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Asymptotic form of the electron-hydrogen scattered wave

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A relationship between the total wave function describing electron-impact ionization of hydrogen and the one representing scattering of two electrons and a proton in the continuum is revealed. On the basis of this relationship, forms of the scattered wave for the ionization process valid in all asymptotic domains are obtained. When all interparticle distances become large, the new wave functions reduce to the well-known Peterkop asymptotic wave function obtained in the hyperspherical approach. In particular, the Peterkop wave function is obtained by direct application of the present approach. This allows one to resolve the long-standing amplitude-phase ambiguity problem, which is an artifact of the hyperspherical approach to the ionization process. The Peterkop wave function is invalid when the two electrons are close to each other. This causes problems in practical calculations even in the domain where all particles are far apart. Our formulation provides a solution to this problem.

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In recent years several powerful time-independent methods for the calculation of energy-differential electron-impact ionization cross sections of hydrogen have emerged including exterior complex scaling (ECS) [1,2], convergent close coupling (CCC) [3,4], and *R*-matrix [5,6] methods. These methods provide an accurate three-body scattering wave function in an ''internal'' region in coordinate space, and the ionization amplitude is extracted by matching to ionization boundary conditions in the asymptotic region. In each method, the extraction process relies on approximate ionization boundary conditions. For example, in the CCC method, the ionization flux is initially obtained by discretizing the target continuum. The ionization amplitude is then constructed by means of a renormalization of the square-integrable positive-energy target states with the true target continuum. Implicit in this approach is the representation of the three-body continuum states as a product of plane and Coulomb waves without electron-electron correlation. A similar approach is being adopted in the *R*-matrix method [15]. In the ECS method an integral representation of the ionization amplitude is used but again the three-body continuum states are approximated, this time by a product of two fixed-charge Coulomb waves for the two free electrons [2]. This yields an ionization amplitude with divergent phase as a function of matching radius although the magnitude of the amplitude converges.

An asymptotic form of the scattered wave for electron-impact ionization of hydrogen for the case when all interparticle distances are large was obtained by Peterkop [7,8] four decades ago but it has not been successfully implemented in these approaches. One reason is that direct numerical solution of the Schrödinger equation for the full hydrogen-ionization problem requires partial-wave analysis of the asymptotic wave function and a suitable partial-wave decomposition of the Peterkop wave function does not exist. The problem is that Peterkop's asymptotic wave function is invalid when the two electrons are close to each other. Thus, for full-scale numerical calculations, a representation of the wave function describing ionization at least in this region as well is necessary. A further difficulty with Peterkop's wave function is that it does not define the ionization amplitude uniquely [9]. This so-called amplitude-phase ambiguity has caused problems in the formal theory of breakup at a very fundamental level.

Therefore a deeper understanding of the asymptotic behavior of the total scattering wave function is crucial in the theory of atomic ionization. The present paper deals with these outstanding problems of quantum dynamics. We show how to resolve the amplitude-phase ambiguity and present analytic forms of the scattered wave in all asymptotic domains relevant to ionization. This removes the above-mentioned problems in practical calculations and makes the correct extraction of observables possible.

Consider scattering of electron e_2 off hydrogen $(p+e_1)$ at energies above the ionization threshold of the atom. We assume that the electrons are distinguishable. The total three-body wave function describing this process satisfies the Schrödinger equation

$$(E-H)\Phi^{+}_{\boldsymbol{k}_1,\boldsymbol{k}_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)=0, \tag{1}$$

where H is the three-body Hamiltonian and $E=k_1^2/2+k_2^2/2$ is the total energy of the system (atomic units are used throughout this work; we also assume that the proton is infinitely heavy compared to the electrons and remains at rest). $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ are the coordinates of the electrons relative to the proton and $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ are their momenta.

The wave function Φ^{+} consists of the incoming initial-channel wave $\Phi^{(\mathrm{in})}$ and the outgoing scattered wave $\Phi^{(\mathrm{sc})+}$: $\Phi^{+}=\Phi^{(\mathrm{in})}+\Phi^{(\mathrm{sc})+}$. With this, a formal solution of Eq. (1) can be written as

$$\Phi^{(\mathrm{sc})+}_{\boldsymbol{k}_1,\boldsymbol{k}_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)=\int d\boldsymbol{r}_1' d\boldsymbol{r}_2' G^{+}(\boldsymbol{r}_1,\boldsymbol{r}_2;\boldsymbol{r}_1',\boldsymbol{r}_2';E+i0) \times \overline{V}\Phi^{(\mathrm{in})}_{\boldsymbol{k}_{\mathrm{in}}}(\boldsymbol{r}_1',\boldsymbol{r}_2'), \tag{2}$$

where $\boldsymbol{k}_{\rm in}$ is the momentum of the incident electron, $\overline{V}$ is the interaction of the incident electron with the target particles, and G^+ is the three-body Green's function.

