What is it good for? The point is that a number of effective and physically transparent methods of studying the quantum structure of a target and mechanisms of scattering of several charged particles is based on the domination of the first approximation of some perturbative series. For example, the method of electron momentum spectroscopy (EMS), the theoretical foundations of which were given in [18, 19, 20], was experimentally implemented nearly 40 years ago [21–24]. In a nutshell, a target is bombarded by a monochromatic electron beam with sufficiently high energy E_0 . A great number of events are produced by the electrons from the incident beam. By using a coincidence circuit, only those events are selected in which an incoming electron, passing by some target electron at a small (at atomic scale) distance, instantly knocks that electron out of a target by means of Coulomb interaction, transferring to the latter a substantial part of its own kinetic energy. The energy and angular distributions of both secondary electrons are measured. Such a process is often called a quasi-elastic (e, 2e) reaction.

In a simplest case of coplanar geometry (when the momentum vectors of the incident and both secondary electrons lie in the same plane), a coincidence circuit registers the final electrons with the energies E_s and E_e outgoing at the angles θ_s and θ_e counted from the incident beam direction (for $\theta_s = \theta_e$ and $E_s = E_e$, the kinematics is symmetrical), thereby defining the momenta of final electrons \mathbf{p}_s and \mathbf{p}_e . Here, we consider the kinematics of quasi-elastic knock-out, which is close to free scattering kinematics with the angle between momenta \mathbf{p}_s and \mathbf{p}_e being approximately 90° and the energies $E_s \sim E_e \sim E_0/2$, i.e., close to those of free scattering. This restriction means that the virtual momen-

tum of a knocked-out electron in a target $q \ll p_s, p_e$ and its ionization potential $|\varepsilon_i| \ll E_s, E_e$.

In the EMS method, the kinematics of a studied pair collision is fixed in such a way as to reduce an effect of many electron system, containing a knocked-out electron, to two simple, yet fundamentally important, factors: a knocked-out electron has definite binding energy ε_i and (at the impact instant) momentum $-\mathbf{q}$ (momentum \mathbf{q} , opposite in direction, is a recoil one received by a final system; such a choice of signs is simply a tribute to the tradition). These quantities are fixed in the experiment by the conservation laws for pair collisions $E_0 + \varepsilon_i = E_s + E_e$ and $\mathbf{p}_0 - \mathbf{q} = \mathbf{p}_s + \mathbf{p}_e$ (a target mass is assumed to be infinitely large). By measuring E_0 , E_s , and E_e , we learn out of which single particle state (an atom orbital in atom or molecule) an electron is knocked out. The momenta \mathbf{p}_s and \mathbf{p}_e are fixed by the energies E_s and E_e and measured solid angles Ω_s and Ω_e . Let us repeat that the conditions under which a quasi-free collision takes place are $|\varepsilon_i| \ll E_s, E_e$ and $q \ll p_s, p_e$. Thus, the quantities ε_i and \mathbf{q} are restored by using a small but well-measured deviation of the kinematics of quasi-elastic (e, 2e) process from the kinematics of a fast electron scattering off a free electron at rest. The momentum \mathbf{q} may be measured by either slightly varying two final electron emission angles in their emission plane, or changing an orientation of incident electron beam with respect to that plane. As a result, the momentum distribution $|\varphi_i(\mathbf{q})|^2$ of a single particle state i with the ionization potential $|\varepsilon_i|$ is measured within virtually the entire range of physically relevant q values from zero to several atomic units.

The theory behind EMS method is based on a plane-wave first Born (impulse) approximation. Until recently, the real contribution of the higher order terms of a corresponding perturbative series was not studied in detail; however, estimating it is extremely important from the point of view of the information capacity of the EMS method. Firstly, a differential cross section of quasi-elastic processes is proportional to Q^{-4} , where $\mathbf{Q} = \mathbf{p}_0 - \mathbf{p}_s$ is the momentum transferred to the system, which is large for these reactions. The higher the energy of an incoming electron, the lower the differential cross section and the harder to measure it experimentally. Therefore, one can talk about “trade-off” energies, at which the contribution of higher Born terms may not be asymptotically small. Second, to assess the applicability of the first order approximation, it is necessary to calculate at least second order terms, and higher Born terms are described by the formally divergent integrals that need to be regularized by extracting in a certain way and then discarding divergent terms. Such a procedure was proposed by Popov [5]; similar results were also obtained by Zorbas [6]. In fact, the values of Sommerfeld Coulomb parameters (Coulomb numbers) of the scattering

channels were taken for the small parameters. Third, in this context it is required to develop a convenient scheme of calculating higher terms of a Born series.

Thus, an estimate of a higher Born terms' contribution to the amplitudes and differential cross sections of multiple ionization processes seems extremely urgent, inasmuch as without it the real value of the method, based on the domination of the first term of a perturbative series, becomes questionable. It should be noted that there is still no consistent investigation into an applicability area of EMS theory. Therefore, simple specific examples of application of the general formalism are considered in this work, in particular, the quasi-elastic reaction of hydrogen atom ionization.

Below, where not otherwise stated, the following atomic units $e = m_e = \hbar = 1$ are used when writing formulas.

1. DETERMINATION OF WAVE FUNCTIONS AND TRANSITION AMPLITUDES IN MULTIPARTICLE SYSTEMS WITH COULOMB INTERACTION

The notations, customary in the scattering theory and adopted in, e.g., [3, 25], are used. Specifically, H denotes the Hamiltonian of a multiparticle quantum system (with a centroidal motion already separated); its resolvent, or the full Green's function of a system, is denoted by $G(z) = (z - H)^{-1}$ and satisfies the LS equation (the second resolvent identity):

$$G(z) = G_\alpha(z) + G_\alpha(z)V^\alpha G(z),$$

where $G_\alpha(z) = (z - H_\alpha)^{-1}$ is the Green's function for the channel α , H_α is the corresponding channel Hamiltonian, and $V^\alpha = H - H_\alpha$ is a sum of the interaction pair potentials between particles that belong to different fragments colliding in the α channel.

A set of relative momenta $\mathbf{p}_{\beta\gamma}$ defining motion of n_α fragments colliding in the α channel is denoted by \mathbf{p}_α , whereas a set of spatial variables conjugate to \mathbf{p}_α are denoted by \mathbf{r}_α . In this case, the relative coordinate of particles i and j is written as \mathbf{r}_{ij} , while their relative momentum as \mathbf{k}_{ij} . Finally, the vector $|\phi_\alpha\rangle$ denotes a product of fragments' bound state wave functions, which define the α channel, with a total binding energy of $-\kappa_\alpha^2$.

In the notations used the unnormalized *in*- and *out*-asymptotes of the α channel have the form $|\phi_\alpha, \mathbf{p}_\alpha\rangle$ so that $H_\alpha|\phi_\alpha, \mathbf{p}_\alpha\rangle = E_\alpha|\phi_\alpha, \mathbf{p}_\alpha\rangle$, where E_α is the respective energy of the channel.

1.1. General Theory of the Wave Operators

As is known, in the case of multiparticle systems with short-range interaction pair potentials, the

asymptotic condition (see, for example, [1, 4, 25]), ensuring the existence of the wave operators $\Omega_{\pm\alpha}$

$$\Omega_{\pm\alpha} = s - \lim_{t \rightarrow \mp\infty} e^{iHt} e^{-iH_\alpha t} |\phi_\alpha\rangle, \quad (1.1)$$

where $s - \lim$ denotes a strong limit (a norm limit) and has the form

$$\int_0^{\mp\infty} dt \left\| V^\alpha e^{-iH_\alpha t} |\phi_\alpha, f_\alpha\rangle \right\| < \infty, \quad (1.2)$$

where $|f_\alpha\rangle$ belongs to the Hilbert functional space $\mathbb{L}^2(\mathbb{R}^{3n_\alpha-3})$ of the channel, does not hold for the potentials decreasing at infinity like $r^{-\gamma}$, $\gamma \leq 1$, in particular, for Coulomb interaction. This is related to the long-range nature of the Coulomb forces, under which the motion never becomes asymptotically free.

A necessary modification to the definition of the wave functions given in Eq. (1.1) was proposed by Dollard [26, 27],

$$\Omega_{\pm\alpha} = s - \lim_{t \rightarrow \mp\infty} e^{iHt} e^{-iH_\alpha t - i\chi_\alpha^\pm(t)} |\phi_\alpha\rangle. \quad (1.3)$$

The operator function $\chi_\alpha^\pm(t)$ commutes with the Hamiltonian H_α and in the momentum representation is the operator of multiplication by the function

$$\chi_\alpha^\pm(\mathbf{p}_\alpha, t) = \text{sgn}(t)(\eta_\alpha \ln|t| + A_\alpha). \quad (1.4)$$

In Eq. (1.4) the quantity

$$\eta_\alpha = \sum_{\beta, \gamma} \eta_{\beta\gamma} = \sum_{\beta, \gamma} \frac{Z_\beta Z_\gamma \mu_{\beta\gamma}}{p_{\beta\gamma}} \quad (1.5.1)$$

denotes the Coulomb parameter (Coulomb number, Sommerfeld parameter) of the α channel equal to the sum of Coulomb parameters of the fragment pair β and γ , $\mu_{\beta\gamma}$ is the reduced mass of these fragments, and

$$A_\alpha = \sum_{\beta, \gamma} \eta_{\beta\gamma} \ln \frac{2p_{\beta\gamma}^2}{\mu_{\beta\gamma}}, \quad (1.5.2)$$

stands for the so-called Dollard phase needed for matching, in the case of two charged particles, the wave function $\langle \mathbf{r} | \Omega_\pm | \mathbf{k} \rangle$ given by Eq. (1.3) and the two-particle Coulomb wave function

$$\psi_c^+(\mathbf{k}, \mathbf{r}) = e^{-\pi\eta/2} \Gamma(1 + i\eta) e^{i\mathbf{k}\mathbf{r}} \times {}_1F_1(-i\eta, 1; i\mathbf{k}\mathbf{r} - i\mathbf{k}\mathbf{r}). \quad (1.6)$$

Another possible representation of the wave functions Ω_α may be derived from Eq. (1.3) by substituting

the Dollard operator $e^{-iH_\alpha t - i\chi_\alpha^\pm(t)}$ for the Muhlerin–Zinnes operator $\mathbb{V}_\alpha^\pm e^{-iH_\alpha t}$ [28–30],

$$\Omega_{\pm\alpha} = s - \lim_{t \rightarrow \mp\infty} e^{iHt} \mathbb{V}_\alpha^\pm e^{-iH_\alpha t} |\phi_\alpha\rangle. \quad (1.7)$$

The operators \mathbb{V}_α^\pm in Eq. (1.7) add a corresponding logarithmic phase to the relative motion plane wave of the charged fragment pair,

$$\langle \rho_\alpha | \mathbb{V}_\alpha^\pm | f_\alpha \rangle = \int \frac{d\mathbf{p}_\alpha}{(2\pi)^{3(n_\alpha-1)}} \quad (1.8)$$

$$\times e^{i\langle \mathbf{p}_\omega, \mathbf{p}_\alpha \rangle \pm i \sum_{\beta\gamma} \ln(\rho_{\beta\gamma} r_{\beta\gamma} \mp \mathbf{p}_{\beta\gamma} r_{\beta\gamma})} f_\alpha(\mathbf{p}_\alpha),$$

where the symbol $e^{i\langle \mathbf{p}_\omega, \mathbf{p}_\alpha \rangle}$ denotes the relative motion plane wave in the channel chosen.

Note that, besides the Muhlerin–Zinnes operator, there are as well other time-independent operators, denoted in what follows as \mathcal{F}_α^\pm , which are asymptotically equivalent to the Dollard operator [28, 31]. This means that

$$\lim_{t \rightarrow \mp\infty} \left\| \left(e^{-iH_\alpha t - i\chi_\alpha^\pm(t)} - \mathcal{F}_\alpha^\pm e^{-iH_\alpha t} \right) | \phi_\alpha, f_\alpha \rangle \right\| = 0; \quad (1.9)$$

hence,

$$\Omega_{\pm\alpha} = s - \lim_{t \rightarrow \mp\infty} e^{iHt} \mathcal{F}_\alpha^\pm e^{-iH_\alpha t} | \phi_\alpha \rangle. \quad (1.10)$$

1.2. Stationary Theory of Coulomb Scattering

Relations (1.6), (1.7), and (1.10), defining the wave operators of multiparticle Coulomb scattering within the framework of the nonstationary theory, can be used to construct the stationary theory of Coulomb scattering. Here, one of the following methods is used: the method of Abel limits [1, 26], Cook's method [26], or the two-Hilbert-space scattering theory [32]. Let us briefly describe these approaches.

The method of Abel limits is based on the following statement [1, 26]: let $v(t)$ be a finite operator function for $t \in [0, \infty]$ with the limit $v_+ = \lim_{t \rightarrow \infty} v(t)$. Then,

$$v_+ = \lim_{\varepsilon \rightarrow 0} \varepsilon \int_0^\infty dt e^{-\varepsilon t} v(t). \quad (1.11)$$

Applying this statement to the operator $e^{iHt} e^{-iH_\alpha t - i\chi_\alpha^\pm(t)} | \phi_\alpha \rangle$, we obtain

$$\Omega_{\pm\alpha} | \mathbf{p}_\alpha \rangle = \lim_{\varepsilon \rightarrow 0} \varepsilon \int_0^\infty dt e^{-\varepsilon t \mp i(Ht - E_\alpha t - A_\alpha)} t^{\pm i\eta_\alpha} | \phi_\alpha, \mathbf{p}_\alpha \rangle \quad (1.12)$$

$$= e^{-\pi\eta_\alpha/2} \Gamma(1 \pm i\eta_\alpha) e^{\pm iA_\alpha}$$

$$\times \lim_{\varepsilon \rightarrow 0} \pm i\varepsilon G^{1 \pm i\eta_\alpha}(E_\alpha \pm i\varepsilon) | \phi_\alpha, \mathbf{p}_\alpha \rangle.$$

Because of the complex power of the Green's function found in Eq. (1.12), it is inconvenient for practical calculation. However [1, 6], the complex power can be transferred to the parameter ε in front of the Green's

function in Eq. (1.12), so that the wave operator is directly expressed through the first power of the full Green's function. To derive a corresponding expression [33] we define the operators $\Omega_{\pm\alpha}^{(0)}(\varepsilon) | \mathbf{p}_\alpha \rangle$ with the help of the relation

$$\Omega_{\pm\alpha}^{(0)}(\varepsilon) | \mathbf{p}_\alpha \rangle = \pm i\varepsilon G(E_\alpha \pm i\varepsilon) | \phi_\alpha, \mathbf{p}_\alpha \rangle. \quad (1.13)$$

This expression can be rewritten in the integral form

$$\Omega_{\pm\alpha}^{(0)}(\varepsilon) | \mathbf{p}_\alpha \rangle = \varepsilon \int_0^\infty dt e^{-\varepsilon t} e^{\mp iHt} e^{\pm iH_\alpha t} | \phi_\alpha, \mathbf{p}_\alpha \rangle, \quad (1.14.1)$$

so that

$$\varepsilon^{\mp i\eta_\alpha} \Omega_{\pm\alpha}^{(0)}(\varepsilon) | \mathbf{p}_\alpha \rangle = \int_0^\infty dt e^{-(t \pm i\eta_\alpha \ln t \pm iA_\alpha)} \quad (1.14.2)$$

$$\times \left[e^{\mp iHt/\varepsilon} e^{\pm iH_\alpha t/\varepsilon} e^{-i\chi_\alpha^\pm(\mathbf{p}_\omega, \mp t/\varepsilon)} \right] | \phi_\alpha \rangle | \mathbf{p}_\alpha \rangle.$$

Taking the limit $\varepsilon \rightarrow 0$ in Eq. (1.14.2) and keeping in mind that the expression in square brackets converges to $\Omega_{\pm\alpha}$, we obtain

$$\lim_{\varepsilon \rightarrow 0} \varepsilon^{\mp i\eta_\alpha} \Omega_{\pm\alpha}^{(0)}(\varepsilon) | \mathbf{p}_\alpha \rangle = \Omega_{\pm\alpha} | \mathbf{p}_\alpha \rangle \int_0^\infty dt e^{-(t \pm i\eta_\alpha \ln t \pm iA_\alpha)} \quad (1.15)$$

$$= \Gamma(1 \mp i\eta_\alpha) e^{\mp iA_\alpha} \Omega_{\pm\alpha} | \mathbf{p}_\alpha \rangle.$$

