Threshold anomaly in *S* scattering with Coulomb charge exchange

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An exact solution to a quantum model for atomic *S* scattering with constant coupling of ionic and covalent states is found. The scattering cross-section anomaly near the ionization threshold is analyzed accurately.

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I. INTRODUCTION

The steplike change of the inelastic-scattering cross section for inelastic channels at the corresponding thresholds is considered to be the best-known anomaly of multichannel scattering of the particles subjected to Coulomb attraction. In this case, due to the condensing Coulomb resonances, the elastic-scattering cross section does not tend to a definite limiting value when approaching the threshold from the below-threshold energy range. Meanwhile, this cross section is well defined above the threshold [1]. Such a picture is based mostly on matching Coulomb asymptotes to the core collision domain functions [2], and it needs confirmation in the framework of alternative approaches. Preference here should be given to models for which an explicit solution can be found. Moreover, these models are necessary in solving the problem of the continuity of the average total scattering cross section at thresholds of inelastic Coulomb channels, which is expected for physical reasons but has not yet been confirmed rigorously [3].

In addition, it should be noted that modern studies of atomic and molecular collisions enable one to obtain experimental and numerical results in a close vicinity to ionic channels thresholds (see [4,5]), which makes it an urgent issue to find suitable and explicitly soluble quantum models.

II. FORMULATION OF THE PROBLEM

A natural target for possible two-state models is Coulomb charge exchange of atoms and, under some restrictions, molecules. In this case, the only essential problem in making a choice is due to the necessity to take into account all the collision orbital angular momenta. However, the specific origin of the anomalies caused by long-range Coulomb forces results in a similar behavior of the anomalies in all orbital channels, as well as in providing one with the opportunity to consider, at the first stage, only *S* scattering.

The argument above leads to a simple model for atomic collision with only one neutral and one ionic state of the system with a minimum set of parameters. The corresponding matrix Schrödinger equation for diabatic amplitudes $\psi_{1,2}$ in the atomic basis is

$$\begin{pmatrix} -\frac{\hbar^2}{2m}\frac{d^2}{dR^2}-\frac{a}{R}+D-E & V \\ V & -\frac{\hbar^2}{2m}\frac{d^2}{dR^2}-E \end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}=0. \tag{2.1}$$

Here R is interatomic separation, m is reduced atomic mass, and $a>0$ and $D>0$ are Coulomb diabatic potential parameters representing the absolute value for the ionic charges product and the diabatic asymptote of the ionic potential, respectively, V is the static coupling independent on R by assumption.

The boundary conditions for our problem should be set considering adiabatic amplitudes $\varphi_{1,2}$ which are uncoupled asymptotically. $\varphi_{1,2}$ are expressed in terms of the diabatic amplitudes $\psi_{1,2}$ by the following rotation formula:

$$\begin{pmatrix}\varphi_1\\ \varphi_2\end{pmatrix}=\begin{pmatrix} \left(\frac{u_2}{u_2-u_1}\right)^{1/2} & \left(\frac{u_1}{u_1-u_2}\right)^{1/2} \\ -\left(\frac{u_1}{u_1-u_2}\right)^{1/2} & \left(\frac{u_2}{u_2-u_1}\right)^{1/2} \end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}, \tag{2.2}$$

where

$$u_{1,2}=\frac{1}{2}\left\{D-\frac{a}{R}\pm\left[\left(D-\frac{a}{R}\right)^2+4V^2\right]^{1/2}\right\} \tag{2.3}$$

are adiabatic potentials of the system. The boundary conditions take the forms

$$\varphi_1(R)=\varphi_2(R)=0, \quad R\to 0, \tag{2.4}$$

$$\varphi_{1,2}(R)=\frac{1}{k_{1,2}^{1/2}}\left[A_{1,2}\exp(i\eta_{1,2}(R)) - B_{1,2}\exp(-i\eta_{1,2}(R))\right], \quad R\to\infty. \tag{2.5}$$

Here $k_{1,2}$ are asymptotic wave vectors for adiabatic channels

$$k_{1,2}=\frac{1}{\hbar}\{2m[E-u_{1,2}(\infty)]\}^{1/2}, \tag{2.6}$$

$\eta_{1,2}(R)$ are the Coulomb phases of the wave-function asymptotes

$$\eta_{1,2}(R)=k_{1,2}R+\frac{1}{k_{1,2}a_{1,2}}\ln(2k_{1,2}R), \tag{2.7}$$

corresponding to the Bohr radii

$$a_{1,2}=\frac{\hbar^2}{ma}\frac{u_1(\infty)-u_2(\infty)}{|u_{1,2}(\infty)|}, \tag{2.8}$$

The coefficients $A_{1,2}$ and $B_{1,2}$ are related by the scattering matrix S,

$$A_1 = S_{1k} B_k , \tag{2.9}$$

which is the main subject of our study. Hence we will restrict our consideration to the continuous spectrum

$$E > u_2(\infty) \tag{2.10}$$

and in particular to the spectrum range near the threshold for inelastic scattering,

$$E_{\text{th}} = u_1(\infty). \tag{2.11}$$

III. EVALUATION OF THE *S* MATRIX

We will seek a solution to the diabatic set of Eqs. (2.1) in the momentum representation

$$\psi_{1,2} = \int_{\mathscr{L}} \exp\left(\frac{i}{\hbar}\, pR \right) \xi_{1,2}(p)\, dp. \tag{3.1}$$