Next we apply a spectral decomposition for the Green's function. To this end we consider another scattering process with the same three particles but one where in the initial channel both electrons are in the continuum (so called $3\rightarrow3$ scattering, as opposed to $2\rightarrow3$ ionization scattering). We take the boundary condition for the wave function Ψ^- describing this process in the form of a Coulomb-distorted three-body plane wave and incoming scattered wave. This wave function of course is also an eigenstate of the same Hamiltonian H, i.e., $(E-H)\Psi^-_{\boldsymbol{k}_1,\boldsymbol{k}_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)=0$. Therefore, it is well suited for our purposes. As it will become clear later, the reason for choosing this form of the total wave function as the basis for decomposition rather than Ψ^+, which consists of the Coulomb three-body plane wave and the outgoing scattered wave, is twofold. First, Ψ^+ would eventually lead to incoming scattered wave $\Phi^{(\rm sc)-}$ instead of outgoing $\Phi^{(\rm sc)+}$ we need. Second, using Ψ^+ we are not able to introduce the ionization amplitude in a standard form.

Thus, making use of the spectral decomposition for the Green's function G^+ in Eq. (2) in terms of the three-body scattering wave function Ψ^-, we arrive at

$$\Phi^{(\rm sc)+}_{\boldsymbol{k}_1,\boldsymbol{k}_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)=\int d\boldsymbol{r}_1' d\boldsymbol{r}_2' \frac{d\boldsymbol{k}_1'}{(2\pi)^3}\frac{d\boldsymbol{k}_2'}{(2\pi)^3} \times\frac{\Psi^-_{\boldsymbol{k}_1',\boldsymbol{k}_2'}(\boldsymbol{r}_1,\boldsymbol{r}_2)\Psi^{-*}_{\boldsymbol{k}_1',\boldsymbol{k}_2'}(\boldsymbol{r}_1',\boldsymbol{r}_2')}{E-k_1'^2/2-k_2'^2/2+i0}\overline{V}\Phi^{(\rm in)}_{\boldsymbol{k}_{\rm in}}(\boldsymbol{r}_1',\boldsymbol{r}_2') +\cdots, \tag{3}$$

where the dots indicate the contributions from all (both three- and two-body) bound states of the Hamiltonian H. The function $(E-k_1'^2/2-k_2'^2/2+i0)^{-1}$ is a propagator describing motion of the electrons in continuum. Defining the ionization amplitude according to

$$f(\boldsymbol{k}_1,\boldsymbol{k}_2)=\int d\boldsymbol{r}_1 d\boldsymbol{r}_2 \Psi^{-*}_{\boldsymbol{k}_1,\boldsymbol{k}_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)\overline{V}\Phi^{(\rm in)}_{\boldsymbol{k}_{\rm in}}(\boldsymbol{r}_1,\boldsymbol{r}_2), \tag{4}$$

we rewrite Eq. (3) in the form

$$\Phi^{(\rm sc)+}_{\boldsymbol{k}_1,\boldsymbol{k}_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)=\int \frac{d\boldsymbol{k}_1'}{(2\pi)^3}\frac{d\boldsymbol{k}_2'}{(2\pi)^3}\frac{f(\boldsymbol{k}_1',\boldsymbol{k}_2')\Psi^-_{\boldsymbol{k}_1',\boldsymbol{k}_2'}(\boldsymbol{r}_1,\boldsymbol{r}_2)}{E-k_1'^2/2-k_2'^2/2+i0} +\cdots. \tag{5}$$

Equation (5) establishes a relationship between the total wave functions of the ionization process and the process of scattering of all three particles of the system in the continuum through the ionization amplitude. We emphasize that this relationship is general for an arbitrary Coulomb three-body system and couples the total wave functions of any $2\rightarrow3$ process within the system with that of the $3\rightarrow3$ process through the corresponding $2\rightarrow3$ breakup amplitude. Equation (5) is our first main result.