As a result, the following chain of equalities is derived:

$$\Omega_{\pm\alpha} | \mathbf{p}_\alpha \rangle = \lim_{\varepsilon \rightarrow 0} \frac{\varepsilon^{\mp i\eta_\alpha}}{\Gamma(1 \mp i\eta_\alpha)} e^{\pm iA_\alpha} \Omega_{\pm\alpha}^{(0)}(\varepsilon) | \mathbf{p}_\alpha \rangle$$

$$= \lim_{\varepsilon \rightarrow 0} \frac{\varepsilon^{\mp i\eta_\alpha}}{\Gamma(1 \mp i\eta_\alpha)} e^{\pm iA_\alpha} (\pm i\varepsilon) G(E_\alpha \pm i\varepsilon) | \phi_\alpha, \mathbf{p}_\alpha \rangle \quad (1.16)$$

$$= \lim_{\varepsilon \rightarrow 0} \frac{e^{-\pi\eta_\alpha/2 \pm iA_\alpha}}{\Gamma(1 \mp i\eta_\alpha)} (\pm i\varepsilon)^{1 \mp i\eta_\alpha} G(E_\alpha \pm i\varepsilon) | \phi_\alpha, \mathbf{p}_\alpha \rangle.$$

For the limit in (1.16) to exist, it is necessary to demand that the structure of the primary (pole or cluster) singularities of the full Green's function be described by [1, 8, 9, 28]

$$G(z) = \sum_\beta u_\beta(z) \langle \phi_\beta | (z - H_\beta)^{-1 \pm i\eta_\beta} + g(z) \quad (1.17)$$

and the choice of the sign in front of $i\eta_\beta$ be fixed by the sign of $\text{Im} z$ (a minus sign for $\text{Im} z > 0$ and vice versa). The β indices in (1.17) are in fact channel indices with $\beta = 0$ ($\kappa_0^2 = 0$) and $\phi_0(\mathbf{k}_0) \equiv 1$ for the channel of a system breakup to N initial particles. The operators $u_\beta(z)$ are called *in*-components of the full Green's function, while the function $g(z)$ is known to be free of singularities $(\pm i\varepsilon)^{-1 \pm i\eta_\beta}$ on the energy shell (though, perhaps,

possesses other types of singularities). Comparison of (1.16) and (1.17) shows that there is a relation,

$$\Omega_{\pm\alpha}|\mathbf{p}_\alpha\rangle = \frac{e^{-\pi\eta_\alpha/2 \pm iA_\alpha}}{\Gamma(1 \mp i\eta_\alpha)} u_\alpha(E_\alpha \pm i0)|\mathbf{p}_\alpha\rangle. \quad (1.18)$$

This result (1.18) is consistent with the definition of the wave operators given in (1.12). To prove this statement by the example with the operator $\Omega_{+\alpha}$, let us consider the identity

$$G^{1+i\eta}(E+i\varepsilon) \equiv \int_{-\infty}^{\infty} \frac{dx}{(-2\pi i)(x-H+i\varepsilon_1)} \frac{1}{(E-x+i\varepsilon_2)^{1+i\eta}}, \quad (1.19)$$

with $\varepsilon_{1,2} > 0$ and $\varepsilon = \varepsilon_1 + \varepsilon_2$. From (1.16), (1.17), and (1.19) it follows that

$$\begin{aligned} \Omega_{+\alpha}|\mathbf{p}_\alpha\rangle &= e^{-\pi\eta_\alpha/2 + iA_\alpha} \Gamma(1+i\eta_\alpha) \\ &\times \lim_{\varepsilon \rightarrow 0} i\varepsilon \int_{-\infty}^{\infty} \frac{dx}{(-2\pi i)} \frac{G(x+i\varepsilon_1)}{(E_\alpha-x+i\varepsilon_2)^{1+i\eta_\alpha}} |\phi_\alpha, \mathbf{p}_\alpha\rangle \quad (1.20) \\ &= e^{-\pi\eta_\alpha/2 + iA_\alpha} \Gamma(1+i\eta_\alpha) I_\alpha u_\alpha(E_\alpha+i0)|\mathbf{p}_\alpha\rangle. \end{aligned}$$

In (1.20)

$$\begin{aligned} I_\alpha &= \lim_{\varepsilon \rightarrow 0} i\varepsilon \int_{-\infty}^{\infty} \frac{dx}{(-2\pi i)} \frac{1}{(x-E_\alpha+i\varepsilon_1)^{1-i\eta_\alpha}} \\ &\times \frac{1}{(E_\alpha-x+i\varepsilon_2)^{1+i\eta_\alpha}} = \frac{1}{\Gamma(1+i\eta_\alpha)\Gamma(1-i\eta_\alpha)}, \quad (1.21) \end{aligned}$$

from which it is easily seen that formula (1.20) is directly transformed into (1.18).

The operators \mathcal{F}_α^\pm are assumed to be finite while formulating the scattering theory in a pair of Hilbert spaces. Then, the following relation holds for the wave operators [31]:

$$\Omega_{\pm\alpha}|\mathbf{p}_\alpha\rangle = \lim_{\varepsilon \rightarrow 0} \pm i\varepsilon G(E_\alpha \pm i\varepsilon) \mathcal{F}_\alpha^\pm |\phi_\alpha, \mathbf{p}_\alpha\rangle. \quad (1.22)$$

With the help of the second resolvent identity and the relation

$$\begin{aligned} &\pm i\varepsilon G_\alpha(E_\alpha \pm i\varepsilon) \mathcal{F}_\alpha^\pm |\phi_\alpha, \mathbf{p}_\alpha\rangle \\ &= \mathcal{F}_\alpha^\pm |\phi_\alpha, \mathbf{p}_\alpha\rangle + G_\alpha(E_\alpha \pm i\varepsilon) [H_\alpha, \mathcal{F}_\alpha^\pm] |\phi_\alpha, \mathbf{p}_\alpha\rangle, \quad (1.23) \end{aligned}$$

expression (1.22) can be rewritten in the form of the modified LS representation

$$\begin{aligned} \Omega_{\pm\alpha}|\mathbf{p}_\alpha\rangle &= \mathcal{F}_\alpha^\pm |\phi_\alpha, \mathbf{p}_\alpha\rangle \\ &+ G(E_\alpha \pm i0) (V^\alpha \mathcal{F}_\alpha^\pm + [H_\alpha, \mathcal{F}_\alpha^\pm]) |\phi_\alpha, \mathbf{p}_\alpha\rangle. \quad (1.24) \end{aligned}$$

The transition operators in the form of the commutators $[H_\alpha, \mathcal{F}_\alpha^\pm]$ were first introduced to scattering theory in [34, 35]. In particular, if the channel α corresponds to the collision of two charged fragments, the

operators $\mathcal{F}_\alpha^\pm |\phi_\alpha\rangle$ can be chosen as $\omega_{\pm\alpha}$; these new wave operators correspond to purely Coulomb scattering on the potential $V_c^\alpha = \frac{Z_{1\alpha} Z_{2\alpha}}{\rho_\alpha}$. In this case, the following expression holds true:

$$\begin{aligned} \Omega_{\pm\alpha}|\mathbf{p}_\alpha\rangle &= \omega_{\pm\alpha}|\mathbf{p}_\alpha\rangle \\ &+ G(E_\alpha \pm i0) (V^\alpha - V_c^\alpha) \omega_{\pm\alpha}|\mathbf{p}_\alpha\rangle, \quad (1.25) \end{aligned}$$

which corresponds to the representations of the multi-channel scattering wave operators in the distorted wave method [3, 28, 36].

In Cook's method, the question of existence of the limit of a function at $t \rightarrow \infty$, defined and continuously differentiable for $t \geq 0$, reduces to that of derivative integrability of this function, since

$$\lim_{t \rightarrow \infty} f(t) = f(0) + \lim_{t \rightarrow \infty} \int_0^t d\tau f'(\tau).$$

As comes to the wave operators, the integrability of the respective operator function's norm on the half-open interval $[0, \infty)$ is exactly the asymptotic condition of their existence [3, 25, 26, 31] and, in the case of short-range pair potentials, this condition has the form given in (1.2). In [31] Cook's method was applied to the wave operator representation of Coulomb scattering in the formulation by Muhlerin–Zinnes, and it was shown that the wave operators $\Omega_{\pm\alpha}|\mathbf{p}_\alpha\rangle$ satisfy LS representation (1.24) with the operators \mathcal{F}_α^\pm replaced by the asymptotic operators \mathcal{V}_α^\pm .

1.3. Transition Amplitudes

By employing the formalism presented above one can describe the singularity structure of the transition operator matrix elements. There are two ways to write the latter:

post

$$T_{\beta\alpha}(z) = \langle \phi_\beta | V^\beta + V^\beta G(z) V^\alpha | \phi_\alpha \rangle \quad (1.26.1)$$

and *prior*

$$\tilde{T}_{\beta\alpha}(z) = \langle \phi_\beta | V^\alpha + V^\beta G(z) V^\alpha | \phi_\alpha \rangle, \quad (1.26.2)$$

with the difference between their matrix elements $\langle \mathbf{p}_\beta | T_{\beta\alpha}(z) - \tilde{T}_{\beta\alpha}(z) | \mathbf{p}_\alpha \rangle$ on the energy shell $z = E_\alpha + i0 = E_\beta + i0$ equal to zero, which is easily verifiable (see, e.g., [25]). The transition operator (in what follows, we consider *post*-form for convenience) by definition is connected to the full Green's function of the problem at hand in the following manner:

$$G(z) = (z - H_\beta)^{-1} |\phi_\beta\rangle T_{\beta\alpha}(z) \langle \phi_\alpha | (z - H_\alpha)^{-1} + \tilde{G}(z),$$

where the function $\tilde{G}(z)$ does not possess cluster singularities of the channels α and β simultaneously (for details, see [3]). The matrix elements (1.26) in the case

of short-range pair potentials define a finite transition amplitude between α and β channels on the energy shell [3, 25], whereas in the case of Coulomb interaction between particles, when pole singularities of the Green's function has the form (1.17), the matrix elements considered possess singularities of the types $(z - E_\alpha)^{i\eta_\alpha}$

and $(z - E_\beta)^{i\eta_\beta}$ (see also [37]). This means that when the parameter z is on the energy shell in both channels ($E_\alpha = E_\beta = E$), the expression of the type

$$t_{\beta\alpha}(\mathbf{p}_\beta, \mathbf{p}_\alpha; E + i0) = \frac{e^{-\pi/2(\eta_\beta + \eta_\alpha)} e^{i(A_\beta + A_\alpha)}}{\Gamma(1 - i\eta_\alpha)\Gamma(1 - i\eta_\beta)} \times \lim_{z \rightarrow E + i0} e^{-i(\eta_\beta + \eta_\alpha)\ln(z - E)} \langle \mathbf{p}_\beta | T_{\beta\alpha}(z) | \mathbf{p}_\alpha \rangle \quad (1.27)$$

is finite. With the help of formulas (1.13) and (1.26), it can be represented in the following way:

$$t_{\beta\alpha}(\mathbf{p}_\beta, \mathbf{p}_\alpha; E + i0) = \frac{e^{-\pi/2(\eta_\beta + \eta_\alpha)} e^{i(A_\beta + A_\alpha)}}{\Gamma(1 - i\eta_\alpha)\Gamma(1 - i\eta_\beta)} \times \lim_{\varepsilon \rightarrow 0} (i\varepsilon)^{i(\eta_\alpha + \eta_\beta)} \begin{cases} \langle \mathbf{p}_\beta, \phi_\beta | V_\beta^\beta \Omega_{+\alpha}^{(0)}(\varepsilon) | \mathbf{p}_\alpha \rangle \\ \langle \mathbf{p}_\beta | \Omega_{-\beta}^{(0)+}(\varepsilon) V_\alpha^\alpha | \mathbf{p}_\alpha, \phi_\alpha \rangle. \end{cases} \quad (1.28)$$

Indeed, expression (1.13), with the help of the second resolvent identity, can be brought to the form

$$\Omega_{\pm\alpha}^{(0)}(\varepsilon) | \mathbf{p}_\alpha \rangle = [I + G(E_\alpha \pm i\varepsilon) V_\alpha^\alpha] | \phi_\alpha, \mathbf{p}_\alpha \rangle,$$

so that

$$\langle \mathbf{p}_\beta, \phi_\beta | V_\beta^\beta \Omega_{+\alpha}^{(0)}(\varepsilon) | \mathbf{p}_\alpha \rangle = \langle \mathbf{p}_\beta | T_{\beta\alpha}(E + i\varepsilon) | \mathbf{p}_\alpha \rangle. \quad (1.29.1)$$

Analogously,

$$\langle \mathbf{p}_\beta | \Omega_{-\beta}^{(0)+}(\varepsilon) V_\alpha^\alpha | \mathbf{p}_\alpha, \phi_\alpha \rangle = \langle \mathbf{p}_\beta | \tilde{T}_{\beta\alpha}(E + i\varepsilon) | \mathbf{p}_\alpha \rangle. \quad (1.29.2)$$

If, for example, the entrance channel of the reaction contains no more than a single charged fragment ($\eta_\alpha = 0$), the amplitude of such a process, taking into account (1.16), can be written in a more customary form via the full wave function Ψ_β^- (\mathbf{p}_β) of the problem's exit channel,

$$t(\mathbf{p}_\beta, \mathbf{p}_\alpha; E + i0) = \langle \Psi_\beta^- | V_\beta^\alpha | \phi_\alpha, \mathbf{p}_\alpha \rangle. \quad (1.30)$$

We now express the S -matrix elements, which by definition are

$$S_{\beta\alpha}(\mathbf{p}_\beta, \mathbf{p}_\alpha) = \langle \mathbf{p}_\beta | \Omega_{-\beta}^+ \Omega_{+\alpha} | \mathbf{p}_\alpha \rangle, \quad (1.31)$$

in terms of the quantities $t_{\beta\alpha}$,

$$\langle \mathbf{p}_\beta | S_{\beta\alpha} | \mathbf{p}_\alpha \rangle = -2\pi i \delta(E_\alpha - E_\beta) t_{\beta\alpha}(\mathbf{p}_\beta, \mathbf{p}_\alpha; E + i0). \quad (1.32)$$

To derive formulas (1.32), let us proceed as follows. In the S -matrix elements (1.31), we write down each of the wave operators in the form of the time limit (1.3)

and the products of limits with for the limit of products. As a result, we obtain

$$\langle \mathbf{p}_\beta | S_{\beta\alpha} | \mathbf{p}_\alpha \rangle = e^{i(A_\alpha + A_\beta)} \lim_{t \rightarrow +\infty} t^{i(\eta_\alpha + \eta_\beta)} \times e^{i(E_\alpha + E_\beta)t} \langle \phi_\beta, \mathbf{p}_\beta | e^{-2iHt} | \mathbf{p}_\alpha, \phi_\alpha \rangle. \quad (1.33)$$

Now, we cast the matrix element in the right hand side of (1.33) down to the integral representation via the Green's function,

$$\langle \phi_\beta, \mathbf{p}_\beta | e^{-2iHt} | \mathbf{p}_\alpha, \phi_\alpha \rangle = \lim_{\varepsilon \rightarrow 0} \int_{-\infty}^{\infty} \frac{dE}{(-2\pi i)} e^{-2iEt} \times \langle \phi_\beta, \mathbf{p}_\beta | G(E + i\varepsilon) | \mathbf{p}_\alpha, \phi_\alpha \rangle, \quad (1.34)$$

and then twice apply to it the second resolvent identity. In this case, from (1.34), it follows that

$$\langle \mathbf{p}_\beta | S_{\beta\alpha} | \mathbf{p}_\alpha \rangle = e^{i(A_\alpha + A_\beta)} (I_1 + I_2), \quad (1.35)$$

$$I_1 = \lim_{t \rightarrow +\infty} t^{i(\eta_\alpha + \eta_\beta)} e^{i(E_\alpha + E_\beta)t} \langle \phi_\beta, \mathbf{p}_\beta | \mathbf{p}_\alpha, \phi_\alpha \rangle, \quad (1.36)$$

$$I_2 = \lim_{t \rightarrow +\infty} \lim_{\varepsilon \rightarrow 0} \int_{-\infty}^{\infty} \frac{dE}{(-2\pi i)} \frac{t^{i\eta_\beta} e^{-i(E - E_\beta)t}}{(E - E_\beta + i\varepsilon)^{1 - i\eta_\beta}} \times \frac{t^{i\eta_\alpha} e^{-i(E - E_\alpha)t}}{(E - E_\alpha + i\varepsilon)^{1 - i\eta_\alpha}} [(E - E_\beta + i\varepsilon)^{-i\eta_\beta} \times \langle \mathbf{p}_\beta | T_{\beta\alpha}(E + i\varepsilon) | \mathbf{p}_\alpha \rangle (E - E_\alpha + i\varepsilon)^{-i\eta_\alpha}]. \quad (1.37)$$

By applying to I_2 the limit relations for the asymptote of the Fourier transformations of generalized functions [1, 38],

$$\lim_{t \rightarrow +\infty} \frac{t^{i\eta} e^{-ixt}}{(x \pm i0)^{1 - i\eta}} = \begin{cases} -2\pi i \delta(x) \frac{e^{-\pi\eta/2}}{\Gamma(1 - i\eta)}, & \text{for } +i0; \\ 0, & \text{for } -i0, \end{cases} \quad (1.38)$$

we find

$$I_2 = -2\pi i e^{-i(A_\alpha + A_\beta)} \delta(E_\alpha - E_\beta) \times t_{\beta\alpha}(\mathbf{p}_\beta, \mathbf{p}_\alpha; E_\alpha + i0). \quad (1.39)$$

The term I_1 in the case of short-range pair potentials is equal to $\delta_{\alpha\beta}$. In the case at hand, when at least one of the Coulomb parameters η_α or η_β does not equal zero, this term equals zero for $\alpha = \beta$ by virtue of the Riemann–Lebesgue lemma (in a weak sense) [1, 3, 26, 39, 40]. From the latter and (1.35), the result given by (1.32) follows.

