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RESONANCES IN THE SCATTERING OF ELECTRONS ON HYDROGEN ATOMS

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The behavior of the cross section for elastic scattering of electrons on hydrogen atoms near the threshold of the 2s excitation level is investigated. The calculations are performed by taking into account strong coupling between the 1s and 2s levels for the incident s and p waves. Narrow resonances in the cross sections have been found below the threshold for the s wave in the singlet state and the p wave in the triplet state.

SMITH, McEachran, and Frazer[1] found a sharp maximum in the elastic scattering cross section of electrons on hydrogen atoms close to the excitation threshold of the 2s level. These authors calculated the cross section by numerical integration of a system of integro-differential equations, taking into account two channels: elastic scattering and the virtual excitation of the 2s level. The authors stated that the obtained maximum may be a Wigner threshold peak.

Ross and Shaw[2,3] showed that it is convenient to investigate the behavior of the cross sections near a new channel with the aid of the matrix M, related to the reaction matrix K by the relation

$$M_{ij} = k_i^{l_i+1/2} (K^{-1})_{ij} k_j^{l_j+1/2}, \qquad (1)$$

where k_i is the momentum, and l_i —the angular momentum of the i-th channel. In the case of a single channel $M = k^{2l+1} \cot \delta$, where δ is the phase shift. Close to the threshold of a new channel, where the cross sections can undergo considerable changes, the elements of the matrix M are smoothly varying functions of the energy.

In the case of two channels with angular momenta $l_1 = l_2 = l$ we have for the elastic scattering in the "old" channel

$$\sigma_l = \frac{4\pi(2l+1)}{k_1^2 + \gamma_l^2}, \qquad k_1^2 \leqslant 2E_0; \qquad (2)$$

$$\gamma_l = \frac{1}{k_1^{2l}} \left(M_{11} - \frac{M_{12}^2}{M_{22} + (-1)^l |k_2|^{2l+1}} \right), \qquad k_2^2 = k_1^2 - 2E_0; \qquad (3)$$

$$\sigma_l = \frac{4\pi(2l+1)(M_{22}^2 + k_2^{4l+2})}{|(M_{11} - ik_1)(M_{22} - ik_2) - M_{12}^2|^2}, \qquad k_1^2 \geqslant 2E_0. \qquad (4)$$

The energy corresponding to the excitation threshold of the 2s level is $E_0 = 0.275$ (in the atomic system of units).

In the effective-radius (ER) approximation account is taken of the first two terms of the expansion of M_{ij} in powers of the energy:

$$M_{ij}(E) = M_{ij}(E_0) + R_{ij}(E_0)(E - E_0). \qquad (5)$$

By integrating with the aid of a BÉSM-2 computer the system of integro-differential equations, taking into account the strong 1s—2s coupling, we have in this paper obtained the functions $M_{ij}(E)$ for $E > E_0$. The equations were solved by a method analogous to that of Marriott,[4] but use was made of different integration formulas. Method XI from Milne's book[5] was used. Close to the threshold ($k_2^2 \leq 0.001$) the values of M_{ij}, which were used to determine $M_{ij}(E_0)$ and the effective radii $R_{ij}(E_0)$, turned out to be practically linear functions of the energy. The values of $M_{ij}(E_0)$ and $R_{ij}(E_0)$ for the singlet (+) and triplet (−) cases, and for the case of no exchange (0) are listed in the table. As is seen from the table, the assump-

State	l	M_{11}	M_{12}	M_{22}	R_{11}	R_{12}	R_{22}
+	0	1.1300	−0.0629	−0.0356	4.82	−4.32	11.54
−	0	0.0301	−0.0017	−0.1206	1.20	−0.06	5.14
0	0	0.9373	−0.3097	0.2042	7.64	−10.68	19.2
+	1	−5.8759	0.00517	−0.00932	−32.56	0.58	−0.69
−	1	1.6653	0.01803	−0.00072	6.0	0.556	−0.354