The increments along the contour $\mathscr{L}$ are assumed to satisfy the following conditions:

$$\xi_{1,2}(p) \exp\left(\frac{1}{\hbar}\, pR \right) \Big|_{\mathscr{L}} = 0, \quad p^2 \xi_{1,2}(p) \exp\left(\frac{i}{\hbar}\, pR \right) \Big|_{\mathscr{L}} = 0. \tag{3.2}$$

Then

$$\frac{d}{dp}\left[\left(\frac{p^2}{2m} + D - E \right) \xi_1 + V \xi_2 \right] + \frac{ia}{\hbar}\, \xi_1 = 0,$$
$$V \xi_1 + \left(\frac{p^2}{2m} - E \right) \xi_2 = 0. \tag{3.3}$$

Introducing dimensionless Coulomb variables and asymptotic parameters

$$z = p(mV)^{-1/2}, \quad r = (mV)^{1/2} R/\hbar, \quad e = E/V, \quad d = D/V, \tag{3.4}$$

$$e_q = \frac{ma^2}{\hbar^2 V}, \quad \kappa = e_q^{1/2}, \tag{3.5}$$

we rewrite Eqs. (3.3) in the form

$$\frac{d}{dz}\left[\left(\frac{z^2}{2} - e + d \right) \xi_1 + \xi_2 \right] + i\kappa \xi_1 = 0,$$
$$\xi_1 + \left(\frac{z^2}{2} - e \right) \xi_2 = 0. \tag{3.6}$$

These equations have the following solution:

$$\xi_1(z) = \frac{\varepsilon(z)}{g(z)} \exp\left(i\kappa \int^z \frac{\varepsilon(z')}{g(z')}\, dz' \right),$$
$$\xi_2(z) = \frac{1}{g(z)} \exp\left(i\kappa \int^z \frac{\varepsilon(z')}{g(z')}\, dz' \right), \tag{3.7}$$

where

$$\varepsilon(z) = e - z^2/2, \quad g(z) = \tfrac{1}{4}(z^2 - z_1^2)(z^2 - z_2^2)$$
$$z_{1,2} = [2(e - \varepsilon_{1,2})]^{1/2}, \tag{3.8}$$
$$\varepsilon_{1,2} = \tfrac{1}{2}[d \pm (d^2 + 4)^{1/2}]; \quad \varepsilon_1 > 0, \quad \varepsilon_2 < 0.$$

As is seen from Eqs. (2.3), (2.6), and (3.4),

$$\varepsilon_{1,2} = u_{1,2}(\infty)/V, \quad z_{1,2} = \hbar k_{1,2} (mV)^{-1/2}. \tag{3.9}$$

Returning to the R representation gives

$$\psi_1(r) = \int_{\mathscr{L}} dz\; e^{izr}\, \frac{\varepsilon(z)}{g(z)} \left(\frac{z - z_1}{z + z_1} \right)^{i\alpha} \left(\frac{z - z_2}{z + z_2} \right)^{i\beta},$$
$$\psi_2(r) = \int_{\mathscr{L}} dz\; e^{izr}\, \frac{1}{g(z)} \left(\frac{z - z_1}{z + z_1} \right)^{i\alpha} \left(\frac{z - z_2}{z + z_2} \right)^{i\beta}. \tag{3.10}$$

Here

$$\alpha = -\frac{\varepsilon_1}{\varepsilon_1 - \varepsilon_2}\, \frac{\kappa}{z_1},$$
$$\beta = -\frac{\varepsilon_2}{\varepsilon_2 - \varepsilon_1}\, \frac{\kappa}{z_2}, \tag{3.11}$$

and, as can be noted,

$$\alpha = -1/k_1 a_1, \quad \beta = -1/k_2 a_2, \tag{3.12}$$

which is in accordance with Eq. (2.8). The $z_{1,2}$ momenta branches are assigned by the formulas

$$z_1 > 0, \quad \alpha < 0, \quad e > \varepsilon_1,$$
$$z_1 = i|z_1|, \quad \alpha = i|\alpha|, \quad \varepsilon_2 < e < \varepsilon_1, \tag{3.13}$$

and

$$z_2 > 0, \quad \beta < 0. \tag{3.14}$$

Due to Eqs. (2.2) and (2.4), solutions (3.10) must satisfy the boundary conditions

$$\psi_1(0) = \psi_2(0) = 0, \tag{3.15}$$

and, according to the asymptotic form of the wave function (2.5), be finite when $R \to \infty$. Thus the physical solution to Eq. (2.1) can be selected using in expressions (3.10) contours such as $\mathscr{L}$ which ensure the restrictions (3.2), (3.15), and (2.5). Conditions (3.2) and the first of Eqs. (3.15) are fulfilled for the contours $\mathscr{L}_1$ arranged as follows (see Fig. 1): $\mathscr{L}_1$ is a simple loop starting at a point **A** on the real axis, which is located either between z_1 and z_2 for $e > \varepsilon_1$ or between 0 and z_2 for $\varepsilon_2 < e < \varepsilon_1$, and circumventing only z_1 and $-z_1$ in the negative direction. $\mathscr{L}_2$ is a simple loop starting at a point **A** on the real axis to the right of z_2, and circumventing only z_2 and $-z_2$ in the negative direction. $\mathscr{L}_3$ is a double loop starting at a point **A** on the real axis to the right of z_2 and circumventing successively only z_2 in the negative direction, z_1 in the positive direction, z_2 in the positive direction, and z_1 in the negative direction.

