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Continuous spectrum of the H atom after confinement

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The study of confinement effects on atomic and molecular systems has been a topic of recent interest [1]. Experimentally it has been possible to insert atoms and molecules within molecular nanocavities. This brings the possibility of employing such as novel structures for different applications, ranging from energy storage and transport to medical use. In addition, depending on the relative sizes, confinement may exert a strong influence on the electronic structure of the guest atom or molecule. This opens up the field for manipulating the spectroscopic properties of the confined atom, which is of great interest in optics and electronics.

In this work we focus in the stability of the atom after it is released from the cavity. If the

confined atom or molecule is stored in order to be used to produce energy or to be transported, it is important to analyze if the atom is stable when the confining environment is removed.
Here we consider the H atom within an impenetrable spherical wall. This simple model reproduces the most important physical features of confinement and the study of the H atom simplifies the computational problem and the possible excitation mechanisms after the system is released. The excited states of the H atom, both in the discrete and the continuous spectra can be obtained very accurately.
We assume that the atom is liberated in a period of time that can be considered small as compared with the dynamics of the atom. Then the sudden approximation can be employed to study the state of the atom after confinement is removed. Within this approach, the time dependent state of the released atom after is expanded in terms of the stationary states of the free Hamiltonian. In this expansion both, the bound states and the Coulomb wave functions need to be included. The linear coefficients provide the amplitude probability of the released atom to reach the corresponding stationary state of the unconfined atom. The values of these coefficients are calculated as the overlap of the confined wave function with the wave function of the unconfined atom.

In Table 1 we show the energy of the three stationary states of the H atom here studied. We

consider hard wall spherical confinement of radius 2 au with the nucleus of the atom fixed at the center of the wall.

In Figure 1 we plot the ionization probability energy distribution of the atom when

confinement is released.

In all of the cases shown, a spread distribution around a principal maximum is obtained. The

value of the energy at the maximum is close and smaller thant the energy of the confined state. The other secondary maxima, obtained at higher energies, are less important. The probability distribution presents several nodes, showing that no electrons with that value of the energy can be emitted.

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