Orbiting-type oscillations in the total charge exchange cross section for the p+H(1s)→(H1s)+p

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A detailed calculation is performed for the charge exchange between protons and hydrogen atoms in the energy range $10^{-2} \leq E \leq 0.7$ eV. Oscillations with an amplitude ~0.1 about the mean value of the cross section are observed in the total cross section. The oscillatory structure of the cross section is ascribed to orbiting near the tops of the centrifugal barriers of the effective potentials of the problem. A phase shift analysis of the charge-exchange cross section is carried out.

INTRODUCTION

A detailed calculation of the charge-exchange reaction of hydrogen atoms in the ground state with deuterons

$$H(1s)+d \rightarrow D(1s)+p \qquad (1)$$

at collision energies E < 0.5 eV has revealed oscillations in the total charge-exchange cross section[1]

It is established in the present paper that analogous oscillations appear in the total cross section of the symmetrical charge exchange

$$H(1s)+p \rightarrow p+H(1s) \qquad (2)$$

at collision energies $10^{-2} \leq E \leq 0.7$ eV. Their period turns out to be approximately constant in momentum scale, and the amplitude amounts in rough approximation to 10% of the averaged cross section. With increasing energy of the relative motion, the oscillations are attenuated (see Fig. 1a).

The general course of the charge-exchange cross section (2) in the collision energy interval $10^{-4} \leq E \leq 5$ eV was calculated by us earlier.[2] In the present paper, the formulation of the problem, the procedure, and the accuracy of the calculation of the scattering phase shifts remained the same as before.

The effective potentials that determine the scattering process (2) (see Fig. 2) have a form that is typical in many respects of atomic collisions: repulsion at short distances, minimum at finite R, and a long-range attraction "tail." The cross section for the scattering by such a potential has a complicated oscillatory structure, which is a consequence of the interference of oscillations of the following types:[3] orbiting, glory, and rainbow. The foregoing oscillations have the usual cause, namely, the presence of bound states in the scattering potential.

The cross section of the charge exchange (2) is determined by two potentials (see Fig. 2). As we shall see later on, their mutual influence leads to a vanishing of the glory phenomenon in the cross section of the charge exchange reaction, which greatly simplifies the analysis of the calculation results.

The oscillations observed in the total charge-exchange cross section (2), due to the quantum analog of the orbiting phenomenon, are well known from the classical theory of scattering.[4] In the interpretation of the results of the calculations, the noted classical analogy turns out to be quite meaningful and helps explain the main features of the behavior of the cross section,

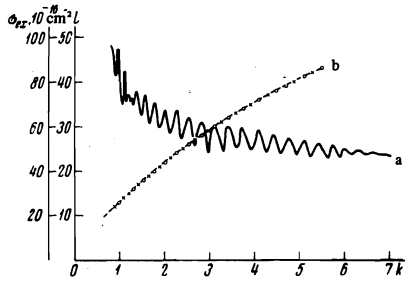

FIG. 1. a) Total cross section of the symmetrical charge exchange H(1s) + p → p + H(1s) as a function of the scattering momentum. The momenta are given in the units of the problem, the cross sections are given in units 10^{-16} cm^2, and E = 1.48 × 10^{-2}k^2 eV. b) Orbital angular momentum as a function of the orbiting momentum k$_l$ defined by the relation (10). The values k = k$_l$ correspond to the maxima (circles) and minima (crosses) of the cross section σ_{ex}(k). In the most interesting region, $1.5 \leqslant k \leqslant 4$, the points corresponding to the pairs of values (l_0, k$_l$) cluster about the straight line l = 7k + 8, which approximates well the curve b in the indicated region.

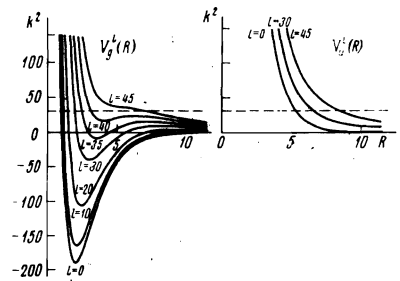

FIG. 2. Effective potentials $V^l_{g,u}(R) = 2MW_{g,u}(R) + l(l+1)/R^2$, describing the charge-exchange process (2). The ordinates are the values of k^2 in the units of the problem. The dashed line marks the boundary of the orbiting region. The weak minimum of the potential $V^0_u(\neq)$ is located at R = 12.55 [7].

namely the positions of the maxima and minima, the number and period of the oscillations, and also the collision-energy region in which they can be observed.