Indeed, the integrands of Eqs. (3.10) are obviously single valued along $\mathscr{L}_1$, therefore Eqs. (3.2) are satisfied since $\mathscr{L}_1$ are closed. The equality $\psi_1(0) = 0$ follows from the relation

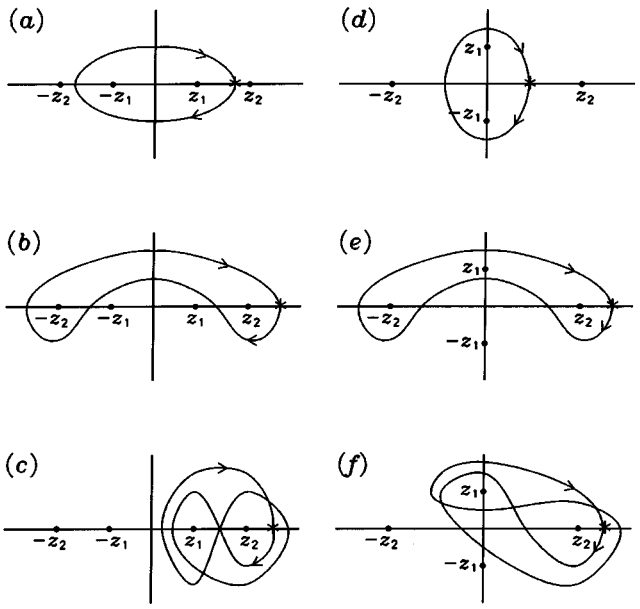

FIG. 1. The integration contours in Eq. (3.10). Curves a, b, and c present the contours $\mathscr{L}_1$, $\mathscr{L}_2$, and $\mathscr{L}_3$ in the case $e>\varepsilon_1$. Curves d, e, and f present the contours $\mathscr{L}_1$, $\mathscr{L}_2$, and $\mathscr{L}_3$ in the case $\varepsilon_2<e<\varepsilon_1$. The asterisk denotes the beginning of the contours, and the arrows indicate the direction of circumventing.

$$\psi_1(0)=\int_{\mathscr{L}} dz\,\frac{\varepsilon(z)}{g(z)}\exp\left(i\kappa\int^{z}\frac{\varepsilon(z')}{g(z')}\,dz'\right)$$
$$=\frac{1}{i\kappa}\left(\frac{z-z_1}{z+z_1}\right)^{i\alpha}\left(\frac{z-z_2}{z+z_2}\right)^{i\beta}\Bigg|_{\mathscr{L}}, \tag{3.16}$$

and from the above-mentioned single valuedness.

The solutions to Eqs. (2.1),

$$\vec{\Psi}_0^{(i)}\equiv\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}_{\mathscr{L}_1}\equiv\begin{pmatrix}\psi_1^{(i)}\\ \psi_2^{(i)}\end{pmatrix}, \tag{3.17}$$

corresponding to the contours $\mathscr{L}_1$, are linearly independent. This follows from the asymptotic behavior of $\psi_{1,2}$ in the limit $R\to\infty$. This behavior is defined by the contributions from branch points into the integrals in Eqs. (3.10), since $\mathscr{L}_1$ can be displaced into the upper half-plane of z so that their tails, after circumventing $z_{1,2}$, were running to $+i\infty$ where the integrand behavior is defined basically by the exponential decrease of $\exp(izr)$.

After assigning the phases to the branching factors in the integrands of Eq. (3.10) at point **A** with the conditions

$$|\arg(z\pm z_1)|<\pi/2,$$
$$\arg(z+z_2)=0,\quad \arg(z-z_2)=\begin{cases}-\pi, & \mathbf{A}\in\mathscr{L}_1\\ 0, & \mathbf{A}\in\mathscr{L}_{2,3},\end{cases} \tag{3.18}$$

we calculate the contributions from the branch points using the well-known Hanckel representation for the γ function.

Above the threshold $e>\varepsilon_1$ the asymptotic behavior of the diabatic vectors (3.17) is given by

$$\vec{\Psi}_0^{(1)}=\begin{pmatrix}1 & 1\\ \frac{1}{\varepsilon_1} & \frac{1}{\varepsilon_1}\end{pmatrix}\begin{pmatrix}\rho z_1^{-1/2} & e^{i[\eta_1(R)+\delta_1]}\\ \rho z_1^{-1/2} & e^{-i(\eta_1(R)+\delta_1)}\end{pmatrix},\quad R\to\infty,$$

$$\vec{\Psi}_0^{(2)}=\begin{pmatrix}1 & 1\\ \frac{1}{\varepsilon_2} & \frac{1}{\varepsilon_2}\end{pmatrix}\begin{pmatrix}\tau z_2^{-1/2} & e^{i[\eta_2(R)+\delta_2]}\\ \tau z_2^{-1/2} & e^{-i[\eta_2(R)+\delta_2]}\end{pmatrix},\quad R\to\infty,$$

$$\vec{\Psi}_0^{(3)}=\begin{pmatrix}1 & 1\\ \frac{1}{\varepsilon_1} & \frac{1}{\varepsilon_2}\end{pmatrix}\begin{pmatrix}\rho\nu z_1^{-1/2} & e^{i[\eta_1(R)+\delta_1]}\\ -\tau\mu z_2^{-1/2} & e^{i[\eta_2(R)+\delta_2]}\end{pmatrix},\quad R\to\infty, \tag{3.19}$$

