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BEHAVIOR OF CROSS SECTIONS NEAR THRESHOLD OF A NEW REACTION IN THE CASE OF A COULOMB ATTRACTION FIELD

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The multichannel effective-radius theory is extended to the case of a Coulomb attractive field. It is shown that this theory leads to the presence of resonances in the cross sections below the threshold of the new reaction. Expressions are obtained for the averaged cross sections, widths, and shifts of the resonances.

INTRODUCTION

BAZ' has considered [1] the behavior of the elastic cross section near the threshold of the first inelastic reaction, and established the existence of resonances in the elastic scattering cross section. The resonances are the result of the fact that at definite energies below the thresholds the particles are able to excite a transition and remain themselves bound on one of the Bohr orbits in the Coulomb field. Such a state is unstable and the particles return to the ground states and move apart. To each of the unstable states there corresponds a resonance maximum (and a minimum) on the cross section curve. The distance between neighboring maxima is approximately equal to the distance between the corresponding Bohr levels. Near the threshold, where this distance is very small, only the cross section averaged over the resonances is of interest. Baz' has shown [1] that the average value of the elastic cross section below the first threshold is equal to the total cross section above the threshold. Fonda and Newton [2-4] investigated the behavior of the cross sections near higher thresholds. They expressed the scattering matrix below threshold in terms of its values above threshold and also demonstrated the continuity of the averaged total cross sections. In the present paper expressions are derived for the discontinuities in the averaged partial cross sections, widths, and shifts of the resonances. It is shown that these expressions are also applicable to the excitation of hydrogenlike ions by electrons, where polarization forces of the type r^{-3} act between the scattered electron and the ion in the excited state at large distances, in addition to the Coulomb forces.

We are considering d parallel nonrelativistic reactions $X(a, b_f) Y_f$, $f = 1, \ldots, d$ near the threshold of a new reaction $X(a, b_t) Y_t$. (Several channels, differing in the momenta of the particles b_t and Y_t can open immediately at this threshold. Accidental coincidence of thresholds of two essentially different reactions are disregarded.) We assume that at these energies there are no reactions in which three or more particles are produced. The particles b_t and Y_t are assumed oppositely charged. The remaining particles may or may not be charged.

We choose r_0 such that only Coulomb forces act between them when $r \geq r_0$. The wave function of the system of particles participating in the reaction is in this region a linear combination of single-particle wave functions in a Coulomb field. The cross section is expressed in terms of the coefficients of these functions, determined by smoothly joining the wave function of the system when $r \geq r_0$ with the same wave function for $r \leq r_0$. In place of the explicit solution for the latter, we shall use the smooth energy dependence of the logarithmic derivative. This, together with the known energy dependence of the Coulomb wave functions, is sufficient to determine the behavior of the cross sections below threshold and their connection with the cross sections above threshold.

1. FUNDAMENTAL EXPRESSIONS

We denote by l, J, m, r, v, and k the diagonal matrices whose elements are the orbital and total momenta, the reduced mass, the distance, the relative velocity, and the wave number of the channel. F(kr) and G(kr) are the regular and irregular Coulomb wave functions [5],

$$\eta = Z_b Z_Y / \hbar v, \qquad \sigma_l = \arg \Gamma(l + 1 + i\eta), \qquad \omega_l = \sigma_l - \sigma_0,$$

s is the spin of the channel.

The wave functions of the system for $r \geq r_0$ can be written in the form of a square matrix[6]

$$\psi = v^{-1/2}(F(kr) + G(kr)K). \quad (1)$$

Different columns in (1) correspond to different linearly independent solutions. Different rows correspond to the wave-function components for different channels. Only components of open channels and of those closed channels whose threshold region is under consideration are included in (1). The wave-function components for the remaining channels attenuate rapidly with increasing r, and when r_0 is sufficiently large their contribution is negligibly small. The channels that are open only above threshold will be called new, and summation over them will be denoted by Σ'. The remaining channels will be called old and the summation denoted by Σ''.