1.4. Distorted Wave Method

By analogy with (1.13), let us introduce into consideration the following operator:

$$\tilde{\Omega}_{\pm\alpha}(\varepsilon) | \mathbf{p}_\alpha \rangle = \pm i\varepsilon G(E_\alpha \pm i\varepsilon) \omega_{\pm\alpha} | \mathbf{p}_\alpha \rangle. \quad (1.40)$$

In (1.40) the wave operators $\omega_{\pm\alpha}$ give rise to distorted waves, which are eigenfunctions of the Hamiltonian $H^\alpha = H_\alpha + U^\alpha$ (cf. (1.25)). They can be written by using definition (1.3):

$$\omega_{\pm\alpha} = s - \lim_{t \rightarrow \mp\infty} e^{iH^\alpha t} e^{-iH_\alpha t - i\chi_\alpha^{(0)\pm}(t)} |\phi_\alpha\rangle. \quad (1.41)$$

The operators $\chi_\alpha^{(0)\pm}(t)$ are defined by the distorting potentials U^α , with

$$\chi_\alpha^{(0)\pm}(t) |\mathbf{p}_\alpha\rangle = \text{sgn}(t) (\eta_\alpha^{(0)} \ln t + A_\alpha^{(0)}) |\phi_\alpha\rangle.$$

The following relation holds:

$$\begin{aligned} \Omega_{\pm\alpha} |\mathbf{p}_\alpha\rangle &= \lim_{\varepsilon \rightarrow 0} \frac{\varepsilon^{\mp i(\eta_\alpha - \eta_\alpha^{(0)})}}{\Gamma(1 \mp i(\eta_\alpha - \eta_\alpha^{(0)}))} \\ &\times e^{\pm i(A_\alpha - A_\alpha^{(0)})} \tilde{\Omega}_{\pm\alpha}(\varepsilon) |\mathbf{p}_\alpha\rangle; \end{aligned} \quad (1.42)$$

this is a generalization of (1.16). Let us prove this relation for the case of the operator $\Omega_{+\alpha}$. Since

$$\tilde{\Omega}_{+\alpha}(\varepsilon) |\mathbf{p}_\alpha\rangle = \varepsilon \int_0^\infty dt e^{-iHt} e^{iH^\alpha t} \omega_{+\alpha} |\mathbf{p}_\alpha\rangle$$

and

$$\lim_{t \rightarrow +\infty} \left(e^{iH^\alpha t} \omega_{+\alpha} - e^{iH_\alpha t + i\chi_\alpha^{(0)+}(-t)} |\phi_\alpha\rangle \right) \rightarrow 0$$

in a strong sense, then

$$\begin{aligned} \tilde{\Omega}_{+\alpha}(\varepsilon) |\mathbf{p}_\alpha\rangle &= \varepsilon \int_0^\infty dt e^{-iHt} e^{iH_\alpha t + i\chi_\alpha^{(0)+}(\mathbf{p}_\alpha, -t)} |\phi_\alpha, \mathbf{p}_\alpha\rangle \\ &+ R(\varepsilon) |\mathbf{p}_\alpha\rangle. \end{aligned} \quad (1.43)$$

Following the same logic, while deriving formulas (1.14)–(1.16), we obtain

$$\begin{aligned} \varepsilon^{-i(\eta_\alpha - \eta_\alpha^{(0)})} \tilde{\Omega}_{+\alpha}(\varepsilon) |\mathbf{p}_\alpha\rangle &= \int_0^\infty dt e^{-t - i(\eta_\alpha - \eta_\alpha^{(0)}) \ln t - i(A_\alpha - A_\alpha^{(0)})} \\ &\times [e^{-iHt/\varepsilon} e^{iH_\alpha t/\varepsilon + i\eta_\alpha \ln t/\varepsilon + iA_\alpha} |\phi_\alpha\rangle] |\mathbf{p}_\alpha\rangle \\ &+ \varepsilon^{-i(\eta_\alpha - \eta_\alpha^{(0)})} R(\varepsilon) |\mathbf{p}_\alpha\rangle. \end{aligned} \quad (1.44)$$

Taking the limit $\varepsilon \rightarrow 0$ in (1.44) and considering that the expression in square brackets converges to $\Omega_{+\alpha}$, we come to the relation

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} \varepsilon^{-i(\eta_\alpha - \eta_\alpha^{(0)})} \tilde{\Omega}_{+\alpha}(\varepsilon) |\mathbf{p}_\alpha\rangle &= \Gamma(1 - i(\eta_\alpha - \eta_\alpha^{(0)})) \\ &\times e^{-i(A_\alpha - A_\alpha^{(0)})} \Omega_{+\alpha} |\mathbf{p}_\alpha\rangle + \lim_{\varepsilon \rightarrow 0} \varepsilon^{-i(\eta_\alpha - \eta_\alpha^{(0)})} R(\varepsilon) |\mathbf{p}_\alpha\rangle. \end{aligned} \quad (1.45)$$

The operator $R(0) |\mathbf{p}_\alpha\rangle$ can be written in terms of the Abel limit

$$\begin{aligned} R(0) |\mathbf{p}_\alpha\rangle &= \lim_{\varepsilon \rightarrow 0} \varepsilon \int_0^\infty dt e^{-iHt} \\ &\times \left(e^{iH^\alpha t} \omega_{+\alpha} - e^{iH_\alpha t + i\chi_\alpha^{(0)+}(-t)} |\phi_\alpha\rangle \right) |\mathbf{p}_\alpha\rangle. \end{aligned} \quad (1.46)$$

The integrand in (1.46) is bounded with its limit equal to zero for $t \rightarrow \infty$. Because of general properties of the Abel limits $R(0) |\mathbf{p}_\alpha\rangle = 0$ and, consequently, expression (1.45) is equivalent to (1.42).

Result (1.42) allows the amplitude given in (1.30) to be rewritten to take a form analogous to (1.28) and (1.27),

$$\begin{aligned} t_{\beta\alpha}(\mathbf{p}_\beta, \mathbf{p}_\alpha; E + i0) &= \frac{e^{-\pi/2(\eta_\beta - \eta_\beta^{(0)})}}{\Gamma(1 - i(\eta_\beta - \eta_\beta^{(0)}))} \\ &\times \lim_{\varepsilon \rightarrow 0} (i\varepsilon)^{-i(\eta_\beta - \eta_\beta^{(0)})} \langle \mathbf{p}_\beta | \tilde{\Omega}_{-\beta}^+(\varepsilon) V^\alpha | \mathbf{p}_\alpha, \phi_\alpha \rangle \\ &= \frac{e^{-\pi/2(\eta_\beta - \eta_\beta^{(0)})}}{\Gamma(1 - i(\eta_\beta - \eta_\beta^{(0)}))} \lim_{z \rightarrow E + i0} (z - E)^{-i(\eta_\beta - \eta_\beta^{(0)})} \\ &\times \langle \zeta_\beta^-(\mathbf{p}_\beta) | [V^\alpha + (V^\beta - U^\beta)G(z)V^\alpha] | \phi_\alpha, \mathbf{p}_\alpha \rangle, \end{aligned} \quad (1.47)$$

where $|\zeta_\beta^-(\mathbf{p}_\beta)\rangle = \omega_{-\beta} |\mathbf{p}_\beta\rangle$. Result (1.47) shows that, if there is a wave function of some set of charged particles in the exit (entrance) channel with the right Coulomb asymptotic form, then their (total) Sommerfeld parameter does not contribute to the general (total) one of the channel during a regularization procedure. An equation of type (1.47) was obtained in [41] in the case of hydrogen atom ionization by a fast electron.

1.5. Conclusions to Section 1

Summarizing Section 1 it can be said that the specific asymptotic form of the Coulomb interaction for large distances between charged fragments gives rise to additional singularities in the scattering amplitudes, which are solutions to the LS equations, when these solutions tend to the energy shell. Outside of this domain these solutions to the LS equations (nonphysical amplitudes) can be dealt with just as in the case of short-range pair potentials.

In order to obtain physical observables, it is required to remove the singularities of the transition amplitudes according to specific prescriptions. Such rules are deduced from representations (1.27) and (1.47). We will below consider an example of how to do that.

2. GENERAL THEORY APPLICATION TO THE PROBLEM OF HYDROGEN ATOM IONIZATION BY A FAST ELECTRON

In what follows we will be mainly concerned with a system of three particles. For its description the Jacobi coordinates \mathbf{r}_γ , \mathbf{p}_γ are used, where \mathbf{r}_γ is the relative coordinate of a pair γ and \mathbf{p}_γ stands for the radius-vector of a third particle relative to the center of mass of this pair. The momenta conjugate to these coordinates will be denoted as \mathbf{k}_γ and \mathbf{p}_γ . The free Hamiltonian of a three-particle system can be written as

$$H_0 = -\frac{1}{2\mu_\gamma}\Delta_{\mathbf{r}_\gamma} - \frac{1}{2n_\gamma}\Delta_{\mathbf{p}_\gamma},$$

where μ_γ is the reduced mass of particles in a pair γ and n_γ is the reduced mass of a pair γ and a third particle.

In such a system, four scattering channels are possible—a bound pair and a free third particle (three channels)—and all three particles are free. A typical example of such a system is the interaction of a charged particle (electron, positron, proton, and so on) with a hydrogen atom. The problem of atomic particle scattering, when there is only Coulomb interaction between particles, is extremely important from the methodological point of view. Firstly, any two-particle problem can here be exactly solved, and in some cases there is a chance to compare approximate result with exact one. Second, according to conventional approaches, a nuclear problem of charged particle scattering can be dealt with once an atomic one is solved [42]. Third, most of the atomic physics' problems (e.g., electron scattering off an atom, or even proton scattering at very small angles) can further be simplified by using a large (infinitely large) nucleus mass. Usually, the nucleus momentum K is not large in such collisions, and its energy $K^2/2M \rightarrow 0$. In the latter case it is possible to consider a problem of two particles scattered in the field of a third (static) particle, where there exists a preferable coordinate system [1, 43, 44]. Here, instead of the coordinates $(\mathbf{r}_\gamma, \mathbf{p}_\gamma)$ it is convenient to introduce the coordinates $(\mathbf{r}_1, \mathbf{r}_2)$ that characterize the positions of light particles relative to a static heavy one, located at the center of coordinates.

2.1. Definitions

In this subsection we mainly adhere to the approach given in [5]. Let us give basic definitions. The hydrogen atom wave function in the initial state is denoted as φ_0 , its binding energy is ε_0 . The Hamiltonian of a system ($e + H$) has the form

$$H = h_{01} + h_{02} + W = H_0 + W, \quad (2.1)$$

where $W = v_{1N} + v_{2N} + v_{12}$ is the overall system potential, and v_{iN} , v_{12} are the potentials of electron interactions with static nucleus (proton) and with each other,

respectively. The total energy of a system is $E = \varepsilon_0 + \frac{p_0^2}{2} = \frac{p_1^2}{2} + \frac{p_2^2}{2}$, where \mathbf{p}_0 is the momentum of an incoming electron, \mathbf{p}_s , \mathbf{p}_e are the momenta of scattered and emitted electrons (this division is conventional, its meaning will shortly become clear).

We apply now the general mathematical provisions stated above to some specific scattering process. The expression for a physical amplitude of the hydrogen atom ionization process from a neutral channel to that of three free charged particles, the so-called (e, 2e) reaction, here is of key value. This amplitude is written, according to (1.27), in the form

$$t(\mathbf{p}_s, \mathbf{p}_e, \mathbf{p}_0; E + i0) = \frac{e^{-\frac{\pi}{2}\eta + iA}}{\Gamma(1 - i\eta)} \lim_{z \rightarrow E + i0} (z - E)^{-i\eta} \langle \mathbf{p}_s, \mathbf{p}_e | T(z) | \mathbf{p}_0, \varphi_0 \rangle. \quad (2.2)$$

In (2.2) η is the full Coulomb parameter (1.5.1)

$$\eta = \eta_s + \eta_e + \eta_{se}; \quad \eta_s = -p_s^{-1}, \quad (2.3)$$

$$\eta_e = -p_e^{-1}, \quad \eta_{se} = |\mathbf{p}_s - \mathbf{p}_e|^{-1},$$

While the Dollard phase A is equal in accordance with (1.5.2)

$$A = \eta_s \ln(2p_s^2) + \eta_e \ln(2p_e^2) + \eta_{se} \ln|\mathbf{p}_s - \mathbf{p}_e|^2. \quad (2.4)$$

The triple differential cross section of (e, 2e) process is written as

$$\frac{d^3\sigma}{dE_s d\Omega_s d\Omega_e} = (2\pi)^{-5} \frac{p_s p_e}{p_0} \times \left(\frac{1}{4} |t^{\text{dir}} + t^{\text{exch}}|^2 + \frac{3}{4} |t^{\text{dir}} - t^{\text{exch}}|^2 \right).$$

Here the momenta directions of outgoing electrons are specified by the solid angles Ω_s and Ω_e . The amplitude t^{dir} (t^{exch}) corresponds to the case of a scattered electron having the momentum \mathbf{p}_s (\mathbf{p}_e), i.e., the momenta are simply interchanged in Eq. (2.2) describing an exchange process.

Take the transition amplitude t in the form given in (1.30) (further we will be considering only t^{dir} omitting an index)

$$t(\mathbf{p}_s, \mathbf{p}_e, \mathbf{p}_0; E + i0) = \langle \Psi_f^-(\mathbf{p}_s, \mathbf{p}_e) | V_i | \mathbf{p}_0, \varphi_0 \rangle. \quad (2.5)$$

In (2.5) $V_i = v_{1N} + v_{12}$ is the interaction potential between an incoming electron and an atom. The initial state of a system is taken to be $|\mathbf{p}_0, \varphi_0\rangle$ and satisfies the Schrödinger equation

$$(H - V_i - E)|\mathbf{p}_0, \varphi_0\rangle = 0, \quad (2.6)$$

with the Hamiltonian H defined in (2.1). A hydrogen atom is electrically neutral; therefore, the matrix element is regular on the energy shell of the entrance channel despite the presence of the incoming electron

plane wave. The scattered wave in the final state $\langle \Psi_f^-(\mathbf{p}_s, \mathbf{p}_e) | = \langle \mathbf{p}_s, \mathbf{p}_e | \Omega_{-f}^\dagger$ includes all interactions between fragments of the final state and satisfies the Schrödinger equation

$$(H - E)|\Psi_f^-(\mathbf{p}_s, \mathbf{p}_e)\rangle = 0. \quad (2.7)$$

The final function possesses the right Coulomb asymptotic form, which follows from the long-range nature of interaction between reaction's final products. That is why representation (2.5) does not have singularities on the energy shell, corresponds to the physical amplitude and does not need further manipulations like regularization to be done.