and condition (2.5) is satisfied automatically. Here the following notations are used:

$$\delta_1=\arg\Gamma(i\alpha)-\beta\,\ln\,\omega,$$
$$\delta_2=\arg\Gamma(i\beta)-\alpha\,\ln\,\omega; \tag{3.20}$$

$$\omega=\frac{z_2+z_1}{z_2-z_1},$$

$$\mu=\exp(-2\pi\alpha)-1, \tag{3.21}$$

$$\nu=\exp(-2\pi\alpha)[\exp(-2\pi\beta)-1];$$

$$\rho=2\,\frac{\varepsilon_1 z_1^{-1/2}}{\varepsilon_2-\varepsilon_1}\exp[\pi(\beta+\alpha/2)]\sinh(\pi\alpha)|\Gamma(i\alpha)|,$$
$$\tau=2\,\frac{\varepsilon_2 z_2^{-1/2}}{\varepsilon_1-\varepsilon_2}\exp(\pi\beta/2)\sinh(\pi\beta)|\Gamma(i\beta)|. \tag{3.22}$$

In the energy range for elastic scattering, $\varepsilon_2<e<\varepsilon_1$, $\vec{\Psi}_0^{(1)}(R)$ increases exponentially with $R\to\infty$, and hence should be omitted. The asymptotic behavior of the rest of the solutions,

$$\vec{\Psi}_0^{(2)}=\begin{pmatrix}1 & 1\\ \frac{1}{\varepsilon_2} & \frac{1}{\varepsilon_2}\end{pmatrix}\begin{pmatrix}\rho z_2^{-1/2} & e^{i[\eta_2(R)+\delta_2]}\\ \rho z_2^{-1/2} & e^{-i[\eta_2(R)+\delta_2]}\end{pmatrix},\quad R\to\infty,$$

$$\vec{\Psi}_0^{(3)}=\begin{pmatrix}1 & 1\\ \frac{1}{\varepsilon_1} & \frac{1}{\varepsilon_2}\end{pmatrix}\begin{pmatrix}0\\ -\rho\mu z_2^{-1/2}e^{i[\eta_2(R)+\delta_2]}\end{pmatrix},\quad R\to\infty, \tag{3.23}$$

satisfy Eq. (2.5). Here exponentially small elements in $\vec{\Psi}_0^{(3)}$ are omitted, and the analytical continuation (3.13) is implied.

We transform the initial basis $\vec{\Psi}_0^{(i)}$ to the symmetrized form $\vec{\tilde{\Psi}}_0^{(i)}$:

$$\vec{\tilde{\Psi}}_0^{(i)}\equiv\begin{pmatrix}\tilde{\psi}_1^{(i)}\\ \tilde{\psi}_2^{(i)}\end{pmatrix};$$
$$\vec{\tilde{\Psi}}_0^{(1,2)}=\vec{\Psi}_0^{(1,2)},\quad \vec{\tilde{\Psi}}_0^{(3)}=\vec{\Psi}_0^{(3)}-\vec{\Psi}_0^{(3)*};\quad e>\varepsilon_1 \tag{3.24}$$
$$\vec{\tilde{\Psi}}_0^{(1)}=\vec{\Psi}_0^{(3)},\quad \vec{\tilde{\Psi}}_0^{(2)}=\vec{\Psi}_0^{(3)*},\quad \varepsilon_2<e<\varepsilon_1 .$$

Using this basis we impose the second condition from the set (3.15) on the solution (3.10). This can be done if the general solution with an arbitrary constant c_1,

$$\vec{\Psi}=\sum_i c_1\vec{\tilde{\Psi}}_0^{(i)}, \tag{3.25}$$

is subjected to the restriction

$$\sum_i c_1\tilde{\psi}_2^{(i)}(0)=0. \tag{3.26}$$

This procedure enables us to introduce a physical basis for the diabatic system of Eqs. (2.1), e.g., in the form

$$\vec{\Psi}^{(1)}=\vec{\tilde{\Psi}}_0^{(1)}-\frac{\tilde{\psi}_2^{(1)}(0)}{\tilde{\psi}_2^{(3)}(0)}\,\vec{\tilde{\Psi}}_0^{(3)},$$

$$\vec{\Psi}^{(2)}=\vec{\tilde{\Psi}}_0^{(2)}-\frac{\tilde{\psi}_2^{(2)}(0)}{\tilde{\psi}_2^{(3)}(0)}\,\vec{\tilde{\Psi}}_0^{(3)},\quad e>\varepsilon_1$$

$$\vec{\Psi}^{(1)}=\vec{\tilde{\Psi}}_0^{(1)}-\frac{\tilde{\psi}_2^{(1)}(0)}{\tilde{\psi}_2^{(2)}(0)}\,\vec{\tilde{\Psi}}_0^{(2)},\quad \varepsilon_2<e<\varepsilon_1. \tag{3.27}$$