The symmetrical matrix K is connected with the cross sections in the following manner:

$$Q^J(i-f) = \frac{\pi}{k_i^2}\frac{2J+1}{2s_i+1}|T_{fi}|^2, \quad (2)$$

$$T = -2i(K^{-1} - i)^{-1}, \quad (3)$$

$$T = e^{-i\omega}[e^{2i\omega} - U]e^{-i\omega}. \quad (4)$$

We have chosen for the matrix T a definition (4) which differs from that used in [6] by the factors $e^{-i\omega}$, so as to simplify the formulas derived later.

The matrix K, as a function of the energy E, has a branch point at the threshold E_t of the new channel. We must separate in the formula for K the terms with the branching from the part that is analytic in the vicinity of the threshold. To this end we use the method employed by Teichmann for elastic scattering [7]. We define the R-matrix [8] by the relation

$$\frac{1}{\sqrt{m}}\psi(r_0) = R\frac{1}{\sqrt{m}}r_0\frac{d}{dr}\psi(r)\Big|_{r=r_0} \quad (5)$$

and, substituting (1) in (5), express K in terms of R,

$$K^{-1} = -\frac{G}{F} + \frac{1}{F\dot{F}} - \frac{1}{\rho^{1/2}F}\left[\rho^{-1}\frac{F}{\dot{F}} - R\right]^{-1}\frac{1}{\dot{F}\rho^{1/2}},$$

$$\rho = kr_0, \qquad F = F(\rho), \qquad G = G(\rho), \qquad \dot{F} = \frac{d}{d\rho}F(\rho). \quad (6)$$

It follows from the solution of the Schrödinger equation in the region $r \leq r_0$ (see [6]) that the R-matrix is analytic in the energy and has only simple poles on the real axis. The branching in (6) is due only to the Coulomb functions, which we therefore express in terms of the functions Ψ and Φ, which are regular in E when r_0 = const [5]:

$$F_l(\rho) = C_l\rho^{l+1}\Phi_l(\rho),$$

$$G_l(\rho) = \frac{\rho^{-l}}{(2l+1)C_l}\Big[\Psi_l(\rho) + \rho^{2l+1}p_l(\eta)\left(\ln 2\rho + \frac{q_l(\eta)}{p_l(\eta)}\right)\Phi_l(\rho)\Big],$$

$$C_l = \frac{2^l C_0}{(2l+1)!}\prod_{s=1}^{l}(s^2+\eta^2)^{1/2}, \qquad C_0 = \left(\frac{2\pi\eta}{e^{2\pi\eta}-1}\right)^{1/2},$$

$$p_l = 2\eta(2l+1)C_l^2/C_0^2, \qquad f(\eta) = {}^1/_2[\psi(i\eta) + \psi(-i\eta)]. \quad (7)$$

$q_l(\eta)/p_l(\eta) - f(\eta)$ is a rational function of η^2, which tends to a constant as $|\eta|^2 \to \infty$.

Substituting (7) in (6) we obtain

$$k^{l+1/2}(2l+1)!!\,C_lK^{-1}C_l(2l+1)!!\,k^{l+1/2} = M - \frac{(2l+1)!!^2}{(2l+1)}k^{2l+1}p_l(\ln k + f(\eta)), \quad (8)$$

where

$$M = \frac{(2l+1)!!}{r_0^{l+1/2}}\Big\{-\frac{\Psi}{(2l+1)\Phi} - \frac{k^{2l+1}p_l}{2l+1}r_0^{2l+1}\left(\ln 2r_0 + \frac{q_l}{p_l} - f(\eta)\right) + \frac{1}{\Phi\overline{\Phi}} - \frac{1}{\Phi}\left[\frac{\Phi}{\overline{\Phi}} - R\right]^{-1}\frac{1}{\overline{\Phi}}\Big\}\frac{(2l+1)!!}{r_0^{l+1/2}},$$

$$\overline{\Phi}_l(\rho) = (l+1)\Phi_l(\rho) + \rho\frac{d}{d\rho}\Phi_l(\rho). \quad (9)$$

The terms $k^{2l+1}p_l$ and $q_l(\eta)/p_l(\eta) - f(\eta)$ contained in (9) are rational functions of k^2 and finite when $k^2 = 0$. The matrix M, which is symmetrical and real on the real axis, is therefore analytic in the vicinity of the threshold.