Further in this work we investigate the asymptotic behavior of $\Phi^{(\rm sc)+}$ based on the relationship (5). Such an approach then allows us to find a wave function valid in all asymptotic domains.

Let us call Ω_0 the asymptotic domain, where all interparticle distances are large, i.e, $r_1\rightarrow\infty$, $r_2\rightarrow\infty$, and $r_3\rightarrow\infty$, where $\boldsymbol{r}_3=\boldsymbol{r}_1-\boldsymbol{r}_2$. In addition, we call Ω_1 (Ω_2) the asymptotic regime, where r_1 (r_2) is limited, but $r_2\rightarrow\infty$ ($r_1\rightarrow\infty$) and $r_3\rightarrow\infty$. Finally, Ω_3 is a domain where two electrons tend to infinity, but with r_3 being limited. Since Ω_1 and Ω_2 are symmetric, it is sufficient to consider only one of them. We introduce notations $\Phi^{(i)+}$ ($\Psi^{(i)-}$) for the leading-order asymptotic terms of $\Phi^{(\rm sc)+}$ (Ψ^-) in $\Omega_i, i=0,1,3$.

For $E>0$ considered, the leading term of Ψ^- in Ω_0 in nonsingular directions was given by Redmond [10]:

$$\Psi^{(0)-}_{\boldsymbol{k}_1,\boldsymbol{k}_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)=e^{i\boldsymbol{k}_1\cdot\boldsymbol{r}_1+i\boldsymbol{k}_2\cdot\boldsymbol{r}_2} \times e^{i/k_1\ln\zeta(\boldsymbol{k}_1,\boldsymbol{r}_1)}e^{i/k_2\ln\zeta(\boldsymbol{k}_2,\boldsymbol{r}_2)}e^{-i/2k_3\ln\zeta(\boldsymbol{k}_3,\boldsymbol{r}_3)}, \tag{6}$$

where $\zeta(\boldsymbol{k},\boldsymbol{r})=kr+\boldsymbol{k}\cdot\boldsymbol{r}$ and $\boldsymbol{k}_3=(\boldsymbol{k}_1-\boldsymbol{k}_2)/2$. Later Alt and Mukhamedzhanov (AM) [11] obtained the main leading term of Ψ^- in Ω_1 and Ω_3:

$$\Psi^{(1)-}_{\boldsymbol{k}_1,\boldsymbol{k}_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)=e^{i\boldsymbol{k}_1\cdot\boldsymbol{r}_1+i\boldsymbol{k}_2\cdot\boldsymbol{r}_2}\phi(-1,\tilde{\boldsymbol{k}}_1,\boldsymbol{r}_1) \times e^{i/k_2\ln\zeta(\boldsymbol{k}_2,\boldsymbol{r}_2)}e^{-i/2k_3\ln\zeta(\boldsymbol{k}_3,\boldsymbol{r}_3)}, \tag{7}$$

$$\Psi^{(3)-}_{\boldsymbol{k}_1,\boldsymbol{k}_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)=e^{i\boldsymbol{k}_1\cdot\boldsymbol{r}_1+i\boldsymbol{k}_2\cdot\boldsymbol{r}_2}e^{i/k_1\ln\zeta(\boldsymbol{k}_1,\boldsymbol{r}_1)} \times e^{i/k_2\ln\zeta(\boldsymbol{k}_2,\boldsymbol{r}_2)}\phi(1/2,\tilde{\boldsymbol{k}}_3,\boldsymbol{r}_3), \tag{8}$$

where the wave function of two-body scattering in the Coulomb field of the third particle is given by

$$\phi(\nu,\tilde{\boldsymbol{k}},\boldsymbol{r})=\Gamma(1-i\nu/\tilde{k})\exp(-\pi\nu/2\tilde{k}) \times {}_1F_1[i\nu/\tilde{k},1;-i\zeta(\tilde{\boldsymbol{k}},\boldsymbol{r})], \tag{9}$$

and ${}_1F_1$ is the confluent hypergeometric function. Local momenta are defined as