Now we can define the physical adiabatic basis $\Phi^{(i)}$ with the corresponding asymptotic amplitudes $A_1^{(i)}$ and $B_1^{(i)}$, and derive an equation for the S matrix,

$$A_1^{(i)}=S_{1k}B_k^{(i)}, \tag{3.28}$$

The values of $\psi_2^{(i)}(0)$ which define the S matrix together with combinations (3.20)–(3.22) obey the relation

$$\psi_2^{(1)}(0)=-\psi_2^{(2)}(0). \tag{3.29}$$

The topological symmetry Eq. (3.29) follows from the relationship

$$\psi_2^{(2)}(0)=\psi_2^{(0)}(0)-\psi_2^{(1)}(0), \tag{3.30}$$

where $\psi_2^{(0)}(0)=0$ is calculated along the contour embracing all four branch points $\pm z_{1,2}$. Note that $\psi_2^{(1,2)}(0)$ are real valued due to the property

$$\xi_2(z)=\xi_2^*(-z^*). \tag{3.31}$$

Thus the boundary conditions determine the S matrix for inelastic collisions in terms of two parameters,

$$\vartheta=\psi_2^{(1)}(0),\quad w=\mathrm{Im}[\psi_2^{(3)}(0)], \tag{3.32}$$

and through a single parameter for elastic collisions,

$$\delta=\arg[\psi_2^{(3)}(0)], \tag{3.33}$$

For the model under consideration these parameters can be found in an explicit form, since the required integrals $\psi_2^{(i)}(0)$ are reduced to the usual integral representation of the hypergeometric Gauss function. With this purpose we rewrite $\psi_2(0)$ in the form

$$\psi_2(0)=\int_{\mathscr{L}}dz\left(\frac{1}{\varepsilon_1}f_1'(z)+\frac{1}{\varepsilon_2}f_2'(z)\right)\exp\{i\kappa(f_1(z)+f_2(z))\}, \tag{3.34}$$

where

$$f_1=\frac{\alpha}{\kappa}\ln\left(\frac{z-z_1}{z+z_1}\right),\quad f_2=\frac{\beta}{\kappa}\ln\left(\frac{z-z_2}{z+z_2}\right), \tag{3.35}$$

and introduce the variable $\zeta=(z-z_{1,2})/(z+z_{1,2})$ into (3.34). The result of the calculation is

$$\psi_2^{(1)}(0)=\frac{\varepsilon_1-\varepsilon_2}{\varepsilon_1\varepsilon_2}\frac{2\pi\alpha\beta}{\kappa}(\omega^2-1)e^{\pi\beta}\omega^{i(\beta-\alpha)}\times F(1-i\alpha,1+i\beta,2,1-\omega^2), \tag{3.36}$$

$$\psi_2^{(3)}(0)=\frac{\varepsilon_1-\varepsilon_2}{\varepsilon_1\varepsilon_2}\frac{4i\alpha\beta}{\kappa}e^{-\pi\alpha}\times\frac{\Gamma(i\alpha)\Gamma(i\beta)\sinh(\pi\alpha)\sinh(\pi\beta)}{\Gamma(1+i\alpha+i\beta)}\times\omega^{-i(\alpha+\beta)}F(i\alpha,i\beta,1+i\alpha+i\beta,1/\omega^2). \tag{3.37}$$

where F is the Gauss function. Here $\psi_2^{(3)}(0)$ for $\varepsilon_2<e<\varepsilon_1$ is specified according to formulas (3.13).

The solution to Eq. (3.28) has the form

$$S=\frac{-1}{1-i\dfrac{\vartheta}{2w}(\mu+\nu)}\begin{pmatrix}\exp(2i\delta_1)\left(1-i\dfrac{\vartheta}{2w}(\mu-\nu)\right) & -i\dfrac{\vartheta}{w}\sqrt{\mu\nu}\exp[i(\delta_1+\delta_2)]\\ -i\dfrac{\vartheta}{w}\sqrt{\mu\nu}\exp[i(\delta_1+\delta_2)] & \exp(2i\delta_2)\left(1+i\dfrac{\vartheta}{2w}(\mu-\nu)\right)\end{pmatrix},\quad e>\varepsilon_1 \tag{3.38}$$

$$S=\exp\{2i[\delta_2+\arg(\mu)-\delta]\},\quad \varepsilon_2<e<\varepsilon_1. \tag{3.39}$$

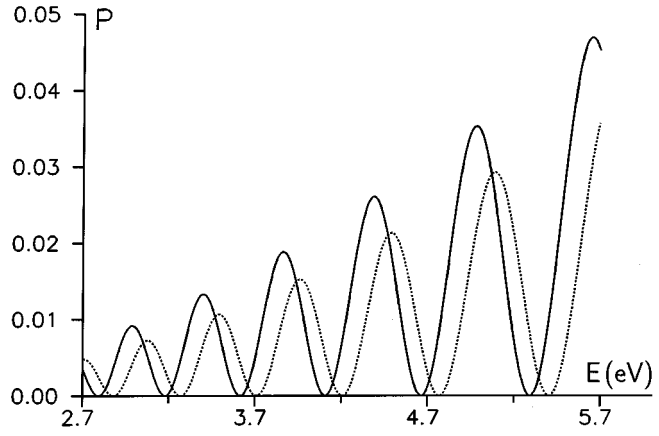

FIG. 2. Nonadiabatic transition probability as a function of collision energy near ionic channel threshold for the $H(1s)+H(2s)\rightarrow H^+ + H^-$ process. Solid line—exact quantum result from Eq. (3.38); dotted line—modified Landau-Zener-Stueckelberg approximation.

Thus the construction of the S matrix in a rigorously unitary form is completed.

Some idea about this result is given by Fig. 2, where the nonadiabatic transition probability $P=|S_{12}|^2$ calculated from Eq. (3.38) is shown along with the modified Landau-Zener-Stueckelberg approximation. The parameters which are used in the calculation correspond to the process $H(1s)+H(2s)\rightarrow H^+ + H^-$, and appear to be in quasiclassical range $e_q \gg d \gg 1$. This gives us an opportunity to use the matching procedure for the construction of a modified Stueckelberg result, taking into account both quantum regions of the collision under consideration, namely the nonadiabatic region in the crossing vicinity, and the adiabatic one near $R=0$. The result of this approach is presented in Fig. 2.

