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CHARACTERISTIC FEATURE OF $2p \to 2s$ TRANSITION IN SPHERICALLY CONFINED HYDROGEN ATOM

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Abstract. The electronic transition $2p \to 2s$ absent in the free hydrogen atom due to the Coulomb degeneracy becomes feasible when the atom is embedded inside a spherical cavity with impenetrable walls. We show, for the first time, that the oscillator strength corresponding to this transition in the confined state attains its maximum value at the characteristic confinement radius of 2 a.u. at which simultaneous degeneracy also takes place between the confined $[ns, (n+1)d]$ levels with $n \geq 2$.

1. INTRODUCTION

Model of spatially confined hydrogen atom (CHA in the text bellow) was introduced in physics in order to simulate the high pressure effects on dipole polarizability of hydrogen gas (Michels et al. 1937). Over the years, this model has been applied in many diverse fields of physics and chemistry. For example, the model of hydrogen atom confined in a hard spherical box was used in the study of partially ionized plasma (Harris et al. 1960) as well thermodynamic properties of non-ideal gases (Graboske et al. 1969) and atoms embedded in neutral media (Tabbert et al. 1997, Saha et al. 2002). Other important applications of confined CHA model deal with the study of hydrogenic impurity in semiconductor nanostructures like quantum dots, quantum wells and quantum well wires (see e.g. Moriarty 2001). An exhaustive account of diverse applications of the CHA model can be found in the available review articles (Jaskólski 1996, Dolmatov et al. 2004).

As compared to the unconfined (free) hydrogen atom, UHA, the superimposition of spatial confinement potential significantly changes the structure of the eigen-spectrum and other properties of the CHA. Hydrogen atom when placed at the center of the spherical well with impenetrable walls, does not exhibit any Coulomb degeneracy of levels. As a consequence of such confinement, the (nl) states with the same quantum number n and $l = 0, 1, \ldots, n-1$ are separated on the energy scale. Thus, newer allowed transitions appear in the CHA absorption spectrum which are generally absent in the UHA.

In this paper we focus on one such transition in the CHA given by $2p \to 2s$ transition and report the corresponding transition energy and oscillator strength as a function of the confinement radius. Our aim is to examine if there exists any characteristic feature in the variation of the chosen spectroscopic properties of the CHA. The paper is organized as follows. In section 2 the theoretical model is outlined. In section 3 we present the results for oscillator strength of $2p \to 2s$ transition and half-lifetime of the $2s$ state. Section 4 closes the paper summarizing the main results.

Atomic units ($m_e = e = \hbar = 1$) are used throughout the paper.

2. THEORY

In the CHA model considered here, the atomic nucleus is placed at the center of spherically symmetric potential well with impenetrable walls. Accordingly, electronic potential is given by

$$V(r) = \begin{cases} -\frac{1}{r}, & r < r_0 \\ \infty, & r \geq r_0 \end{cases} . \tag{1}$$

Spherical symmetry of the potential (1) allows factorization of the wave function into the radial and angular parts: $\Psi(\mathbf{r}) = \frac{1}{r} P_{nl}(r) Y_{lm}(\theta, \phi)$. Radial wave function is the solution of the radial Schrödinger equation

$$\left\{ -\frac{1}{2} \left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} \right] + V(r) \right\} P_{nl}(r) = 0 \tag{2}$$

with the imposed Dirichlet boundary condition

$$P_{nl}(r_0) = 0 \tag{3}$$

and requirement of the condition at $r = 0$ given by $P_{nl}(0) = 0$.

3. RESULTS AND DISCUSSION

3. 1. OSCILLATOR STRENGTH FOR $2p \to 2s$ TRANSITION

The required eigenvalue problem (2)-(3) is solved applying Numerov-Cooley method (Numerov 1933, Cooley 1961) with given accuracy $\epsilon = 1 \cdot 10^{-9}$ and 50000 grid points at every confinement radius value r_0. For more details on the method and avoiding the singularity at the origin see e.g. (Jensen 1983). Oscillator strength for $2p \to 2s$ transition in dipole approximation is given by

$$f = \frac{2}{3} \Delta E S_{2p \to 2s} \,, \tag{4}$$

where

$$S_{2p \to 2s} = \left| \int_0^{r_0} r P_{2p}(r) P_{2s}(r) dr \right|^2 \tag{5}$$

and ΔE is a transition energy

$$\Delta E = E_{2s} - E_{2p} \,. \tag{6}$$

All the spectroscopic properties stated above are the functions of confinement radius.

