Two band model for a semiconductor quantum dot

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Two band model for a semiconductor quantum dot has been developed. Energy eigenvalues and the wavefunctions have been calculated for the dot of radius, \(a\). Our calculation shows that energy eigenvalues which become discrete due to the quantum confinement depends on \(a\). The band gap between two bands has been found \(a\)-dependent and it increases on decreasing the size of the dot. The calculated wavefunctions and energy eigenvalues are aimed to use for computing the size dependent static dielectric constant of the quantum dot. The computed wavefunctions and energy eigenvalues and preliminary calculations of dielectric constant are presented in this paper.

Keywords: Quantum dot, Energy eigenvalues, Wavefunctions, Band gap, Dielectric constant

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1 Introduction

The properties of semiconductor quantum structures with reduced dimensions have been the subject of many experimental and theoretical investigations in the past decade\(^1\)-\(^6\). The system is interesting from the point of view of basic physics, with the carriers being confined to an essentially zero dimensional structure\(^7\). It is their quantum mechanical properties that are of interest rather than their nanoscale size, although the former are indeed a function of the later. Quantum confinement (QC) plays an important role in altering the optical and transport properties of semiconductor materials with reduced dimensions. The transition from micro to nano can lead to number of changes in physical properties. According to the confinement, they are termed as quantum well, quantum wire, and quantum dot (QD), in which the carriers are confined to the one, two and three dimensions, respectively. With the miniaturization of a solid, quantum and interface effect becomes increasingly important. As a result, the band structure of a nanometric semiconductor changes: the band gap expands, the core level shifts, the bandwidth revises, and the sublevel separation within a band increases\(^8\). The QD, zero dimensional structure, is also termed as semiconductor nanocrystallite or artificial atom because, due to the small dimensions of the dot, level spacing is correspondingly high\(^9\). QC causes the band gap to expand which reduces the dielectric constant and enhances the coulomb interaction among electrons, holes and shallow impurities in nanometric structures.

The exciton binding energy also increases. Reduction in the static dielectric constant becomes significant as the size of the quantum confined physical system such as wires and dots approach the nanometre range\(^1\).

Penn model has been used to perform the calculation of bulk static dielectric constant\(^8\),\(^9\). In past, the calculations of dielectric constant have been performed with the use of semi empirical method or by considering the pseudopotential method\(^2\)\(^-\)\(^6\). But the validity of this assumption, which postulates the use of fitted parameters in a size regime of a few nanometers, is not clear and has been questioned in recent studies\(^3\). In view of this, we developed a self-consistent two band model aimed to calculate the static dielectric constant of spherical semiconductor nanocrystallite of radius \(a\). Extended zone scheme has been used to represent the model where the band gap lies at the zone boundary. Instead of inventing a new specialized approach for nanostructures, we formulate the problem such that the same conceptual methods and sophistication with which bulk solids have been successfully treated in the past can be applied to the nanostructures. In order to study the near edge properties of semiconductor QD, what one typically needs to know about such system includes the energy eigenvalues and eigenfunction near the band-edge states i.e. the conduction band (CB) minimum and the valence band (VB) maximum\(^11\). Our method is exact in that the solutions are obtained from a single particle Hamiltonian. The aim of our work is to investigate the size dependence properties of a QD and to compare them with the available data.
2 Calculations

Our approach is similar to the Penn model developed for a bulk semiconductor, in which the actual energy bands of a semiconductor are replaced by those of a nearly free electron gas. Dielectric function, in Penn model, depends only on the average bulk energy gap that can be determined from the optical data. We consider QD as a sphere of radius, \( a \).

For a spherically symmetric QD, the single particle Hamiltonian

\[ H\Psi = E\Psi \]  

... (1)

can be expressed as follows;

\[ \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d\Psi}{dr} \right) + \frac{2m}{\hbar^2} \left( E - V(r) - \frac{l(l+1)\hbar^2}{2mr^2} \right) \Psi = 0 \]  

... (2)

Solution of Eq. (2) can be written in the form of spherical Bessel function \( j_l(kr) \), which for QD must vanish at the boundary. The potential energy can be expanded as:

\[ V(r) = \sum_g V_g e^{ig\theta} = \sum_g \sum_l V_g j_l(2l+1)j_l(gr)P_l(\cos \theta) \]  

... (3)

where the symbols have their usual meanings. \( \vec{g} \) is reciprocal lattice vector, which can be given by \( g = 2k_F \). In analogy to Penn model, two wavefunctions for QD can be taken as:

\[ R^\pm(r) = A^\pm j_l(kr) + B^\pm j_l(k'r) \]  