FUNDAMENTAL EQUATIONS

In the two-level approximation of the method of perturbed stationary states, the problem of calculating the charge-exchange cross section for the process (2) reduces to a solution of two one-dimensional radial Schrödinger equations (in units e = ħ = m = 1, 1/m = 1/m$_e$ + 1/2M$_p$)

$$\frac{d^2}{dR^2}\chi^l_{g,u}(R)+[k^2-V^l_{g,u}(R)]\chi^l_{g,u}(R)=0, \qquad (3)$$

where

$$V^{l}_{g,u}(R)=2M[W_{g,u}(R)-W_{g,u}(\infty)]+[K_{gg,uu}(R)-K_{gg,uu}(\infty)]+\frac{l(l+1)}{R^2},$$
$$k^2=2ME,\ M=M_p/2m, \quad (4)$$

m_e and M_p are respectively the masses of the electron and the proton, and E is the energy of the relative motion in c.m.s.

The terms $W_g(R)$ and $W_u(R)$ (the eigenvalues of the two-center problem) and the adiabatic corrections to the terms $K_{gg}(R)$ and $K_{uu}(R)$ (matrix elements of the kinetic-energy operator of the nuclei in terms of the wave functions of the two-center problem), together with the centrifugal potential $l(l+1)/R^2$, form two sets of effective potentials $V_g^l(R)$ and $V_u^l(R)$, which are represented in Figs. 2a and 2b. The scattering phase shifts $\delta_g^l(k)$ and $\delta_u^l(k)$, calculated from Eqs. (3), enable us to find the cross section for the charge exchange of the reaction (2):

$$\sigma_{ex}(k)=\frac{\pi}{k^2}\sum_{l=0}(2l+1)\sin^2\Delta^l(k), \quad (5)$$

where

$$\Delta^l(k)=\delta_g^l(k)-\delta_u^l(k). \quad (6)$$

CALCULATION RESULTS

Figures 3a–3c show the phase shifts $\delta_g(l)\equiv\delta_g^l(k)$, $\delta_u(l)\equiv\delta_u^l(k)$ and $\Delta(l)\equiv\Delta^l(k)$ as functions of the angular orbital momentum l at certain fixed values of E. We note the characteristic features of these functions, which determine the behavior of the cross section. First, the presence of maxima on the plots of the phase shifts $\delta_g(l)$ and $\delta_u(l)$ indicate that the total elastic-scattering cross section for the process (2)

$$\sigma=\frac{2\pi}{k^2}\sum_{l=0}(2l+1)(\sin^2\delta_g^l+\sin^2\delta_u^l) \quad (7)$$

will contain glory oscillations, which are ensured by phases satisfying the quasiclassical condition $\partial\delta_g(l)/\partial l=0$.[4-6] It is seen from Fig. 3c that the functions $\Delta(l)$ decrease monotonically, and consequently the glory phenomenon is missing from the charge exchange cross section (5).

The orbiting region is characterized by a strong dependence of the scattering phase shift on l.[3,4] It follows from Fig. 3 that this behavior of $\Delta(l)$ is determined completely by the phase shifts $\delta_g(l)$, and therefore the orbiting oscillations will be present both in the total cross section (7) and in the charge-exchange cross section (5), and their position depends only on the potential $V_g(R)$.

The family of the functions $\Delta^l(k)$ is shown in Fig. 4. With decreasing k, these functions tend to the values

$$\Delta^l(0)=\pi(n_g^l-n_u^l), \quad (8)$$

where n_g^l and n_u^l are equal respectively to the numbers of the bound states in the potentials $V_g^l(R)$ and $V_u^l(R)$. As is well known,[7] $n_g^0=20$ and $n_u^0=2$, and accordingly $\Delta^0(0)=18\pi$. It is quite remarkable that the approximate equality $\Delta^0(0)\approx 18\pi$ turns out to be true in a very wide range of values of k (Fig. 3c). As l increases, n_u^l vanishes and n_l becomes equal to $\Delta^l(0)/\pi=n_g^l$, i.e., it is equal to the number of levels in the potential $V_g^l(R)$. The number of bound states n_l decreases with increasing l and the last discrete level vanishes at $l=36$.

The abrupt jumps of the phase shifts $\Delta^l(k)$ at certain values of k offer evidence of the presence of quasistationary states in the potentials $V_g^l(R)$ (it is obvious that their energy cannot exceed the height of the centrifugal barrier). The number of quasistationary states n_l^* does not exceed three and the last of them vanishes at $l=42$ together with the vanishing of the minimum in the potential $V_g^l(R)$.