$$\tilde{\boldsymbol{k}}_1=\boldsymbol{k}_1+\frac{1}{2k_3r_3}\frac{\hat{\boldsymbol{k}}_3+\hat{\boldsymbol{r}}_3}{1+\hat{\boldsymbol{k}}_3\cdot\hat{\boldsymbol{r}}_3}, \tag{10}$$

$$\tilde{\boldsymbol{k}}_3=\boldsymbol{k}_3-\frac{1}{k_1r_1}\frac{\hat{\boldsymbol{k}}_1+\hat{\boldsymbol{r}}_1}{1+\hat{\boldsymbol{k}}_1\cdot\hat{\boldsymbol{r}}_1}-\frac{1}{k_2r_2}\frac{\hat{\boldsymbol{k}}_2+\hat{\boldsymbol{r}}_2}{1+\hat{\boldsymbol{k}}_2\cdot\hat{\boldsymbol{r}}_2}. \tag{11}$$

When Ω_1 or $\Omega_3\rightarrow\Omega_0$ the AM wave functions smoothly transform to the Redmond wave function as the local corrections to momenta become negligible. All significant leading terms of Ψ^- in Ω_1 and Ω_3 of the lowest order have been found by Mukhamedzhanov and Lieber (ML) [12]. The AM wave functions (7) and (8) correspond to the main term of the ML function in the relevant domain.

Let us proceed now to the asymptotic behavior of $\Phi^{(\rm sc)+}$. The standard procedure proposed by Peterkop [7–9] is to

write Eq. (1) in six-dimensional hyperspherical coordinates. Then in Ω_0, in the leading order, one has

$$\Phi^{(\mathrm{sc})+}_{\boldsymbol{k}_1,\boldsymbol{k}_2}(\boldsymbol{r}_1,\boldsymbol{r}_2) \overset{\Omega_0}{\to} A(\hat{\omega}) R^{-5/2} e^{i\kappa R + i\gamma \ln(\kappa R)}, \tag{12}$$

where $R=(r_1^2+r_2^2)^{1/2}$ is a hyperradius, $\hat{\omega}=(\hat{\boldsymbol{r}}_1,\hat{\boldsymbol{r}}_2,\alpha)$ is a five-dimensional hyperangle, with $\alpha=\arctan(r_2/r_1)$, $\kappa=(2E)^{1/2}$, and the Coulomb parameter γ is given by

$$\gamma=\frac{1}{\kappa}\left[\frac{1}{\cos\alpha}+\frac{1}{\sin\alpha}-\frac{1}{\sqrt{1-\hat{\boldsymbol{r}}_1\cdot\hat{\boldsymbol{r}}_2\,\sin 2\alpha}}\right], \tag{13}$$

and $A(\hat{\omega})$ is the ionization amplitude. As it is seen, the Peterkop asymptotic wave function is not valid in the region where $\boldsymbol{r}_1 \simeq \boldsymbol{r}_2$. Another drawback of the Peterkop wave function consists in an amplitude-phase ambiguity problem, when some part of $A(\hat{\omega})$ can be moved to the phase factor and the resulting wave function is still a solution to the original equation [9]. Accordingly, the remainder $A'(\hat{\omega})$ can equally well be called an ionization amplitude. Thus, generally speaking, the hyperspherical approach is not capable of uniquely identifying the ionization amplitude. We will fix this problem later, unambiguously relating the ''hyperspherical'' definition of the ionization amplitude to its standard quantum-mechanical one given by Eq. (4).

We now investigate the behavior of $\Phi^{(\mathrm{sc})+}$ in Ω_0 using Eq. (5). Since contributions from all components of Ψ^- involving bound states exponentially decrease in this domain, the only surviving contribution to $\Phi^{(\mathrm{sc})+}$ comes from the continuum part of Ψ^-, the leading term of which is given by the Redmond wave function $\Psi^{(0)-}$. Therefore, we get from Eq. (5) a fundamental asymptotic relationship,

$$\Phi^{(0)+}_{\boldsymbol{k}_1,\boldsymbol{k}_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)=\int \frac{d\boldsymbol{k}_1'}{(2\pi)^3}\frac{d\boldsymbol{k}_2'}{(2\pi)^3}\frac{f(\boldsymbol{k}_1',\boldsymbol{k}_2')\Psi^{(0)-}_{\boldsymbol{k}_1',\boldsymbol{k}_2'}(\boldsymbol{r}_1,\boldsymbol{r}_2)}{E-k_1'^2/2-k_2'^2/2+i0}. \tag{14}$$

