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# Calculation of oscillator strength and the effects of electric field on energy states, static and dynamic polarizabilities of the confined hydrogen atom

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## ABSTRACT

In this study, we investigate the effect of an electric field on energy states of a spherical quantum dot with infinite confining potential using the perturbation method. We also perform the static dipole and dynamic dipole polarizabilities. In addition, the oscillator strengths have been calculated for the dipole transitions between higher unperturbed states. The results show that impurity and dot radius have an important effect on the Stark shift, and the effect of electric field is insensitive in small dot radii. For the excited states the Stark shift from the first-order increases linearly with the increase of electric field strength. On the other hand, the Stark shift from the first-order decreases with increasing of the magnetic quantum number. A very important future is that, for dot radius region  $1.8 a_B \leq R \leq 7a_B$ , the static dipole polarizabilities change very quickly. In addition, it is found that as the dot radius increases, the photon energy corresponding to the singularity of dynamic dipole polarizability decreases.

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## 1. Introduction

Thanks to considerable progress in micro-fabrication has made it possible to produce zero-dimensional quantum dots (QDs) with various size and shapes such as sphere, box, disc and cylinder. The charge carriers of QDs, electrons and holes, have been confined in three-dimensions. The special confinement causes remarkable changes in the properties of the confined systems such as energy spectrum, polarizability, electrical, optical and so on. Due to their small size and potential applications in microelectronic and optoelectronic devices, a number of authors have devoted to study the electronic structure, binding energies and optical properties of QDs [1–15].

Recently, both from theoretical and from experimental point of view, the studies made on the effects of an external electric field in QDs have drawn a considerable attention. That is, external electric fields have become the subject of interest for studying of the physical properties in QDs. As is well known, the external electric field can destroy the symmetry of the system and can provide much valuable information about the confined systems. The application of an electric field causes a shift on the energy states

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of QD, called Stark effects, and also a polarization of the carrier distribution. These effects produce important changes in the energy spectra of the carriers. Therefore, many researchers have studied the effects of electric field on the confined systems using different methods such as variational [16–20], perturbation [21–23], compact density approach [24–27] and other methods [28–31]. However, in above mentioned studies the effects of the electric field on the binding energies were investigated for the ground ( $l = 0$ ) and the first excited state ( $l = 1$ ).

Dipole polarizability studies are important for investigating the effects of pressure on the atom, the theoretical description of interatomic interactions, the electron atom scattering and the optical properties of materials. Static and dynamic dipole polarizabilities depend on the behavior of the wavefunction of system. Dutt et al. [32] and Xu et al. [33] calculated the static dipole polarizability of the confined hydrogen atom inside a spherical box with impenetrable wall. The oscillator strength for the transition  $1s-2p$  and the static dipole polarizability for the  $1s$  ground state of hydrogen-like atoms confined at the center of a spherical box were computed by Laughlin [34] and Burrows and Cohen [35] using Rayleigh–Schrödinger perturbation theory and analytical methods. Montgomery [36] studied the static and dynamic polarizabilities for the ground state of hydrogen atom confined at the center of an impenetrable cavity using variational perturbation theory. Similarly, Saha et al. [37], Banerjee et al. [38], Sen [39] and Aquino [40] carried out the calculations of the transitions energies, the

oscillator strength and the static dipole polarizability for the confined hydrogen atom within an impenetrable spherical box. Detailed analysis for the static and dynamic dipole polarizabilities of the ground and excited states of the confined hydrogen atom were performed by Cohen et al. [41] and Motapon et al. [42] using variational-perturbation approach with a mapped Fourier grid method and the variational method on a B-spline basis set. In 2012, Montgomery and Sen [43] investigated in detail the ground state static and dynamic polarizabilities for a hydrogen atom confined at the center of a spherical box with penetrable walls. Extensive theoretical studies have been performed for the calculation of the static and dynamic polarizabilities related to the free atoms. However, to our knowledge, there are a few studies related to calculations of the stark shift and oscillator strength for the excited states of the confined hydrogen atom. A systematic study on the stark shift, oscillator strength and dipole polarizabilities is still lacking. Therefore, studies in this field are still important for theoretical researchers and practical applications.

In the present study, we calculate the unperturbed wavefunctions and energy eigenvalues of the ground and excited states using a variational optimization approach which is a combination of the Quantum Genetic Algorithm (QGA) and the Hartree-Fock Roothaan (HFR) method. Also, the Stark shift from the first-and the second-order as a function of the electric field strength, the static and dynamic dipole polarizabilities for the 1s ground state and the oscillator strength for the transitions between the excited states are investigated as a function of the dot radius by the perturbation calculations.

## 2. Theory

Within the framework of an effective mass approximation, in the presence of an electric field, the Hamiltonian of a hydrogen atom confined by an impenetrable spherical box of radius  $R$  is given by

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 - \frac{e^2}{\epsilon r} + V_C(r) + |e|Fr \cos \theta, \tag{1}$$

where  $m^*$ ,  $\epsilon$  and  $e$  are the effective mass of electron, the static dielectric constant of the medium and the charge of electron, respectively.  $F$  is the strength of electric field applied along the  $z$ -direction,  $r$  is the distance between electron and impurity and  $\theta$  is the angle between the position vector and the electric field in  $z$ -direction.  $V_C(r)$  is the spherical confining potential:  $V_C(r) = 0$  for  $r < R$  and  $V_C(r) = \infty$  for  $r \geq R$ ,  $R$  is the dot radius. When the fourth term on the right of Eq. (1) is compared with the magnitude of the unperturbed Hamiltonian, this term can be calculated perturbatively because of the relatively small, but it may be important. In this case, the Hamiltonian given in Eq. (1) can be rewritten as

$$H = H^{(0)} + H^{(1)} \tag{2}$$

with

$$H^{(0)} = -\frac{\hbar^2}{2m^*}\nabla^2 - \frac{e^2}{\epsilon r} + V_C(r) \tag{3}$$

and

$$H^{(1)} = |e|Fr \cos \theta \tag{4}$$

where  $H^{(0)}$  is the unperturbed Hamiltonian and  $H^{(1)}$  is the perturbation Hamiltonian.

