DIFFERENTIAL CAPTURE PROBABILITY OF ELECTRON IN PROTON-HYDROGEN COLLISION AT LOW ENERGIES

GURUDAS CHATTERJEE AND N. C. SIL

DEPARTMENT OF THEORETICAL PHYSICS,

INDIAN ASSOCIATION FOR THE CULTIVATION OF SCIENCE,

JADAVPUR, CALCUTTA, INDIA.

ABSTRACT. Electron capture in proton-hydrogen collision at 3° scattering angle (laboratory system) has been investigated, using a two state approximation. The system of two protons and an electron forms a hydrogen-molecular-ion, with variable internuclear distance. In the present paper only the lowest symmetric and anti-symmetric states of H_2^+ are considered and the protons with their associated electron-cloud are scattered differently in these two cases. The two different scattering amplitudes are each associated with a time dependent phase which develops differently for the symmetric and anti-symmetric states. Finally the amplitudes in different phases interfere and determine the probability of capture. The numerical computation of capture probability in the present paper shows a very good agreement with experiment regarding the position of maxima and minima, in the energy range 1.1 to 0.45 Kev. Below 0.45 Kev the present result shows more rapid fluctuations, in capture probability which are however, not found in the experimental curve.

INTRODUCTION

The proton-hydrogen atom charge transfer problem has been largely investigated, both theoretically and experimentally in recent years. Previous theoretical studies, on the differential cross sections at fixed scattering angle, were made by Bates and McCarrol (1962) and Mukherjee and Sil (1962), using a 'two-state approximation' in impact parameter method. Theoretical calculations show a resonant variation of capture probability against the incident energy of the proton. The probability reaches the value one at the peeks and zero at the valleys. The experimental findings of Helbig and Everhart (1965) show a similar variation of capture probability with several peaks and valleys, but the probabilities neither reach the maximum value one, nor drop to zero. This deviation from theoretical result was found more prominent near the lower energies. Moreover there is a marked disagreement between those theoretical results and experimental findings in respect of the position of maxima and minima.

The discrepancies were thought of as due to the neglect of the coupling of the excited states. Accordingly calculations were done by Bates and Williams (1964) using a 'three state approximation''. Another theoretical result was put forward

by Basu, Sil and Bhattacharyya (1965), using a variational method and taking four atomic states $1S$, $2S$ around each proton. Both of these calculations show a decrease of the capture probability at the peak and increase of the same at the valley, thus in qualitative agreement with the experiment of Everhart.

Recently, F. J. Smith (1964) pointed out the failure of the impact parameter method at low energies and developed the wave treatment of the same problem. Taking into consideration only two states in his calculations, he finds a considerable decrease in the oscillation of capture probability at low energies. Further, after introducing a correction due to coupling with the excited state $2p\pi_u$ (from the calculations of Bates and Williams) in this two state calculations, he finds a good agreement regarding the position of resonances.

Another theoretical treatment, in connection with the scattering problem of $He^+ - He$ system, has been introduced by Marchi and Smith (1965). They have emphasized the need for the separate treatment for the motion of the two nuclei in two separate fields due to symmetric and antisymmetric states of ion-atom pair. In our problem we allow the two protons to move in their respective classical orbits under the potential due to symmetric and antisymmetric states of hydrogen molecular ion. In order that the protons may be scattered through a fixed angle, each of the two potentials gives rise to a separate set of impact parameter, distance of closest approach and the classical cross section of scattering. The square root of the classical cross section is assumed to be the scattering amplitude in the respective state. Each amplitude is associated with a certain phase which is determined by the time dependent motion of the electrons in the field of the two protons. In the calculation of the phase, the effect of motion of the protons in their actual trajectory (rather than the approximate assumption that protons move in straight paths) has also been considered. Finally, the two amplitudes with their appropriate phase interfere and exhibits capture phenomena at a particular angle.

Atomic units are used in all calculations of this paper.

THEORY

If Ψ is the wave function of a system composed of two protons A and B placed at the points R_A and R_B and an electron at r, then we can expand Φ in terms of molecular wave functions as

$$\Psi = \sum_i F_i(R)\psi_i(R, r),$$

where, $$R = |R| = |R_A - R_B|, \text{ and } \Psi_i(R, r)$$

is the molecular wave function with the nuclear separation distance R considered momentarily at rest.

