Investigation of electron and hydrogenic-donor states confined in a permeable spherical box using B-splines

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Abstract
Effects of quantum size and potential shape on the spectra of an electron and a hydrogenic-donor at the center of a permeable spherical cavity have been calculated, using linear variational method. B-splines have been used as basis functions. By extensive convergence tests and comparing with other results given in the literature, the validity and efficiency of the method were confirmed.

Keywords: quantum dots, permeable cavity, B-spline technique, potential shape effects

1. Introduction
Semiconductor QDs\(^1\) due to their high potential for applications in photonics and quantum information technology have attracted considerable attention since years ago [1]. Performing single dot spectroscopy and using appropriate theoretical models lead to substantial progress in understanding their electronic, optical and spinning properties [2-4]. One of the most important and effective models for studying QDs is the model of confined particles that is used in this paper. This model reconstructs behaviors and characteristics of QDs, properly [5, 6].

Nowadays, researchers can construct nanocrystals in different shapes [7-9]. This requires the study of the quantum confinement effects which in addition to confined quantum systems size depend on their shape, too [10, 11]. Although the single-electron spectrum plays a vital role in the QDs structures, an impurity can change significantly the spectrum of a single-electron under appropriate QDs structures. Impurities in semiconductors affect their optical, electronic and transmission properties [12]. So far, most investigations into the QDs are conducted on impermeable cavities, while permeable cavities are more realistic.

In this paper, spectra of a single-electron and a donor in the center of a permeable spherical cavity with different confinement potentials have been probed. The effects of potential-shape and quantum-size on the electron and donor spectra have been investigated. Effective atomic units are used throughout this paper. B-splines have been used as basis functions, which can easily perform the trial wave functions with appropriate boundary conditions. B-splines, due to their high efficiency, have been applied successfully to studying various confined quantum systems [11-17]. To learn more about these functions, the reader can refer to [17, 18].

2. Model and method
Characteristics of a confined quantum system reflect the form of its confining potential. In this paper, permeable spherical cavity is investigated so that \( V(r) \), the confining potential, is determined as follows

\[
V(r) = \begin{cases} 
V_0 & \text{if } r \geq R_0 \\
\alpha r^K & \text{if } r < R_0 
\end{cases} \quad ; \quad \alpha = \frac{V_0}{R_0^K} ,
\]

where \( V_0 \) is the barrier height of confining potential whose value depends on the desired quantum dot. \( K \) determines the shape of the potential. \( R_0 \) is the radius of the permeable cavity. For further information about this confining potential, the reader can refer to [19].

The effective mass approximation is used. Regarding the symmetric potential, we examine the following Schrodinger equation

\[
-\frac{\hbar^2}{2m^*} \frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} - \frac{w}{r} + V(r) U_{n,l}(r) = E_{n,l} U_{n,l}(r) ,
\]

where \( m^* \) is the effective mass of the electron, \( l \) is the orbital angular momentum quantum number, \( w \) is the width of the well, and \( E_{n,l} \) is the energy of the state. The solutions of this equation are the energy eigenvalues and wave functions of the system.
where $w=0$ and $w=1$ are for the electron and the donor, respectively. Effective atomic units are used throughout this paper and the length unit is 1 au = 104 Å and energy unit is 1 au = 10.4 MeV. Linear variational method is used for solving this problem. For this purpose, we have expanded the radial function $U_{n,l}(r)$, in terms of B-splines as

$$U_{n,l}(r) = \sum_{i=1}^{N} c_{i}^{nl} B_{i,k}(r),$$

where $B_{i,k}(r)$ is the B-spline of order $k$. $N$ is the number of B-splines used to expand the radial function.

