SLOW COLLISIONS IN A SYSTEM OF THREE BODIES INTERACTING ACCORDING TO COULOMB'S LAW. II. SYMMETRIC CHARGE EXCHANGE

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Submitted May 20, 1969

Zh. Eksp. Teor. Fiz. 57, 2084–2094 (December, 1969)

The scattering phase shifts and cross sections for the process of symmetric charge exchange $p + H(1s) \to H(1s) + p$ are determined by the perturbed stationary states method for collision energies between 10^{-5} and 5 eV. The phase shifts are determined on the basis of the phase function method, which yields the values with a prescribed accuracy. For a specific physical problem, the results obtained permit us to derive some general regularities in the behavior of the partial phase shifts and cross sections, to elucidate the limits of applicability of the Born approximation for calculation of these quantities, and also to illustrate the features of transition from low collision energies to high collision energies. In the antisymmetric $2p\sigma$ state of the molecular hydrogen ion H_2^+, a weakly bound state with a binding energy $J \sim 4 \times 10^{-4}$ eV is found to exist for a large equilibrium distance between the nuclei, $R_0 \sim 12.55$ atomic units.

INTRODUCTION

THE problem of the scattering of a proton by a hydrogen atom

$$p + H(1s) \to H(1s) + p \qquad (1)$$

is the simplest example of scattering in a three body system interacting according to Coulomb's law. The reaction (1) has intrinsic interest, but in addition, the features of more general problems of a similar type can be traced through this example.

In the calculation of the cross sections for the process (1), the method of partial waves is the most systematic;[2-4] it is especially good for low-energy collisions, when the number of waves that make a contribution to the cross section is comparatively small. Within the framework of this approximation, the partial amplitudes and phases can be calculated classically by the formulas[5,6], or, if the phases are small one may use the Born approximation.[7] In much earlier researches, the method of the impact parameter was also used.[2,8] Under natural limitations, both methods give a reasonable approximation without, however, defining its limits.

For slow collisions, the most systematic realization of the partial wave method is the method of perturbed stationary states (PSS),[2,3] the correct application of which to processes of type (1) became possible after the exact solution of the problem of two centers.[9-12] In the present work, within the framework of the PSS method, the phases and cross sections are calculated for the reaction (1) without any further approximations. The phase function method, developed comparatively recently, has been used in the calculations. This method is being developed intensively and two monographs have already been devoted to it;[13,14] however, it has been applied only comparatively rarely in practical calculations.

METHOD OF PERTURBED STATIONARY STATES

In the problem of three bodies interacting according to Coulomb's law, the variables in the Schrödinger equation are completely separated in the Jacobian coordinates,[1,15] which makes it possible to separate the motion of the center of inertia of the system as a whole, the relative motion of nuclei with masses M_1 and M_2 (the vector $\mathbf{R}$) and motion of the third particle M_3 (the electron) relative to the center of mass of the nuclei M_1 and M_2 (the vector $\mathbf{r}$). After separation of the motion of the center of inertia in the PSS method, the wave function

$$\Psi(\mathrm{R}, \mathbf{r}) = \sum_{\{n\}} \chi_n(\mathrm{R})\varphi_n(R, \mathbf{r}) \qquad (2)$$

in expanded in the complete set $\{n\}$ of eigenfunctions $\varphi_n(R; \mathbf{r})$ of the problem of two centers, i.e., the problem of the motion of a particle M_3 in the field of two fixed nuclei M_1 and M_2, separated by a distance R. In the case of symmetric charge exchange for low-energy collisions, the resonance character of the process makes it possible to limit ourselves to the two-level approximation, i.e., to keep in the sum (2) only the two lowest states of the system of H_2^+: $1s\sigma$ (even) and $2p\sigma$ (odd).[16]

Under these assumptions, the cross section of process (1) is computed by the formula[3,4]

$$\sigma_{ex}(k) = \sum_{l=0}^{\infty} \sigma_l(k) = \frac{\pi}{k^2} \sum_l (2l+1)\sin^2(\delta_g^l - \delta_u^l), \qquad (3)$$

where $\sigma_l(k)$ is the partial cross section of the resonant charge exchange, and δ_g^l and δ_u^l are the partial phases of scattering, which are determined from the equation

$$\frac{d^2}{dR^2}\chi_{g,u}^l(R) + [k^2 - V_{g,u}^l(R)]\chi_{g,u}^l(R) = 0. \qquad (4)$$

