Whispering gallery and surface mode of electrons in lateral and corrugated quantum dots

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Abstract
Quantum dots (QDs) are fundamental elements in the applications related to light–matter interaction, such as solar cells, lasers and sensors. Moreover, some modes of electrons including whispering galley modes (WGMs) and surface modes can be incorporated in many electronic systems, in high Q-resonators, and quantized reflection/transmission. Therefore, controlling and manipulating their energy spectra is vital. Here, we investigate energy spectra as well as WGM and surface mode of electrons in lateral and corrugated QDs. Although, lateral QDs are usually modelled by a 2D harmonic oscillator (with zero thickness), we show that even very small thickness of dots can change their energy spectra, also they can contain surface mode of electrons. Moreover, we investigate WGM in deformed QDs, and the dots which contain corners in their outermost region, and show that some degenerated points would be created. Meanwhile, in the corrugated QDs, the wavefunction would be distributed in the specific teeth based on its energy level.

1. Introduction
Semiconductor QD can be considered as an artificial atom since its electronic band structure shows similar properties of atomic orbitals, such as filling s, p, d, ... orbitals [1–5]. Whispering gallery mode (WGM) of electrons is an electronic state in QD which is highly interested in electronic lenses and sensors. Analogous to its optical counterpart, WGM of electrons can be achieved in different structures and configurations: inducing a p–n junction by a scanning tunneling probe, WGM can be created in Graphene [6], Oligothiophene nano-rings act as a WGM for electronic resonator [7], and WGM is proposed in relativistic quantum chaos [8]. Beside, using high spatial resolution optical spectroscopy, WGMs are depicted in InP/GaInP QDs which can be in the resonance of Wigner Molecules (crystallization of electrons in a confined structure with a few amounts of electrons) ground state [9–11].

Studying the effect of size, shape and structure of QD on its energy spectra and electronic distribution is essential in both theoretical study and their functionalities. Less than a (size) limit, energy levels of a semiconductor crystallite differ from those of bulk materials, and depends on size, shape as well as the material [12]. The size of the QD can change the band-gap of colloidal QD [13], and with core–shell structure of a QD, its energy levels can be manipulated [14]. Besides, [15] studies the effect of shape and size of QD on the electron and hole energy states for 3D InAs/GaAs QDs of different geometrical shapes such as tetrahedral, pyramidal, and icosahedral geometries.

Another interesting mode of electrons is surface modes which can appear in, for example, molybdenum disulfide (MoS2) nanoflake. Its associated conductivity behaves mostly as a 2D mode rather than 3D, depends firmly on the thickness of MoS2 nanoflakes [16]. Also, surface-plasmon (SP) mode can propagate in ultra-sharp convex grooves of gold, by applying electron beam along the axis of the grooves [17].

Analogous to the electronic distribution in the semiconductor QDs, optical response of semiconductor particles can be manipulated by changing the size and shape. Silicon is a suitable material for measurement of intensity, color and position of visible light, due to its bandgap. However, [18] shows that hourglass-shaped
silicon nanowire can be used for detection of near infrared (NIR), and short-wave infrared (SWIR) light. Also, near unity absorption can be achieved in the optical frequency range, by changing the shape of semiconductor particle in an array of these particles [19]. Localized surface plasmons (LSPs) can be excited in the nanoparticles at visible/near infrared frequencies. However, [20] introduces the excitation of LSPs at lower frequencies in a periodic textured metallic disk which induces WGMs, make it suitable for biosensing by exciting multipolar resonances with high Q-factor values, and on-chip integration.

In this paper, we show the controlling of energy spectra of QDs with different shapes, specifically, the electronic distribution on the surface of the dots including WGMs and surface modes. We investigate the energy spectra of a lateral QD (which is usually considered as a 2D harmonic oscillator), and show that the thickness of the dot can considerably affect the energy spectra. Besides, some states with quantum number associated to the height of the QD are detected (referred to z-state or surface mode) which can interfere with energy spectra and create degenerated states. We depict energy spectra of a QD which contain two and four corners at its outermost area, and show that two-folded and four-folded degeneracy would be created in the energy levels, respectively, at higher angular momentum, while they are distinguishable at the lower angular momentum. We depicts the wavefunction related to the electronic WGMs in a corrugated QD containing asymmetry teeth which would be distributed selectively in a tooth or teeth, based on its energy level.

2. Lateral quantum dot

The Schrödinger equation can be solved, numerically [21, 22], which provides the possibility to study the electronic band structure of any complex shaped semiconductor QDs. Here, we study QDs with different shapes which are symmetrical in azimuthal direction. The Quantum Dot and surrounding area are InP and GaAs with effective mass of electrons 0.08 \( m_e \) and 0.067 \( m_e \), respectively while the applied potential on the QD and surrounding area are 0 and 0.2 eV, respectively.

Lateral QD (in which its height is much smaller than the length) is usually considered as a 2D harmonic oscillator. However, here we show that even very small thickness of the dot can effectively change its energy

Figure 1. Energy spectra of QDs with (a) larger and (b) smaller heights.
spectra. Moreover, some electronic states along the surface of the dot would be appeared, which are (closely) degenerated to the other states with the same angular momentum. Figure 1 shows energy spectra of two QDs with different heights while their lengths are almost identical. In this figure, the states with nonzero quantum number associated to the z-direction (across the height) is shown by red and blue colors. First energy level as well as second, third, . . . energy levels of different angular momentum are connected to each other by dashed lines. It shows that by increasing the height of the QD, the distance between these dashed lines are decreased while their bending as well as the number of eigenvalues for each angular momentum are increased, which are the signs of
deviation of QD from 2D harmonic oscillator. We note that when the energy splittings become closer to each other, coulomb interaction can cause the higher energy levels become below of the lower energy levels. For instance, some WGMs with angular momentum $m = 2$ and $m = 3$ can occur between the two lowest energy levels s- and p-states $[23]$. Moreover, the slope of the z-states and their energy splitting are slightly less than the states in their vicinity, which cause the energy levels interfere, and some degenerated points be created.

