SOME FEATURES OF THE THRESHOLD BEHAVIOR OF THE CROSS SECTIONS FOR EXCITATION OF HYDROGEN BY ELECTRONS DUE TO THE EXISTENCE OF A LINEAR STARK EFFECT IN HYDROGEN

M. GAĬLITIS and R. DAMBURG

Physics Institute, Academy of Sciences, Lithuanian S.S.R.

Submitted to JETP editor December 15, 1962

J. Exptl. Theoret. Phys. (U.S.S.R.) **44**, 1644-1649 (May, 1963)

In the case of short-range forces the cross sections for inelastic transitions near the threshold (provided that one particle is charged in the final state) depend on the energy as $k_f^{2l_f+1}$ where k_f and l_f are the momentum and the angular momentum in the final state.[11] If $l_f = 0$ the cross sections in the old channels at the threshold energy possess a singularity of the peak or step type.[6] It is shown that upon excitation of the hydrogen atom by electrons these laws are violated because of the strong polarization interaction between the electron moving away and the hydrogen atom in the excited state. The cross sections near the threshold oscillate. The inelastic cross sections tend to zero only at energies of the order of the relativistic splitting between the levels.

INTRODUCTION

FOR a given total angular momentum L the cross sections which we are considering are given by

$$Q^L(i-f) = \frac{\pi}{k_i^2}\frac{2L+1}{2l'+1}|T_{fi}|^2, \tag{1}$$

where l' is the angular momentum of the atom in the initial state and k_i is the momentum of the incident electron. If the interactions of the particles in the channels attenuate exponentially with the distance, then the T matrix can be represented in the form (cf. [1])

$$T = k^{l+1/2}\frac{-2i}{M - ik^{2l+1}}k^{l+1/2}, \tag{2}$$

where k and l are the diagonal matrices of the momenta and the angular momenta in the channels, and M is the symmetric matrix which has no branch points as a function of the energy.

Near the threshold energy E_t, M can be expanded in powers of $E - E_t$. Confining ourselves to two terms, we obtain the effective-radius approximation which has been previously investigated for eH scattering.[2] Confining ourselves to the first term only, we obtain the law of the threshold behavior of the cross sections

$$Q(i-f) \sim k_f^{2l_f+1}, \tag{3}$$

which follows from the left-hand factor in (2), and the existence of a peak or step for $l_f = 0$, which follows from the numerator in (2).

Equation (2) breaks down for eH scattering; this is a direct consequence of the existence of the linear Stark effect in the hydrogen atom.

Because of the degeneracy of the excited states of hydrogen with respect to l' the hydrogen atom in the excited state takes on, in the field of the scattered electron, a constant dipole moment which is independent of the distance of the electron from the atom. The interaction energy of the electron with the dipole moment depends on the distance of the electron r as $1/r^2$. It is added to the centrifugal energy $l(l+1)/r^2$, and a term $\lambda(\lambda+1)/r^2$ with nonintegral λ appears in the Schrödinger equation instead of the usual centrifugal term. For small L, λ is complex. Expression (2) is replaced by another expression in which nonintegral (or complex) λ appear instead of l.

1. FUNDAMENTAL EXPRESSIONS

Let us obtain the analog of (2) for eH scattering. To find the cross sections it is necessary to solve a Hartree-Fock type system of equations.[3]

$$\mathscr{L}\psi = V\psi \tag{4}$$

with the following boundary conditions at infinity:

$$\psi(r) \sim \frac{1}{\sqrt{k}}e^{-i(kr-\pi l/2)} - \frac{1}{\sqrt{k}}e^{i(kr-\pi l/2)}S, \tag{5}$$

$$T = 1 - S. \tag{6}$$

In (5) ψ is a quadratic matrix whose columns are different linearly-independent solutions

$$\mathcal{L} = d^2/dr^2 - l(l+1)/r^2 + k^2. \quad (7)$$

The matrix of the potentials V contains terms of two types. First, terms which decrease exponentially with increasing r, including all exchange terms. Second, multipole terms of the type β/r^s. Let us choose r_0 such that for $r \geq r_0$ we can assume all exponentially decreasing terms in V and all rows in ψ corresponding to closed channels (with the exception of those whose threshold we are considering[1)]) to vanish. We assume that an exact solution of the system (4) is known in the region $r \leq r_0$ and investigate the matching of this solution with that for $r \geq r_0$. For $r \geq r_0$ the system (4) will be of finite order, owing to the vanishing of the functions corresponding to the closed channels. The matrix of the potentials V will contain only multipole terms. These will include dipole terms $-\alpha/r^2$ connecting channels with equal k^2. The remaining terms will either themselves decrease faster than $1/r^2$ or will be dipole terms d/r^2 connecting channels with different k^2, and will therefore contribute to the polarization potential which decreases faster than $1/r^2$.[2)] In order to explain the role of the terms α/r^2, we discard for $r \geq r_0$ all the remaining terms which decrease much faster. Then, for $r \geq r_0$, (4) reduces to