IV. SCATTERING CROSS SECTION. THRESHOLD ANOMALIES

Let us now consider the scattering cross sections for neutral particles (channel 2) near the ionization threshold using Eqs. (3.38) and (3.39). We begin by introducing limiting values of the cross sections for elastic (σ_e) and inelastic (σ_r) scattering:

$$\sigma_{e+}=\frac{\pi}{k_2^2}\,|1-S_{22}|^2, \quad \sigma_{r+}=\frac{\pi}{k_2^2}\,(1-|S_{22}|^2), \quad e\rightarrow\varepsilon_1+0. \tag{4.1}$$

$$\sigma_{e-}=\frac{2\pi}{k_2^2}\,[1-\mathrm{Re}(S)], \quad e\rightarrow\varepsilon_1-0. \tag{4.2}$$

In order to calculate them, we need the following asymptotic expressions. For $e\rightarrow\varepsilon_1+0$:

$$F(i\alpha,i\beta,1+i\alpha+i\beta,1/\omega^2)=-2i\lambda\,\frac{\Gamma(1+i\alpha+i\beta_0)}{\Gamma(1+i\alpha)}\times\Psi(1+i\beta_0,2,-2i\lambda),$$
$$F(1-i\alpha,1+i\beta,2,1-\omega^2)=\Phi(1+i\beta_0,2,-2i\lambda). \tag{4.3}$$

For $e\rightarrow\varepsilon_1-0$:

$$F(i\alpha,i\beta,1+i\alpha+i\beta,1/\omega^2)=-2i\lambda\,\frac{\Gamma(1-|\alpha|+i\beta_0)}{\Gamma(1-|\alpha|)}\left(\Psi(1+i\beta_0,2,-2i\lambda)+\frac{\pi e^{i\pi|\alpha|}}{\sin(\pi|\alpha|)\Gamma(i\beta_0)}\,\Phi(1+i\beta_0,2,-2i\lambda)\right). \tag{4.4}$$

Here

$$\lambda=2\,\frac{\varepsilon_1}{\varepsilon_1-\varepsilon_2}\left(\frac{e_q}{2(\varepsilon_1-\varepsilon_2)}\right)^{1/2},$$
$$\beta_0=\frac{\varepsilon_2}{\varepsilon_1-\varepsilon_2}\left(\frac{e_q}{2(\varepsilon_1-\varepsilon_2)}\right)^{1/2}, \tag{4.5}$$
$$|\alpha|=\frac{\varepsilon_1}{\varepsilon_1-\varepsilon_2}\left(\frac{e_q}{2|e-\varepsilon_1|}\right)^{1/2}\rightarrow\infty$$

and $\Phi(1+i\beta_0,2,-2i\lambda)$ and $\Psi(1+i\beta_0,2,-2i\lambda)$ are confluent hypergeometric functions. Equations (4.3) and (4.4) result from a representation of the Gauss function in terms of an integral over a simple loop [6] (see the Appendix). The asymptotes for the required elements of the S matrix are obtained from Eqs. (3.38) and (3.39) using Eqs. (4.3) and (4.4) as follows:

$$S_{22}=\frac{1-iK[2\exp(\pi\beta_0)-\exp(-\pi\beta_0)]}{1+iK\,\exp(-\pi\beta_0)}\exp\{2i[\lambda+\arg\,\Gamma(1+i\beta_0)]\}, \quad e\rightarrow\varepsilon_1+0 \tag{4.6}$$

where

$$K=\frac{1}{2}\,\frac{e^{i\lambda}\Phi(1+i\beta_0,2,-2i\lambda)}{\mathrm{Im}\left(e^{i\lambda}\,\dfrac{\Psi(1+i\beta_0,2,-2i\lambda)}{\Gamma(1-i\beta_0)}\right)} \tag{4.7}$$

and

$$S=-\exp\left\{-2i\ \arg\left(\Psi(1+i\beta_0,2,-2i\lambda)+\frac{\pi e^{i\pi|\alpha|}}{\sin(\pi|\alpha|)\Gamma(i\beta_0)}\,\Phi(1+i\beta_0,2,-2i\lambda)\right)\right\},\quad e\to\varepsilon_1-0. \tag{4.8}$$

In addition, the simplifying relationship between Φ and the confluent hypergeometric function Ψ can be used (see [6]),

$$\Phi(1+i\beta_0,2,-2i\lambda)=-2e^{\pi\beta_0-i\lambda}\ \mathrm{Re}\left(e^{i\lambda}\,\frac{\Psi(1+i\beta_0,2,-2i\lambda)}{\Gamma(1-i\beta_0)}\right) \tag{4.9}$$

resulting in the following explicit expressions for the scattering cross sections above the ionization threshold:

$$\sigma_{e+}=\frac{4\pi}{k_2^2}\,(e^{2\pi\beta_0}\cos^2\{\arg[\Psi(1+i\beta_0,2,-2i\lambda)]\}+(1-e^{2\pi\beta_0})\sin^2\{\lambda+\arg[\Gamma(1+i\beta_0)]\})-\sigma_{r+},$$

$$\sigma_{r+}=\frac{4\pi}{k_2^2}\,e^{2\pi\beta_0}(1-e^{2\pi\beta_0})\cos^2\{\arg[\Psi(1+i\beta_0,2,-2i\lambda)]+\lambda+\arg[\Gamma(1+i\beta_0)]\}. \tag{4.10}$$

Both cross sections are finite, and the inelastic one has the form typical to twofold localized Landau-Zener transitions.