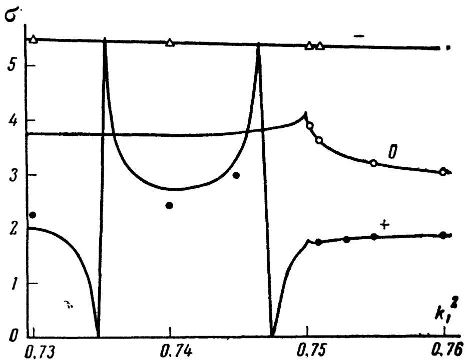

FIG. 1. Elastic scattering cross sections of the s wave in the singlet (+), triplet (-) cases, and in the case without exchange (0) (in units of πa_0^2). Curves – effective-radius approximation; points – exact calculation.

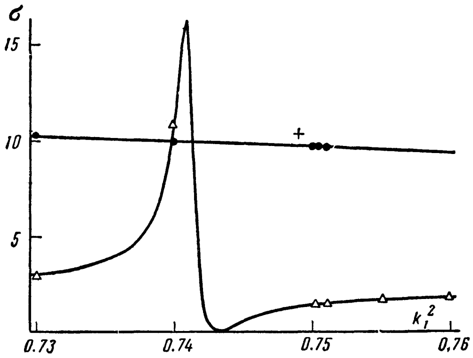

FIG. 2. Elastic scattering cross sections of the p wave (in units of πa_0^2). Curve (+) – singlet cross section in the effective-radius approximation, multiplied by a factor of 50. Curve (–) – triplet cross section, calculated by taking into account three terms of the expansion. Points – exact calculation.

tion of Shaw and Ross [2] that the nondiagonal radii are considerably smaller than the diagonal radii is not fulfilled in all cases.

In Fig. 1 the s cross section in the ER approximation is compared with the exact values obtained below the threshold by Smith, McEachran, and Frazer, [1] and above the threshold in this paper. Two narrow resonances are seen in the singlet case. The analysis carried out by Ross and Shaw [2] shows that the resonance nearer to the threshold, appearing between the limits $R_{22}^{-2} < k_2^2 < 0$, is real. The vanishing of the elastic cross section in this case corresponds to a pole of the S matrix in the new channel (without account of the strong coupling).

The second resonance is, according to Ross and Shaw, [2] artificial. In the region where it occurs account must be taken of higher terms in the expansion of the M matrix; these terms we estimate to be extremely large (of the order of $10-10^3$). Account of the following two terms of the expansion leads to an insignificant shift of the resonance close to the threshold, and to almost complete agreement between the σ_0^+ cross section with the results obtained by Smith, McEachran, and Frazer [1] for k_1^2 equal to 0.745 and 0.74. At lower energies the use of the expansion becomes more difficult because of the necessity to take into account additional terms of the series.

In the triplet case the ER approximation is applicable in a large region. In the interval $0.25 \le k_1^2 \le 1.44$ the cross section σ_0^- in the ER approximation differs from the exact values by no more than 0.6 percent. The threshold effect is determined by the sign of γ_0 at the threshold. This quantity is in all cases positive, thus indicating a peak. In the triplet case, the peak is unnoticeable on the scale used in the figure.

Figure 2 shows the p cross sections. The cross section σ_1^+ is calculated in the ER approximation. In calculating σ_1^- three terms of the expansion were included. The coefficients of $(E - E_0)^2$ were found from the results obtained above the threshold for $k_2^2 \le 0.02$. They are 16.0, 5.2, and 6.0 for M_{11}, M_{12}, and M_{22} respectively. The contribution from the third term is small, but it is precisely this contribution which leads to the appearance of a sharp resonance (this is particularly true for M_{22}).

Thus, the use of the M matrix makes it possible to join the cross section above and below threshold. We note that the maxima observed by Smith, McEachran, and Frazer [1] are below the threshold. The resonances are seen to be very narrow, and their experimental confirmation is therefore difficult. Some indications of a maximum close to the threshold were observed by Brackmann, Fite, and Neynaber. [6] It must be noted that for complete comparison with experiment allowance for the effect of the coupling with the 2p state is essential.

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