It follows from (3) and (8) that

$$T = k^{l+1/2}(2l+1)!!\,C_l\frac{-2i}{M - (2l+1)!!^2p_lk^{2l+1}\tau/(2l+1)} \times C_l(2l+1)!!\,k^{l+1/2}, \quad (10)$$

$$\tau = \ln k + f(\eta) + i\pi/(e^{2\pi\eta} - 1). \quad (11)$$

The factor $(2l+1)!!$ has been singled out because $(2l+1)!!\,C = 1$ in the absence of a Coulomb field, when (10) goes over into formula (22) of Ross and Shaw [8].

The only term with a branch point in (10) is the diagonal matrix τ. The only elements of this matrix not analytic near the threshold are those corresponding to the new channels. They are all the the same and in the direct vicinity of the threshold they are equal to $(a|k_t| \ll 1)$

$$\tau_{tt}^a = \ln\frac{1}{a} - i\pi \quad (E > E_t), \quad \tau_{tt}^b = \ln\frac{1}{a} + \pi y \quad (E < E_t),$$

$$a = \frac{\hbar^2}{me^2|Z_{b_t}Z_{Y_t}|}, \quad y = \operatorname{ctg}\frac{\pi}{a\varkappa}, \quad k_t = i\varkappa \text{ for } E < E_t. \quad (12)^*$$

*ctg = cot.

2. BEHAVIOR OF CROSS SECTIONS NEAR THE THRESHOLD OF ONE NEW CHANNEL

In this section and in the following we consider the region of energies near threshold, where M can be regarded as constant and equal to M_t, the value at threshold, and where formula (12) can be used for τ_{tt}. Eliminating M_t from (10), we relate T below threshold (T^b) with T above threshold (T^a):

$$T^b = [T^{a-1} + i\eta C_0^{-2}(\tau^a - \tau^b)]^{-1}. \quad (13)$$

All the elements of the matrix $\tau^a - \tau^b$ are proportional to $E - E_t$, except $\tau^a_{tt} - \tau^b_{tt} = -\pi(y+i)$. Neglecting the former and assuming that $\lim_{E\to E_t} 2\eta_t C_0^{-2}(\eta_t) = -1/\pi$, we obtain

$$T^b = (T^{a-1} + Y)^{-1}. \quad (14)$$

The matrix Y contains only one nonvanishing element $Y_{tt} = i(y+i)/2$, enabling us to simplify (14):

$$T^b_{fi} = T^a_{fi} - \frac{T^a_{ft}T^a_{ti}}{T^a_{tt}} + \frac{T^a_{ft}T^a_{ti}}{(T^a_{tt})^2}\frac{-2i}{y+i-2i(T^a_{tt})^{-1}}. \quad (15)$$

The quantity y is a periodic function of $1/a = \hbar/a\sqrt{2m_t(E_t - E)}$. Therefore T^b and all the cross sections oscillate near threshold, assuming identical values at those energies for which $1/a\kappa$ differ by an integer. The form of the cross-section curve depends on T^a. If $\mathrm{Re}\, T^a_{tt} \ll 1$, then the values of T^b_{fi} are constant and approximately equal to T^a_{fi} at energies for which y differs noticeably from $-2\,\mathrm{Im}(T^a_{tt})^{-1}$. The cross sections are then equal to the corresponding cross sections above threshold. When $y \approx -2\,\mathrm{Im}(T^a_{tt})^{-1}$, the cross sections vary rapidly. The width of the resonance Γ and its shift Δ (if the latter is small) with respect to the value of $E_t - E = \hbar^2(2m_t a^2 n^2)^{-1}$ are given by the expressions

$$\frac{\Gamma}{D} = \frac{1}{2\pi}[2\,\mathrm{Re}\, T^a_{tt} - |T^a_{tt}|^2] = \frac{1}{2\pi}\sum_j{}'' |T^a_{tj}|^2,$$

$$\frac{\Delta}{D} = \frac{1}{2\pi}\mathrm{Im}\, T^a_{tt}, \quad (16)$$

where $D = 2\sqrt{2m_t}\, a\,(E_t - E)^{3/2}/\hbar$ is the distance between resonances.

