

A Theoretical Study of Electronic Energy States in Semiconducting Nano Particles

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ABSTRACT

An engineered nano particle may be defined as any intentionally produced particle that has a characteristic dimension from 1 to 100 nm. Substances at the nano scale can sometimes contradict common sense by behaving erratically and emerging new properties.

An electron in the conduction band of a particle is nearly free to move inside the particle and this situation can be pictured as an “Electron inside a finite depth potential well”. The energy equations for this system can be derived by applying the “Time Independent Schrödinger equation” and corresponding boundary conditions in terms of one and three dimensions. In this study we have employed computer software and numerical root finding methods to obtain the numerical values of the legitimate energy states. According to these numerical solutions, we could demonstrate that, the number of allowed energy states and the spacing between adjacent levels inside a semiconducting nano particle depend on both particle size and the magnitude of the attractive potential. The energy levels obtained by this method were plotted and compared with reported experimental observations and they are in good agreement.

1. INTRODUCTION

A nearly free electron in the conduction band of a particle can be described to be a one that is free to move inside the particle but cannot move out due to the attraction imposed on it from the ion core. Hence this situation can be pictured as an “electron inside a finite depth potential well”. By applying the Schrödinger equation for these electrons inside a finite depth potential well in terms of one and three dimensions, the wave functions which describe the behaviour of the electrons can be obtained. “Energy equation of the system” can be derived by applying the boundary conditions to these wave functions. The numerical solutions of these energy equations will yield the allowed energy states for the electrons inside the well. Therefore the energy states calculated for the finite depth potential well will reveal the electronic structure of the conduction band of the particle.

2. CALCULATION OF ENERGY STATES OF ONE DIMENSIONAL FINITE POTENTIAL WELL

For a one dimensional finite depth potential well of width $2a$, with an electron confined to a constant attractive potential ($-v_0$), by applying the one dimensional Schrödinger equation [1] yields,

$$\frac{d^2\Psi}{dx^2} + \alpha^2\Psi = 0 \quad , \quad \text{where } \alpha^2 = \frac{2m}{\hbar^2} (|v_0| - |E|)$$

Above equation results in the following wave function inside the well when ($|v_0| > |E|$)

$$\Psi(x) = A \sin \alpha x + B \cos \alpha x \quad (1)$$

By applying the one dimensional Schrödinger equation for outside the well,

$$\frac{d^2\Psi}{dx^2} - \beta^2\Psi = 0 \quad , \quad \text{where } \beta^2 = \frac{2m|E|}{\hbar^2} > 0$$

Result in the following wave function outside the well.

$$\Psi(x) = C e^{-\beta x} + D e^{\beta x} \quad (2)$$

where A, B, C, D are arbitrary constants.

2.1 Energy States of the System

Boundary conditions for the system are that $\Psi(x)$ and $\frac{d}{dx}\Psi(x)$ should be continuous at the boundaries. By applying these boundary conditions to the above wave functions yield:

$$\alpha \tan \alpha a = \beta \quad (3)$$

$$\alpha \cot \alpha a = -\beta \quad (4)$$

Equations (3) and (4) represent the energy equations of one dimensional finite potential well. These equations can be solved numerically or graphically to obtain the allowed energy states of the system. The standard way of solving these equations are based on graphical methods in which the points of intersection of two graphs would yield the legitimate energy values of the system. Instead of using complex graphical methods, it is much convenient to employ a programming language such as “Fortran” from which numerical values of the legitimate energy states can be obtained following the numerical root finding methods like “Newton-Raphson method”

$$\text{Taking } y^2 = \alpha^2 a^2 \text{ and } t = \frac{2m v_0 a^2}{\hbar^2} ;$$

The equations (3) and (4) can be changed to the following forms:

$$y^2 + y^2 \tan^2 y - t = 0 \quad (5)$$

$$y^2 + y^2 \cot^2 y - t = 0 \quad (6)$$

Then the Energy values will be given by:

$$E = v_0 \left(1 - \frac{y^2}{t} \right) \quad (7)$$

The obtained numerical solutions in this method are highly accurate than the results from the graphical methods. These numerical values would reveal the electronic structure of the one dimensional particle.

2.2 Variation of Probability of Finding the Electron Inside and Outside the Well

The probability density is determined by the respective wave function such that,

$$\rho(x) = [\Psi(x)].[\Psi(x)]^* = |\Psi(x)|^2$$

For example, two states are given below.