Here

$$k^2 = 2ME,$$

$$V^l_{g,u}(R) = 2M[W_{g,u}(R) - W_{g,u}(\infty)] + [K_{g,u}(R) - K_{g,u}(\infty)] + \frac{l(l+1)}{R^2},$$

$$M = \frac{M_0}{m}, \quad \frac{1}{M_0} = \frac{1}{M_1} + \frac{1}{M_2}, \quad \frac{1}{m} = \frac{1}{M_3} + \frac{1}{M_1 + M_2}, \tag{5a}$$

$W_g(R)$ and $W_u(R)$ are the even and odd terms, respectively of the two-center problem in the set of units $\hbar = e = m = 1$, and

$$K_{g,u}(R) = \int d\mathbf{r}\, \varphi_{g,u}(R; \mathbf{r})(-\Delta_R)\varphi_{g,u}(R; \mathbf{r})$$

are the diagonal matrix elements of the operator of nuclear motion over wave functions of the two-center problem.[10,12]

The asymptote of the potentials $V(R)$ is the following:

as $R \to 0$

$$V_g{}^l(R) = \frac{2M}{R} + \frac{l(l+1)}{R^2}, \tag{5b}$$

$$V_u{}^l(R) = \frac{2M}{R} + \frac{2 + l(l+1)}{R^2}; \tag{5c}$$

as $R \to \infty$

$$V^l_{g,u}(R) = \frac{l(l+1)}{R^2} - \frac{9M}{2R^4}.$$

METHOD OF CALCULATION

In the computation of the partial phase shifts $\delta^l_{g,u}$ the phase function method is used,[13,14] which makes it possible to reduce the linear equation of second order (4) for the wave function $\chi(R)$ to a nonlinear equation of first order for the phase function $\delta(R)$:

$$\frac{d}{dR}\delta^l_{g,u}(R) = -\frac{1}{k} V^l_{g,u}(R)\sin^2[kR + \delta^l_{g,u}(R)] \tag{6}$$

with the initial conditions as $R \to 0$ that are obtained from Eq. (6) with account of the asymptote of the potentials (5b):

$$\delta_g{}^l(R) = kR(a + bR),$$

$$a = -\frac{(2S+1) + \sqrt{4S-1}}{2S}, \quad b = -\frac{M(1+a^2)}{1 + (1+a)S}, \tag{7}$$

$$S = l(l+1).$$

For δ^l_u one must make the substitution

$$S = l(l+1) \to S = 2 + l(l+1)$$

in the expansion of (7). The desired scattering phases $\delta^l_{g,u}$ are determined from the relation

$$\delta^l_{g,u} = \delta^l_{g,u}(\infty) + \pi l/2. \tag{8}$$

Equation (6) was integrated in the energy range $R = 10^{-5}$–5 eV; the features of the calculation are discussed in Appendix I.

DISCUSSION OF RESULTS

1. Figures 1 and 2 show the scattering phases δ^l_g and δ^l_u for different collision energies. These are smooth functions, similar to what are discussed in[3,17]. For low-energy collisions ($E \leq 0.1$ eV), the phase $\delta^l_g = \delta_g(l)$ becomes a discontinuous function of the orbital momentum l: from its initial value $\delta^0_g \approx 18\pi$[1] with increase in l it decreases to zero in jumps, equal to $k\pi$, where $k = 0$ and 1.

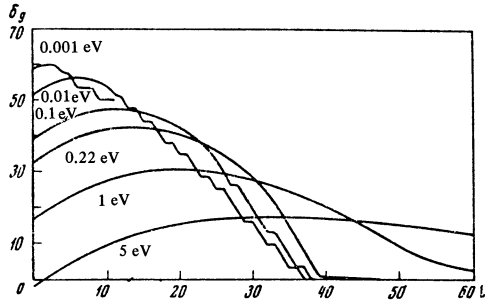

FIG. 1. Scattering phases $\delta_g{}^l(k) = \delta_g(l)$ in the even channel as functions of the orbital momentum l for different collision energies E. For $E \leq 0.1$ eV, the function $\delta_g(l)$ becomes a step function.