The resonances are very close together near threshold, so that interest attaches to the cross sections averaged over the resonances

$$\overline{Q} = \frac{1}{D}\int_{E-D/2}^{E+D/2} Q(E)\,dE = \frac{1}{\pi}\int_{-\infty}^{+\infty} Q(y)\frac{dy}{1+y^2}. \quad (17)$$

Formula (16) expresses T^b_{fi} in the form $\alpha + \beta/(y-\gamma)$ and (17) reduces to the integral

$$\frac{1}{\pi}\int_{-\infty}^{+\infty}\left(\alpha + \frac{\beta}{y-\gamma}\right)\left(\alpha^* + \frac{\beta^*}{y-\gamma^*}\right)\frac{dy}{1+y^2}$$

$$= \frac{1}{\mathrm{Im}\,\gamma}\frac{|\beta|^2}{|\gamma+i|^2} + \left|\alpha - \frac{\beta}{\gamma+i}\right|^2,$$

$$\mathrm{Im}\,\gamma = 2|T^a_{tt}|^{-2}\mathrm{Re}\, T^a_{tt} - 1 = |T^a_{tt}|^{-2}\sum_j{}''|T^a_{tj}|^2 > 0. \quad (18)$$

Using (2), (15), and (18), we obtain

$$\overline{Q^{bJ}(i-f)} = Q^{aJ}(i-f) + \frac{\pi}{k_i^2}\frac{2J+1}{2s_i+1}\frac{|T^a_{ft}|^2|T^a_{ti}|^2}{\sum_j''|T^a_{tj}|^2}$$
$$= Q^{aJ}(i-f) + \frac{Q^{aJ}(i-t)\,Q^{aJ}(t-f)}{\sum_j'' Q^{aJ}(t-j)}. \quad (19)$$

Expression (19) shows that all averaged cross sections decrease abruptly at the threshold with increasing energy. The distribution of the jumps between the cross sections does not depend on the initial state and is equal to the distribution of the inelastic jumps in the averaged cross sections in scattering, where the new channel is the initial one. The behavior of the jumps in the averaged cross sections is analogous to their behavior in the compound-nucleus model. The sum of all the jumps is equal to the cross section of the new channel, i.e., the total cross section is continuous on the threshold. The latter was proved by Baz'[1] and by Fonda and Newton[2-4] by averaging the imaginary part of the scattering amplitude.

3. BEHAVIOR OF CROSS SECTIONS NEAR THE THRESHOLD OF SEVERAL NEW CHANNELS

If the particles b_t and Y_t have proper momenta, then, for the same threshold several (n) channels with different particle momentum for a constant total momentum J open up immediately. This case differs but little from the case considered in Sec. 2. Formula (14) remains in force, but the diagonal matrix Y now contains n equal non-zero elements $i(y+i)/2$. Expression (15) assumes the form

$$T^b_{fi} = T^a_{fi} - \sum_{mm'}{}' T^a_{fm}[\hat{T}^{-1}]_{mm'}T^a_{m'i}$$
$$+ \sum_{mm'}{}' T^a_{fm}\left[\frac{-2i}{(y+i-2i\hat{T}^{-1})\hat{T}^2}\right]_{mm'}T^a_{m'i}. \quad (20)$$

Here $\hat{T}$ is a symmetrical matrix of rank n, containing the T^a-matrix elements relating the new channels only. Using the orthogonal matrix B that diagonalizes $\hat{T}$

$$B^{-1}\hat{T}B = t \equiv (t_k\delta_{kj}), \quad B^{-1} = B^T, \quad (21)$$

we transform (20) into

$$T^b_{fi} = T^a_{fi} - \sum_{mm'}{}' T^a_{fm}\, [\hat{T}^{-1}]_{mm'} T^a_{m'i} + \sum_k{}' \Theta_{ik}\Theta_{fk} \frac{-2i}{(y + i - 2it_k^{-1})\, t_k^2};$$
$$\Theta_{jk} = \sum_m{}' T^a_{jm} B_{mk}. \qquad (22)$$