The identity of A and B gives rise to two sets of wave functions, symmetric and antisymmetric, corresponding to the interchange of A and B in the hamiltonian.

For small velocities of the incident proton it is a reasonable approximation to take in the sum only two terms, viz., the lowest states in the symmetric and anti-symmetric distribution of electron cloud in hydrogen molecular ion.

Thus in this two state approximation Ψ is written as

$$\Psi = F_S(R)\psi_S(R, r) + F_a(R)\psi_a(R, r)$$

For large R, the molecular wave functions transform to the linear combinations of the ground state atomic wave functions $\psi_{A,B}(r)$ i.e. wave functions of the electron around the proton A or the proton B. The functions $F_{S,a}(R)$ take up the form $\exp (i\mathbf{k} \cdot \mathbf{R}) + f_{S,a}(\theta)\{\exp(ikR)\}/R$ for large R, so that the scattered wave is given by

$$\psi_{SC} = \frac{1}{\sqrt{2}} \frac{e^{ikR}}{R} \left[\{\psi_A(r) + \psi_B(r)\} f_S(\theta) e^{i\{\eta_S(t)\}}_{t-\infty} \right.$$

$$\left. + \{\psi_A(r) - \psi_B(r)\{ f_a(\theta) e^{i\{\eta_a(t)\}}_{t-\infty} \right] \qquad \ldots (1)$$

We assume that the amplitude $f_{S,a}(\theta)$ is the positive square root of the classical cross section $\sigma_{S,a}{}^{cl}(\theta)$ which is connected with impact parameter $b_{S,a}$ and scattering angle θ, by the relation,

$$\sigma_{S,a}{}^c (\theta) = b_{S,a} \left(\frac{db}{d\theta}\right)_{S,a} \operatorname{cosec}\theta.$$

It is to be noted that we have introduced in the asymptotic form of Ψ the phase factors $\exp[i \{\eta_{S,a}(t)]$ which determine the dissociation of molecular wave functions $\psi_{S,a}(R, r)$ to either $\psi_A(r)$ or $\psi_B(r)$ after infinite separation of the protons. The electron has been originally attached to the proton A before the collision starts and we may associate this initial condition to $[\eta_{S,a}(t)]_{t=-\infty} = 0$ (Time is measured from the instant when the two protons are close to each other). The phase factors have been obtained from the time dependent wave equation of the electron in the field of the two protons, (cf. Smith, F. T. 1965)

$$\eta_{S,a}(t) = \int_{-\infty}^{t} \epsilon_{S,a}[R(t)]dt \qquad \ldots (2)$$

where $\epsilon_{S,a}$ is the electronic energy in the ground state of symmetric and antisymmetric cloud of hydrogen molecular ion.

Collecting the coefficient of ψ_B from the equation (1) and squaring it, we get the capture cross section. This capture cross section divided by the sum of the cross sections of scattering and capture gives the capture probability,

$$P_C = \frac{1}{2} \left[1 - \frac{2\sqrt{\sigma_S{}^{cl} \cdot \sigma_a{}^{cl}}}{\sigma_S{}^{cl} + \sigma_a{}^{cl}} \cos \{\eta_S(\infty) - \eta_a(\infty)\} \right] \qquad \ldots (3)$$

CALCULATIONS AND RESULTS

We have from (2)

$$\eta_{S,a}(\infty) = \int^{\infty} \epsilon_{S,a}[R(t)]dt$$

$$= 2 \int_{(r_0)_{S,a}}^{\sim} \epsilon_{S,a}[R]\left(\frac{dt}{dR}\right)_{S,a} dR \qquad \dots \ (4)$$

$\left(\dfrac{dR}{dt}\right)_{S,a}$ are given by the well known classical relation,

$$\left(\frac{dR}{dt}\right)^{2}_{S,a} = v_0^2 \left[1 - \frac{2}{T}\left\{\epsilon_{S,a}(R) + \frac{1}{R} + 0.5\right\} - \frac{b_{S,a}^2}{R^2}\right]$$

and $(r_0)_{S,a}$ are the distances of closest approach, so that for $R = r_0$, $(dR/dt) = 0$. v_0^2 is the velocity and T the kinetic energy of the incident proton in laboratory system of coordinates.

The table of $\epsilon_{S,a}(R)$ at equal intervals of R has been calculated by H. Wind (1965), and $b_{S,a}$ have been plotted against energy by F. J. Smith (1965).