It is easy to understand the reason for such a behavior of $\delta_g(l)$ if we use the asymptotic expansions of the scattering phases δl for the potential[3,7]

$$V(R) = \frac{l(l+1)}{R^2} - \frac{\alpha}{R^4}.$$

For $l = 0$ (a = scattering length)

$$k\,\mathrm{ctg}\,\delta_0 = -\frac{1}{a} + \frac{\pi\alpha}{3a^2}k + \frac{2\alpha}{3a}k^2 \ln\frac{\alpha k^2}{16}, \tag{9a}$$

and for $l \neq 0$

$$k^2\,\mathrm{ctg}\,\delta_l = \frac{(2l+3)(2l+1)(2l-1)}{\pi\alpha}. \tag{9b}$$

It follows from (9b) that as $k \to 0$, the phase $\delta_g(l)$ can only take on values that are multiples of π. On the other hand, as $l \to \infty$, according to the general rule, $\delta_g(l) \to 0$. These requirements can be compatible only if, beginning with some $l = L$ (which is determined by the region of applicability of Eq. (9b)), the phase $\delta_g(l)$ decreases by jumps that are multiples of π.

This tendency is noted even more sharply in the plot of $\Delta l = \delta_g(l) - \delta_u(l)$, inasmuch as the phase shifts Δl in the zeroth approximation correspond to scattering by an exponentially decreasing potential. The results of the calculations for $E = 10^{-3}$ are shown in Table I.

2. The graphs of $\delta_u(l)$ for different k show characteristic features of another type, which are determined by the form of the potential $V_u(R)$. The antisymmetric term $V_u(R)$ has a repulsive character almost everywhere, with the exception of a weak minimum for $R_0 = 12.55$ of depth $D = 6.079 \times 10^{-5}$ a.u. $= 1.65 \times 10^{-3}$ eV. In accord with this, the phases $\delta_u(l)$ are negative[2] for small l, but in the region of large l they have a weak positive maximum. For a decrease in k, this maximum increases and shifts into the region of small l. For $E = 10^{-5}$ eV we have $\delta^0_u = 3.748$. According to the Levinson theorem, this means that in the antisymmetric state $2p\sigma$ of molecular hydrogen ion H_2^+ there exists a

[1] For $l = 0$ and $k = 0$, by Levinson's theorem,[13,14] $\delta_g = n\pi$, where n is the number of bound states of the electron in the potential V_g. For the symmetric term of the system H_2^+, the value of $n = 18$.

[2] The connection between the sign of the phase δ and the sign of the potential V is clearly seen from Eq. (6).

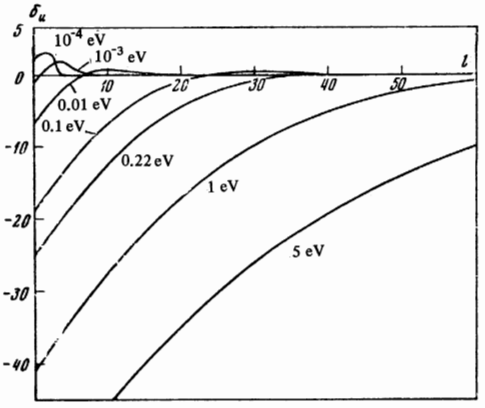

FIG. 2. Scattering phases $\delta_u{}^l(k) = \delta_u(l)$ in the odd channel. As $E \to 0$, $\delta_u{}^0(k) > \pi$, which indicates the existence of a metastable level in the odd potential $W_u(R)$ of the H_2^+ system.