The Schrödinger equation for the unperturbed Hamiltonian  $H^{(0)}$  is given by

$$H^{(0)}\psi_i^{(0)} = E_i^{(0)}\psi_i^{(0)}, \tag{5}$$

where  $\psi_i^{(0)}$  and  $E_i^{(0)}$  are the eigenfunction and eigenvalue of the unperturbed Hamiltonian  $H^{(0)}$  corresponding  $i$ th state. In HFR

approximation, the spatial part of the normalized wavefunction can be expressed as linear combination of basis sets,  $\chi$ , as follow:

$$\psi_i^{(0)} = \sum_{k=1}^{\omega} c_{ik}\chi_{q_k}(\zeta_k, \vec{r}) \tag{6}$$

where  $i$  and  $q_k$  denote the quantum numbers of the atomic orbitals and the basis sets.  $\omega$ ,  $c_{ik}$  and  $\zeta_k$  are the size, expansion coefficients and screening parameters of basis sets, respectively. The principle, orbital and magnetic quantum numbers of  $\chi_{q_k}$  are denoted by  $n_k$ ,  $l_k$  and  $m_k$ , respectively. For the first-order energy correction, the Schrödinger equation is given by

$$H^{(1)}\psi_i^{(0)} = E_S^{(1)}(i)\psi_i^{(0)} \tag{7}$$

in which  $E_S^{(1)}(i)$  is the correction energy of  $i$ th state and it is sometimes called as the Stark energy. After substituting Eqs. (4) and (6) into Eq. (7), one can obtain the first-order Stark correction energy for the excited states as follow:

$$E_S^{(1)}(i) = |e|F\sqrt{\frac{4\pi}{3}}\sum_k^{\omega}\sum_{k'}^{\omega'}c_{in_kl_km_k}^*c_{in'_kl'_km'_k}\sum_{L=L_{\min}}^{L_{\max}}\langle l_km_k|l'_km'_k|LM\rangle Q_{n_k+n'_k}( \zeta_k + \zeta_{k'}R) \tag{8}$$

where  $L_{\min} = \max\{|l-l'|, |m-m'|\}$ ,  $L_{\max} = l+l'$  and  $\langle lm|l'm'|LM\rangle$  with  $L \geq M$  and  $M = |m-m'|$  are Gaunt coefficients and calculated by the method presented in Ref. [44]. The integral  $Q_N(\alpha, R) = \int_0^R x^N e^{-\alpha x} dx$ .

The first-order energy correction to the non-degenerate ground state ( $n=1$ ) will be zero due to well-defined parity of the state, that is,  $E_S^{(1)}(1s) = |e|F\langle \psi_{100}^{(0)}|r \cos \theta|\psi_{100}^{(0)}\rangle = 0$ . However, the 1s ground state has a Stark correction from the second-order, and the second-order correction in perturbation series is given by [45]

$$E_S^{(2)}(1s) = e^2 F^2 \sum_{n>1} \frac{|\langle \psi_{np}^{(0)}(\vec{r})|r \cos \theta|\psi_{100}^{(0)}(\vec{r})\rangle|^2}{E_{100}^{(0)} - E_{np}^{(0)}} \tag{9}$$

Polarizability is important because of establishing a relationship between the refractive index which is a macroscopic quantity and the polarizability which is a microscopic one. If an external electric field is applied on the dot, the center of the negative charge distribution shifts. As a result of this, electronic polarizability occurs. One may obtain the magnitude of dipole moment by differentiating Eq. (9) according to the electric field [32]

$$D = -\frac{\partial E_S^{(2)}(1s)}{\partial F} = \alpha_D F \tag{10}$$

Here, the term  $\alpha_D$  is the static dipole polarizability for the 1s ground state. When an atom is exposed to a time-independent electric field along the  $z$ -axis, this is called as static case and the polarizability of the static case is given by [32,34]

$$\alpha_D = 2e^2 \sum_{n>1} \frac{|\langle \psi_{np}^{(0)}(\vec{r})|r \cos \theta|\psi_{100}^{(0)}(\vec{r})\rangle|^2}{E_{np}^{(0)} - E_{100}^{(0)}} \tag{11}$$

The summation over  $n$  in Eqs. (9) and (11) includes all states including the continuum wavefunctions. The accurate evaluation of the integrals over all continuum states is very complex for the present numerical capability [43]. The dominant contribution to the 1s dipole polarizability comes from the 1s–2p transition, since 2p state which is closest to the state 1s. Therefore, in our study, this sum was terminated after two cases including 1s–2p and 1s–3p transitions, and we calculated the static dipole polarizability from four different expressions. Firstly, we evaluated the static polarizability from Eq. (11), and secondly, the static polarizability was computed from the following two different expressions suggested by Kirkwood [46] and Buckingham [47]

$$\alpha_D^K = \frac{4}{9}\langle r^2 \rangle^2 \tag{12}$$

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