The elastic cross section has no limiting value for $e\to\varepsilon_1-0$ because of the condensing resonances. When approaching the threshold, σ_{e-} behavior is given by

$$\sigma_{e-}=\frac{4\pi}{k_2^2}\,\frac{\{[x-Y]\tan(\pi|\alpha|)+X\}^2}{\{[x-Y]\tan(\pi|\alpha|)+X\}^2+\{[y+X]\tan(\pi|\alpha|)+Y\}^2}, \tag{4.11}$$

where

$$\begin{aligned}X&=\pi\ \mathrm{Re}[\Phi(1+i\beta_0,2,-2i\lambda)\Gamma^{-1}(i\beta_0)],\\ Y&=\pi\ \mathrm{Im}[\Phi(1+i\beta_0,2,-2i\lambda)\Gamma^{-1}(i\beta_0)],\\ x&=\mathrm{Re}[\Psi(1+i\beta_0,2,-2i\lambda)],\\ y&=\mathrm{Im}[\Psi(1+i\beta_0,2,-2i\lambda)].\end{aligned} \tag{4.12}$$

The resonances are located at energies satisfying the equation

$$\tan\pi|\alpha|=-\frac{Y}{y+X}. \tag{4.13}$$

In a sufficient vicinity of the threshold they are represented by the Coulomb series

$$E_n=u_1(\infty)-\frac{1}{2(n+\Delta)^2}\,E_q, \tag{4.14}$$

where

$$\Delta=-\frac{1}{\pi}\,a\ \tan\left(\frac{Y}{y+X}\right), \tag{4.15}$$

and E_q is the energy unit

$$E_q=\left(\frac{\varepsilon_1}{\varepsilon_1-\varepsilon_2}\right)^2\frac{ma^2}{\hbar^2}. \tag{4.16}$$

Averaging σ_{e-} over the energy interval covering a single resonance in between two adjacent zeros of σ_{e-}, and using the relationship (4.9) for Φ and Ψ hyperfunctions as in the derivation of Eq. (4.10), gives an explicit relationship

$$\langle\sigma_{e-}\rangle=\sigma_{e+}+\sigma_{r+}. \tag{4.17}$$

Equations (4.10)–(4.12) provide a complete description of the Coulomb anomaly in the scattering cross sections near the threshold of the inelastic channel. The relationship in (4.17) answers the question about the correlation between the result of the regularization procedure applied to the Coulomb cross section (4.11) and the quantum-mechanical statement about the continuity of the total scattering cross section as a function of collision energy.

V. CONCLUSION

Equation (4.10) is remarkable not only as a rigorous quantum-mechanical result, but also in view of apparent opportunities for generalizations of the model considered. One of them is associated with the Landau-Zener form of the cross section σ_{r+}, which testifies to the localized nature of the transition. In the case of weak dependence of the state coupling upon interatomic separation, the S matrix can be obtained by performing matching procedures using adiabatic generalizations of the model studied. When the state coupling behaves exponentially, matchings of solutions to the exponential model [7] and those to model (2.1) are possible.

Another possibility for generalization relates to the scattering with nonzero angular momenta. It is provoked by the qualitative nature of the famous conclusion that the Coulomb anomaly takes the same form for all orbital states [2,3]. The corresponding explicit result seems to be essential, and probably can be obtained for the intersection model considered above. The type of possible total cross section can even be

predicted, keeping in mind the localized nature of the transitions. Just as in the energy range allowing the semiclassical description, the threshold cross section should be formed mainly by the momenta for which the intersection is classically accessible [8].

The above arguments imply that accurate analytical results can be obtained for realistic models of atomic scattering near thresholds of ion formation. One of these models used for chemi-ionization collisions includes the exchange interaction of ionic and covalent states, and is described by the equation

$$\begin{pmatrix} -\frac{\hbar^2}{2m}\frac{d^2}{dR^2}-\frac{a}{R}+D-E & V\exp\left(-\frac{R}{R_0}\right) \\ V\exp\left(-\frac{R}{R_0}\right) & -\frac{\hbar^2}{2m}\frac{d^2}{dR^2}-E \end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}=0,$$

where R_0 is the characteristic atomic distance.

The chemi-ionization is the collision process with far-off crossing $R_* \gg R_0$ ($R_*=a/D$) that causes the stratification of the transition region into two separate pieces in the vicinity of R_0 and R_*. The quantum Demkov model with diabatic splitting $D-a/R_0$ is adequate to describe the transitions near R_0. The exact solution of the Coulomb intersection problem (20) with $V\exp(-R/R_0)$ coupling may be used in the vicinity of R_*. Being in the main quasiclassical due to inequality $e_q \gg 1$, the real atomic collisions admit the matching of exact quantum solutions in the vicinities R_0 and R_*, with quasiclassical adiabatic wave functions for the region between these vicinities. Additive matchings near $R=0$ and in the asymptotic region $R\to\infty$ provide the conditions (3.15), and also the physical limit $E\to D$ for the inelastic cross section.

In the R_0 region, the basis set of exact solutions which is necessary for the matchings may be constructed of Meijer functions [7]. Solutions (20) along four independent contours going around the branch points $\pm z_{1,2}$ form the basis set in the R_* region.