The first (lowest) even energy level is obtained by solving the equation (5) and the values of α and β can be calculated using the relationships (1) and (3). By applying boundary conditions, the wave function for three regions can be defined piecewise as follows:

$$\Psi(x) = \begin{cases} Ce^{\beta x} & ; x < -a \\ \cos \alpha x & ; -a \leq x \leq a \\ Ce^{-\beta x} & ; x > a \end{cases}$$

Similarly the second energy level is obtained by solving the equation (4) and hence this energy level is odd. By applying boundary conditions, the wave function can be defined piecewise as follows:

$$\Psi(x) = \begin{cases} De^{\beta x} & ; x < -a \\ \sin \alpha x & ; -a \leq x \leq a \\ -De^{-\beta x} & ; x > a \end{cases}$$

Probability functions corresponding to the above wave functions can be plotted and it can be shown that the “Quantum tunneling effect” is significant when the particle size is below 20 nm.

2.3 Three Dimensional Finite Depth Spherical Potential Well

By applying the three dimensional Schrödinger equations to a spherically symmetric finite potential well, we can obtain the wave functions of an electron inside a particle.

Standard wave functions which describe the above situation are spherical Bessel functions $j_\ell(\rho)$ and Hankel functions of the first kind [2]. Spherical Bessel functions yield the radial part of the wave function $R_\ell(\rho)$ of an electron inside the well.

Applying boundary conditions at $\rho = a$ to above wave functions, energy equation of the system can be obtained as follows,

$$k_1 \frac{[j_{\ell-1}(k_1 a) - j_{\ell+1}(k_1 a)]}{j_{\ell}(k_1 a)} + \left(\frac{1}{a} + k_2 \right) = 0$$

$$\text{where } k_1^2 = \left[\frac{2m}{\hbar^2} (|v_0| - |E|) \right] \text{ and } k_2^2 = \left[\frac{2m}{\hbar^2} (|E|) \right].$$

Unlike in the one dimensional case, three dimensional energy equation contain both Radial and angular momentum components. In order to obtain allowed energy values of this system, it is recommendable to employ the computer software “Matlab” and the root finding method, “Bisection Method” [3]. Numerical solutions obtained in this manner will pave the way to understand the electronic structure of the particle.

3. RESULTS AND DISCUSSION

Variation of the number of allowed energy states with the particle size of a one dimensional nanoparticle is shown in figure 1, for $v_0 = -1$ eV when the particle sizes are 5 nm, 10 nm, 50 nm.

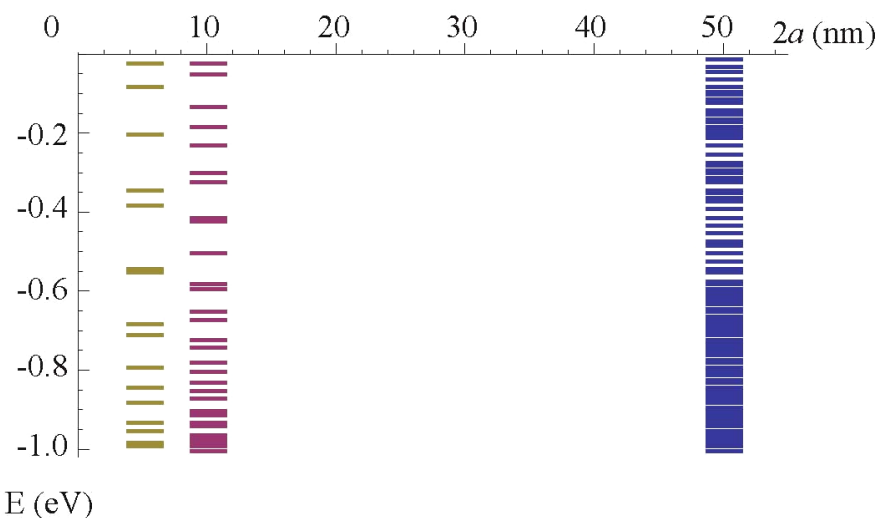


Figure1: Variation of energy levels with the particle size for $|v_0| = 1$ eV

It is clearly seen in figure 1, when the particle size is increased, the number of energy levels are increased and the gaps between adjacent levels are decreased. This has been established very well in the literature by experimental observations [4].

The variation of energy levels with the attractive potential of a one dimensional nano particle is shown in figure 2, for $v_0 = -3$ eV when the particle sizes are 5 nm, 10 nm, 50 nm respectively.