In the cross section $\sigma_{ex}(k)$ these quasistationary states become manifest as narrow resonances (they are not shown in Fig. 1a because of their large number). The positions of these resonances can be easily determined from Fig. 4, and the relative height can be calculated from the formula for the partial cross sections

$$\sigma_{ex}^l=\pi(2l+1)/k^2. \quad (9)$$

The width of the resonances decreases exponentially as the vertex of the centrifugal barrier of the potentials $V_g^l(R)$ is approached, and in the vicinity of the vertex of the barrier it becomes comparable with the distance between the levels. As follows from Fig. 4, in this region the phase shifts $\Delta^l(k)$ still vary rapidly enough to ensure a resonant behavior of the cross section, but slowly enough to make the width of the resonance appreciable.

The principal statement of this paper is that the oscillations in the cross section $\sigma_{ex}(k)$, represented in Fig. 1a, are accounted for by the singularities of the scattering process near the vertex of the centrifugal barriers of the potentials $V_g^l(R)$, and consequently by

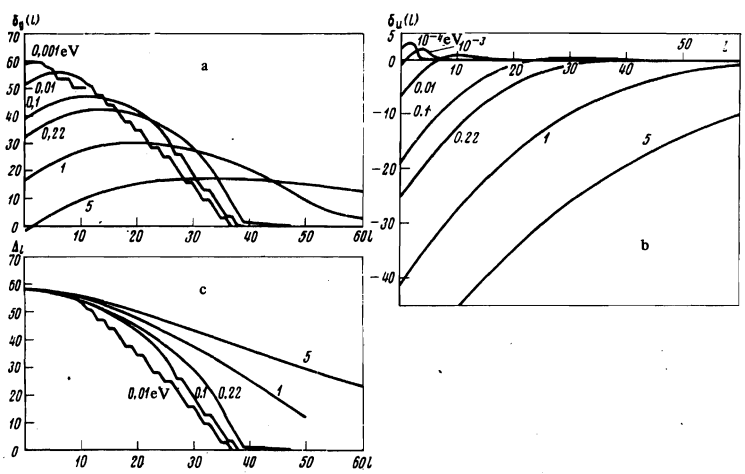

FIG. 3. Scattering phase shifts as functions of the orbital angular momentum at a fixed collision energy. a) The phase shifts $\delta_g(l)\equiv\delta_g^l(k)$. From the displacements of the maxima of the maxima of the curves we can determine the period of the glory oscillation in the elastic cross section (7), which ($\Delta k\sim 1$) turns out to be approximately three times larger than the period of the orbiting oscillations ($\Delta k\approx 0.3$). b) The phase shifts $\delta_u(l)\equiv\delta_u^l(k)$. In the region of the orbiting momenta ($1\leqslant k\leqslant 5$) and at a value of the orbital angular momenta corresponding to them (see Fig. 1b), the phase shifts $\delta_u^l(k)$ are small and are practically constant, so that they do not influence the structure of the orbiting oscillations. c) The functions $\Delta^l=\delta_g(l)-\delta_u(l)$ decrease monotonically with increasing l, and this explains the absence of glory oscillations in the charge-exchange cross sections (2).