In order to evaluate the above integral we use an asymptotic form of the plane wave (see, e.g., Ref. [9])

$$e^{i\boldsymbol{k}r} \overset{r\to\infty}{\sim} \frac{2\pi}{ikr}[\delta(\hat{\boldsymbol{k}}-\hat{\boldsymbol{r}})e^{ikr}-\delta(\hat{\boldsymbol{k}}+\hat{\boldsymbol{r}})e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}]. \tag{15}$$

After inserting Eq. (6) into Eq. (14) and using Eq. (15) we are left with a two-dimensional integral. Taking the residue at $k_1'=(\kappa^2-k_2'^2)^{1/2}$, the position of the pole singularity for one of the integrals, and evaluating the other by means of the stationary-phase method [13] at the stationary-phase point $k_2'=k_1' r_2/r_1$, we arrive at

$$\Phi^{(0)+}_{\boldsymbol{k}_1,\boldsymbol{k}_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)=\frac{\sqrt{2\pi i}}{(2\pi)^3}f\left(\frac{\kappa}{R}\boldsymbol{r}_1,\frac{\kappa}{R}\boldsymbol{r}_2\right)\frac{\kappa^{3/2}}{R^{5/2}}e^{i\kappa R+i\gamma\ln(\kappa R)+i\sigma}, \tag{16}$$

with

$$\sigma=\frac{1}{\kappa}\left[\frac{\ln(2\cos^2\alpha)}{\cos\alpha}+\frac{\ln(2\sin^2\alpha)}{\sin\alpha}-\frac{\ln(1-\hat{\boldsymbol{r}}_1\cdot\hat{\boldsymbol{r}}_2\,\sin 2\alpha)}{\sqrt{1-\hat{\boldsymbol{r}}_1\cdot\hat{\boldsymbol{r}}_2\,\sin 2\alpha}}\right]. \tag{17}$$

Thus, the asymptotic form of $\Phi^{(\mathrm{sc})+}$ in Ω_0 comes as a result of the intimate relationship between the total wave functions describing two different scattering processes within the same three-body system. Most importantly, our derivation leads to an unambiguous amplitude-phase form, which allows us to uniquely express the ''hyperspherical'' ionization amplitude $A(\hat{\omega})$ in terms of the standard definition of the ionization amplitude $f(\boldsymbol{k}_1,\boldsymbol{k}_2)$:

$$A(\hat{\omega})=\frac{\sqrt{2\pi i}}{(2\pi)^3}\kappa^{3/2}f\left(\frac{\kappa}{R}\boldsymbol{r}_1,\frac{\kappa}{R}\boldsymbol{r}_2\right)e^{i\sigma}. \tag{18}$$

Let us now proceed to Ω_1. By definition, here r_1 is limited as compared to r_2 and r_3. Therefore, it cannot, strictly speaking, be used as an asymptotic parameter. However, we have another pair of asymptotically large parameters, namely, ρ and r_3, where $\boldsymbol{\rho}=(\boldsymbol{r}_1+\boldsymbol{r}_2)/2$ is the coordinate of the center of mass of the electrons. Let us introduce for $\boldsymbol{\rho}$ its canonical conjugate momentum $\boldsymbol{q}=\boldsymbol{k}_1+\boldsymbol{k}_2$. Since the leading continuum term of Ψ^- in Ω_1 is given by the AM wave function $\Psi^{(1)-}$, one can write from Eq. (5) [16]

$$\Phi^{(1)+}_{\boldsymbol{k}_1,\boldsymbol{k}_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)\sim\int\frac{d\boldsymbol{q}'}{(2\pi)^3}\frac{d\boldsymbol{k}_3'}{(2\pi)^3}\frac{f(\boldsymbol{k}_1',\boldsymbol{k}_2')\Psi^{(1)-}_{\boldsymbol{k}_1',\boldsymbol{k}_2'}(\boldsymbol{r}_1,\boldsymbol{r}_2)}{E-q'^2/4-k_3'^2+i0}. \tag{19}$$