Some of z-states with quantum number $z = 1$, and different values of $(r, m)$ are shown in figure 2, for both of the QDs which are studied in figure 1. With increasing the quantum number $r$, the higher harmonics appear along the length of dots, while with increasing $m$, the wavefunction distributions move toward the corner.

Figure 3(a) shows energy spectra of a QD for which its height is 13.4 times less than its length. It shows that the z-states emerge very close to the applied potential. With decreasing the thickness more, these states would disappear from the energy spectra. Figure 3(b) shows all of the possible z-states in the dot. The energy levels of these states are close to the applied voltage, leading them less confined to the QD, as it is obvious from their spatial wavefunction distribution. These states can have application in effective interaction between outcoming signal and QD as well as quantized refraction and transmission spectra, and surface conductance.

Figure 4. WGMs in spherical, deformed QDs and QDs with a corner in its outermost area.
3. Corrugated quantum dot with corners

In this section we manipulate the energy spectra and electronic wavefunction distribution in a QD containing a corner or corners in its outermost area. Figure 4 shows electronic WGMs in a spherical QD, slightly deformed spherical QD, and QD with a corner, associated to the first three eigenvalues of angular momentum $m = 20$. It shows that slightly deformed spherical QD changes the spatial distribution of wavefunctions, smoothly. However, creating a corner in QD causes the spatial distribution of all of the three WGMs concentrate at the corner. Therefore, by manipulating the shape of QD we can control the position of the electronic distributions, as well as their energy spectra. Figure 5(a) shows energy levels of first 12 eigenvalues of different angular momentum $m$ related to a QD with two corners at its outermost area (hyperbolic- or hourglass-like shape). The energy spectra reveals two-folded degeneracy, at higher $m$, while at lower $m$, they are 12 distinguished energy levels. The pair of energy levels, with lower angular momentums become degenerated faster with respect to $m$, which can be attributed to the size of corner and spatial distribution of related wavefunctions. In order to show the process of the degeneracy, figure 5(b) depicts the spatial distribution of wavefunction related to the first pair of energy levels. It reveals that at lower $m$, the amount of distribution is equally distributed in the corners, while with increasing the $m$, the amount of one side would be reduced and the other side would be increased, until that the wavefunction would be distributed only in one side. It is also possible to use asymmetry corners in order to lift the degeneracy, tune the splitting of the energy levels as well as the amount of wavefunction distribution in each corner.

Figure 6(a) shows the first 12 eigenenergies of a QD with 4 corners, which contains four-fold (closely) degenerated states at higher values of $m$, although the position of the two corners in the center is different from...
the side corners, geometrically. The wavefunctions related to the 1st, 5th and 9th eigenvalues with \( m = 20 \) are shown in figure 6(b), which have (local) radial quantum numbers \( r = 1 \), \( r = 2 \) and \( r = 3 \), respectively.

4. Corrugated quantum dot with teeth

In this section we study wavefunction and energy levels of corrugated QD containing unequal teeth (figure 7). With setting the length, width, number and distance between the teeth one can tune the energy levels and wavefunction distribution in the structure. Figure 7 (top row) depicts the eigenfunction of first eigenvalue of different angular momentum. With increasing \( m \), the distribution approaches to the base of teeth, while with increasing the \( m \) more, the wavefunction would be confined only in the longest tooth, which is related to the lowest energy level of the related \( m \). This selective behaviour of electronic distribution can be utilized in applications such as single photon detection and q-bits.

Figure 7 (bottom row) shows some of the eigenfunctions of \( m = 24 \), in which the wavefunction of each eigenvalue is distributed alternately in different teeth. The wavefunction related to the lowest energy level would be distributed to the longest tooth, while other distributions would be in the same or different tooth/teeth, based on their energy levels.

5. Conclusion

Energy spectra including Whispering gallery and surface mode of electron are studied in QDs with different geometrical shape. In lateral QD, we showed that the height of the dot can effectively change the energy spectra,
and even for a very small thickness comparing to the length, some states with quantum number related to the height of the dot, can be created. These states interfere with the other energy spectra and can create a degeneracy, due to their different energy splittings and slopes with respect to the angular momentum. We depicted two-folded and four-folded degeneracy in energy spectra of QDs containing 2 and 4 corners, respectively, in the outermost area. Besides, the position of wavefunction distribution related to the WGMs could be controlled by the location of the corners. We investigated energy spectra of a corrugated QD containing asymmetry teeth, and revealed that the electronic wavefunctions would be distributed selectively in the teeth based on their energy levels: for the lowest energy level related to $m=24$, it would be distributed to the longest tooth, while for the other energy levels, the distribution would be in the same or other tooth/teeth.

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**Figure 7.** Eigenfunctions of corrugated QD related to the first eigenvalue of different angular momentums (top series), and related to the eigenvalues of $m = 24$ (below series).
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