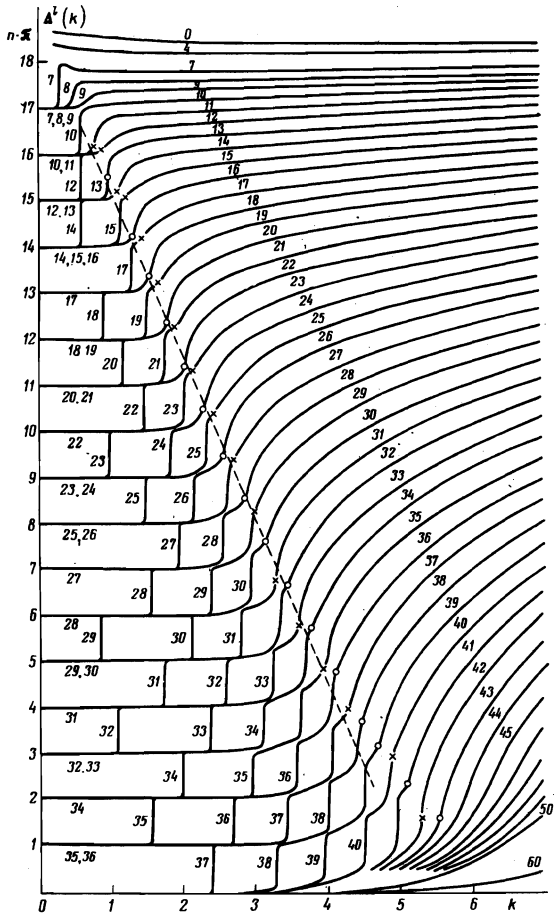

FIG. 4. The function $\Delta^l(k)$. As $k \to 0$ we have $\Delta^l(0) = \pi n_l$, where n_l is equal to the number of bound states in the effective potential $V_{ex}(R)$. The number of abrupt jumps at small k is equal to the number n^*_l of the quasistationary states ($n^*_l \leqslant 3$). When the highest stationary level falls in the orbiting region ($k \approx k_l$), the phase shifts $\Delta^l(k)$ take on values $\Delta^l_{max}(k_l) \approx \pi(n_l + n_l^* + \frac{1}{2})$ (these points are marked by circles). The crosses designate the values $\Delta^l_{min}(k_l) \approx \pi(n_l + n_l^*)$ at collision energies satisfying the orbiting condition (10), but not coinciding with the energy of the quasistationary state. The values of the phase shifts $\Delta^l(k_l)$ for $1 \leqslant k \leqslant 4$ and $10 \leqslant l \leqslant 36$ cluster about the straight line $\Delta^l(k_l) = 59.7 - 11k$, or, taking into account the relation between l_0 and k_l (Fig. 1b), $\Delta^l(k_l) \approx 23\pi - \pi l/2$. From the slope of the straight line $\Delta^l(k_l)$ we can estimate the period of the orbiting oscillations, namely $\Delta k \approx \pi/11 \approx 0.28$.

the singularities of the behavior of the scattering phase shifts in the corresponding region of collision energies (Fig. 4).

OSCILLATIONS IN THE TOTAL CHARGE EXCHANGE CROSS SECTION IN THE ORBITING PHENOMENON

The orbiting phenomenon in classical scattering by potentials $V^l_g(R)$ occurs at collision momenta satisfying the condition

$$k_l^2 = 2MV^l_g(R_l), \tag{10}$$

where the values of R_l correspond to the vertex of the centrifugal barrier and are determined by the equation

$$\frac{\partial}{\partial R} V^l_g(R_l) = 0. \tag{11}$$

The set of points obtained in this manner in the (l, k) plane lies on a smooth curve (Fig. 1b). It is easy to verify that the values of k_l practically coincide with the

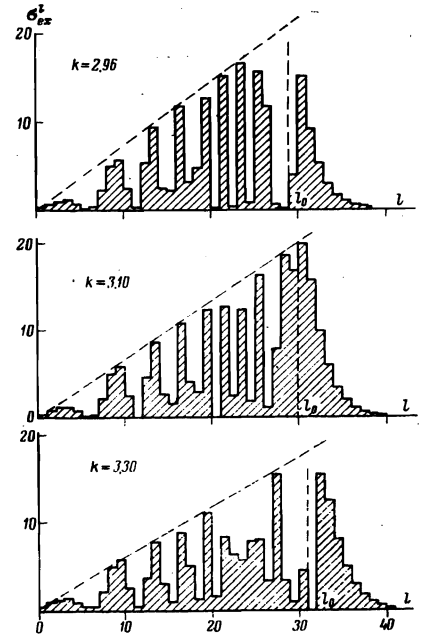

FIG. 5. Partial analysis of the total charge exchange cross section $\sigma_{ex}(k)$ at values k = 3.10 (maximum of the cross section), k = 2.96, and k = 3.30 (the two neighboring minima). The values l_0 determined from the orbiting condition (10) at these values of the energy are respectively 30, 29, and 31 (see also Fig. 1b). The character of the histograms on both sides of these values of l_0 is essentially different. The partial cross sections σ^l_{ex} in a small vicinity of the values of $l \lesssim l_0$ correspond to rainbow scattering.

positions of the maxima and minima in the charge-exchange cross section.