Variation of Schrödinger radial wave function is as follows:

$$\left( -\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + \frac{\nu}{r} + V(r) - E_{nl} \right) U_{n,l}(r) B_{j}(r) = 0$$

for $j = 1, ..., N$

Integral form of the last equation is as follows:

$$\sum_{i=1}^{N} c_{i}^{nl} \int_{0}^{R} \left[ \frac{1}{2} \frac{d B_{i}(r)}{dr} \frac{d B_{j}(r)}{dr} \right] +$$

$$\left( \frac{l(l+1)}{2r^2} + \frac{\nu}{r} + V(r) - E_{nl} \right) \int_{0}^{R} B_{i}(r) B_{j}(r) dr = 0$$

for $j = 1, ..., N$

Equation (5) is a generalized eigenvalue equation as

$$H_{i,j} C = E_{ij} C,$$

where $H_{i}$ and $S$ are Hamiltonian and overlap matrices, respectively. The energy eigenvalues and the corresponding eigenstates can be obtained by diagonalizing the Hamiltonian matrix.

The sequence of the knot points is adopted as

$$0 = t_{1} = ... = t_{k} < t_{k+1} = ... < t_{j} = ... = t_{j+k-3} = R_{0} < ... < t_{N+k-2} <,$$

$$t_{N+k-1} = t_{N+k} = R_{\text{max}}.$$

We use multiple-knot technique to satisfy the boundary conditions. $N$ is the number of basis functions. $R_{\text{max}}$ should be chosen large enough to represent the distribution of all desired states. In this paper, for insurance, we have selected $R_{\text{max}} = 5R_{0}$, although it could be smaller than that. Also, $k$, the order of B-splines, is equal to 7.

The numerical-solution program is written in FORTRAN, and the subroutines of ARPACK and LAPACK libraries are exploited for diagonalizing the overlap matrix.

### 3. Results and discussion

Regarding the high localization of B-splines, banded Hamiltonian and overlap matrices are obtained. Execution time is very short. To check the validity and the efficiency of the method, extensive convergence tests for various shapes of the confining potential have been performed. Some results for some lower energy levels of a donor in a quantum dot of $V_{0}=80au^{*}$ and $R_{0}=3au^{*}$ with $K=1$ and $K=\infty$, are shown in tables 1 and 2, respectively. As we can see, the convergence in these states is very fast, especially in the case of $K=\infty$ (because the potential shape of this case is simpler).

In table 3, we have compared our results for some of the lowest energy levels with those of Zhu et al [19]. Here, following Zhu, our results are normalized with the lowest energy levels with those of Zhu et al [19].

We believe that our results are reliable. $K$ determines the shape of the confining potential, therefore according to table 3, energy-level structure alters as $K$ changes from 1 to $\infty$. These changes also are shown in figure 1. As shown in this figure, with $K$ increasing, the energy levels decrease. Also the potential-shape affects the level ordering. Intersection between levels 2s and 3d, 3p and 4f; and also 3s, 4d and 5g together, is shown in figure 1. For $K$ approximately 7 and above, changes in energy levels become relatively slower and noticeable changes are not observed anymore. So, it can be realized that the potential shape is very impressive on the electronic structure of QDs.

In figure 2, effects of the existence of a donor in QDs on three of the lowest energy levels of a single-electron...
of the single-electron. With comparing table 4 with table 5 that the existence of a donor.

Table 3. Confined-electron (n=0) and confined-donor (n=1) spectra normalized by E_{30}(n=0) for QDs of V_0=80au* and R_0=3au*. The data in the brackets are the values obtained by Zhu et al. [19]. (The value of E_{30} (n=0) is equal to 4.6822366, 13.3240493, 23.1900360, 39.1098012au* for K=∞, 4, 2, and 1, respectively).