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)+\alpha}{r^2} + k^2\right)\psi = 0. \quad (8)$$

Here α is a symmetric matrix which connects only channels with equal energy. Its diagonal elements are zeros. The values of α are cited in Seaton's paper.[4]

A more general solution of Eq. (8) can be found (cf. [4]). We introduce the matrix A which diagonalizes $l(l+1) + \alpha$:

$$A^{-1}[l(l+1)+\alpha]A = a \equiv \lambda(\lambda+1), \quad (9)$$

where a is a diagonal matrix. Then $\psi = A\varphi$, where for φ we have two systems of independent solutions:

$$I = -i\sqrt{\pi kr/2}\,H^{(2)}_{\lambda+1/2}(kr) \underset{r\to\infty}{\sim} e^{-i(kr-\pi\lambda/2)},$$
$$O = i\sqrt{\pi kr/2}\,H^{(1)}_{\lambda+1/2}(kr) \underset{r\to\infty}{\sim} e^{i(kr-\pi\lambda/2)}. \quad (10)$$

---

1)Channels whose threshold is being considered are called new, while open channels below the threshold are referred to as old.

2)This is strictly true in the adiabatic approximation. If an electron is at rest at a distance r from an atom in state a, then its energy in the second approximation is

$$\sum_{b\neq a}\left(\frac{d_{ab}}{r^2}\right)\frac{1}{E_a-E_b}\left(\frac{d_{ba}}{r^2}\right) \sim \frac{1}{r^4}.$$

Dipole terms connecting channels with equal energies should not appear here, and must therefore be considered separately.

From (10) we can obtain the more general solution of (8) in the form

$$\psi = A\left(\frac{1}{\sqrt{k}}I - \frac{1}{\sqrt{k}}OS'\right). \quad (11)$$

Multiplying (11) from the right by $\exp(-i\pi\lambda/2)A^{-1} \times \exp(i\pi l/2)$, we obtain a solution which for large r behaves like (5) with

$$S = e^{i\pi l/2}Ae^{-i\pi\lambda/2}S'e^{-i\pi\lambda/2}A^{-1}e^{i\pi l/2}. \quad (12)$$

The matrix S′ can be found by smoothly matching (11) at $r = r_0$ with the solution of (4) in the region $r \leq r_0$. It is convenient to take the matching condition in the form of a matrix equation which is satisfied at $r = r_0$ by an arbitrary solution of (4) in the region $r \leq r_0$:[5]

$$\psi(r_0) = Rr_0\frac{d}{dr}\psi(r)|_{r=r_0}. \quad (13)$$

The function (11) must also satisfy Eq. (13). Substituting (11) in (13), we express S′ in terms of R:

$$S' = \left[\frac{e^{-i\pi(\lambda+1/2)}}{\sin\pi(\lambda+1/2)} - k^{-\lambda-1/2}Mk^{-\lambda-1/2}\right]^{-1}$$
$$\times\left[\frac{e^{i\pi(\lambda+1/2)}}{\sin\pi(\lambda+1/2)} - k^{-\lambda-1/2}Mk^{-\lambda-1/2}\right], \quad (14)$$

where

$$M = -\frac{k^{2\lambda+1}}{\sin\pi(\lambda+1/2)}\frac{J_{-\lambda-1/2}(kr_0)}{J_{\lambda+1/2}(kr_0)} + \frac{2}{\pi}\frac{k^{2\lambda+1}}{J_{\lambda+1/2}(kr_0)J'_{\lambda+1/2}(kr_0)}$$
$$+\frac{2}{\pi}\frac{k^{\lambda+1/2}}{J'_{\lambda+1/2}(kr_0)}\left[\frac{J_{\lambda+1/2}(kr_0)}{J'_{\lambda+1/2}(kr_0)} - \bar{R}\right]^{-1}\frac{k^{\lambda+1/2}}{J'_{\lambda+1/2}(kr_0)}, \quad (15)$$

$$J'_{\lambda+1/2}(\rho) = \tfrac{1}{2}J_{\lambda+1/2}(\rho) + \rho\frac{d}{d\rho}J_{\lambda+1/2}(\rho), \quad (16)$$
$$\bar{R} = A^{-1}RA. \quad (17)$$

The values of $k^{\lambda+1/2}J_{-\lambda-1/2}(kr_0)$, $k^{-\lambda-1/2} \times J_{\lambda+1/2}(kr_0)$, and $k^{-\lambda-1/2}J'_{\lambda+1/2}(kr_0)$ as functions of k^2 have no singularities for finite k^2. The matrix R as a function of the energy has only simple poles on the real axis, since according to [5]

$$R_{ij} = \sum_\varkappa \frac{\gamma_{\varkappa i}\gamma_{\varkappa j}}{E_\varkappa - E}. \quad (18)$$

For this reason it is possible to expand the symmetric matrix M as a function of the energy near the threshold E_t in powers of $E - E_t$ (if $|E - E_t|$ is less than the distance from E_t to the nearest pole of the matrix M).