To each pair of values (l_0, k_l) on the plots of $\Delta^l(k)$ corresponds a point $\Delta^l(k_l)$, and the aggregate of the points clusters about a straight line (Fig. 4). At values of k_l corresponding to the orbiting condition (10), the quantities $\Delta^l(k_l)$ take on in succession, with successive increase of l, the values $\Delta^l_{max}(k_l) \approx \pi(n_l + n_l^* + 1/2)$ and $\Delta^l_{min}(k_l) \approx \pi(n_l + n_l^*)$. This means that at values k_l, corresponding to Δ^l_{max}, the quasistationary level is indeed in the vicinity of the vertex of the centrifugal barrier. Approximately similar resonance conditions repeat themselves with an interval $\Delta l = 2$ (see Fig. 4). With increasing l, the discrete levels of the initial potential well $V^0_g(R)$ become quasistationary levels of the potential $V^l_g(R)$, and with further increase of l they are crowded out into the continuous spectrum, bypassing the vicinity of the vertex of the centrifugal barrier. From this it follows, in particular, that the number of the orbiting oscillations approximately coincides with the number of discrete levels in the potential $V^0_g(R)$.

With decreasing collision energy ($k \leq 1$), the periodicity of the oscillations is violated and they gradually degenerate into narrow resonances. At $k \gtrsim 5$, when only above-the-barrier scattering is possible, the orbiting oscillations go over into rainbow scattering oscillations,[3] the amplitude of which decreases rapidly.

A partial analysis of the oscillations (see Fig. 5) shows that actually the vibrational structure of the cross section is ensured also at $k < 5$ by a superposition of the orbiting oscillations and the rainbow oscillations, so that a group of several waves takes part in the formation of the maximum (minimum) of the cross section.

As seen from Fig. 5, the value $l_0 = l(k_l)$ serves as a

boundary on both sides of which the structure of the partial cross sections $\sigma_{ex}^{l}(k)$ is quite different. At $l < l_0$, the set of quantities σ_{ex}^{l} forms a stepwise and rather irregular function of the orbital angular momentum l, and at $l > l_0$ there is formed a stable picture, which becomes more and more definite with increasing k.[2] The partial cross section σ_{ex}^{l} in a small vicinity of $l \lesssim l_0$ correspond to rainbow scattering.

CONCLUSION

The reaction (2) is a rather rare example of a real quantum scattering problem, which can be formulated and solved with the required accuracy. The collision-energy range $10^{-2} \leq E \leq 0.7$ eV, in which this reaction has been investigated in the present paper, is quite interesting for numerous applications, but the approximate calculation methods must be employed here with great caution. The results of the calculations presented in this paper will illustrate this statement, which incidentally is quite well known.[3,6] Of particular interest to us is the fact that even a simple analysis of the form of the potentials that enter in the Schrödinger equation makes it possible to explain rather subtle features of the structure of the quantum-mechanical scattering cross section.

A characteristic feature of the symmetrical charge-exchange reaction (2) is the possibility of expressing its cross section in the form (5). This means that $\sigma_{ex}(k)$ can be represented as a result of scattering by a certain "exchange" potential $V_{ex}(R)$, which generates a set of scattering phase shifts $\Delta^{l}(k)$. Certain properties of $V_{ex}(R)$ follow already from Fig. 3c. Thus, the monotonic character of the functions $\Delta^{l}(k)$ means that the potential $V_{ex}(R)$ is finite at $R \to 0$, and the weak dependence of $\Delta^{l}(k)$ on k at $l \to 0$ offers evidence that $V_{ex}(R)$ depends on the collision energy in a certain special manner. The latter circumstance imposes a rather definite limitation on the form of the exchange potential, for which it is customary in the impact-parameter approximation to assume the expression $V_{ex} = V_g(R) - V_u(R)$.[6,8,9]

The effect investigated, with symmetrical charge exchange (2) as a particular example, is sufficiently general and appears in more complicated charge-exchange reactions, for example in reaction (1). In these cases, however, its interpretation is not so lucid, for to describe the process (1) it is necessary to have already three sets of phase parameters instead of the single $\Delta^{l}(k)$ in the case of reaction (2).

The orbiting oscillations should arise always in low-energy scattering (for energies lower than the depth of the well and of the order of the height of the centrifugal barrier) by sufficiently powerful potentials, containing several bound states. With increasing collisions, the oscillations vanish, but when a new charge-exchange reaction channel is open, for example

$$H(nl)+p \to p+H(nl), \tag{2a}$$

they should appear again at collision energies somewhat higher than threshold. In this sense, the orbiting oscillations can be regarded as a threshold effect.

The vibrational structure of the cross section and its connection with the classical scattering problem was apparently first investigated by Vogt and Wannier[10] for the potential $V(R) = -\alpha/R^4$. Similar problems were considered also by Munn, Mason, and Smith,[3], who discussed in sufficient detail the accuracy and limits of applicability of the quasiclassical approximation in problems of this type.

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