In the above equation $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, $\boldsymbol{k}_1'$, and $\boldsymbol{k}_2'$ are kept as shorthand notations and given by

$$\boldsymbol{r}_1=\boldsymbol{\rho}+\boldsymbol{r}_3/2,\quad \boldsymbol{r}_2=\boldsymbol{\rho}-\boldsymbol{r}_3/2, \tag{20}$$

$$\boldsymbol{k}_1'=\boldsymbol{q}'/2+\boldsymbol{k}_3',\quad \boldsymbol{k}_2'=\boldsymbol{q}'/2-\boldsymbol{k}_3'. \tag{21}$$

Now we calculate the integrals in Eq. (19) in analogy with the procedure we used in Ω_0. Taking into account that $2\rho^2+r_3^2/2=r_1^2+r_2^2\equiv R^2$ and $q'^2/2+2k_3'^2=k_1'^2+k_2'^2\equiv\kappa^2$ one can show that the six-dimensional integral in Eq. (19) has a stationary-phase point at $\boldsymbol{q}'=2\kappa\boldsymbol{\rho}/R$ and $\boldsymbol{k}_3'=\kappa\boldsymbol{r}_3/2R$. Evaluating the integrals and transforming the answer back to the conventional $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ variables we arrive at the final result

$$\Phi^{(1)+}_{\boldsymbol{k}_1,\boldsymbol{k}_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)\sim\frac{\sqrt{2\pi i}}{(2\pi)^3}f\left(\frac{\kappa}{R}\boldsymbol{r}_1,\frac{\kappa}{R}\boldsymbol{r}_2\right)\frac{\kappa^{3/2}}{R^{5/2}}e^{i\kappa R}\phi(-1,\tilde{\boldsymbol{k}}_1',\boldsymbol{r}_1)\times\exp\left[\frac{iR}{\kappa r_2}\ln\left(\frac{2\kappa r_2^2}{R}\right)-\frac{iR}{\kappa r_3}\ln\left(\frac{\kappa r_3^2}{R}\right)\right], \tag{22}$$

where we used the fact that at the stationary-phase point $\boldsymbol{k}_1'=\kappa\boldsymbol{\rho}/R+\kappa\boldsymbol{r}_3/(2R)=\kappa\boldsymbol{r}_1/R$ and, similarly, $\boldsymbol{k}_2'=\kappa\boldsymbol{r}_3/R$ [17].

For the asymptotic behavior of $\Phi^{(\mathrm{sc})+}$ in Ω_3 a similar argument leads to

$$\Phi^{(3)+}_{\boldsymbol{k}_1,\boldsymbol{k}_2}(\boldsymbol{r}_1,\boldsymbol{r}_2)=\frac{\sqrt{2\pi i}}{(2\pi)^3}f\left(\frac{\kappa}{R}\boldsymbol{r}_1,\frac{\kappa}{R}\boldsymbol{r}_2\right)\frac{\kappa^{3/2}}{R^{5/2}}e^{i\kappa R}\phi(1/2,\tilde{\boldsymbol{k}}'_3,\boldsymbol{r}_3)\times\exp\left[\frac{iR}{\kappa r_1}\ln\left(\frac{2\kappa r_1^2}{R}\right)+\frac{iR}{\kappa r_2}\ln\left(\frac{2\kappa r_2^2}{R}\right)\right]. \tag{23}$$

New local momenta in Eqs. (22) and (23) are given by

$$\tilde{\boldsymbol{k}}'_1=\frac{\kappa}{R}\boldsymbol{r}_1+\frac{R}{\kappa r_3^3}\boldsymbol{r}_3, \tag{24}$$

$$\tilde{\boldsymbol{k}}'_3=\frac{\kappa}{2R}\boldsymbol{r}_3-\frac{R}{\kappa}\left(\frac{\boldsymbol{r}_1}{r_1^3}+\frac{\boldsymbol{r}_2}{r_2^3}\right). \tag{25}$$

Since

$$\phi(-1,\tilde{\boldsymbol{k}}'_1,\boldsymbol{r}_1)\overset{r_1\to\infty}{\sim}\exp\left[\frac{iR}{\kappa r_1}\ln\left(\frac{2\kappa r_1^2}{R}\right)\right], \tag{26}$$

where we took into account that as r_1 also becomes large the second term in Eq. (24) becomes negligible, Eq. (22) transforms to Eq. (16) when $\Omega_1\to\Omega_0$. The same is true also for Eq. (23) when $\Omega_3\to\Omega_0$.