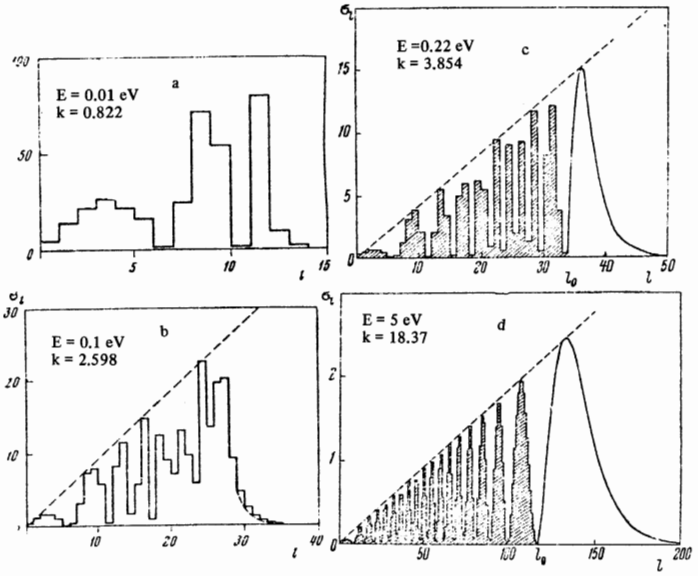

FIG. 3. Partial cross sections $\delta_l(k)$ as functions of the orbital momentum l for different collision energies E. For $E < 0.1$ eV, this is a stepwise function (a); for $E \geq 0.1$ eV, a characteristic smooth fall-off is noted b( ); for E = 0.22 eV, a region of smooth change of σ_l-(c); for E = 5 eV, this region is greatly expanded and simultaneously, the step-wise function for $l < l_0$ approximates a periodic function (d).

weakly bound state at large distances between the nuclei. This fact can be interesting chemically, and evidently has not previously been noted. In the approximation of the Morse potential, the binding energy J of this level is equal to[3)]

$$J = 1.5 \cdot 10^{-5} \text{ a.u.} = 4 \cdot 10^{-4} \text{ eV}. \quad (10)$$

3. Figure 3 shows graphs of the partial cross sections $\sigma_l(k)$ for different values of k. It follows from them that in the general case there exists two regions of l in which $\sigma_l(k)$ depends on l in essentially different fashion. For $l < l_0$, this is a stepwise function, having 18 maxima; for $l > l_0$, it is a smooth function, having a maximum and a characteristic fall off (Fig. 3, c-d). For $k < 3$, the second region appears (Fig. 3b) and for further decrease of k, the number of maxima of the stepwise function also decreases (Fig. 3a). In the limit $k \to 0$, a single partial wave $\sigma_0(k)$ is preserved and we obtain pure s-scattering.

Conversely, with increase im k, the contribution of the partial cross sections $\sigma_l(k)$ from the region $l > l_0$ also increases. Simultaneously, in the region $l < l_0$,

Table I

l	δ_g^l	δ_u^l	δ_B	Δ_l	σ_l
0	$18\pi + 1.132$	−0.721	—	$19\pi - 1.283$	42.9
1	$19\pi - 0.841$	0.519	—	$19\pi - 1.360$	134
2	$19\pi - 0.033$	1.413	—	$19\pi - 1.501$	232
3	$19\pi + 0.222$	$\pi - 1.228$	—	$18\pi + 1.450$	321
4	$19\pi + 0.011$	$\pi - 1.276$	—	$18\pi + 1.286$	389
5	$18\pi + 1.404$	1.077	—	$18\pi + 0.327$	52.6
6	$18\pi + 0.515$	0.513	—	$18\pi + 0.002$	0.002
7	$17\pi - 0.301$	0.297	—	$17\pi + 0.004$	0.009
8	$17\pi + 0.194$	0.194	—	$17\pi + 10^{-5}$	$\sim 10^{-6}$
9	$17\pi + 0.135$	0.135	—	$17\pi + 10^{-6}$	$\sim 10^{-8}$
10	$16\pi + 0.099$	0.099	0.095	$16\pi + 10^{-8}$	$\sim 10^{-8}$
11	$16\pi + 0.074$	0.074	0.072	$16\pi + 10^{-6}$	$\sim 10^{-8}$
12	$15\pi + 0.058$	0.058	0.056	$15\pi + 10^{-7}$	$\sim 10^{-11}$

Note: The Born phase δ_B is computed from Eq. (9b). The partial cross sections σ_l are given in natural area units $(\hbar/me^2)^2 = 0.28 \times 10^{-6}$ cm^2.

[3)]This level is metastable, inasmuch as the transition from it to the highly excited vibrational levels of the system H_2^+ in the ls σ state is made very difficult from the small overlap of the wave functions of the nuclear motion. It is of interest to make clear the role of this level in biological molecules for the structure of which long-range order is characteristic.

the jumps in the function $\sigma_l(k)$ become ordered and begin to approach a periodic function more strongly than in the histogram (Fig. 3d).

The graphs that have been shown permit us to follow smoothly the features of transition from low-energy collisions to high-energy ones. In particular, it follows from them that for $E > 5$ eV, the total cross section $\sigma(k)$ can be estimated in the following way:

$$\sigma(k) \approx \frac{\pi(l_0+1)^2}{2k^2} + \int_{l_0}^{\infty} \sigma_l \, dl, \quad (11)$$

i.e., by averaging over the region $0 \leq l \leq l_0$ and integrating over the range $l > l_0$. In previous works, it was done in this way,[5,6] and σ_l was computed by the WKB method.