The consequences of (22) are similar to those of (15): near the threshold the cross sections oscillate and assume identical values when $1/a\kappa$ differ by integers. If $\mathrm{Re}\, t_k \ll 1$, then for energy values when y differs appreciably from all the $-2\, \mathrm{Im} t_k^{-1}$ the cross sections are approximately equal to their values above threshold. When $y \approx -2\, \mathrm{Im}\, t_k^{-1}$ resonances are observed. Their widths and shift are

$$\frac{\Gamma_k}{D} = \frac{1}{2\pi} [2\, \mathrm{Re}\, t_k - |t_k|^2] \approx \frac{1}{2\pi} \sum_j{}'' |\Theta_{jk}|^2, \quad \frac{\Delta_k}{D} = \frac{1}{2\pi} \mathrm{Im}\, t_k. \qquad (23)$$

In analogy with (19) we obtain

$$\overline{Q^{bJ}(i-f)} - Q^{aJ}(i-f) = \frac{\pi}{k_i^2} \frac{2J+1}{2s_i+1} \sum_{k,\varkappa}{}' \frac{\Theta_{ik}\Theta^*_{i\varkappa}\Theta_{fk}\Theta^*_{f\varkappa}}{t_k - t_k t^*_\varkappa + t^*_\varkappa}$$
$$= \frac{\pi}{k_i^2} \frac{2J+1}{2s_i+1} \sum_{k,\varkappa}{}' \frac{\Theta_{ik}\Theta^*_{i\varkappa}\Theta_{fk}\Theta^*_{f\varkappa}}{\sum_j{}'' \Theta_{jk}\Theta^*_{j\varkappa}} \sum_m{}' B_{mk} B^*_{m\varkappa}. \qquad (24)$$

As in the case of one new channel, all the averaged cross sections decrease abruptly on the threshold with increasing energy, inasmuch as the right half of (24) is always positive. This can be readily verified by representing it in the form

$$\sum_{k,\varkappa}{}' \frac{a_k a^*_\varkappa}{1 - S_k S^*_\varkappa}, \quad |S_k| < 1$$

and expanding the denominator in a series. The sum of all the jumps is equal to the sum of the cross sections of the new channels. The form of (24) is more complicated than that of (19) because of the superposition of the neighboring resonances. In the important case when the sections of the new channels are small, i.e., the elements T^a_{jk} relating the old and the new channels are small and, in accord with (23), the resonances are narrow, Eq. (24) simplifies greatly. The terms with $k \neq \kappa$ in (24) are then much smaller than the terms with $k = \kappa$, and

$$\overline{Q^{bJ}(i-f)} - Q^{aJ}(i-f) = \frac{\pi}{k_i^2} \frac{2J+1}{2s_i+1} \sum_k{}' \frac{|\Theta_{ik}|^2 |\Theta_{fk}|^2}{\sum_j{}'' |\Theta_{jk}|^2}. \qquad (25)$$

4. THRESHOLD BEHAVIOR OF THE EXCITATION CROSS SECTIONS OF HYDROGENLIKE IONS BY ELECTRONS

Owing to the degeneracy of the levels of the hydrogenlike ion with different momenta, a strong polarization interaction exists between the electron and the ion in the excited state. This interaction decreases as $1/r^2$ with increasing distance between the electron and the ion.[1)] It is therefore impossible to choose r_0 such that the electron-ion interaction reduces to a Coulomb interaction when $r > r_0$, and the derivation presented above for the threshold behavior does not apply. We shall show that an account of the polarization interaction does not change the threshold behavior of the ion excitation cross sections, in contrast with the case of the excitation of hydrogen atoms, where the threshold behavior depends essentially on the polarization.

In analogy with [9] we choose r_0 such that Eq. (4) of [9] reduces when $r \geq r_0$ to

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)+\alpha}{r^2} + \frac{2Z}{r} + k^2\right)\psi = 0, \qquad (26)$$

where Z is the ion charge. The solution of (26) has the form $\psi = A\varphi$, with two systems of independent solutions existing for φ:

$$I_\lambda = -ie^{-\pi\eta/2} e^{-i\rho} (2\rho)^{\lambda+1}\, U_2(\lambda + 1 - i\eta,\ 2\lambda + 2,\ 2i\rho) \underset{\rho\to\infty}{\sim} \exp\{-i(\rho - \pi\lambda/2 - \eta \ln 2\rho)\},$$
$$O_\lambda = ie^{-\pi\eta/2} e^{-i\rho} (2\rho)^{\lambda+1}\, U_1(\lambda + 1 - i\eta,\ 2\lambda + 2,\ 2i\rho) \underset{\rho\to\infty}{\sim} \exp\{i(\rho - \pi\lambda/2 - \eta \ln 2\rho)\}. \qquad (27)$$