<table>
<thead>
<tr>
<th>K, w</th>
<th>1s</th>
<th>2p</th>
<th>3d</th>
<th>2s</th>
<th>4f</th>
<th>3p</th>
<th>5g</th>
<th>4d</th>
<th>6h</th>
<th>3s</th>
</tr>
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<tbody>
<tr>
<td>0, 0</td>
<td>0.111162 (0.111)</td>
<td>0.2273989 (0.228)</td>
<td>0.3740937 (0.374)</td>
<td>0.4445730 (0.445)</td>
<td>0.5499046 (0.550)</td>
<td>0.6719899 (0.672)</td>
<td>0.7539510 (0.754)</td>
<td>0.9313124 (0.931)</td>
<td>0.9856003 (0.986)</td>
<td>1.0000000 (1.000)</td>
</tr>
<tr>
<td>1, 2</td>
<td>0.1789060 (0.179)</td>
<td>0.3346981 (0.335)</td>
<td>0.5105117 (0.511)</td>
<td>0.5482880 (0.548)</td>
<td>0.7026626 (0.703)</td>
<td>0.7548913 (0.755)</td>
<td>0.9087907 (0.909)</td>
<td>0.9719886 (0.972)</td>
<td>1.1272343 (1.069)</td>
<td>1.1272343 (1.069)</td>
</tr>
<tr>
<td>1, 1</td>
<td>0.4252727 (0.424)</td>
<td>0.6088612 (0.609)</td>
<td>0.7404954 (0.740)</td>
<td>0.7695202 (0.770)</td>
<td>0.8847747 (0.885)</td>
<td>0.9149210 (0.915)</td>
<td>1.0000000 (1.000)</td>
<td>1.1097173 (1.020)</td>
<td>1.0496078 (1.050)</td>
<td>1.1244554 (1.124)</td>
</tr>
</tbody>
</table>

Figure 1. Energy levels of a donor in QDs of V_0=30au* with R_0=3au* as a function of K.

Table 4. Energy levels of a donor in QDs of V_0=60au* with K=∞.

<table>
<thead>
<tr>
<th>R_0</th>
<th>1s</th>
<th>2p</th>
<th>3d</th>
<th>2s</th>
<th>4f</th>
<th>3p</th>
<th>5g</th>
<th>4d</th>
<th>6h</th>
<th>3s</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.0</td>
<td>-0.1788754 (0.178)</td>
<td>2.9715350 (2.971)</td>
<td>8.4214575 (8.421)</td>
<td>1.4000033 (1.400)</td>
<td>5.6738219 (5.674)</td>
<td>3.0062008 (3.006)</td>
<td>8.4568884 (8.457)</td>
<td>4.8487860 (4.848)</td>
<td>6.9539245 (6.954)</td>
<td></td>
</tr>
<tr>
<td>3.0</td>
<td>-0.4338350 (0.434)</td>
<td>1.0150885 (1.015)</td>
<td>3.4801252 (3.480)</td>
<td>0.4341033 (0.434)</td>
<td>2.3452376 (2.345)</td>
<td>1.2011866 (1.201)</td>
<td>3.6594087 (3.659)</td>
<td>2.6000418 (2.600)</td>
<td>3.0336823 (3.034)</td>
<td></td>
</tr>
<tr>
<td>4.0</td>
<td>-0.4843313 (0.484)</td>
<td>0.3839526 (0.384)</td>
<td>1.7696202 (1.769)</td>
<td>0.1258778 (0.126)</td>
<td>1.1920808 (1.192)</td>
<td>0.5845781 (0.585)</td>
<td>1.9651491 (1.965)</td>
<td>1.0840227 (1.084)</td>
<td>1.6453125 (1.645)</td>
<td></td>
</tr>
<tr>
<td>5.0</td>
<td>-0.4968957 (0.497)</td>
<td>0.1252038 (0.125)</td>
<td>0.020957 (0.021)</td>
<td>0.0002508 (0.000)</td>
<td>0.6736623 (0.673)</td>
<td>0.3113255 (0.311)</td>
<td>1.1879801 (1.188)</td>
<td>0.6401268 (0.640)</td>
<td>1.0061699 (1.006)</td>
<td></td>
</tr>
<tr>
<td>7.0</td>
<td>-0.4998822 (0.499)</td>
<td>-0.0552678 (0.055)</td>
<td>0.3758642 (0.376)</td>
<td>-0.0894981 (0.089)</td>
<td>0.2465598 (0.247)</td>
<td>0.0908974 (0.091)</td>
<td>0.5278011 (0.528)</td>
<td>0.267633 (0.267)</td>
<td>0.4602550 (0.460)</td>
<td></td>
</tr>
<tr>
<td>10.0</td>
<td>-0.4999994 (0.499)</td>
<td>-0.1134570 (0.113)</td>
<td>0.0868808 (0.087)</td>
<td>-0.1191941 (0.119)</td>
<td>0.0459911 (0.046)</td>
<td>-0.0086339 (0.008)</td>
<td>0.1968319 (0.197)</td>
<td>0.0852079 (0.085)</td>
<td>0.1836115 (0.183)</td>
<td></td>
</tr>
<tr>
<td>20.0</td>
<td>-0.5000000 (0.500)</td>
<td>-0.1249880 (0.125)</td>
<td>-0.0500059 (0.050)</td>
<td>-0.1249950 (0.125)</td>
<td>-0.0517311 (0.052)</td>
<td>-0.0054018 (0.005)</td>
<td>-0.0059930 (0.006)</td>
<td>-0.0020162 (0.002)</td>
<td>0.0085733 (0.009)</td>
<td></td>
</tr>
</tbody>
</table>