The method of successive approximations in the scattering theory is based on the LS integral equation for the operator $T(z)$, and in the case of several charged particles it has a number of distinctive features. First, it is a choice of potentials in the initial and final states which we treat as a perturbation. This choice is dictated, as a rule, by physical conditions of the scattering problem and, to some extent, by intuition of a researcher. For example, in our case this is V_i , though, if we would have considered a problem of ionization of a singly charged hydrogen-like ion, then the scheme based on expression (1.25) should have to be chosen: thereby, we would have considered the Coulomb wave of an incoming particle instead of the plane one in the initial state, avoiding regularization of the entrance channel. Second, the higher Born terms are described by divergent integrals for $z \rightarrow E + i0$ as a result of the long-range nature of Coulomb forces. Physically, the divergences mean that the plane waves of scattered particles are not their asymptotical states. Let us elaborate a bit on this point.

Off the energy shell, the final three-particle state is sought as a solution to the equation

$$\begin{aligned} |\Psi_f^-(\mathbf{p}_s, \mathbf{p}_e; z)\rangle &= |\mathbf{p}_s, \mathbf{p}_e\rangle \\ &+ G_0^-(z)W|\Psi_f^-(\mathbf{p}_s, \mathbf{p}_e; z)\rangle, \end{aligned} \quad (2.8)$$

or

$$(z - H)|\Psi_f^-(\mathbf{p}_s, \mathbf{p}_e; z)\rangle = (z - H)|\mathbf{p}_s, \mathbf{p}_e\rangle,$$

which follows from (1.13). The free Green's operator $G_0^\pm(z)$ is taken in the form

$$G_0^\pm(z) = (z - H_0)^{-1}, \quad (2.9)$$

with the plus or minus sign fixed by the sign of imaginary part of z parameter. Expression (2.8) can be represented in the equivalent form

$$|\Psi_f^-(\mathbf{p}_s, \mathbf{p}_e; z)\rangle = [1 + G^-(z)W]|\mathbf{p}_s, \mathbf{p}_e\rangle, \quad (2.10)$$

where $G^\pm = (z - H)^{-1}$ is the full Green's operator.

From (2.5) and (2.8), a plane-wave Born perturbative series follows:

$$T(\mathbf{p}_s, \mathbf{p}_e; z) = \sum_{n=0}^{\infty} T_n(\mathbf{p}_s, \mathbf{p}_e; z), \quad (2.11)$$

$$T_n(\mathbf{p}_s, \mathbf{p}_e; z) = \langle \mathbf{p}_s, \mathbf{p}_e | [WG_0^+(z)]^n V_i | \mathbf{p}_0, \varphi_0 \rangle.$$

The term with index $n = 0$ corresponds to the first Born approximation (FBA)

$$T_0(\mathbf{p}_s, \mathbf{p}_e) \equiv \text{FBA} = \langle \mathbf{p}_s, \mathbf{p}_e | V_i | \mathbf{p}_0, \varphi_0 \rangle. \quad (2.12)$$

In formulas (2.11) and (2.12), the symbol T is deliberately used instead of t , since now all the terms of a Born series for $n \geq 1$ contain singularities at $z \rightarrow E + i0$. An interesting question arises as to at which step the regular expression given in (2.5) is replaced by a singular one (2.11)? The answer to this is that it happens exactly when we start replacing the exact three-point wave function in (2.8) by the sum of successive plane-wave terms. It should be recalled that the scattering theory in the case of short-range pair potentials is constructed out of a quite physical assumption, that entire space can be considered as a sum of well separated domains: small ones where particles, in fact, interact, and a vast one where they move freely between collisions, including motion at (infinitely) large mutual distances (see, e.g. [25]). An incoming wave packet is always much larger than an atom, thus permitting consideration of a small part of that packet within a range, set by the atom size, as a plane wave. Whereas in the case of Coulomb potentials everything is exactly opposite: the sizes of any wave packet are always less than the interaction region, and the packet itself is to enter boundary conditions of a stationary problem, which is inconvenient. Thus, the singularities of the scattering amplitude are the price to pay for fitting the well developed scattering theory with short-range pair potentials to the problems of scattering of charged particles. This situation somehow resembles renormalizations in quantum electrodynamics, although there the singularities are related with the hypothesis of point-like relativistic particles and, apparently, with unjustified application of the interaction representation to describing the processes of their scattering. Even there the basis of plane waves is inadequate for to the posed problem.

2.2. Regularization of the Singular Matrix Elements

Now we will show how the calculation scheme based on expression (2.2) can be applied to the regularization procedure (removal of the singularities) of the Born series' terms. Let us consider one of the possible ways of extracting the exponent $e^{i\text{Im}(z-E)}$ out of a series (2.11) that is meant to compensate for the same

exponent in (2.2). Consider the term $T_1(\mathbf{p}_s, \mathbf{p}_e; z)$. The following relation is then valid:

$$T_1(\mathbf{p}_s, \mathbf{p}_e; z) = R_1(\mathbf{p}_s, \mathbf{p}_e; z)T_0(\mathbf{p}_s, \mathbf{p}_e) + \tilde{T}_1(\mathbf{p}_s, \mathbf{p}_e; z), \quad (2.13)$$

where

$$R_1(\mathbf{p}_s, \mathbf{p}_e; z) = \int \frac{d^3 k_s}{(2\pi)^3} \frac{d^3 k_e}{(2\pi)^3} \frac{\langle \mathbf{p}_s, \mathbf{p}_e | W | \mathbf{k}_s, \mathbf{k}_e \rangle}{z - k_s^2/2 - k_e^2/2}, \quad (2.14)$$

$$\tilde{T}_1(\mathbf{p}_s, \mathbf{p}_e; z) = \int \frac{d^3 k_s}{(2\pi)^3} \frac{d^3 k_e}{(2\pi)^3} \frac{\langle \mathbf{p}_s, \mathbf{p}_e | W | \mathbf{k}_s, \mathbf{k}_e \rangle}{z - k_s^2/2 - k_e^2/2} \times [T_0(\mathbf{k}_s, \mathbf{k}_e) - T_0(\mathbf{p}_s, \mathbf{p}_e)]. \quad (2.15)$$

By analogy,

$$T_2(\mathbf{p}_s, \mathbf{p}_e; z) = R_2(\mathbf{p}_s, \mathbf{p}_e; z)T_0(\mathbf{p}_s, \mathbf{p}_e) + R_1(\mathbf{p}_s, \mathbf{p}_e; z)\tilde{T}_1(\mathbf{p}_s, \mathbf{p}_e; z) + \tilde{T}_2(\mathbf{p}_s, \mathbf{p}_e; z), \quad (2.16)$$

where

$$R_2(\mathbf{p}_s, \mathbf{p}_e; z) = \int \frac{d^3 k_s}{(2\pi)^3} \frac{d^3 k_e}{(2\pi)^3} \frac{\langle \mathbf{p}_s, \mathbf{p}_e | W | \mathbf{k}_s, \mathbf{k}_e \rangle}{z - k_s^2/2 - k_e^2/2} \times R_1(\mathbf{k}_s, \mathbf{k}_e; z), \quad (2.17)$$

$$\tilde{T}_2(\mathbf{p}_s, \mathbf{p}_e; z) = \int \frac{d^3 k_s}{(2\pi)^3} \frac{d^3 k_e}{(2\pi)^3} \frac{\langle \mathbf{p}_s, \mathbf{p}_e | W | \mathbf{k}_s, \mathbf{k}_e \rangle}{z - k_s^2/2 - k_e^2/2} \times R_1(\mathbf{k}_s, \mathbf{k}_e; z)[T_0(\mathbf{k}_s, \mathbf{k}_e) - T_0(\mathbf{p}_s, \mathbf{p}_e)] + \int \frac{d^3 k_s}{(2\pi)^3} \frac{d^3 k_e}{(2\pi)^3} \frac{\langle \mathbf{p}_s, \mathbf{p}_e | W | \mathbf{k}_s, \mathbf{k}_e \rangle}{z - k_s^2/2 - k_e^2/2} \times [\tilde{T}_1(\mathbf{k}_s, \mathbf{k}_e) - \tilde{T}_1(\mathbf{p}_s, \mathbf{p}_e)], \quad (2.18)$$

and so forth. By induction it can be shown that

$$R_{n+1}(\mathbf{p}_s, \mathbf{p}_e; z) = \int \frac{d^3 k_s}{(2\pi)^3} \frac{d^3 k_e}{(2\pi)^3} \times \frac{\langle \mathbf{p}_s, \mathbf{p}_e | W | \mathbf{k}_s, \mathbf{k}_e \rangle}{z - k_s^2/2 - k_e^2/2} R_n(\mathbf{k}_s, \mathbf{k}_e; z), \quad (2.19)$$

$$R \equiv 1,$$

$$\tilde{T}_{n+1}(\mathbf{p}_s, \mathbf{p}_e; z) = \sum_{k=0}^n \int \frac{d^3 k_s}{(2\pi)^3} \frac{d^3 k_e}{(2\pi)^3} \frac{\langle \mathbf{p}_s, \mathbf{p}_e | W | \mathbf{k}_s, \mathbf{k}_e \rangle}{z - k_s^2/2 - k_e^2/2} \times R_k(\mathbf{k}_s, \mathbf{k}_e; z)[\tilde{T}_{n-k}(\mathbf{k}_s, \mathbf{k}_e; z) - \tilde{T}_{n-k}(\mathbf{p}_s, \mathbf{p}_e; z)], \quad (2.20)$$

$$\tilde{T}_0(\mathbf{p}_s, \mathbf{p}_e; z) \equiv T_0(\mathbf{p}_s, \mathbf{p}_e).$$

Summing up the Born terms, we obtain from (2.11)

$$T(\mathbf{p}_s, \mathbf{p}_e; z) = R(\mathbf{p}_s, \mathbf{p}_e; z)\tilde{T}(\mathbf{p}_s, \mathbf{p}_e; z). \quad (2.21)$$

Here the function $R(\mathbf{p}_s, \mathbf{p}_e; z)$ satisfies the equation

$$R(\mathbf{p}_s, \mathbf{p}_e; z) = 1 + \int \frac{d^3 k_s}{(2\pi)^3} \frac{d^3 k_e}{(2\pi)^3} \times \frac{\langle \mathbf{p}_s, \mathbf{p}_e | W | \mathbf{k}_s, \mathbf{k}_e \rangle}{z - k_s^2/2 - k_e^2/2} R(\mathbf{p}_s, \mathbf{p}_e; z) \quad (2.22)$$

and is singular on the energy shell, that is, for $z \rightarrow E + i0$.

The function $R(\mathbf{p}_s, \mathbf{p}_e; z)$ is closely related to the full Green's function of the scattering problem, namely,

$$R(\mathbf{p}_s, \mathbf{p}_e; z) = \langle \mathbf{p}_s, \mathbf{p}_e | G_0^{-1}(z)G(z) | \mathbf{r}_1 = 0, \mathbf{r}_2 = 0 \rangle, \quad (2.23)$$

and for $z \sim E$ has a structure of the type [5, 45]

$$R(\mathbf{p}_s, \mathbf{p}_e; z) = (z - E)^{in} r(\mathbf{p}_s, \mathbf{p}_e; z) + \tilde{R}(\mathbf{p}_s, \mathbf{p}_e; z), \quad (2.24)$$

with the function $r(\mathbf{p}_s, \mathbf{p}_e; z)$ being regular on the energy shell, and the function $\tilde{R}(\mathbf{p}_s, \mathbf{p}_e; E + i0) = 0$. Proof of the statement given in (2.24) is given in the Appendix (see also [46]).

2.3. First Born Approximations in the Distorted Wave Method

The specific forms of writing LS equations are numerous, which is connected with the introduction of different distorting potentials into the potential groups of the initial and final states (see the general theory in subsection 1.4). Let us dwell on this point in more detail. The matrix element of the operator $t(E + i0)$ in (2.2) can be written in two equivalent forms. The first representation is expressed through the proper three-particle Hamiltonian function (1.33) $\Psi^-(\mathbf{p}_s, \mathbf{r}_1; \mathbf{p}_e, \mathbf{r}_2)$, which is asymptotically characterized by two electrons in the continuum with the features of a converging spherical wave

$$t(\mathbf{p}_s, \mathbf{p}_e; +i0) = \langle \Psi^-(\mathbf{p}_s, \mathbf{p}_e) | W - V_i | \psi_i^+(\mathbf{p}_0) \rangle, \quad (2.25)$$

and the second one via the analogous function $\Psi_0^+(\mathbf{p}_0, \mathbf{r}_1; \mathbf{r}_2)$ that describes asymptotically electron 2 in the initial state and electron 1 in the continuous spectrum with the features of a diverging spherical wave

$$t(\mathbf{p}_s, \mathbf{p}_e; E + i0) = \langle \psi_f^-(\mathbf{p}_s, \mathbf{p}_e) | W - V_f | \Psi_0^+(\mathbf{p}_0) \rangle. \quad (2.26)$$

The wave functions of the final $\psi_f^\pm(\mathbf{p}_s, \mathbf{r}_1; \mathbf{p}_e, \mathbf{r}_2)$ and initial $\psi_i^\pm(\mathbf{p}_0, \mathbf{r}_1; \mathbf{r}_2)$ states satisfy the Schrödinger equation

$$\left(\frac{p_s^2}{2} + \frac{p_e^2}{2} - H_0 - V_f \right) | \psi_f^\pm \rangle = 0, \quad (2.27)$$

$$\left(\varepsilon_0 + \frac{p_0^2}{2} - H_0 - V_i \right) | \psi_i^\pm \rangle = 0.$$

The choice for the initial V_i and final V_f potentials, as well as an approximation for the three-particle wave function $|\Psi\rangle$, defines in both cases the model of calculating the amplitude. Various models and calculations can be found in [47–50 and others]. Most of those works use the formulas presented in (2.25) and (2.26), which help, as a rule, to obtain various approximations of the distorted waves. In this approximation the first thing to be accounted for is the probable distortions of the plane waves corresponding to fast initial and final electrons. For this, it is convenient to divide the potential v_{12} to internal short-range v_{12}^{in} and peripheral v_{12}^{out} parts either by introducing some cutoff radius R or proceed in the way proposed in, e.g., [1]. Let us set $V_i = v_{12}^{\text{out}} + v_{1N} + v_{2N}$. To simplify description of the interaction between an incoming electron and an atom, we replace $v_{1N} + v_{12}^{\text{out}} \rightarrow \tilde{v}_0$ and consider the motion of the incident electron in the field with a short-range potential \tilde{v}_0 . Taking into account such a substitution, the expression in (2.25) is transformed to take the following form:

$$t(\mathbf{p}_s, \mathbf{p}_e; z) \approx \langle \Psi^-(\mathbf{p}_s, \mathbf{p}_e) | v_{12}^{\text{in}} | \chi_0^+(\mathbf{p}_0), \varphi_0 \rangle, \quad (2.28)$$

where $\varphi_0(\mathbf{r}_2)$ is the ground state wave function of a hydrogen atom and $\chi_0^+(\mathbf{p}_0, \mathbf{r}_1)$ stands for the distorted wave of an incoming electron. Note that the effective short-range potential \tilde{v}_0 tends to zero at sufficiently large distances between an electron and an atom and, therefore, the distorted wave asymptotically transforms to the plane one, as it should be for a charged particle scattered off a neutral system.

As it follows from (2.28), while replacing the real potential $v_{1N} + v_{12}^{\text{out}}$ with the effective central potential, we neglect possible transformations of the atom wave function, for instance, polarization. More refined models can be constructed within a framework set by formula (2.26).