Substituting (14) in (12) and (6), we find

$$T = 1 - e^{i\pi l/2}Ae^{-i\pi\lambda}A^{-1}e^{i\pi l/2}$$
$$+ e^{i\pi l/2}Ae^{-i\pi\lambda/2}k^{\lambda+1/2}$$

$$\times \frac{-2i}{M - ik^{2\lambda+1}e^{-i\pi\lambda}/\cos\pi\lambda} k^{\lambda+1/2}e^{-i\pi\lambda/2}A^{1}e^{i\pi l/2}. \qquad (19)$$

Expression (19) is the analog of (2) for eH scattering.

In deriving (19) we have neglected the relativistic splitting $\Delta\epsilon$ of the energies of the new channels. If this splitting is taken into account, the functions (10) will be solutions of (8) only in the region $r \ll r_1$ where the difference between the terms $l(l+1)r^{-2}$ for different channels is considerably larger than $\Delta\epsilon$:

$$r_1^2 \approx 2(L+1)/\Delta\varepsilon. \qquad (20)$$

Equation (12) remains in force if it is possible to replace the functions (10) at the boundary of this region by $\exp[\mp i(kr - \pi\lambda/2)]$. The condition for the latter is:

$$|k'^2 r_1^2| \gg (L+1)^2, \qquad (21)$$

where k is the momentum of the electron in the new channels. From (20) and (21) follows the condition for the applicability of (19):

$$2|k'^2|/\Delta\varepsilon \gg L+1. \qquad (21')$$

2. BEHAVIOR OF THE CROSS SECTIONS NEAR THE THRESHOLD

Let us consider the range of energies near the threshold, where condition (21′) is fulfilled. The first term in (19) does not depend on the energy and differs from zero only for transitions between degenerate states. It is caused by the constant phase shift in the asymptotic behavior of the Hankel functions of the type $\exp[i(kr - \pi\lambda/2)]$ relative to $\exp[i(kr - \pi l/2)]$.

The threshold behavior of the cross sections depends on the magnitudes of the eigenvalues $a = \lambda(\lambda+1)$ of the matrix $l(l+1) + \alpha$ for the new channels. If among the a there are no negative values less than $-1/4$, then all

$$\lambda = -1/2 + \sqrt{1/4 + a} \qquad (22)$$

are real and the excitation cross sections of all the new channels near the threshold depend approximately equally on the energy as

$$Q \sim k'^{2\lambda_{min}+1}, \qquad (23)$$

independently of the angular momenta in each of the degenerate channels. λ_{min} is the smallest λ for the new channels. If $-1/2 < \lambda_{min} < 1/2$ all the cross sections of the "old" channels will have discontinuities—a peak or a step, the shape of these being, however, different than in the paper of Baz′.[6] Whereas in [6] the peak or the step are produced by the tangency of two parabolas $(E_t - E)^{1/2}$ $(E < E_t)$ and $(E - E_t)^{1/2}$ $(E > E_t)$ at $E = E_t$, here the curves $(E_t - E)^{\lambda_{min}+1/2}$ and $(E - E_t)^{\lambda_{min}+1/2}$ are tangent.

If the a include values smaller than $-1/4$, the behavior of the cross sections changes considerably. The corresponding $\lambda + 1/2 = i\nu$ is an imaginary number $|k'^{\lambda+1/2}| = 1$, and no element of the T matrix tends to zero at the threshold. At the same time all the cross sections near the threshold are different from zero. Their threshold behavior is affected by the term which enters in (19)

$$k'^{2\lambda+1} = \exp(2i\nu \ln k'),$$

which oscillates as a function of $\ln k'$. This gives rise to oscillations of all cross sections both above and below the threshold.

If only one $a < -1/4$, then the cross sections near the threshold take on equal values for E for which

$$\nu \ln|E - E_t| = 2\pi n + \text{const} \qquad (24)$$

both above and below the threshold (with different constant terms; n is an integer).

The oscillations of the cross sections below the threshold are caused by the presence of an infinite set of bound states in the attraction field, which at large distances is of the form a/r^2 with $a < -1/4$[7].[3)] The energy spectrum of these states for small $E_t - E$ is of the form (24), independent of the behavior of the field at small r. To each of these bound states on the cross section curves there corresponds, in accordance with [8], a resonance maximum (and minimum). If the matrix elements of the M matrix connecting the old and new channels are small, then the resonance maxima are narrow and have the shape given by the Breit-Wigner formula. Between neighboring resonances there exists a plateau where the cross sections change little. The oscillations of the cross sections above threshold are caused by the oscillations of the elastic scattering cross sections in the field which has at large distances the form a/r^2 $(a < -1/4)$, since in accordance with Levenson's theorem[9] at small energies the phase δ tends to $n\pi$, where n is the number of bound states.