Figure 2. Comparison between the three lowest energy levels of a donor (n=1) and a single-electron (n=0) in QDs of V_0=60au* with K=∞ as a function of R_0.

The spectrum are shown. Energy levels of a donor and a single-electron in QDs of V_0=60au* with K=∞ is shown in tables 4 and 5, respectively. It is seen in figure 2 and by comparing table 4 with table 5 that the existence of a donor in QDs decreases the corresponding energy levels of the single-electron. With R_0 decreasing, the differences between corresponding energy levels increase. Also, as shown in table 3, the introduction of a donor changes the ordering of s and d states. This phenomenon depends on the potential shape and for different K, the ordering of the levels is not the same. Therefore, the existence of a donor in QDs, effectively changes the energy levels.
are approximately corresponding to one another.

According to figure 4, some levels, like values of energy levels undergo negligible changes. Lower levels that mean $V_0$ affects higher levels more than too. In this case, higher levels undergo more changes than seen that with $R_0=2\,\text{au}^*$ we have plotted the energy levels of a donor in QDs of $K=\infty$ as a function of $R_0$.

In table 6, energy levels of a donor in QDs of $K=60\,\text{au}^*$ with $K=\infty$. For example, the crossover of $R_0=3\,\text{au}^*$ with $V_0=40\,\text{au}^*$ decreases. Also, readily seen that with $V_0=40\,\text{au}^*$ the energy levels of the free relevant states occurs as $K=\infty$.

In figure 3 the energy levels of a donor in QDs of $V_0=40\,\text{au}^*$ with $K=\infty$ are shown as a function of $R_0$. It is readily seen that with $R_0$ increasing, the energy levels decrease. Also, $R_0$ has obvious effects on the ordering. For example, the crossover of $2s$, $3d$, and $3s$ with $4d$ states occurs as $R_0$ changes. These kinds of changes are observable from table 4, too. As QDs get bigger, the values of energy levels tend to constant numbers that are approximately the energy levels of the free relevant particle.

In table 6, energy levels of a donor in QDs of $R_0=3\,\text{au}^*$ with $K=\infty$. In figure 4 we have plotted the energy levels of a donor in QDs of $R_0=2\,\text{au}^*$ with $K=\infty$, as a function of $V_0$. In fact, the amount of $V_0$ depends on the desired quantum dot. It is seen that with $V_0$ increasing, the energy levels increase, too. In this case, higher levels undergo more changes than lower levels that mean $V_0$ affects higher levels more than lower levels. For $V_0$ approximately $30\,\text{au}^*$ and above, the values of energy levels undergo negligible changes. According to figure 4, some levels, like $2s$, $3d$ and $3s$, $4d$ are approximately corresponding to one another.

4. Summary

In this paper, we have examined the spectra of a single-electron and a donor in the center of a permeable cavity, using B-splines. The variational approach we employed here produced energy eigenvalues with high accuracy at low computational cost. We tried to precisely obtain the effects of quantum-size and potential-shape on the spectra of a single-electron and a donor in the center of a permeable spherical cavity. The size and shape effects on the low-lying states were probed. Also, the effects of a present donor on the single-electron spectrum in QDs were investigated. Considering these effects was useful in electronic device applications.

Due to diverse and new forms of QDs, studying the confined quantum systems with different shapes has attracted considerable attention over the last decade. Regarding the validity and the efficiency of the method applied here, we can extend it to investigate QDs with more realistic shapes.
References