We consider now the total wave function of a system $|\Psi^-(\mathbf{p}_s, \mathbf{p}_e)\rangle$, which is an eigenfunction of the Hamiltonian given in (2.7). We divide all the potentials to internal and peripheral parts and introduce the asymptotic Green's function,

$$G_{\text{as}}^{\pm}(z) = [z - H_0 - v_{12}^{\text{out}} - v_{1N}^{\text{out}} - v_{2N}^{\text{out}}]^{-1}.$$

This is done in order to correctly apply the Faddeev reduction of the total wave function,

$$|\Psi^-\rangle = |\Psi_{1,2}^-\rangle + |\Psi_{12}^-\rangle, \quad (2.29)$$

which is impossible to consistently carry out for the Coulomb potentials, because of the noncompactness of the kernels of integral equations obtained [1]. Now,

the following system of equations can formally be written for its components:

$$\begin{cases} (z - H_0 - v_{1N} - v_{2N} - v_{12}^{\text{out}}) |\Psi_{1,2}^-\rangle \\ = (v_{1N}^{\text{in}} + v_{2N}^{\text{in}}) |\Psi_{12}^-\rangle \\ (z - H_0 - v_{1N}^{\text{out}} - v_{2N}^{\text{out}} - v_{12}) |\Psi_{12}^-\rangle = v_{12}^{\text{in}} |\Psi_{1,2}^-\rangle. \end{cases} \quad (2.30)$$

By using the operator equation $t_{12}^{\text{in}}(z) = v_{12}^{\text{in}} + v_{12}^{\text{in}} G_{\text{as}}^+(z) t_{12}^{\text{in}}$ and taking into account only one complete pair collision between incoming and target electrons, we obtain from (2.28), (2.29), and (2.30) for the direct amplitude of (e, 2e) reaction the approximate expression

$$\begin{aligned} t(\mathbf{p}_s, \mathbf{p}_e; z) \\ \approx \int \frac{d^3 p}{(2\pi)^3} \langle \Psi^-(\mathbf{p}_s, \mathbf{p}_e) | t_{12}^{\text{in}}(z) | \chi_0^+(\mathbf{p}_0), \mathbf{p} \rangle \varphi_0(\mathbf{p}). \end{aligned} \quad (2.31)$$

The function $|\Psi^-(\mathbf{p}_s, \mathbf{p}_e)\rangle$ in (2.31) satisfies the wave equation

$$\left(\frac{p_s^2}{2} + \frac{p_e^2}{2} - H_0 - v_{1N} - v_{2N} - v_{12}^{\text{out}} \right) \times |\Psi^-(\mathbf{p}_s, \mathbf{p}_e)\rangle = 0 \quad (2.32)$$

and turns into a product of two Coulomb waves only if a peripheral interaction v_{12}^{out} is neglected. In this case we get the so-called off-shell impulse approximation of distorted waves (off-shell DWIA [24]),

$$\begin{aligned} T(\mathbf{p}_s, \mathbf{p}_e; z) \\ \approx \int \frac{d^3 p}{(2\pi)^3} \langle \varphi^-(\mathbf{p}_s), \varphi^-(\mathbf{p}_e) | t_{12}^{\text{in}}(z) | \chi_0^+(\mathbf{p}_0), \mathbf{p} \rangle \varphi_0(\mathbf{p}), \end{aligned} \quad (2.33)$$

where $|\varphi^-(\mathbf{p}_i)\rangle$ is the Coulomb function of a continuous spectrum.

Once again, we pay attention to the replacement of t by T in (2.33). They coincide for $z \rightarrow E + i0$ only to a zero order approximation in the potential v_{12}^{out} . Their complete relation should be found in the context of general formula (1.47).

The majority of used approximations follow from formula (2.31). Among them are the one discussed above, the half-off-shell factorized impulse approximation of distorted waves (see [51]), and its variant called the eikonal impulse approximation (EWIA [22, 52]). If, on the other hand, only peripheral parts of all the potentials v_s^{out} are left in (2.32), we obtain the so-called quasi-classical eikonal impulse approximation (EWIA-SC [53, 54]). This model is sufficiently simple for the distortion effect to be estimated if the total energy is not asymptotically large.

Finally, neglecting in (2.32) all the potentials and also taking $\tilde{v}_0 = 0$, the plane-wave impulse approxi-

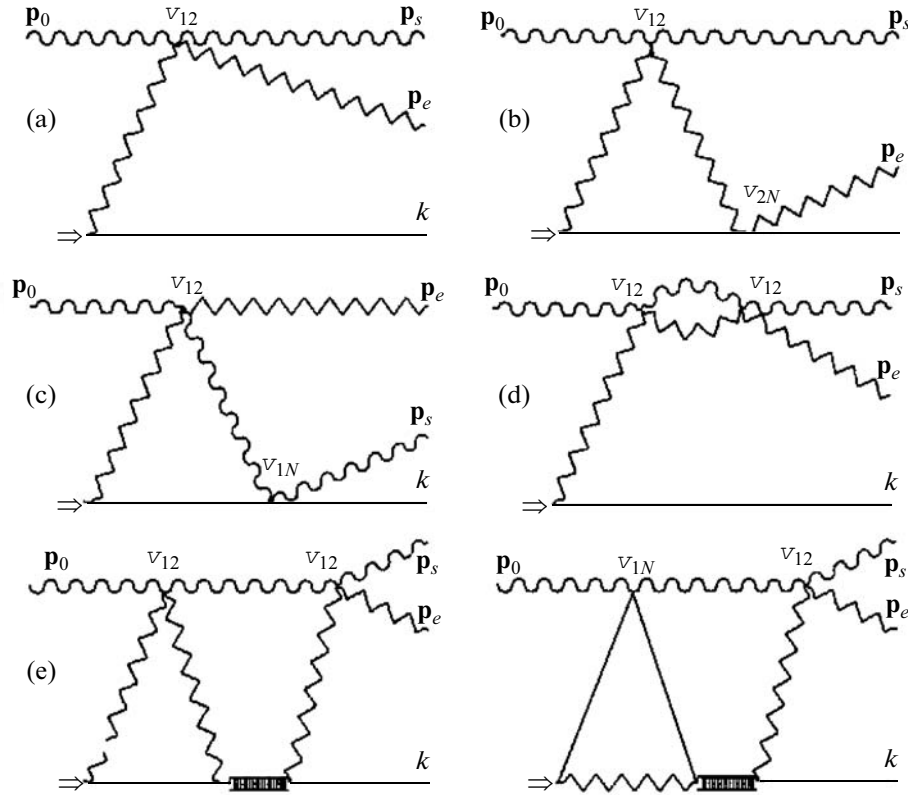


Fig. 1. Nonrelativistic diagrams visualizing the first- and second-order processes for the reaction $H(e, 2e)H^+$: (a) FBA, (b) TS1, (c) TS2₂₁, (d) TS2₂₂, and (e) TS2₁.

mation (PWIA) is obtained. The differential cross section is proportional to the square of the absolute value of the hydrogen wave function in the impulse approximation (this quantity is also called a momentum distribution)

$$\frac{d^3\sigma}{dE_s d\Omega_e d\Omega_s} \propto |\varphi_0(\mathbf{q})|^2, \quad \mathbf{q} = \mathbf{p}_s + \mathbf{p}_e - \mathbf{p}_0. \quad (2.34)$$

Despite the apparent simplicity of representation (2.31), its usefulness in real calculations is rather limited. First, it is almost impossible to evaluate an “internal” pair amplitude t_{12}^{in} , since there is a Green’s function $G_{as}^+(E)$ in the LS equation that cannot be written in any sensible way without further simplifications. Second, there is considerable uncertainty in the definition of the potential \tilde{v}_0 . Third, even if these complexities are somehow overcome, the matrix element in (2.31) is still a nine-dimensional integral.

In the first two subsections of this section, we were mainly concerned with a Born series; however, in the scattering theory with short-range potentials, the so-called iterations of the Faddeev equations (also known as the Watson or Born–Faddeev series) can be consid-

ered, in which each term includes different particles consecutively interacting by means of pair amplitudes [1, 2]. We have already referred in this subsection to this representation of the scattering amplitude. In particular, a customary plane-wave impulse approximation widespread in the calculations

$$PWIA = \frac{e^{-\frac{\pi}{2}\eta_{se} + iA_{se}}}{\Gamma(1 - i\eta_{se})} \lim_{z \rightarrow E + i0} (z - E)^{-i\eta_{se}} \times \langle \mathbf{p}_s, \mathbf{p}_e | t_{12}(z) | \mathbf{p}_0, \varphi_0 \rangle \quad (2.35)$$

is exactly the first term of such a series. Another example is expression (2.31), which can also be viewed as the first term of a series of such type. As a matter of fact, this is the distorted wave method, which appears to be more informative regarding the scattering mechanisms.

So why do we devote the primary attention to a Born series that involves potentials in the knots of a diagrammatical representation (Fig. 1) rather than pair amplitudes? A diagram of the term of a Born–Faddeev series contains consecutive blocks, in which two particles interact via a pair amplitude, with a third particle being free. Such a situation is never realized in the scattering theory of particles with Coulomb inter-

action because of the absence of asymptotic freedom. Of course, the successive iterations of a system of Faddeev equations can formally be written off the energy shell, followed by extracting singular and regular parts in each pair amplitude, owing to the fact that the pair Coulomb amplitudes have analytic expressions off the energy shell (see, e.g., [55–57]), and then proceed to work with this expansion. However, even in the second order, the numerical implications of such a program look quite problematic.

Indeed, the properties of the solutions to the resolvent-type equations, which include also Faddeev equations, allow one to formulate a procedure of calculating the square of the absolute value of physical transition amplitude (1.27),

$$|t_{\beta\alpha}(\mathbf{p}_\beta, \mathbf{p}_\alpha; E + i0)|^2 = \left| \frac{e^{-\pi/2(\eta_\beta + \eta_\alpha)}}{\Gamma(1 - i\eta_\alpha)\Gamma(1 - i\eta_\beta)} \right|^2 \lim_{z \rightarrow E + i0} |\langle \mathbf{p}_\beta | T_{\beta\alpha}(z) | \mathbf{p}_\alpha \rangle|^2.$$

Since, for $\text{Im}z > 0$, the Faddeev equations possess unique solution, the limiting procedure allows, at least formally, evaluating a physically observable cross section of the process, proportional to the square of the absolute value of the amplitude. However, this procedure is not suitable for the case of approximating the amplitude T by its iterations within a frame of a Watson series. Let us show this by an example demonstrating the second order iteration. The matrix elements of the type $I_{\beta\alpha} = \langle \mathbf{p}_\beta | t_\beta(z) G_0(z) t_\alpha(z) | \mathbf{p}_\alpha \rangle$, with the variable z on the energy shell, are represented as

$$I_{\beta\alpha} \approx (z - E)^{i\eta_\alpha} A_{\beta\alpha} + (z - E)^{i\eta_\beta} B_{\beta\alpha}$$

(see, e.g., [12, 13]). Summing up the first and second iterations we can easily verify that compensation of these singularities with the help of (1.27) is impossible and, calculating the cross section in this way, reveal that it diverges on the energy shell (!).

From this point of view, the approximation PWIA also seems an inadequate theoretical tool. Indeed, as is shown in [58], even if in (2.2) we succeed in extracting a pair amplitude $t_{12}(z)$ out of $T(z)$ as a separate term and

regularize it, i.e., extract the singularity $(z - E)^{i\eta_{se}}$, we will not obtain the standard PWIA because of three-particle factors, including singular ones, emerging before the matrix element (cf. (2.2) and (2.35)). Thus, in order to formally obtain PWIA, we have to neglect the Sommerfeld electron–ion parameters in the factors before the matrix element after extracting $t_{12}(z)$ out of $T(z)$, i.e., to assume $\eta_s = \eta_e = 0$ in (2.2). Leaving aside the question of justifying such a procedure from the mathematical point of view, note that, in the case of a quasi-elastic (e, 2e) reaction, a kinematics in which a pair of Sommerfeld parameters— η_{se} , η_e and η_s —are quantities of the same order is realized. Evidently, the latter does not permit an approximation $\eta_s = \eta_e = 0$ to be justified by any physical reasoning.

The discussion above shows that if, from the very beginning, the required Coulomb singularities are not extracted in the amplitude defined by the LS equation, then all the attempts at constructing approximate expressions for the charged particle scattering amplitudes are doomed to failure. One feasible procedure is discussed in the next section, and another, based on the method of effective charges, is given in [46, 59, 60].

2.4. Second Plane-Wave Born Approximation for the Amplitude of Quasi-Elastic (e, 2e) Reaction on a Hydrogen Atom

The results of subsection 2.2 show that the role of a small parameter while expanding the amplitude in a Born series is practically played by the channel Sommerfeld parameters, which are unambiguously related to the Coulomb potentials. Leaving terms of no higher than the first order in the expansion of expression (2.2) in a series over parameters η_i , we obtain the expression for the physical amplitude in the second plane-wave Born approximation (since the potentials are already included in the term T_0),

$$t_1(\mathbf{p}_s, \mathbf{p}_e, \mathbf{p}_0; E + i0) \equiv t_{\text{SBA}} = \left(1 - \frac{\pi\eta}{2} + iA - iC\eta \right) T_0(\mathbf{p}_s, \mathbf{p}_e) \quad (2.36)$$

$$+ \lim_{z \rightarrow E + i0} [T_1(\mathbf{p}_s, \mathbf{p}_e; z) - i\eta T_0(\mathbf{p}_s, \mathbf{p}_e) \ln(z - E)],$$

where $C = 0.577215\dots$ is the Euler constant. For the operator $T(z)$, we choose its *prior*-form (1.26.2) (hereinafter, we omit a tilde sign for convenience), in which we choose $V^\alpha = v_{1N} + v_{12}$. Then, the following chain of computations is valid:

$$T(z) = (v_{1N} + v_{12}) + WG_0^+(z)T(z) = (v_{1N} + v_{12}) + WG^+(z)(v_{1N} + v_{12}).$$

From the first equality, it follows that

$$(1 - v_{2N}G_0^+(z))T(z) = (v_{1N} + v_{12}) + (v_{1N} + v_{12})G_0^+(z)T(z)$$

or

$$T(z) = [1 - v_{2N}G_0^+(z)]^{-1} \times [(v_{1N} + v_{12}) + (v_{1N} + v_{12})G_0^+(z)T(z)] = [1 - v_{2N}G_0^+(z)]^{-1} [(v_{1N} + v_{12}) + (v_{1N} + v_{12})G^+(z)(v_{1N} + v_{12})]. \quad (2.37)$$

Using the known representation of the full Green's function in the form of expansion over a spectrum of eigenfunctions of the total Hamiltonian H , let us write

the matrix element $\langle \mathbf{p}_s, \mathbf{p}_e | T(z) | \mathbf{p}_0, \varphi_0 \rangle \equiv T(\mathbf{p}_s, \mathbf{p}_e; z)$ of the operator $T(z)$ in (2.37) in the form

$$T(\mathbf{p}_s, \mathbf{p}_e; z) = \langle \mathbf{p}_s, \varphi^-(\mathbf{p}_e; z') | v_{1N} + v_{12} | \mathbf{p}_0, \varphi_0 \rangle + \sum_{\alpha} \frac{\langle \mathbf{p}_s, \varphi^-(\mathbf{p}_e; z') | v_{1N} + v_{12} | \Psi_{\alpha}^- \rangle \langle \Psi_{\alpha}^- | v_{1N} + v_{12} | \mathbf{p}_0, \varphi_0 \rangle}{z - E_{\alpha}} \quad (2.38)$$

$$z' = z - \frac{p_s^2}{2}.$$

In (2.38) $|\Psi_{\alpha}^- \rangle$ is a three-particle wave function of the problem (with the features of a converging spherical wave in the case of at least one electron being in a continuous spectrum), while $\langle \varphi^-(\mathbf{p}_e; z') | = \langle \mathbf{p}_e | [1 - v_{2N} g_0^+(z')]^{-1}$.

At this point the meaning behind the terms “first plane-wave Born approximation,” “second plane-wave Born approximation,” etc., when considering the three-body problem in which there are both bound states and free electrons should be discussed. Only processes with only one or two consecutive potential interaction of free electrons are taken into consideration. Since in what follows we consider the case with all the momenta \mathbf{p}_0 , \mathbf{p}_s , and \mathbf{p}_e being sufficiently large, as well as the transferred momentum $\mathbf{Q} = \mathbf{p}_0 - \mathbf{p}_s$ (so-called quasi-elastic (e, 2e) processes or the method of electron momentum spectroscopy, which was mentioned in the Introduction, the details of this method are also given in reviews [61, 62]), the following assumptions and approximations are put forward:

—we neglect the terms in which coordinates corresponding to fast particles enter intermediate bound states, since the probability of a fast particle “residing” for some time in a bound state is rather small; and

—we leave only those elementary processes of the second order that decrease with increasing energy no faster than $Q^{-2} p_i^{-1}$ ($i = 0, s, e$).