As we mentioned earlier the Peterkop asymptotic wave function becomes invalid when $r_1\to\infty$ and $r_2\to\infty$, but $\boldsymbol{r}_1\to\boldsymbol{r}_2$. This limit point is not actually in Ω_0, but is in Ω_3. However, the $\boldsymbol{r}_1\simeq\boldsymbol{r}_2$ problem has been associated with the Peterkop wave function (and hence Ω_0), since in practical calculations of ionization cross sections one has to turn $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ around each other (e.g., in partial-wave analysis), and therefore unavoidably crossing the Ω_3 domain when $r_1\simeq r_2$. Thus, it is not possible to separate, in practice, the domains Ω_0 and Ω_3. The conclusion is that one has to use in this case an asymptotic wave function valid both in Ω_0 and Ω_3, and such a function is given by Eq. (23). This resolves the $\boldsymbol{r}_1\simeq\boldsymbol{r}_2$ problem.

Summarizing, a simple relationship between the total wave function describing a breakup process in a Coulomb three-body system (called the $2\to3$ process) and the one representing another process within the same system, of scattering of the three particles in the continuum ($3\to3$ process) through the corresponding $2\to3$ breakup amplitude, is revealed. On the basis of this relationship, forms of the scattered wave for electron-impact ionization of hydrogen valid in all asymptotic domains are given. When all interparticle distances become large, the new wave functions reduce in the leading order to the well-known Peterkop wave function obtained in the hyperspherical approach. In particular, the Peterkop function is obtained by direct application of the present approach in the domain when all interparticle separations are large. This allows one to resolve the long-standing amplitude-phase ambiguity problem, which is an artifact of the hyperspherical approach to the ionization process. The Peterkop asymptotic wave function is invalid when two electrons are at the same position relative to the proton. This causes problems in practical calculations even in the domain where all particles are wide apart. Our formulation provides a solution to this problem.

The presented wave functions can be directly used in calculations of ionization of hydrogen or any hydrogenlike ion by electron or positron impact. However, the problems considered in this work, and approach to them, are not specific to the electron-hydrogen ionization. The relationships (5), (14), and (19) are general for any atomic and nuclear three-body breakup scattering. Generalization of the particular results to these processes and more details of calculations will be given elsewhere.

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[1] M. Baertschy, T.N. Rescigno, W.A. Isaacs, X. Li, and C.W. McCurdy, Phys. Rev. A **63**, 022712 (2001).
[2] M. Baertschy, T.N. Rescigno, and C.W. McCurdy, Phys. Rev. A **64**, 022709 (2001).
[3] I. Bray and A.T. Stelbovics, Phys. Rev. Lett. **70**, 746 (1993).
[4] I. Bray, D.V. Fursa, A.S. Kheifets, and A.T. Stelbovics, J. Phys. B **35**, R117 (2002).
[5] K. Bartschat, E.T. Hudson, M.P. Scott, P.G. Burke, and V.M. Burke, J. Phys. B **29**, 115 (1996).
[6] M.P. Scott, T. Stitt, N.S. Scott, and P.G. Burke, J. Phys. B **35**, L323 (2002).
[7] R.K. Peterkop, Izv. Akad. Nauk Latv. SSR, Ser. Fiz. Tekh. **9**, 79 (1960).
[8] R.K. Peterkop, Zh. Eksp. Teor. Fiz. **43**, 616 (1962) [Sov. Phys. JETP **14**, 1377 (1962)].
[9] R.K. Peterkop, *Theory of Ionization of Atoms by Electron Impact* (Colorado Associated University Press, Boulder, 1977).
[10] P.J. Redmond (unpublished), described in Ref. [14].
[11] E.O. Alt and A.M. Mukhamedzhanov, Phys. Rev. A **47**, 2004 (1993).
[12] A.M. Mukhamedzhanov and M. Lieber, Phys. Rev. A **54**, 3078 (1996).
[13] N. Bleistein and R.A. Handelsman, *Asymptotic Expansions of Integrals* (Dover Publications, New York, 1986).
[14] L. Rosenberg, Phys. Rev. D **8**, 1833 (1973).
[15] P.G. Burke (private communication).
[16] In general, in this domain the contribution from the bound states must be retained; however, we skip this part of the asymptotic wave function which is well known (see, e.g., Ref. [9]) and give only the continuum part.
[17] For brevity we keep for the values of the momenta at the stationary-phase point the old notations used so far for the variables.