We use for the hypergeometric functions the notation of Morse and Feshbach [10] and the expansions of [5,11]

$$F(\lambda + 1 - i\eta,\ 2\lambda + 2,\ 2i\rho) = (-2\eta)^{-2\lambda-1} \rho^{-2\lambda-1} e^{i\rho} \Gamma(2\lambda+2)\, y_1,$$
$$F(-\lambda - i\eta,\ -2\lambda,\ 2i\rho) = \Gamma(-2\lambda)\, e^{i\rho} y_2,$$
$$y_1 = \sum_{p=0}^{\infty} a_p (2Zr)^{(p+2\lambda+1)/2} J_{p+2\lambda+1}(2\sqrt{2Zr}),$$
$$y_2 = \sum_{p=0}^{\infty} b_p (2Zr)^{(p+2\lambda+1)/2} J_{p-2\lambda-1}(2\sqrt{2Zr}),$$
$$a_p = b_p = 0 \ \text{ if } \ p < 0, \qquad a_0 = b_0 = 1,$$
$$a_p = -[(p + 2\lambda)\, a_{p-2} - a_{p-3}]/(2\eta)^2 p,$$
$$b_p = -[(p - 2\lambda - 2)\, b_{p-2} - b_{p-3}]/(2\eta)^2 p. \qquad (28)$$

If we represent ψ for $r \geq r_0$ in the form

$$\psi = k^{-1/2} A\, (I - OU'), \qquad (29)$$

we obtain for the matrix U an expression similar to Eq. (12) of [9]:

$$U = e^{i\pi l/2} A e^{-i(\pi\lambda/2 + \sigma_0)} U' e^{-i(\pi\lambda/2+\sigma_0)} A^{-1} e^{i\pi l/2}. \qquad (30)$$

We express, in accord with (5), (27), and (28),

[1)]For the formulation of the problem and for the definition of the quantities a, A, and λ used here see [9].

the matrix U′ in terms of R and U_1, and U_2 from (27) in terms of Y_1 and y_2 from (28), obtaining the expression

$$U' = -\frac{\Gamma(\lambda+1+i\eta)}{\Gamma(\lambda+1-i\eta)} - 2i\frac{\Gamma(\lambda+1+i\eta)}{\Gamma(\lambda+1)e^{\pi\eta/2}}k^{\lambda+1/2}$$

$$\times\left[M - \frac{2\pi}{\sin 2\pi\lambda}\frac{\Gamma(\lambda+1+i\eta)e^{-i\pi(\lambda+1/2)}k^{2\lambda+1}}{\Gamma(-\lambda+i\eta)\Gamma^2(\lambda+1)}\right]^{-1}$$

$$\times\frac{\Gamma(\lambda+1+i\eta)k^{\lambda+1/2}}{\Gamma(\lambda+1)e^{\pi\eta/2}}, \quad (31)$$

which replaces (10)[2)], where M [which differs from that given by (9)] depends on E only through R and y_1 and y_2, so that it is analytic near the threshold E_t. In the region near the threshold, where M can be regarded as constant and the asymptotic expansion can be used for $\Gamma(\lambda_t + 1 + i\eta_t)$, it follows from (30) and (31) that

$$U^b_{fi} = U^a_{fi} - \sum_{mm'}{}' U^a_{fm}\left[\frac{1}{\hat{U} - \exp\{i(\pi l - 2\pi/a\varkappa)\}}\right]_{mm'} U^a_{m'i}, \quad (32)$$

where $\hat{U}$ is a symmetrical matrix of rank n, containing the matrix elements of U^a connecting new channels only. Upon substitution of (4) Eq. (32) coincides with (20), so that the results of Sec. 3 are applicable also in the case of excitation of hydrogenlike ions by electrons.

2)For diagonal elements with integral λ it is necessary to go in the square brackets to the limit $\lambda \to$ integer, since M also contains the term $(\sin 2\pi\lambda)^{-1}$. We then obtain the expression in the denominator of (10).

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