We consider now the function $|\varphi^-(\mathbf{p}_e; z') \rangle = [1 - g_0^-(z') v_{2N}]^{-1} |\mathbf{p}_e \rangle$. It satisfies the equation $(z' - h_{02} - v_{2N}) |\varphi^-(\mathbf{p}_e; z') \rangle = (z' - p_e^2/2) |\mathbf{p}_e \rangle$ (cf. (2.8)) and for $z' = p_e^2/2$ or $z = E$ turns into the equation for the Coulomb function with the features of a converging spherical wave. It is easy to show that $\langle \varphi_0 | \varphi^-(\mathbf{p}_e; z') \rangle \rightarrow 0$ for $z \rightarrow E$, as required for the eigenfunctions that belong to different parts of the two-particle Hamiltonian's spectrum. Thus, in the first term of the sum given in (2.38), we can omit the term corresponding to the interaction v_{1N} even in spite of the regularization represented by Eq. (2.2). Now the physical meaning of choosing the initial potential V^{α} is clear. This matrix

element should be zero, as there is no energy transfer through an infinitely massive body.

Next, we represent formally the Coulomb function of the continuous part of a spectrum $\langle \varphi^-(\mathbf{p}_e; z') |$ in terms of the expansion in a series over potential v_{2N} and keep only two terms. Then it can be written as

$$\langle \mathbf{p}_s, \varphi^-(\mathbf{p}_e; z') | \approx \langle \mathbf{p}_s, \mathbf{p}_e | (1 + v_{2N} g_0^+(z')). \quad (2.39)$$

Substituting into a part of the first term left in (2.38) only the vector $\langle \mathbf{p}_s, \mathbf{p}_e |$ from (2.39), we obtain FBA

$$\begin{aligned} \text{FBA} &\equiv T_0(\mathbf{p}_s, \mathbf{p}_e) \\ &= \langle \mathbf{p}_s, \mathbf{p}_e | v_{12} | \mathbf{p}_0, \varphi_0 \rangle = \frac{4\pi}{(\mathbf{p}_0 - \mathbf{p}_s)^2} \varphi_0(\mathbf{q}). \end{aligned} \quad (2.40)$$

FBA is graphically presented as a diagram in Fig. 1a. Recall that the normalized wave function of the hydrogen atom ground state is $\varphi_0(\mathbf{q}) = 8\sqrt{\pi}/(q^2 + 1)^2$.

The second term in (2.39), after being substituted in (2.38), describes the so-called two-step (TS1) mechanism, in which atomic electron 2, after collision with incoming electron 1, returns to an ion and a secondary interaction takes place (Fig. 1b). This is a part of the second Born approximation and corresponds to the atomic electron wave distortion to the second order inclusively,

$$\begin{aligned} \text{TS1} &= \langle \mathbf{p}_s, \mathbf{p}_e | v_{2N} g_0^+ \left(z - \frac{p_s^2}{2} \right) v_{12} | \mathbf{p}_0, \varphi_0 \rangle \\ &= -\frac{4\pi}{(\mathbf{p}_0 - \mathbf{p}_s)^2} \int \frac{d^3 \mathbf{x}}{(2\pi)^3} \frac{\varphi_0(\mathbf{q} + \mathbf{x})}{z - \frac{p_s^2}{2} - \frac{(\mathbf{p}_e + \mathbf{x})^2}{2}} \frac{4\pi}{x^2}. \end{aligned} \quad (2.41)$$

Integral (2.41) has a logarithmic singularity at $x \sim 0$, if $z \rightarrow E + i0$.

The second term in (2.38) is an obvious candidate for the second Born approximation. In the literature it is called the TS2 mechanism, and it describes two consecutive interactions of incoming electron 1 with a system. Let us analyze the sum in (2.38). First of all, we exclude from consideration the intermediate bound states of an ion H^- , since such matrix elements will be negligibly small in the case of quasi-elastic (e, 2e) processes. Then, in the sum, we single out the group of functions $|\Psi_{\alpha}^- \rangle$ with one asymptotically free electron and another one being bound. As in the SBA term considered we already have two consecutive interactions, the free electron is assumed to be a plane wave.

In other words, $|\Psi_\alpha^-\rangle = |\mathbf{p}, \varphi_g\rangle$, $g \rightarrow (n, l, m)$. We denote this sum as TS2₁ (Fig. 1e). Then

$$\begin{aligned} \text{TS2}_1 &= \sum_g \int \frac{d^3 \mathbf{x}}{(2\pi)^3} \frac{4\pi}{(\mathbf{p}_0 - \mathbf{p}_s - \mathbf{x})^2} \\ &\times \frac{[F_g(\mathbf{x}) - \delta_{n1}] \varphi_g(\mathbf{q} + \mathbf{x}) 4\pi}{z - \varepsilon_g - \frac{(\mathbf{p}_0 - \mathbf{x})^2}{2} + i0} \frac{4\pi}{x^2}. \end{aligned} \quad (2.42)$$

In (2.42),

$$F_g(\mathbf{x}) = \int \frac{d^3 \mathbf{y}}{(2\pi)^3} \varphi_0(\mathbf{y}) \varphi_g^*(\mathbf{y} + \mathbf{x}). \quad (2.43)$$

Note that this integral does not diverge for arbitrary number g at $z \rightarrow E + i0$, due to the mutual compensation of zeros in the numerator and denominator at $x = 0$.

Furthermore, in sum (2.38) the intermediate states with two asymptotically free electrons (continuum) should be isolated. Analogously, we assign $|\Psi_\alpha^-\rangle = |\mathbf{p}, \varphi^-(\mathbf{p}')\rangle$ with subsequent replacement of the Coulomb wave for the plane one. As a result, we obtain

$$\text{TS2}_2 = \text{TS2}_{21} + \text{TS2}_{22},$$

where

$$\begin{aligned} \text{TS2}_{21} &= - \int \frac{d^3 \mathbf{x}}{(2\pi)^3} \frac{4\pi}{(\mathbf{p}_0 - \mathbf{p}_s - \mathbf{x})^2} \\ &\times \frac{\varphi_0(\mathbf{q} + \mathbf{x}) 4\pi}{z - \frac{p_e^2}{2} - \frac{(\mathbf{p}_s + \mathbf{x})^2}{2} + i0} \frac{4\pi}{x^2} \end{aligned} \quad (2.44)$$

and

$$\begin{aligned} \text{TS2}_{22} &= \varphi_0(\mathbf{q}) \int \frac{d^3 \mathbf{x}}{(2\pi)^3} \frac{4\pi}{(\mathbf{p}_0 - \mathbf{p}_s - \mathbf{x})^2} \\ &\times \frac{1}{z - \frac{(\mathbf{p}_s + \mathbf{x})^2}{2} - \frac{(\mathbf{p}_e - \mathbf{x})^2}{2} + i0} \frac{4\pi}{x^2}. \end{aligned} \quad (2.45)$$

The terms TS2₂₁ and TS2₂₂ are shown in the form of diagrams in Figs. 1c and 1d. Both integrals (2.44) and (2.45) diverge on the energy shell.

Thus, we constructed the amplitude $T_1(\mathbf{p}_s, \mathbf{p}_e; z)$ in formula (2.36) and it equals

$$\begin{aligned} T_1(\mathbf{p}_s, \mathbf{p}_e; z) &\equiv \text{SBA} \\ &= \text{FBA} + \text{TS1} + \text{TS2}_1 + \text{TS2}_{21} + \text{TS2}_{22}. \end{aligned} \quad (2.46)$$

Note that the terms TS1, TS2₂₁, and TS2₂₂ are responsible for the final electron plane wave distortion up to the second order and enter in a symmetrical manner with respect to all three channels. The term TS2₁ bears some information about processes related to indirect Coulomb distortions in the atom itself under the influence of an incoming electron (which is

connected with $\chi^+(\mathbf{p}_0)$). As expected, SBA provides information equivalent to formula (2.31). This amount of information may be less than that contained in (2.31); nonetheless, it is more specific and leaves no ambiguity in treating distorted waves.

Closely related transformations were carried out in [49]; however, the authors did not encounter a divergence problem by using the so-called closure approximation, which substantially alters the asymptotic condition. This approximation allows estimation of the average contribution of intermediate excitations into the cross section of the process under consideration. For this, we proceed with replacing $E_\alpha \rightarrow \bar{\varepsilon} > -0.5$ in the sum given in (2.38) and account for the completeness condition of the eigenfunctions $|\Psi_\alpha^-\rangle$

$$\sum_\alpha |\Psi_\alpha^-\rangle \langle \Psi_\alpha^-| = I.$$

As a result of these manipulations, the sum in (2.38) is reduced to the expression

$$\begin{aligned} \sum_\alpha \dots &= \int \frac{d^3 \mathbf{x}}{(2\pi)^3} \frac{4\pi}{(\mathbf{p}_0 - \mathbf{x})^2} \frac{4\pi}{(\mathbf{p}_s - \mathbf{x})^2} \frac{1}{E - \bar{\varepsilon} - \frac{x^2}{2} + i0} \\ &\times [\int d^3 \mathbf{r}_1 \tilde{\varphi}^{-*}(\mathbf{p}_e, \mathbf{r}_1) e^{i(\mathbf{p}_0 - \mathbf{p}_s)\mathbf{r}_1} \tilde{\varphi}_0(\mathbf{r}_1) \\ &- \int d^3 \mathbf{r}_1 \tilde{\varphi}^{-*}(\mathbf{p}_e, \mathbf{r}_1) e^{i(\mathbf{x} - \mathbf{p}_s)\mathbf{r}_1} \tilde{\varphi}_0(\mathbf{r}_1) \\ &- \int d^3 \mathbf{r}_1 \tilde{\varphi}^{-*}(\mathbf{p}_e, \mathbf{r}_1) e^{-i(\mathbf{x} - \mathbf{p}_0)\mathbf{r}_1} \tilde{\varphi}_0(\mathbf{r}_1)] \end{aligned} \quad (2.47)$$

(the tilde sign here stands for the coordinate representation of the Coulomb function). Keeping in mind that the momentum p_e is large, we assume in (2.47) that the Coulomb wave is approximately a plane one with simultaneous substitution $\mathbf{x} \rightarrow (\mathbf{p}_e - \mathbf{x})$. Finally, we obtain

$$\begin{aligned} \text{CA} &= \int \frac{d^3 \mathbf{x}}{(2\pi)^3} \frac{4\pi}{(\mathbf{p}_0 - \mathbf{p}_s - \mathbf{x})^2} \frac{1}{E - \bar{\varepsilon} - \frac{(\mathbf{p}_s + \mathbf{x})^2}{2} + i0} \frac{4\pi}{x^2} \\ &\times [\varphi_0(q) - \varphi_0(\mathbf{p}_e - \mathbf{x}) - \varphi_0(\mathbf{q} + \mathbf{x})]. \end{aligned} \quad (2.48)$$

In integral (2.48) there is already no divergence problem, if, for example, $\bar{\varepsilon}$ lies somewhere within a discrete part of the Coulomb spectrum, or even is a small and positive quantity. The first two terms in square brackets in (2.48) correspond to the sum of mechanisms TS2₁ + TS2₂₂, whereas the third one corresponds to the mechanism TS2₂₁.

In the closure approximation, only the term TS1(z) needs to be regularized,

$$t_{\text{clos}} \approx [1 - R_e(z)] \text{FBA} + \text{TS1}(z) + \text{CA}, \quad (2.49)$$

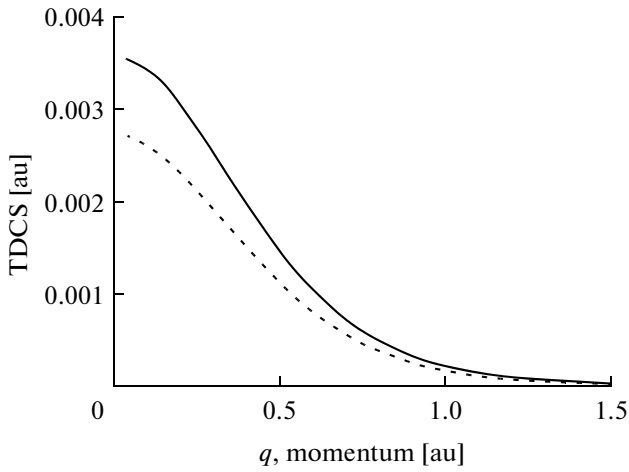


Fig. 2. Triple differential cross section of the quasi-elastic reaction $H(e,2e)H^+$ as a function of recoil momentum q within FBA (solid curve) and PWIA (dashed curve), on a linear scale. $E_0 = 2013.6$ eV.

where

$$R_e(z) = i\eta_e \ln(z - E) + \eta_e \left(\frac{\pi}{2} + iC \right) - i\eta_e \ln(2p_e^2).$$

2.5. Calculation of Differential Cross Sections. Discussion

The kinematics of ionization experiments with a helium target carried out recently by a Japanese group [63] has been chosen for the calculations and estimates. In these experiments the angle of each electron is fixed at 45° with respect to an incoming electron. One of the detectors registering secondary electrons

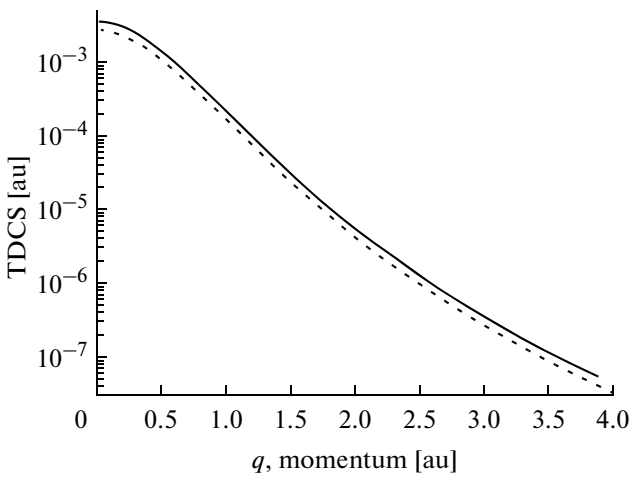


Fig. 3. The same as in Fig. 2 on a logarithmic scale.

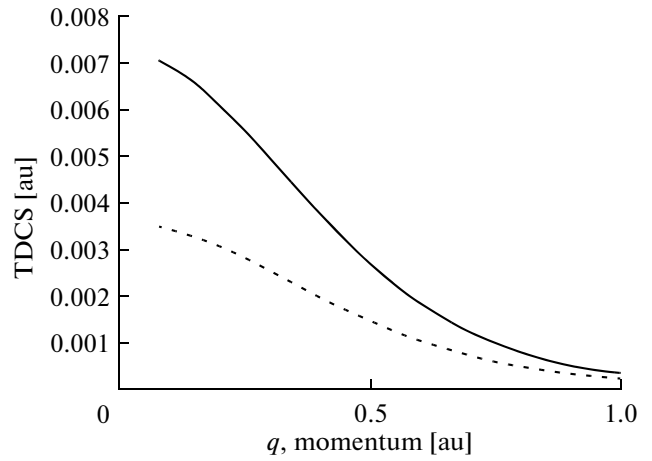


Fig. 4. Triple differential cross section of the quasi-elastic reaction $H(e,2e)H^+$ as a function of recoil momentum q within FBA (dashed curve) and $SBA^{\text{simple}} = FBA + TS1 + TS2_{21} + TS2_{22}$ (solid curve) on a linear scale. $E_0 = 2013.6$ eV.

was circled in the direction transverse to the plane made up of velocity vectors of the incident and another secondary electron. In this kinematics $p_s^2 = p_e^2 = 2E_s$, $p_0^2 = 2(2E_s + \varepsilon_0)$ and Φ is the angle between the vectors \mathbf{p}_s and \mathbf{p}_e . Here

$$\begin{aligned} q^2 &= |\mathbf{p}_0 - \mathbf{p}_s - \mathbf{p}_e|^2 \\ &= 4E_s \left(\cos\Phi + 2 - 2\sqrt{1 + \frac{\varepsilon_0}{2E_s} + \frac{\varepsilon_0}{2E_s}} \right). \end{aligned} \quad (2.50)$$

The angle Φ is related to the polar angle α of the electron momentum relative to the scattering plane by the relation $\cos\Phi = 0.5(1 - \cos\alpha)$ with the phase chosen so that the minimal value q is realized under the condition that all the electrons are in the same plane. This value tends to zero for $E_s \rightarrow \infty$, but for finite E_s it is finite as well. For example, if $E_s \gg \varepsilon_0$, then $q_{\min} \approx \varepsilon_0/(2\sqrt{E_s})$. Equality (2.50) provides the relation between the angles and momentum q , which is used in calculations of various matrix elements while deriving momentum profiles in the variable q .