... (4)

where + and – refer to the conduction band and valence band, respectively. The analytical solution of Eq. (2), with the use of Eq. (3) and the wavefunctions expressed in Eq. (4), is not possible. In order to have simple workable two band model, we consider the case of \( l=0 \) for which Eq. (4) reduces to

\[ R^\pm(r) = A^\pm \sin \left( \frac{kr}{kr} \right) + B^\pm \sin \left( \frac{k'r}{k'r} \right) \]  

... (5)

Eq. (5) leads to

\[ \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR^\pm}{dr} \right) + \frac{2m}{\hbar^2} \left( E - \sum_g V_g j_0(gr) \right) R^\pm = 0 \]  

... (6)

Energy eigenvalues, which are discretised due to QC for the QD, can be evaluated by applying the variational method:

\[ \delta \left[ R \left\{ \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \frac{2m}{\hbar^2} \left[ \sum_g V_g j_0(gr) \right] R \right\} - E \left\langle R \right| R \right] = 0 \]  

... (7)

which with the use of Eq. (5) results into:

\[ \begin{bmatrix} \varepsilon_k^d - E \frac{2V_I^3}{ag} \\ \frac{2V_I^3}{ag} \varepsilon_{k'}^d - E \end{bmatrix} \begin{bmatrix} A^d \\ B^d \end{bmatrix} = 0 \]  

... (8)

Here

\[ \varepsilon_k^d = \frac{\hbar^2 k^2}{2m} + \frac{2V_I}{ag} I_1 \]  

... (9a)

\[ \varepsilon_{k'}^d = \frac{\hbar^2 k'^2}{2m} + \frac{2V_I}{ag} I_2 \]  

... (9b)

The superscript \( d \) stands for the QD and \( I_1, I_2 \), and \( I_3 \) are defined as:

\[ I_1 = \int_0^\frac{\pi}{2} \sin^2(kr) \sin(gr) \frac{dr}{r} \]  

... (10a)

\[ I_2 = \int_0^\frac{\pi}{2} \sin^2(k'r) \sin(gr) \frac{dr}{r} \]  

... (10b)

\[ I_3 = \int_0^\frac{\pi}{2} \sin(2gr) + \sin(2k'r) - \sin(2k'r) \frac{dr}{4r} \]  

... (10c)

Eq. (8) gives:

\[ E^\pm = \frac{1}{2} \left[ \varepsilon_k^d + \varepsilon_{k'}^d + \sqrt{\left(\varepsilon_k^d + \varepsilon_{k'}^d\right)^2 + E_g^2} \right] \]  

... (11)

where, again, the superscript + and – refer to conduction band \( (k > k_F) \) and valence band \( (k < k_F) \), respectively. \( k_F \) is Fermi wave vector. The band gap of the QD in our case is defined by
\[ E_g = \frac{4V_g I_3}{ag} = \frac{2I_3}{ag} \] \quad \ldots (12)

\[ E_g^b = 2V_g \] is the average band gap of the bulk semiconductor. \( E_g^b \) in Penn model has been taken to be 4.8 eV for Si, which is determined by using the values \( \in (0) = 12 \). The coefficients \( A^\pm \) and \( B^\pm \) can be determined from Eq. (8) along with normalization condition:

\[ \langle R^+ | R^+ \rangle = 1 \] \quad \ldots (13)

Evaluation of Eq. (13) gives:

\[ \frac{3}{2} \left( \frac{|A^\pm|^2}{(ka)^2} + \frac{|B^\pm|^2}{(k'a)^2} \right) = 1 \] \quad \ldots (14)

Eqs (8) and (13) yield:

\[ A^\pm = \frac{\sqrt{3}}{1 + (\alpha_k^\pm)^2} \] \quad \ldots (15a)

\[ B^\pm = \frac{\sqrt{3}}{1 + (\alpha_k^\pm)^2} \frac{E_g^b}{2} \] \quad \ldots (15b)

where

\[ \alpha_k^\pm = \frac{E_g^b}{2} \left( \frac{1}{E_k^\pm - \varepsilon_{kF}^\pm} \right) \] \quad \ldots (16)

The \( E^\pm, A^\pm \) and \( B^\pm \) are expressed in manner similar to that used in Penn model.

