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Excitation of Atomic Hydrogen by Protons

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ABSTRACT

S - state excitation cross sections for proton-hydrogen atom collisions are calculated by a non-adiabatic method.

In this letter we consider excitation of hydrogen atoms according to reactions of the type.

$$p + H(1s) \rightarrow p + H(ns) \tag{1}$$

using a generalization of the nonadiabatic theory of Temkin (1). Let $\underline{r}$ and $\underline{R}$ be the position vectors of the electron and incident proton relative to the (stationary) target proton. Above a few keV we may safely apply the impact parameter method which allows us to take $\underline{R} = \underline{\rho} + \underline{v}t$ where $\underline{v}$ is the velocity of the incident proton and t is the time chosen such that at t = o the protons have a minimum separation, $\underline{\rho}$. The electronic wave function $\Psi(\underline{r},t)$ satisfies the time-dependent Schroedinger equation (in atomic units)

$$\left\{\frac{1}{2}\nabla^2 + i\frac{\partial}{\partial t} + \frac{1}{r} + \frac{1}{|\underline{r}-\underline{R}|} - \frac{1}{R}\right\}\Psi(\underline{r},t) = 0 \tag{2}$$

We have retained the interproton potential so that at large separations the perturbation tends rapidly to zero.

Since we are here interested only in the excitation of s-states it is natural to approximate Ψ by

$$\Psi \simeq \frac{1}{r}\Phi(r,t) = \frac{1}{r}\left(\sum_n + \int dk\right)\alpha_n(t)R_{ns}(r)\exp(-i\epsilon_n t) \tag{3}$$

where $\frac{1}{r}R_{ns}(r)$ is the normalised hydrogenic s-state with principal quantum number n and binding energy ϵ_n. Substituting (3) in (2) and integrating over the angular variables gives

$$\left\{\frac{1}{2}\frac{\partial^2}{\partial r^2} + i\frac{\partial}{\partial t} + \frac{1}{r} + V(r,t)\right\}\Phi(r,t) = 0 \tag{4}$$

where

$$\left.\begin{aligned} V(r,t) &= 0, \quad r < R \\ &= \frac{1}{r} - \frac{1}{R}, \quad r > R \end{aligned}\right\} \tag{5}$$

Equation (4) must be solved subject to the boundary conditions

$$\lim_{r \to 0} \Phi(r,t) = \lim_{r \to \infty} \Phi(r,t) = 0 \tag{6}$$

and for a hydrogen atom initially in the 1s state we must also have

$$\lim_{t \to -\infty} \left\{ e^{i\epsilon_{1s} t} \Phi(r,t) \right\} = R_{1s}(r) \tag{7}$$

The problem defined above for $\Phi(r,t)$ closely resembles the zeroth order problem of Temkin's nonadiabatic theory. As in Temkin's application, equation (4) has a clear physical interpretation. Initially the electron sees only the charge of the target proton. However, when the electron cloud is penetrated by the incident proton, the electron sees a doubly charged nucleus. Thus a temporary helium atom is formed which decays as the moving proton emerges from the electron cloud.

The excitation emplitudes $\alpha_n(t)$ can be obtained directly from equation (3)

$$\alpha_n(t) = e^{i\epsilon_n t} \int_0^\infty R_{ns}(r)\, \Phi(r,t)\, dr \tag{8}$$

or, by making use of equation (4) they can be written in the integral form

$$\alpha_n(t) = \delta_{n1} + i \int_{-\infty}^{t} dt' \, e^{i\epsilon_n t'} \int_{R(t')}^{\infty} R_{ns}(r)\, V(r,t')\, \Phi(r,t')\, dr \tag{9}$$

The boundary conditions at infinity, (6) and (7), are awkward to handle numerically and it was found more convenient to make the transformations

$$\Phi = e^{-i\epsilon_{1s} t} \chi , \quad \tau = \tan^{-1}\left(\frac{vt}{\rho}\right) , \quad \xi = \tan^{-1}(r) \tag{10}$$

thus placing the entire problem within a box $-\frac{\pi}{2} \leq \tau \leq \frac{\pi}{2}$, $0 \leq \xi \leq \frac{\pi}{2}$.

The boundary conditions on χ may now be simply stated

$$\chi(\xi, -\tfrac{\pi}{2}) = 2\tan(\xi)\exp(-\tan\xi) \tag{11}$$

$$\chi(0, \tau) = \chi(\tfrac{\pi}{2}, \tau) = 0 \tag{12}$$

The finite (central) difference equation corresponding to (4) is

$$A\chi = K \tag{13}$$

where A is a tri-diagonal complex matrix, χ is a column vector representing the solution at some value of τ and K depends on previous values of τ. Using a non-itterative technique developed by one of us (E. S.) (2) equation (13) may be directly inverted and $\chi(\xi, \tau_i)$ obtained from a knowledge of $\chi(\xi, \tau_{i-1})$. Since the initial condition at $\tau = -\frac{\pi}{2}$ is given by (11) we can develope a numerical solution over the entire region $-\frac{\pi}{2} \leq \tau \leq \frac{\pi}{2}$.

Calculations were performed on the Laboratory's IBM 7094/7040 using a 400 x 400 point mesh on the ξ, τ plane. The unitarity requirement

$$\int_0^{\pi/2} |\chi(\xi, \tau)|^2 \sec^2\xi \, d\xi \tag{14}$$

was confirmed to a very high degree of accuracy except for values of τ close to $\pi/2$ where it was occasionally violated by as much as 2%. This was due to an accumulated instability in χ which greatly inhibited the convergence of the excitation probabilities $|\alpha_n(\tau)|^2$ when computed using equation (8). However, the instability had an insignificant effect on the values of $|\alpha_n(t)|^2$ computed from (9) which depends on the entire history of χ rather than upon its instantaneous value.

The excitation cross sections, computed from

$$Q\,(1s,n) = 2\int_0^\infty \rho\, d\rho\, \left|\alpha_n(\gamma = \pi/2)\right|^2 \tag{15}$$

using the $\alpha_n(\pi/2)$ obtained from (9) are given in the table. Q_I corresponds to the s-wave contribution to the ionization cross section and was computed from

$$Q_I = 2\int_0^\infty \rho\, d\rho\, \left\{1 - \sum_{n=1}^{\infty} \left|\alpha_n(\pi/2)\right|^2\right\} \tag{16}$$

where the complete sum was formed by extrapolating the computed results above $n = 7$.

1. A. Temkin, Phys. Rev. 126, 130 (1962)

2. A. Temkin and E. C. Sullivan, NASA Technical Note D-1702 (unpublished)

Excitation Cross Sections in Units of $\left(\pi a_0^2/n^3\right)$

n \ E(kev)	25	50	100	200	400	800
2	1.68	1.17	.716	.395	.209	.108
3	1.22	.827	.521	.269	.141	.0725
4	1.10	.741	.445	.238	.125	.0639
5	1.05	.705	.412	.225	.118	.0604
6	1.03	.687	.402	.219	.114	.0587
7	1.01	.676	.394	.215	.113	.0576
Q_I	.269	.222	.133	.0718	.0370	.0188