For E =1 eV, both components in Eq. (11) give about the same contribution to the cross section $\sigma(k)$; however, for $E > 1$ eV, the contribution from the range $l > l_0$ begins to dominate.

4. Figure 4 shows the dependence of the total cross section $\sigma(k)$ on the energy of relative motion E. The divergence between our results and the typical values of Dalgarno and Yadav[6] is reasonable if we take into account the approximations made in their research (averaging for small l, the quasi-classical phase calculation, discarding of the matrix elements K_g and K_u).

The reason for the difference of the theoretical calculations from the experimental data[18] is discussed in[5].

We now consider the fact that the character of the dependence of $\sigma_{ex}(t)$ on the collision energy changes for E =0.1 eV. This effect is produced by a change in character of the function Δ_l: for $E < 0.1$ eV, it becomes stepwise and at the same time, the second region $l > l_0$ vanishes in the partial cross sections

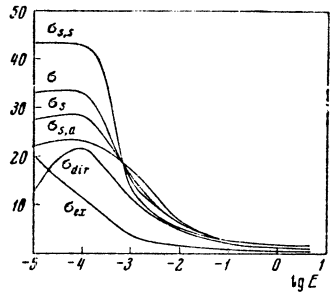

FIG. 4. Various types of cross sections for the process of symmetric charge exchange with account of proton statistics. For E > 0.1 eV, account of spin states of the particles does not affect the value of the total cross section.

$\sigma_l(k)$ (see Figs. 1 and 3b).

However, even for energy $E = 10^{-5}$ eV ($T \sim 0.1°K$) the region of pure s-scattering is still not reached, inasmuch as the four phases (l—0, 1, 2, 3) make contributions to the cross section at this energy. For E > 0.1 eV, the formula

$$\sigma_{ex}(k) \approx A + B \lg E, \tag{12}$$

is fulfilled satisfactorily; this has already been discussed in the literature.[8,19] We note that as $k \to 0$, Eq. (12) no longer holds, since it follows from the relation (9a) that $\sigma(k) \to$ const here.

5. The cross section of the charge exchange $\sigma_{ex}(k)$, the cross section of elastic scattering $\sigma_{dir}(k)$ and the total cross section $\sigma(k)$[4,5]

$$\sigma(k) = \sigma_{ex}(k) + \sigma_{dir}(k) = \\ = \frac{2\pi}{k^2} \sum_l (2l+1)(\sin^2\delta_g^l + \sin^2\delta_u^l) \tag{13}$$

completely determine the scattering process (1) without account of proton statistics.

For low-energy collisions, it is necessary to consider the spin states of the protons. In this connection, two total cross sections $\sigma_{s,s}(k)$ and $\sigma_{s,a}(k)$ appear for the singlet and triplet states of two protons[3,5]

$$\sigma_{s,s}(k) = \frac{4\pi}{k^2}\left\{\sum_{\text{even}}(2l+1)\sin^2\delta_g^l + \sum_{\text{odd}}(2l+1)\sin^2\delta_u^l\right\}, \tag{14a}$$

$$\sigma_{s,a}(k) = \frac{4\pi}{k^2}\left\{\sum_{\text{odd}}(2l+1)\sin^2\delta_g^l + \sum_{\text{even}}(2l+1)\sin^2\delta_u^l\right\}. \tag{14b}$$

Only the total cross section is measured experimentally:[3,5]

$$\sigma_s(k) = \frac{1}{4}\sigma_{s,s}(k) + \frac{3}{4}\sigma_{s,a}(k), \tag{15}$$

and is averaged over the initial and summed over the final spin states of the two protons. In practical applications, the transport cross section[3]

$$\sigma_t = 2\pi \int_0^\pi \sigma(\theta)(1-\cos\theta)\sin\theta\, d\theta \tag{16}$$

is also encountered, which, after expansion in partial waves and symmetrization, takes the form

$$\sigma_t(k) = \frac{4\pi}{k^2}\left\{\left(\frac{3}{4}\sum_{\text{even}} + \frac{1}{4}\sum_{\text{odd}}\right)(l+1)\sin^2(\delta_u^l - \delta_g^{l+1}) \right. \\ \left. + \left(\frac{3}{4}\sum_{\text{odd}} + \frac{1}{4}\sum_{\text{even}}\right)(l+1)\sin^2(\delta_g^l - \delta_u^{l+1})\right\}. \tag{17}$$