In Figs. 2–5 and 9–12 [64], the calculation results for contributions coming from both the separate SBA mechanisms of a hydrogen atom ionization reaction and the SBA in general are shown. The calculations were carried out at the energy $E = 2013.6$ eV (1 keV per each final electron). Such a choice of final electron energies is governed by the experiments [63].

In Figs. 2 and 3, the main approximations of the first order, FBA and PWIA, are presented. Since the ground state of a hydrogen atom is the $1s$ state, the cross section is a finite quantity for $q \rightarrow 0$. In the case of higher angular states— p , d , f —the cross section

will tend to zero at small q . It is this visual difference in the angular profiles of electron momentum distributions in a target that endows the electron momentum spectroscopy with methodological power.

In Figs. 4 and 5, the results of the cross section calculations, which include, along with FBA, contributions coming from some mechanisms of the second order—TS1, TS2₂₁, TS2₂₂ (their sum with FBA is denoted as SBA^{simple})—are shown. They noticeably overestimate FBA calculations at both small and large q values, though there is a range of $1.5 \leq q \leq 2.5$, in which the curves practically coincide. Recall that these mechanisms give rise to the fast electron plane wave distortions in the final state. The mechanisms TS2₂₁ and TS1 are responsible for the distortion of one of the secondary electron plane waves by the nuclear field, whereas TS2₂₂ corresponds to wave distortion caused by their Coulomb repulsion. A contribution from this mechanism reduces the cross section compared to FBA calculations, while the Coulomb interaction of proton and electrons considerably increases it. This is surprising, since the energies of electrons are sufficiently large ($p_s = p_e \sim 10$) for the Coulomb parameters (or Sommerfeld parameters) η_i to be considered rather small.

It should be noted that, in the case of a hydrogen atom, there are a number of analytical tests allowing one not only to check the quality of numerical calculations but also to draw definite conclusions about the quality of the second Born approximation in the case of Coulomb interactions between particles. Let us turn back to the first term in (2.38). This matrix element can be evaluated analytically (we denote it as the CWBA—Coulomb wave Born approximation):

$$\begin{aligned} \text{CWBA} &= \langle \mathbf{p}_s, \varphi^-(\mathbf{p}_e) | \nabla_{12} | \mathbf{p}_0, \varphi_0 \rangle \\ &= \text{FBA} e^{-\pi\eta_e/2} \Gamma(1+i\eta_e) \left[\frac{Q^2 + (1-ip_e)^2}{1+q^2} \right]^{i\eta_e} \\ &\quad \times \left[1 + i\eta_e \left(1 - \frac{(1-ip_e)(1+q^2)}{(1-ip_e)^2 + Q^2} \right) \right]. \end{aligned} \quad (2.51)$$

In formula (2.40) $\eta_e = -1/p_e$. The matrix element PWIA is also calculated analytically:

$$\begin{aligned} \text{PWIA} &= \langle e^{i\mathbf{P}_{se}\mathbf{r}_{12}} \tilde{\varphi}^-(\mathbf{p}_{se}, \mathbf{r}_{12}) | \nabla_{12} | \mathbf{p}_0, \varphi_0 \rangle \\ &= \text{FBA} \times e^{-\pi\eta_{se}/2} \Gamma(1+i\eta_{se}) \left[\frac{\frac{1}{4}(\mathbf{p}_0 - \mathbf{q})^2 - p_{se}^2}{Q^2} \right]^{i\eta_{se}}, \end{aligned} \quad (2.52)$$

where $\mathbf{P}_{se} = \mathbf{p}_s + \mathbf{p}_e$, $\mathbf{p}_{se} = (\mathbf{p}_s - \mathbf{p}_e)/2$, and $\eta_{se} = 1/2p_{se}$.

The second order plane-wave approximations to expressions (2.51) and (2.52) are obtained from their

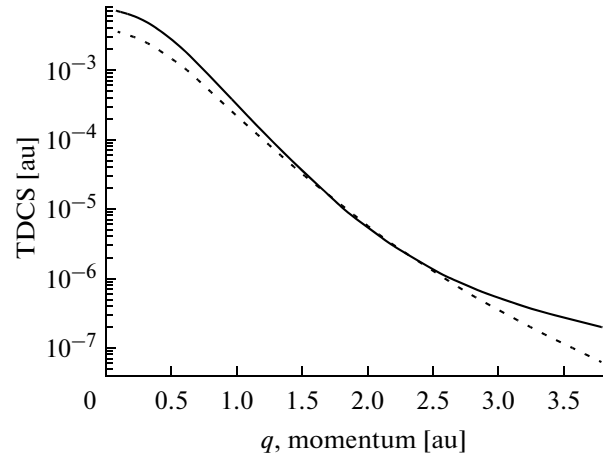


Fig. 5. The same as in Fig. 4 on a logarithmic scale.

expansion in a Taylor series over Sommerfeld parameters η_e and η_{se} , respectively:

$$\begin{aligned} \text{CWBA} &\approx \text{FBA} \cdot \left[1 - \frac{\pi\eta_e}{2} - iC\eta_e \right. \\ &\quad \left. + i\eta_e \left(1 - \frac{(1-ip_e)(1+q^2)}{(1-ip_e)^2 + Q^2} \right) + i\eta_e \ln \frac{Q^2 + (1-ip_e)^2}{1+q^2} \right], \end{aligned} \quad (2.53)$$

$$\begin{aligned} \text{PWIA} &\approx \text{FBA} \times \left[1 - \frac{\pi\eta_{se}}{2} - iC\eta_{se} \right. \\ &\quad \left. + i\eta_{se} \ln \frac{\frac{1}{4}(\mathbf{p}_0 - \mathbf{q})^2 - p_{se}^2}{Q^2} \right]. \end{aligned} \quad (2.54)$$

Note that **absolutely the same results** are obtained in the case of applying a regularization procedure for $z \rightarrow E + i0$:

$$\begin{aligned} \text{CWBA} &\approx \left(1 - \frac{\pi\eta_e}{2} + iA_e - iC\eta_e \right) \text{FBA} \\ &\quad + \lim_{z \rightarrow E+i0} [\text{TS1}(z) - i\eta_e \text{FBA} \ln(z-E)], \end{aligned} \quad (2.55)$$

$$\begin{aligned} \text{PWIA} &\approx \left(1 - \frac{\pi\eta_{se}}{2} + iA_{se} - iC\eta_{se} \right) \text{FBA} \\ &\quad + \lim_{z \rightarrow E+i0} [\text{TS2}_{22}(z) - i\eta_{se} \text{FBA} \ln(z-E)]. \end{aligned} \quad (2.56)$$

Recall that the Dollard phases are $A_e = \eta_e \ln(2p_e^2)$ and $A_{se} = \eta_{se} \ln(4p_{se}^2)$. The integrals TS1(z) and

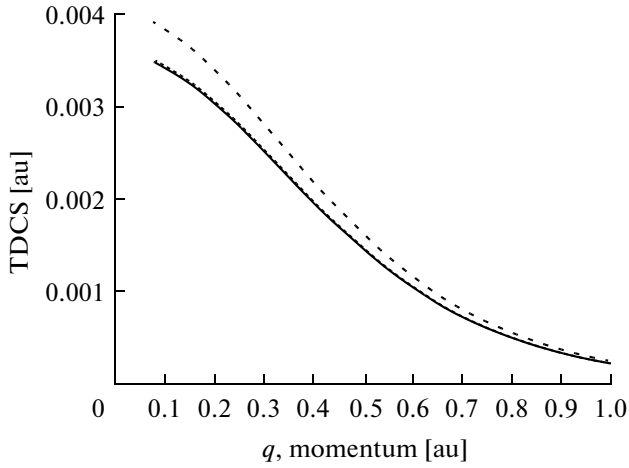


Fig. 6. Triple differential cross section of the quasi-elastic reaction $H(e,2e)H^+$ as a function of recoil momentum q within the following approximations: second order to CWBA (upper dashed curve), third and higher orders to CWBA (lower dotted curve), and exact CWBA (lower curves, almost indiscernible in the picture). $E_0 = 2013.6$ eV.

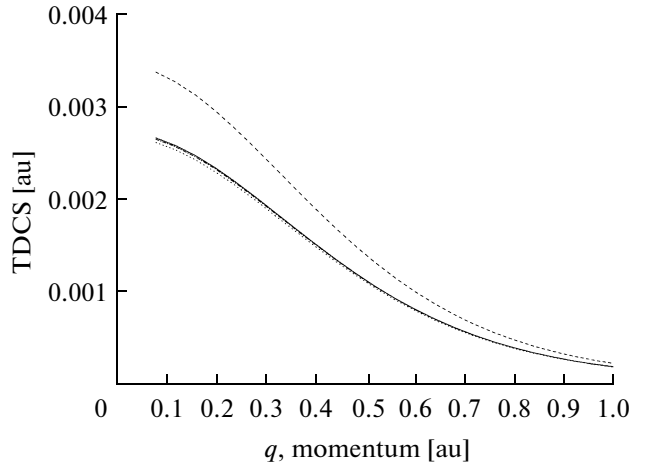


Fig. 7. Triple differential cross section of the quasi-elastic reaction $H(e,2e)H^+$ as a function of recoil momentum q within the following approximations: second order to PWIA (upper dashed curve), third and higher orders to PWIA (lower dotted curve), and exact PWIA (lower curves, almost indiscernible in the picture). $E_0 = 2013.6$ eV.

$TS_{22}(z)$ are related to the so-called Lewis-type integrals [65] and calculated analytically,

$$\begin{aligned} TS1(z \rightarrow E + i0) &= -\frac{4\pi}{Q^2} \int \frac{d^3x}{(2\pi)^3} \\ &\times \frac{\varphi_0(\mathbf{q} + \mathbf{x})}{z - \frac{p_s^2}{2} - \frac{(\mathbf{p}_e + \mathbf{x})^2}{2}} \frac{4\pi}{x^2} \\ &= \text{FBA} i\eta_e \left[1 - \frac{(1 - ip_e)(1 + q^2)}{(1 - ip_e)^2 + Q^2} \right. \\ &\left. + \ln \frac{Q^2 + (1 - ip_e)^2}{1 + q^2} + \ln \frac{(z - E)}{2p_e^2} \right], \end{aligned} \quad (2.57)$$

$$\begin{aligned} TS_{22}(z \rightarrow E + i0) &= \varphi_0(\mathbf{q}) \int \frac{d^3x}{(2\pi)^3} \\ &\times \frac{4\pi}{(\mathbf{Q} + \mathbf{x})^2} \frac{1}{z - E + 2\mathbf{p}_{se}\mathbf{x} - x^2 + i0} \frac{4\pi}{x^2} \\ &= \text{FBA} \cdot i\eta_{se} \left[\ln \frac{\frac{1}{4}(\mathbf{p}_0 - \mathbf{q})^2 - p_{se}^2}{Q^2} + \ln \frac{(z - E)}{4p_{se}^2} \right]. \end{aligned} \quad (2.58)$$

By further expanding expressions (2.51) and (2.52) in terms of Sommerfeld parameters, the higher Born approximations can be derived. The results of calculation in the framework of these approximations are

demonstrated in Figs. 6 and 7 [66]. The curves showing the differential cross section in the FBA and CWBA approximations almost coincide within a sufficiently wide range of recoil momentum q . The same can be said about approximations beginning from the third order one. Only the second Born approximation is notably different (!). The same picture is reproduced in the case of the impulse approximation. From this, a paradoxical conclusion follows that accounting for the wave distortion mechanisms within the SBA framework only leads to worsening, rather than improvement, of the results. This negative effect should entirely be attributed to the quality of the continuous spectrum Coulomb function's approximation by the plane wave: for this, taking into account only two terms of a Taylor series is obviously insufficient.

It is curious that a similar result is obtained by using in (2.25) the so-called BBK function (or 3C) [15] for the final state,

$$\begin{aligned} \Psi_{3C}^-(\mathbf{p}_s, \mathbf{p}_e; \mathbf{r}_1, \mathbf{r}_2) \\ = e^{-i\mathbf{p}_{se}\mathbf{r}_{12}} \tilde{\varphi}^-(\mathbf{p}_s, \mathbf{r}_1) \tilde{\varphi}^-(\mathbf{p}_e, \mathbf{r}_2) \tilde{\varphi}^-(\mathbf{p}_{se}, \mathbf{r}_{12}). \end{aligned} \quad (2.59)$$

When expanded in a series over Coulomb numbers up to the first order inclusive, the function in (2.59) gives exactly (FBA + SBA^{simple}). Corresponding calculations are presented in Fig. 8 (done by C. Dal Capello). As can be seen, the results of application of the BBK function practically coincide with those using FBA.

The contributions coming from intermediate excitations $n = 1, 2$ (Figs. 9, 10) almost do not change the cross section for small q . At the same time, the effect of $2s$ and $2p$ waves is clearly noticeable at medium momenta q .

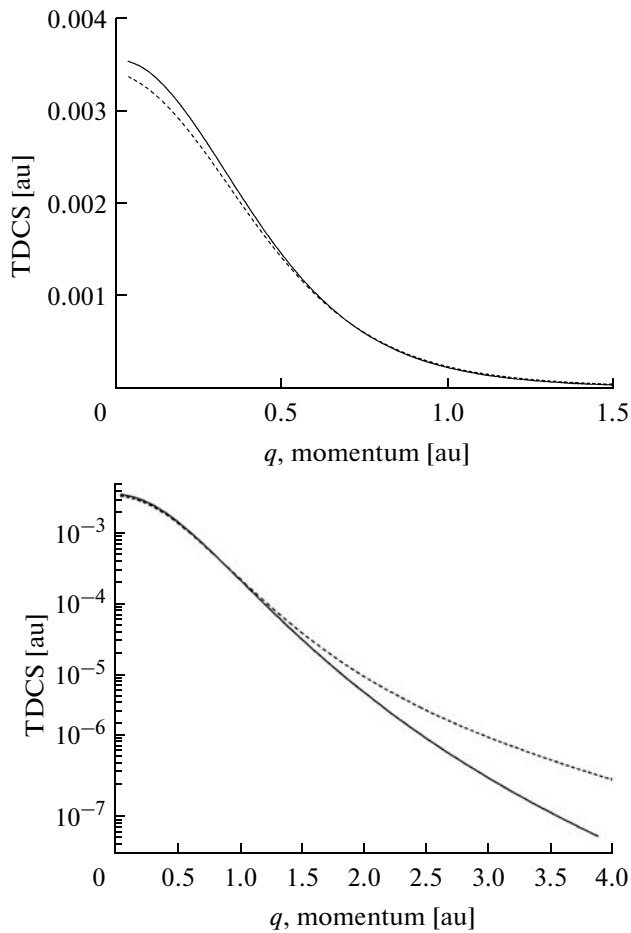


Fig. 8. Triple differential cross section of the quasi-elastic reaction $H(e,2e)H^+$ as a function of recoil momentum q within FBA (solid curve) and BBK (dashed curve). $E_0 = 2013.6$ eV.

Remember that the contributions from intermediate states are usually related to the reaction of a neutral atom to an incoming electron, first of all, to the atom polarization, which is described exactly by $2p$ excited state. It is the transition $1s \rightarrow 2p$ that dominates in the photoionization reaction. In the case of the $(e, 2e)$ reaction at large initial energies, the transitions $1s \rightarrow ns$ ($n \geq 2$) are not forbidden. However, as calculations reveal, in the case of quasi-symmetric geometry chosen, they do not make a noticeable contribution to SBA within almost the entire range of variation of momentum q , just as the transition $1s \rightarrow 2p$. Only an elastic channel in the intermediate state makes an appreciable contribution for $q > 3$, which is usually connected with a distortion of the incoming electron plane wave in the initial state due to multiparticle effects [48].