To describe the collisions with any angular momentum, the centrifugal repulsion must be included. As a result difficulties arise only in a situation when the turning points R_t are in the transition regions. At $R_t \simeq R_0$ the correct description can be made when using the wave functions which satisfy the physical boundary condition for $R\to 0$ as in [7].

The case $R_t \simeq R_*$ is a standard problem. Probably the rigorous solution for it may be found analytically, although the contribution of these momenta to the total cross section can be estimated in the framework of the localized transition idea according to formula (4.10).

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APPENDIX

We consider the hypergeometric Gauss function $F(a,b,1+a+b,z)$, $z=\exp(2i\lambda/a)$, in the limit $|a|\to\infty$. We begin from the integral representation for this function [6],

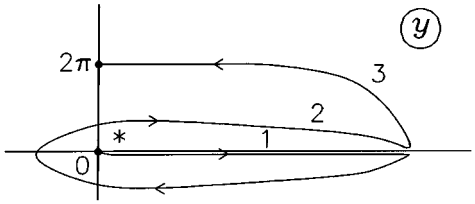

FIG. 3. The integration contour C in Eq. (A.3) and its deformation in the case $\mathrm{Re}(a)<0$. Parts C_1, C_2, and C_3 of the whole contour C are labeled 1, 2, and 3. The asterisk denotes the branch point $y=-2i\lambda/a$.

$$F(a,b,1+a+b,z)=\frac{e^{-i\pi a}}{2\pi i}\,\frac{\Gamma(1-a)\Gamma(1+a+b)}{\Gamma(1+b)}\,I, \qquad \text{(A1)}$$

where I is the contour integral

$$I=\oint t^{a-1}(1-t)^b(1-tz)^{-b}\,dt. \qquad \text{(A2)}$$

The integration contour in (A2) is a simple loop starting at a point $t=1$ and circumventing the branch point $t=0$ in the positive direction. The branch point $t=1/z$ is outside this loop. After the variable change $t=\exp(y)$, the integral I is written in the form

$$I=\int_C e^{ay}(1-e^y)^b(1-e^{y+(2i\lambda/a)})^{-b}\,dy, \qquad \text{(A3)}$$

where the contour C connects the points $y=0$ and $y=2\pi i$

In the case $\mathrm{Re}(a)<0$, the branch point $y_0=-2i\lambda/a$ lies in the upper half-plane of complex variable y, and the integration contour C circumvents this point in the negative direction. After the deformation shown in Fig. 3 the contour C can be partitioned into three parts: C_1 is a straight line starting at the point $y=0$ and going along the real axis to $y\to+\infty$; C_2 is a simple loop starting at $y=+\infty$ and circumventing the branch points $y=0$ and $y=y_0$ in the negative direction; and C_3 connects the points $y=+\infty$ and $y=2\pi i$. In accordance with this partition, the integral I is represented as a sum of three terms: $I=I_1+I_2+I_3$, where the integrand is a single-valued function along the contour C_2.

The principal contribution to integrals I_1 and I_2 comes from a small vicinity of y which is of the order of $1/a$ in the limit $|a|\to\infty$, $\mathrm{Re}(a)<0$. Calculating these contributions, we obtain

$$I_1=\int_0^{+\infty} e^{ay}y^b(y+2i\lambda/a)^{-b}\,dy$$

$$=\frac{2i\lambda}{a}\,\Gamma(1+b)\Psi(1+b,2,-2i\lambda), \qquad \text{(A4)}$$

$$I_2=\oint_{C_2} e^{ay}y^b(y+2i\lambda/a)^{-b}\,dy$$

$$=\frac{4\pi b\lambda}{a}\,\Phi(1+b,2,-2i\lambda), \qquad \text{(A5)}$$

where Ψ and Φ are confluent hypergeometric functions. The principal contribution to the integral I_3 from the vicinity of the point $y=2\pi i$ has the form

$$I_3 = -e^{2\pi i a}\int_0^{+\infty} e^{a\varepsilon}\varepsilon^b(\varepsilon+2i\lambda/a)^{-b}\,d\varepsilon = -e^{2\pi i a}I_1. \tag{A6}$$

As a result, we obtain

$$\frac{i\Gamma(1+a)}{2\lambda\Gamma(1+a+b)}F(a,b,1+a+b,1+2i\lambda/a) = \Psi(1+b,2,-2i\lambda) - \frac{\pi}{\Gamma(b)}\frac{e^{-i\pi a}}{\sin(\pi a)} \times \Phi(1+b,2,-2i\lambda), \quad |a|\to\infty, \quad \mathrm{Re}(a)<0. \tag{A7}$$

In the case $\mathrm{Re}(a)\geqslant 0$, $a\neq i|a|$, contour C can be partitioned into two contours: contour $\tilde{C}_1$, starting at the point $y=0$ and going to $y=-\infty$, and contour $\tilde{C}_3$, starting at $y=-\infty$ and going to the point $y=2\pi i$. The contributions of these contours to integral I are similar to those of I_1 and I_3 as before, and this leads to

$$\frac{i\Gamma(1+a)}{2\lambda\Gamma(1+a+b)}F(a,b,1+a+b,1+2i\lambda/a) = \Psi(1+b,2,-2i\lambda), \quad |a|\to\infty, \quad \mathrm{Re}(a)\geqslant 0, \quad a\neq i|a|. \tag{A8}$$

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