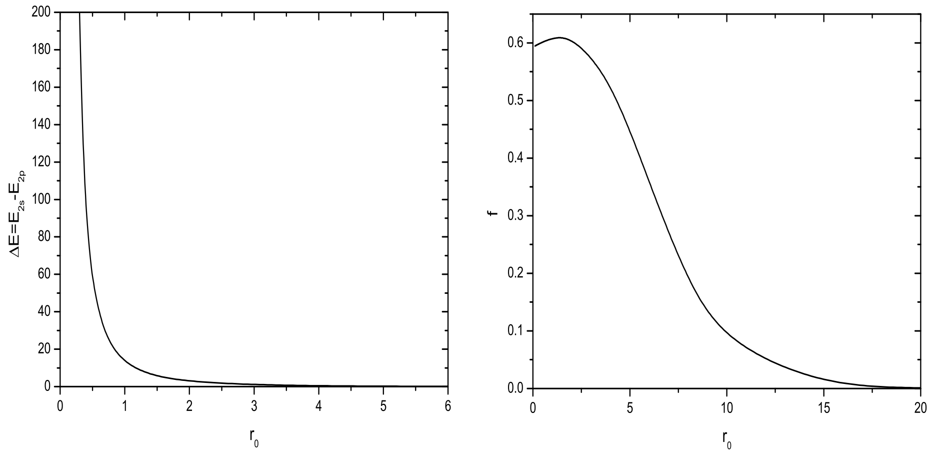

Figure 1: Transition energy (left panel) and oscillator strength (right panel) of the $2p \rightarrow 2s$ transition as a function of confinement radius.

Our results for transition energy and oscillator strength are shown in Figure 1. It is evident that the transition energy ΔE is a monotonically decreasing function of r_0.In the limit of infinite confinement radius the CHA energy levels approach the UHA levels, and $2s$ and $2p$ states become degenerate. In this limit, as given by (4), the oscillator strength approaches zero. It is interesting to note that this quantity is increasing function at small r_0 values which passes through a maximum value and then decreases at larger values of confinement radius. This behavior is reasonable since transition energy is decreasing function and quantity $S_{2p\rightarrow 2s}$ is increasing function of r_0. The oscillator strength maximal value is at $r_0 = 2$, the same value at which the simultaneous degeneracy occurs (see e.g. Scherbinin et al. 1997) between the confined states given by the pairs $[ns, (n+1)d]$ with $n \geq 2$.

3. 2. HALF-LIFETIME OF $2s$ STATE

In dipole approximation $2s$ state of the UHA has an infinite lifetime due to the fact that (1) transition $2s \rightarrow 1s$ is forbidden in this approximation, (2) transition $2s \rightarrow 2p$ is absent due to Coulomb degeneracy (transition energy is zero). In the CHA, the first transition is still not allowed, but the second transition becomes feasible giving the way of $2s$ state radiative decay. Half-lifetime τ (in s) of the CHA $2s$ state is determined by

$$\tau = \frac{1}{P_{2s\rightarrow 2p}}\,, \tag{7}$$

where transition probability for spontaneous emission $2s \rightarrow 2p$ is given by

$$P_{2s\rightarrow 2p} = C(\Delta E)^3 S_{2s\rightarrow 2p}\,. \tag{8}$$

Here, C is a constant $C = 2.1417 \cdot 10^{10} s^{-1}$ and $S_{2s\rightarrow 2p}$ and ΔE are given by the same expressions (5) and (6) as for absorption $2p \rightarrow 2s$.

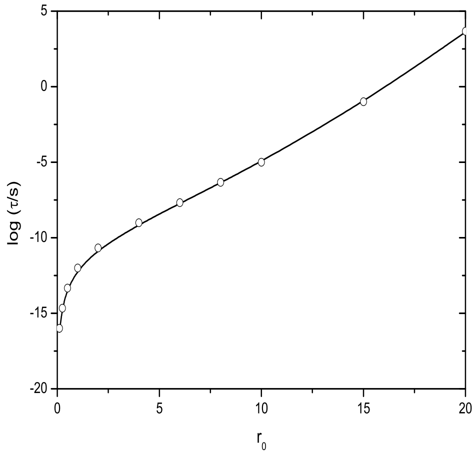

Figure 2: Half-lifetime of $2s$ state of CHA as a function of confinement radius. Line: present calculation, open circle (○): results from (Goldman et al. 1992).

In Figure 2 the $\log \tau$ is shown as a function of confinement radius r_0 together with the other available estimates (Goldman et al. 1992).

4. SUMMARY

The oscillator strength for $2p \rightarrow 2s$ absorption transition in the CHA at different confinement radius values is reported for the first time in the literature. A characteristic feature showing its maximum value at $r_0 = 2$ has been demonstrated numerically. It is of interest to examine the oscillator strength for other transitions $(nl) \rightarrow (n, l \pm 1)$, not appearing in the UHA, and check if the similar behavior is also displayed therein.

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