In Figs. 11 and 12, the results of SBA calculations in the closure approximation are presented. In this version of the latter, an incoming electron plane wave distortion by a proton field in the final state is considered, along with the averaged effect of the intermediate states

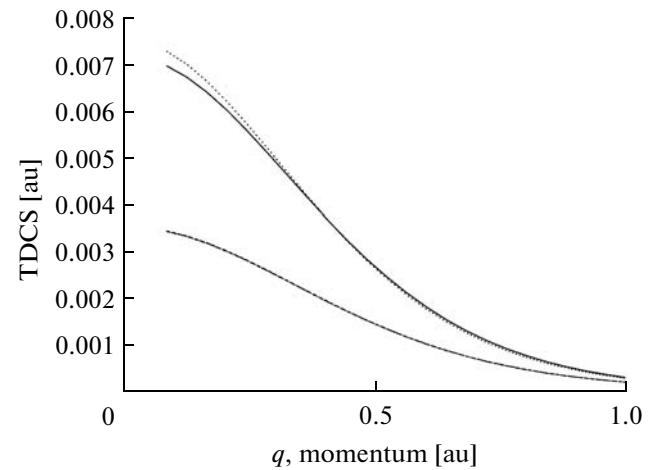


Fig. 9. Triple differential cross section of the quasi-elastic reaction $H(e,2e)H^+$ as a function of recoil momentum q within the following approximations: FBA (lower dashed curve), FBA + $1s$ (lower dash-dotted curve), SBA^{simple} (upper solid curve), and $SBA^{\text{simple}} + 1s + 2s + 2p$ (upper dotted curve) on a linear scale. $E_0 = 2013.6$ eV.

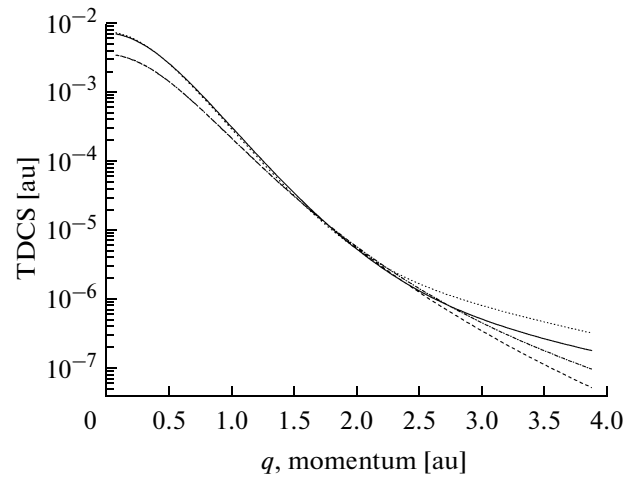


Fig. 10. The same as in Fig. 9 on a logarithmic scale.

according to (2.36). The quantity $\bar{\epsilon}$ may vary in atomic units from -0.5 to $+\infty$. As it follows from the calculations, the cross section curves almost coincide at small q within a wide range of variation of parameter $\bar{\epsilon}$ and are located closer to FBA than to SBA. At the same time, differences at large values of q become increasingly appreciable. While moving an “average point” $\bar{\epsilon}$ around a spectrum of intermediate excitations, the cross section tends to shift toward FBA, which fact is, from our standpoint, positive for this rather rough approximation. It

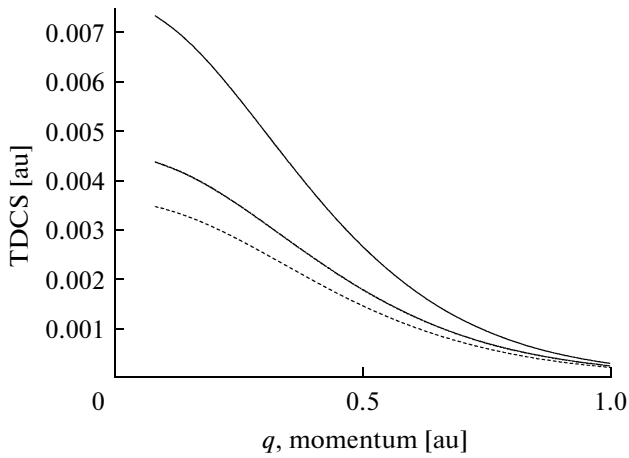


Fig. 11. Triple differential cross section of the quasi-elastic reaction $H(e,2e)H^+$ as a function of recoil momentum q within the following approximations: FBA (lower dashed curve), closure approximation with $\bar{\epsilon} = -0.2$ (middle curve with short strokes), $\bar{\epsilon} = 3$ (middle dash-dotted curve), $\bar{\epsilon} = 10$ (middle dotted curve), and $SBA^{\text{simple}} + 1s + 2s + 2p$ (upper solid curve) on a linear scale. $E_0 = 2013.6$ eV.

should also not be forgotten that the cross section itself, at the end of the range of momentum q , is almost four orders of magnitude smaller than at the beginning of that diapason. Overall, the closure approximation is closer to FBA than to $(FBA + SBA^{\text{simple}})$ at small q , which finding suggests that it is useful for practical calculations. Moreover, if one takes into account the negative effect caused by the TS1 contribution (see Fig. 6) to the total distortion of an incoming electron plane wave, then, apparently, a rather less contribution from the CA term to the cross section at small q is to be expected, what is consistent with the calculations presented in Fig. 9.

2.6. Conclusions to Section 2

Let us briefly formulate the results obtained in this section.

(1) Using the specific example of quasi-elastic reaction $H + e \rightarrow H^+ + 2e$, the possibility to regularize singular integrals, describing higher Born terms, which is provided by the general theory of few charged particle scattering, is shown to exist. A numerical calculation of the cross section of this reaction is carried out in the second order of perturbation theory.

(2) The regularization theory of divergent integrals of a perturbative series yields a result that coincides with expansion in a Taylor series over Sommerfeld parameters in those cases in which analytical solutions are possible.

(3) Taking into account the intermediate continuum while carrying out computations of the second

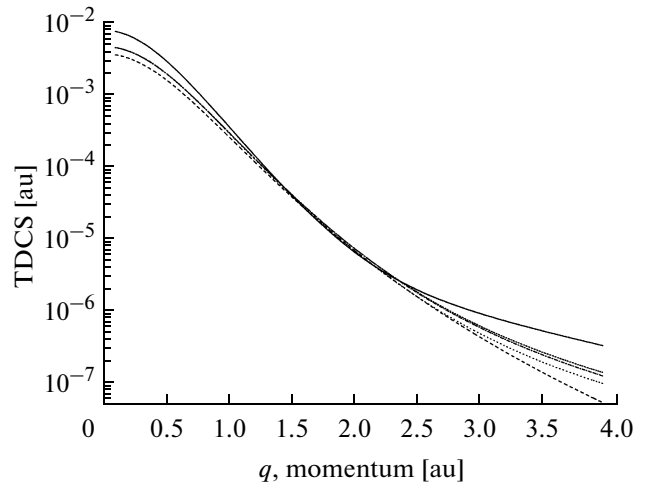


Fig. 12. The same as in Fig. 11 on a logarithmic scale.

order effects reduces the quality of the approximation in the case of quasi-elastic knockout processes at collision energies that are not asymptotically large, what is demonstrated with the test examples. It is necessary to take into account at least the third order effects, or to do calculations with distorted waves, or not to take into account the mechanisms TS1, TS2₂₁, and TS2₂₂ at small momenta q . The latter hypothesis served as a basis for choosing the calculation scheme in [67].

(4) At an initial energy of ~ 2 keV, taking into account the intermediate excitations of atomic discrete states weakly affects the shape of the curve for the differential cross section at small recoil momenta q . However, when increasing q , it becomes more noticeable, mainly due to elastic rescattering against a background of considerable decrease of the cross section itself calculated in FBA. This confirms the validity of the “frozen core” model at large collision energies and small recoil momenta.

(5) The closure approximation gets us closer to FBA, rather than simply SBA, within a wide range of momenta q and parameters $\bar{\epsilon}$.

Yet another important conclusion can be drawn—that 1 keV per one outgoing electron is enough, at least for hydrogen, to speak of the overwhelming dominance of the first Born approximation FBA, which carries basic information about a target wave function, up to $q \approx 2$. At higher momenta q , it is necessary to take into account the wave distortions, including elastic rescattering of a projectile electron off a target (FBA curve + $1s$ in Fig. 10), though this is what is usually done in the most distorted wave method calculations.

APPENDIX

Let us substitute representation (2.24) in (2.22) and rewrite the equation in the form

$$\begin{aligned}
 & (z - p_s^2/2 - p_e^2/2)^{i\eta(\mathbf{p}_s, \mathbf{p}_e)} r(\mathbf{p}_s, \mathbf{p}_e; z) + \tilde{R}(\mathbf{p}_s, \mathbf{p}_e; z) \\
 &= 1 + r(\mathbf{p}_s, \mathbf{p}_e; z) \int \frac{d^3 k_s}{(2\pi)^3} \frac{d^3 k_e}{(2\pi)^3} \langle \mathbf{p}_s, \mathbf{p}_e | W | \mathbf{k}_s, \mathbf{k}_e \rangle \\
 & \quad \times (z - k_s^2/2 - k_e^2/2)^{-1 + i\eta(\mathbf{p}_s, \mathbf{p}_e)} \\
 & \quad + \int \frac{d^3 k_s}{(2\pi)^3} \frac{d^3 k_e}{(2\pi)^3} \frac{\langle \mathbf{p}_s, \mathbf{p}_e | W | \mathbf{k}_s, \mathbf{k}_e \rangle}{(z - k_s^2/2 - k_e^2/2)} \\
 & \quad \times [r(\mathbf{k}_s, \mathbf{k}_e; z)(z - k_s^2/2 - k_e^2/2)^{i\eta(\mathbf{k}_s, \mathbf{k}_e)} \\
 & \quad - r(\mathbf{p}_s, \mathbf{p}_e; z)(z - k_s^2/2 - k_e^2/2)^{i\eta(\mathbf{p}_s, \mathbf{p}_e)}] \\
 & \quad + \int \frac{d^3 k_s}{(2\pi)^3} \frac{d^3 k_e}{(2\pi)^3} \frac{\langle \mathbf{p}_s, \mathbf{p}_e | W | \mathbf{k}_s, \mathbf{k}_e \rangle}{(z - k_s^2/2 - k_e^2/2)} \tilde{R}(\mathbf{k}_s, \mathbf{k}_e; z).
 \end{aligned} \tag{A.1}$$

The matrix element $\langle \mathbf{p}_s, \mathbf{p}_e | W | \mathbf{k}_s, \mathbf{k}_e \rangle$ includes a sum of three terms of the same type. Let us consider one of them,

$$\langle \mathbf{p}_s, \mathbf{p}_e | v_{1M} | \mathbf{k}_s, \mathbf{k}_e \rangle = (2\pi)^3 \delta(\mathbf{p}_e - \mathbf{k}_e) \frac{-4\pi}{|\mathbf{p}_s - \mathbf{k}_s|^2}, \tag{A.2}$$

and calculate the master integral,

$$I_e = \int \frac{d^3 k_s}{(2\pi)^3} \frac{-4\pi}{|\mathbf{p}_s - \mathbf{k}_s|^2} (z - p_s^2/2 - k_e^2/2)^{-1 + i\eta}. \tag{A.3}$$

We proceed with replacing $\mathbf{k}_s = \mathbf{p}_s - \mathbf{x}$, and, by evaluating a trivial integral over angular variables, we obtain

$$\begin{aligned}
 I_e &= \frac{-1}{i\pi p_e \eta} \int_0^\infty \frac{dx}{x} [((z - E + p_e x - x^2/2)^{i\eta} \\
 & \quad - (z - E - p_e x - x^2/2)^{i\eta}] \\
 & \quad - \frac{(p_e^2/2)^{i\eta}}{i\pi p_e \eta} \int_{-\infty}^\infty \frac{dx}{x} (\gamma + 2x - x^2)^{i\eta}; \\
 & \quad \gamma = \frac{(z - E)}{p_e^2/2}; \quad \text{Im}\gamma > 0.
 \end{aligned} \tag{A.4}$$

We use the known transformation

$$\frac{1}{\Gamma(\alpha)} \int_0^\infty t^{-1+\alpha} e^{-tx} dt = x^{-\alpha}; \quad \text{Re}x > 0; \quad \text{Re}\alpha > 0.$$

Then

$$\begin{aligned}
 I_e &= -2 \frac{(p_e^2/2)^{i\eta}}{\pi p_e \eta} \frac{e^{-\pi\eta/2}}{\Gamma(-i\eta)} \\
 & \times \int_0^\infty t^{-1-i\eta} e^{i\gamma t} dt \int_0^\infty \frac{dx}{x} e^{-ix^2} \sin(2xt).
 \end{aligned} \tag{A.5}$$

The integral over x is equal to $\sqrt{t} e^{-\pi/4} {}_1F_1(1/2, 3/2; it)$ and (A.5) turns to

$$\begin{aligned}
 I_e &= -2 \frac{(p_e^2/2)^{i\eta}}{\sqrt{i\pi p_e \eta}} \frac{e^{-\pi\eta/2}}{\Gamma(-i\eta)} \\
 & \times \int_0^\infty t^{-1/2-i\eta} e^{i\gamma t} {}_1F_1(1/2, 3/2; it) dt.
 \end{aligned} \tag{A.6}$$

The integral over t is a textbook one,

$$\begin{aligned}
 & \int_0^\infty d\rho \exp(-\beta\rho) \rho^\nu {}_1F_1(\alpha, \gamma; \lambda\rho) \\
 &= \frac{\Gamma(\nu+1)}{\beta^{\nu+1}} {}_2F_1\left(\nu+1, \alpha; \gamma; \frac{\lambda}{\beta}\right);
 \end{aligned}$$

$$\text{Re}\beta > \text{Re}\lambda,$$

and, as a result of calculations,

$$\begin{aligned}
 I_e &= -2 \frac{(p_e^2/2)^{i\eta}}{\sqrt{\pi p_e \eta}} \frac{\Gamma(1/2 - i\eta)}{\Gamma(-i\eta)} \gamma^{-1/2 + i\eta} \\
 & \times {}_2F_1\left(\frac{1}{2} - i\eta, \frac{1}{2}; \frac{3}{2}; -\frac{1}{\gamma}\right).
 \end{aligned} \tag{A.7}$$

Using the formula for the hypergeometric function transformation under an argument inversion, we finally obtain

$$\begin{aligned}
 I_e &= \frac{\eta_e}{\eta} \left[(z - E)^{i\eta} - \frac{(p_e^2/2)^{i\eta}}{\sqrt{\pi}} \frac{\Gamma(1/2 - i\eta)}{\Gamma(-i\eta)} \right. \\
 & \left. \times {}_2F_1\left(\frac{1}{2} - i\eta, -i\eta; 1 - i\eta; \gamma\right) \right].
 \end{aligned} \tag{A.8}$$

Carrying out analogous calculations for other potentials in the sum W , for $z \rightarrow E + i0$, we derive

$$I_e + I_s + I_{se} \approx (z - E)^{i\eta} - \frac{B}{\sqrt{\pi}} \frac{\Gamma(1/2 - i\eta)}{\Gamma(1 - i\eta)} + O(\gamma), \tag{A.9}$$

where

$$B = \frac{\eta_e E_e^{i\eta} + \eta_s E_s^{i\eta} + \eta_{se} E_{se}^{i\eta}}{\eta},$$

which needs to be proved.

Note that it is necessary to ensure convergence of all the integrals in (A.1) at infinitely large values of integration variables. This is achieved by the formal

replacement $\eta \rightarrow \eta + i\lambda$, $\lambda \rightarrow +0$ and demanding that the functions r and \tilde{R} are sufficiently fast decaying. In the final expressions, it is possible to take $\lambda = 0$, as was done while calculating integral (A.5). Moreover, from (A.1) it follows that $\tilde{R}(\mathbf{p}_s, \mathbf{p}_e; E + i0) = 0$, since the last integral found in the sum in the right hand side of the equality is regular by definition.

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