**3 Results and Discussion**

As can be seen from the Eqs (5), (11), (15), (16), both the wavefunction and energy eigenvalue depend on \( a \). The \( a \)-dependence of wavefunctions appears through coefficients \( A^\pm, B^\pm \) and energy eigenvalue which depends on \( a \) through integrals \( I_1, I_2, \) and \( I_3 \). We compute our wavefunction and energy eigenvalues as a function of \( k \) for different \( a \)-values for Si-QD, which is parameterized in terms of \( E_g^b = 4.8 \) eV, Fermi energy \( \varepsilon_{kF} = 12.6 \) eV and \( k_F = 8 \times 10^{-7} \) cm. The probability amplitudes \( |\psi^+|^2 \) and \( |\psi^-|^2 \) are plotted against \( kr \) for two values of \( a = 0.5 \) nm and 0.75 nm in Fig. 1 for \( k = 0.95 k_F \). The \( a \)-dependence of probability amplitudes (PA) can clearly be seen from Fig. 1, where increase in \( a \) reduces the PA. It is interesting to note that PA of both CB and VB decline faster on increasing \( r \) and for \( r \) close to \( a \) of QD, PA of CB becomes smaller than that of VB. This suggests that near the zone boundary, probability of finding an electron in CB is higher than that of finding in VB for \( r \) closer to zero. While for \( r \) close to \( a \), chances of finding an electron in VB are more than that of finding in CB. We also computed the PA of CB and VB for \( k \) near zone centre \( (k = 0.05 k_F) \) reflecting the probability of being an electron in the conduction band is very much higher than that in the valence band, for all values of \( r \). We, therefore, plotted PA of CB band only in Fig. 2. The PA of CB for \( k \) near to the zone centre is larger than that for \( k \) near zone boundary. Also the slope of PA versus \( kr \) curve of CB is larger for \( k \) near zone boundary. Further, PA for both CB and VB vanishes whenever \( kr \) becoming integer multiple of \( \pi \), which is determined by choice of \( a \).

The computed \( E^\pm / \varepsilon_{kF} \) plotted as a function of reduced wavevector for two values of \( a \) in Fig. 3. Curve-A and curve-B for \( a = 0.5 \) nm represent the CB and VB, respectively for \( a = 0.5 \) nm. Curve-C and curve-D are plotted for \( a = 0.75 \) nm. Though the \( a \)-dependence of both CB and VB is seen for all values of \( k \), it is more profound for \( k \)-values near the zone boundary (Fig. 3). The CB shifts upwards and the VB comes down on energy scale on reducing \( a \). This results in an increase in band gap as size of QD
reduces, which is in agreement with the experimental findings. Difference in energies of CB and VB is more pronounced at and near the zone boundary. It is also to be mentioned that for very large value of $a$, $E_g$ reduces to $E_g^b$.

Our computed wavefunctions and energy eigenvalues are used to calculate the size dependent dielectric function of a QD. The dielectric function for a quantum dot can be given as:

$$
\varepsilon(a, \omega) = 1 + \sum_{k, k'} \frac{f_k (1 - f_{k'})}{E_{k'}^z - E_k^z - \hbar \omega + iy'} \int d^3r \left| \psi_k^e (r') \right|^2 \psi_k^e (r') \psi_{k'}^e (r') e^{i r' r} + \Delta E / E_g \right)^n \right)
$$

where, $f_k$ is Fermi distribution function.

$$
\nu^o(r, r') = \frac{e^2}{|r - r'|} \quad \ldots (17)
$$

is bare Coulomb potential.

Our calculation of $\varepsilon(a, \omega)$ for $\omega = 0$ is under progress. The computed result will be published in our forthcoming publication. The preliminary calculation from our calculation suggests that computed $\varepsilon(a)$ can approximately filled to

$$
\varepsilon(a) = 1 + \frac{\varepsilon_b - 1}{1 + (\Delta E / E_g)^n} \quad \ldots (18)
$$

where, $\varepsilon_b$ is the bulk value of the dielectric constant. The exponent $n$ depends on parameters defining a semiconductor. We find that $n$ varies from 1.2 to 1.6 for elemental semiconductors such as Si. The Eq. (18) is in agreement with calculations reported by Wang and Zunger$^5$.

4 Conclusion

Our simple two band model calculation suggests that both energy eigenvalues and wavefunctions depend on $a$. The $a$-dependence of wavefunctions has been found more prominent than that of energy eigenvalue. Both PA and $E_g$ increase on decreasing $a$. The PA for $k$ near the zone centre exhibits stronger $r$ dependence than that for $k$ near the zone boundary. The $a$-dependence of wavefunction and energy eigenvalue leads to $a$-dependence of various properties including, dielectric function of a QD.

This is to be mentioned that our approach, as against the earlier reported calculations of wavefunctions, energy eigenvalues and dielectric function, is self consistent.

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References