The integrand in (4) has a singularity at the lower limit. The behaviour of the integrand near the lower limit is like that of $x^{-\frac{1}{2}}$ near the origin. We have employed a method, as given in the book 'Methods of Mathematical Physics' by Jeffreys and Jeffreys (1962) for the evaluation of the integral near the lower limit. The integration in the rest of the range is done by Simpson's method. Next we substitute the value of $[\eta_S(\infty) - \eta_a(\infty)]$ in (3). We also substitute the values of $\sigma_{S,a}{}^c$ from the work of F. J. Smith. This gives the expression for P_c.

The capture probability calculated in this paper is presented in fig. 1 in solid line. The experimental curve of Everhart and the curve giving the results of the theoretical calculations in two state approximation by F. J. Smith are also shown for comparison.

It is seen that regarding the positions of maxima and minima, good agreement with experiment is obtained in the range 0.45 to 1.1 Kev. Below 0.45 Kev, the calculated capture probability shows more frequent oscillations which have not been observed in the experiment of Everhart *et al.*, The more frequent oscillation of capture probability in our results in the energy range 0.45 to 0.1 Kev is due to the rapid variation of the phase difference $[\eta_S(\infty) - \eta(\infty)]$. This tendency of more rapid oscillations with decreasing energy is also found in the theoretical results of Bates and Williams (1964), down to 0.25 Kev.
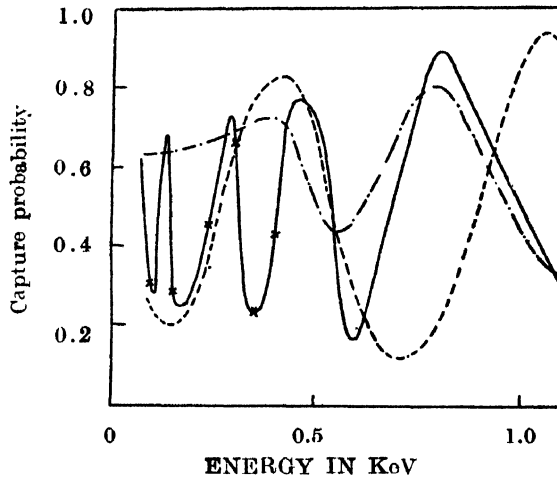
Fig. 1. Capture probability against the incident energy of the proton (in Lab. system).
— — — — — theoretical curve of F.J. Smith (1964) by two-state-calculations. His three state calculation with the inclusion of $2p\pi u$ shows better agreement with experiment.

—·—·—·— experimental curve of Helbig and Everhart. (1965) States

— — —·— —— theoretical curve by the present authors, with actual points of calculation indicated only below 0.5 kev energy to show extrapolation particularly at 0.12 Kev energy.

Above 1.1 Kev our theoretical curve begins to be out of phase with the corresponding experimental curve, this may be due to the neglect of the higher excited states of H_2^+. F. J. Smith finds an encouraging agreement with experiment by considering the correction in capture probability due to the $2p\pi_u$ state. The work to incorporate the same effect in our method is in progress.

ACKNOWLEDGMENTS

REFERENCES

Bates, D. R., and McCarrol, R., 1958, *Proc. Roy. Soc. (London)*, A **245**, 175,.

Bates, D. R. and Williams, D. A., 1964, *Proc. Phys. Soc., (London)*, **83**, 425,.

Basu, D., Sil, N. C. and Bhattacharya, D. M., 1966, *Phys. Rev.* **144**, 1, 56.

Helbig, H. F., and Everhart, E., 1965, *Phys. Rev.* **140**, 715.

Jeffreys and Jeffreys, 1962, *Methods of Mathematical Phys.*, Third Edition, 289.

Mukherjee, S. C., and Sil, N. C., 1962, *Indian J. Phys.*, **36**, 622.

Marchi, R. P. and Smith, F. T., 1965, *Phy. Rev.*, **139**. 1025.

Smith, F. J., 1964, *Proc. Phys. Soc.*, **84**, 889.

Wind, H., 1965, *J. Chem. Phys.*, **42**, 2371.

— — — —, 1965, *Thesis on "Electric Field Dissociation of* H_2^+*"*. (private communication by the courtesy of Dr. Wind.).