Table II

	σ_{ex}^D	σ_{ex}	σ_{dir}	σ	σ_s	$\sigma_{s,s}$	$\sigma_{s,a}$	σ_s^{dif}
10^{-5}	—	20,3	11	33	26	42	21	30
10^{-4}	—	11,4	22	34	29	44	24	17
10^{-3}	—	3,27	11	14	16	12	17	6,7
10^{-2}	—	0.933	4.5	5.4	5.7	4.9	5.9	2.0
0,1	0,60	0.622	1.7	2.3	2.2	2.5	2.1	1.2
0,22	—	0.518	1.6	2,1	2.2	1.9	2.3	0.99
1	0,47	0.454	1.2	1.6	1.6	1.6	1.6	0.89
5	—	0.372	0.87	1.2	1.2	1.2	1.2	0.74

Note: The cross sections are given in units of 10^{-14} cm^2, σ_{ex}^D are the values from [6].

Figure 4 shows some of these cross sections as a function of the collision energy and Table II gives the numerical values. It is seen from them that for energy of 1 eV, account of proton statistics does not change the total cross section.

CONCLUSION

In problems of similar type, two sources of error exist: in the choice of the initial approximation and in the calculation of the cross sections within the framework of the given approximation. In the present research, it has been possible to avoid errors of the second type, since, within the PSS method, the cross sections and the phases for process (1) are computed with the specified accuracy without any additional approximations. Therefore, the results can be used for the estimate of the errors of other, approximate methods of calculation of the phases and cross sections of the process of symmetric charge exchange.

The completed study is principally of methodological interest, since hydrogen is generally in the molecular rather than atomic state at low collision energies. However, this classical problem of scattering theory allows us to have a feeling for the general features of the process of scattering in three-body system interacting according to Coulomb's law.

The proof of the existence of a bound state of the system H_2^+ at large internuclear distances should be especially noted.

We take this occasion to express our thanks to V. V. Babikov for numerous consultations, and also to S. S. Gershteĭn for constant interest and for discussions, to T. M. Peck who kindly lent us the tables of terms.

APPENDIX I

In the practical calculation of phases from Eq. (6), specific difficulties arise which must be emphasized here.

One of these is that the phase functions $\delta_g^l(k)$ have a stepwise character in the presence of bound states as $k \to 0$.[13,14] This gives rise to considerable difficulties in the integration of the more natural phase equations, which use Bessel functions, and it is necessary to integrate Eq. (6) in place of them. For this equation, the limit of integration R_0 is shifted appreciably in the direction of large R. Finally, the phases $\delta_{g,u}^l$ were calculated from the formula

$$\delta_{g,u}^l = \delta_{g,u}^l(R_0) + \frac{\pi l}{2} + h^l(R_0), \tag{A.1}$$

where the correction

$$h'(R_0)=+\frac{1}{2kR_0}\left[l(l+1)+\frac{3M}{2R_0^2}\right]+\frac{1}{(2kR_0)^2}\left[l(l+1)+\frac{9M}{2R_0^2}\right]$$
$$\times\sin 2(kR_0+\delta^0)+\frac{2}{(2kR_0)^3}\left[l(l+1)-\frac{9M}{R^2}\right]\cos 2(kR_0+\delta_0), \quad (A.2)$$
$$\delta_0=\delta(R_0),$$

takes into account the contribution to the phase $\delta^l_{g,u}$ from the region $R_0 \le R < \infty$, and R_0 is determined from the condition of convergence of the expansion (A.2) ($kR_0 > 1$) for the additional condition

$$\delta'(R_0) \leqslant 10^{-2}. \quad (A.3)$$

These conditions guarantee the given accuracy $\epsilon \le 10^{-2}$ in the calculation of the separate phases $\delta^l_{g,u}$ and the accuracy $\epsilon \le 10^{-3}$ in the calculation of Δ_l.