3. BEHAVIOR OF THE CROSS SECTIONS NEAR THE EXCITATION THRESHOLD OF THE 2s AND 2p STATES

In this case the eigenvalues of the matrix $l(l+1) + \alpha$ corresponding to the new channels are (cf. [4])

[3)]Because of condition (21′) the number of oscillations in the cross sections is finite, since (24) is not applicable when $|E - E_t| \sim (L+1)\Delta\varepsilon$ and smaller.

$$a_0 = L(L+1),\ a_\pm = L(L+1) + 1 \pm \sqrt{(2L+1)^2 + 36}. \quad (25)$$

If $L = 0$, there is no value a_0. For $L \leq 2$, $a_- < -1/4$. Therefore, all partial cross sections Q^L with $L \leq 2$ near the threshold oscillate. For $L \geq 3$ all a are positive, $\lambda_{min} > 1/2$. The cross sections $Q^L(1s-2s)$ and $Q^L(1s-2p)$ near the threshold tend to zero following the law (23). The elastic scattering cross section $Q^L(1s-1s)$ has no discontinuities of the peak or step type at the threshold.

When $L \leq 2$ the cross sections for transitions between the degenerate states 2s and 2p oscillate near the threshold. For $L \geq 3$ they tend to

$$Q_0^L(i-f) = \frac{\pi}{k'^2}\frac{2L+1}{2l'_i+1}|T_{fi}^{(0)}|^2, \quad (26)$$

where

$$T^{(0)} = 1 - e^{i\pi l/2}Ae^{-i\pi\lambda}A^{-1}e^{i\pi l/2}$$

is independent of the energy. Utilizing (25) and the explicit expressions for the matrix A, we find that for $L \gg 1$

$$Q_0^L(2s-2p) = 72\frac{\pi}{k'^2}\left[\frac{1}{L} + O\left(\frac{1}{L^2}\right)\right],$$

$$Q_0^L(2s-2s) = 648\frac{\pi}{k'^2}\left[\frac{1}{L^3} + O\left(\frac{1}{L^4}\right)\right]. \quad (27)$$

Summing Q^L over L, we obtain the total cross sections

$$Q(i-f) = \frac{\pi}{k'^2}\Omega(i-f). \quad (28)$$

Making use of (28) and (21′) for $\Omega(2s-2p)$ for $k'^2/\Delta\epsilon \gg 1$, we obtain Seaton's formula[10]

$$\Omega(2s-2p) = 72\left[\ln\frac{4k'^2}{\Delta\varepsilon} - \mu\right]. \quad (29)$$

When $k'^2/\Delta\epsilon \gg 1$, the values of $\Omega(2s-2s)$ and μ near the threshold are almost constant, since the sum Q_0^L with $L \geq 3$ is considerably larger than the oscillating Q^L with $L \leq 2$. With increasing principal quantum number n, the matrix elements of the dipole moment connecting the new channels increase, and the number of angular momenta L for which the cross sections Q^L oscillate increases. For $n = 3$ the cross sections oscillate when $L \leq 4$.

[1] M. H. Ross and G. L. Shaw, Ann. Phys. **13**, 147 (1961).

[2] R. Damburg and R. Peterkop, Proc. Phys. Soc. 80, 1073 (1962); JETP **43**, 1765 (1963), Soviet Phys. JETP **16**, 1247 (1963).

[3] I. C. Percival and M. J. Seaton, Proc. Camb. Phil. Soc. **53**, 654 (1957).

[4] M. J. Seaton, Proc. Phys. Soc. **77**, 174 (1961).

[5] A. M. Lane and R. G. Thomas, Rev. Modern Phys. **30**, 257 (1958).

[6] A. I. Baz', JETP **33**, 923 (1957), Soviet Phys. JETP **6**, 709 (1958).

[7] L. D. Landau and E. M. Lifshitz, Quantum Mechanics, Pergamon, 1958.

[8] A. I. Baz', JETP **36**, 1762 (1959), Soviet Phys. JETP **9**, 1256 (1959).

[9] N. Levenson, Kgl. Danske Videnskab Selskab. Mat.-fys. Medd. **25**, No. 9 (1949).

[10] M. J. Seaton, Proc. Phys. Soc. **A68**, 457 (1955); V. M. Burke and M. J. Seaton, Proc. Phys. Soc. **77**, 199 (1961).

[11] E. P. Wigner, Phys. Rev. **73**, 1002 (1948).

Translated by Z. Barnea
263