In integration in the range $R \le 20$, the tables of Peck[11] were used for the terms $W_g(R)$ and $W_u(R)$ and the tables of Hunter et al.[16] for the matrix elements $K_g(R)$ and $K_u(R)$. In the range $R > 20$, we used the asymptote of the terms[21]

$$W_{g,u}(R)=E_0(R)\mp{}^1/_2\Delta E(R), \quad (A.4)$$
$$E_0(R)=-\frac{9}{4R^2}-\frac{15}{2R^6}-\frac{213}{4R^7}-\frac{7755}{64R^8}-\frac{1773}{2R^9}-\frac{86049}{16R^{10}}, \quad (A.5)$$
$$\Delta E(R)=\frac{4}{e}Re^{-R}\left[1+\frac{1}{2R}-\frac{25}{8R^2}-\frac{131}{48R^3}-\frac{3923}{384R^4}\right]. \quad (A.6)$$

As the collision energy E increases, it is necessary in the calculation of $\sigma(k)$ to sum over a large number of partial cross sections $\sigma_l(k)$ (see Fig. 3). Practically speaking, summation is carried out in Eq. (3) only over a finite number of partial cross sections:

$$\sigma(k)=\sum_{l=0}^{L}\sigma_l(k)+\Delta\sigma(k), \quad (A.7)$$

where L is determined from the condition

$$\delta_g{}^L=\delta_u{}^L\approx\delta_B{}^L\approx 0{,}1, \quad (A.8)$$

and the Born phase δ^L_B is given by Eq. (9b) (see Table I).

In the range $L \le l < \infty$, the asymptotic formula (b) for the scattering phase $\delta^l_{g,u}$ is already well satisfied and the contribution $\Delta\sigma(k)$ to the total cross section $\sigma(k)$ can be estimated analytically:

$$\Delta\sigma(k)=\int_L^\infty\sigma_l(k)\,dl\approx\frac{\pi^3\alpha^2k^2}{32L^4}, \quad (A.9)$$
$$\alpha=9M/2.$$

This contribution is negligibly small ($\sim 10^{-3}$ of the total cross section $\sigma(k)$). For collision energies $E > 10^{-4}$ eV, the value of L can be estimated from the formula

$$L\approx{}^3/_2l_0\approx 30\,k^{3/5}. \quad (A.10)$$

The given estimates determine the accuracy of the results within the framework of the PSS method in the two-level approximation. This approximation is reasonable for small collision energies, although the distances between the protons of the H_2^+ system is large in comparison with the energy of the emitted proton. However, the exact limits of the method are currently unknown, although certain estimates exist for them.[6]

APPENDIX II

In some cases, in the calculation of the phases σ_l from Eq. (4), the regions of applicability of the quasiclassical and Born approximation overlap. This can be shown directly by comparing the two expressions:

$$\delta_{KB}{}^l=\int_{r_0}^\infty\left[k^2-\frac{(l+1/2)^2}{r^2}-U(r)\right]^{1/2}dr-\int_{r_0}^\infty\left[k^2-\frac{(l+1/2)^2}{r^2}\right]^{1/2}dr, \quad (A.11)$$

$$\delta_B{}^l=-\frac{\pi}{2k}\int_0^\infty U(r)[j_l(kr)]^2\,dr. \quad (A.12)$$

(Here $r_0=(l+1/2)/k$, $j_l(kr)=J_{l+1/2}(kr)$ is the spherical Bessel function of half-integral order.) For large l and small k, the turning point $r_0 \gg 1$, and in this region, the condition of applicability of the Born approximation $U(r) \ll k^2$ is satisfied for rapidly decaying potentials. Using this condition, and also the quasiclassical asymptote of the functions $j_l(kr)$ for large l[21]

$$J_{l+1/2}(kr)=\sqrt{\frac{2k}{\pi r}}\left[k^2-\frac{(l+1/2)^2}{r^2}\right]^{-1/4}\cos\left(\int_{r_0}^r\sqrt{k^2-\frac{(l+1/2)^2}{r^2}}\,dr-\frac{\pi}{4}\right), \quad (A.13)$$

in both cases we obtain the same formula

$$\delta_l\approx\frac{1}{2}\int_{r_0}^\infty U(r)\left[k^2-\frac{(l+1/2)^2}{r^2}\right]^{-1/2}dr. \quad (A.14)$$

In our specific case, $U(r)=-\alpha/r^4$. Calculating the integral, we obtain the relation

$$\delta_l=\pi\alpha k^2/8(l+1/2)^3, \quad (A.15)$$

which is practically the same as Eq. (9b).

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Translated by R. T. Beyer
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