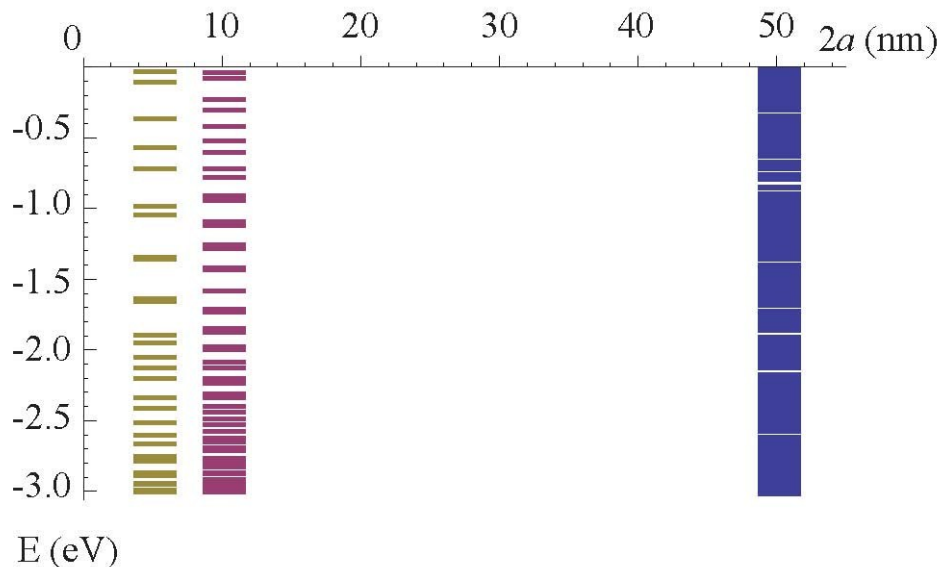


Figure 2: Variation of energy levels with the particle size for $|v_0| = 3\text{eV}$

It is very clearly seen in figure 2, when comparing with figure 1, that the attractive potential v_0 determines the number of energy levels. Therefore the number of allowed energy states inside a one dimensional particle depend on both particle size and the value of the potential. When the particle size exceeds the nano range, energy spectrum becomes almost continuous & formation of energy bands can be expected. This is seen in the case of 50nm particle in figure 2.

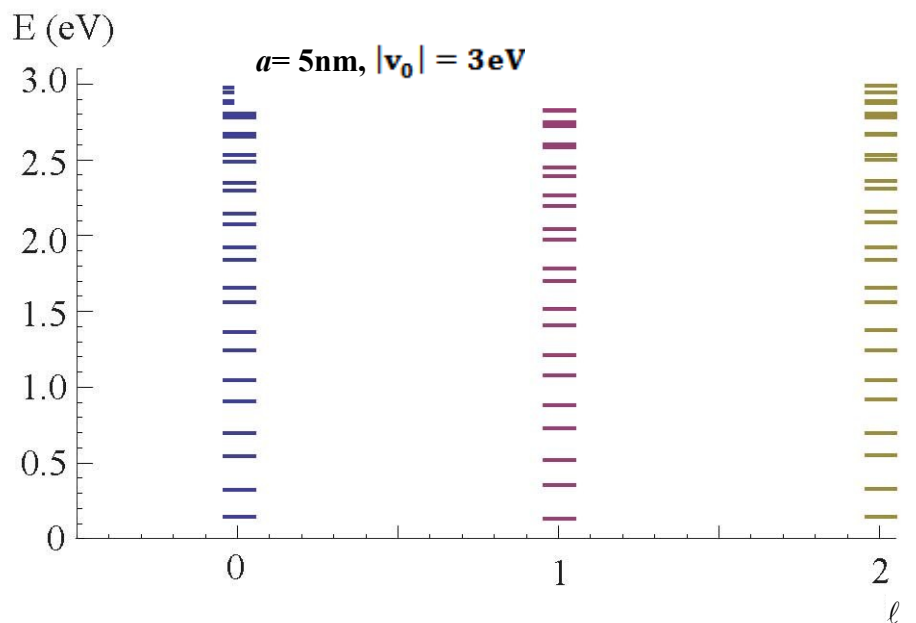


Figure 3: Variation of energy levels with the angular momentum quantum number l (for $2a = 10\text{ nm}$, $|v_0| = 3\text{ eV}$)

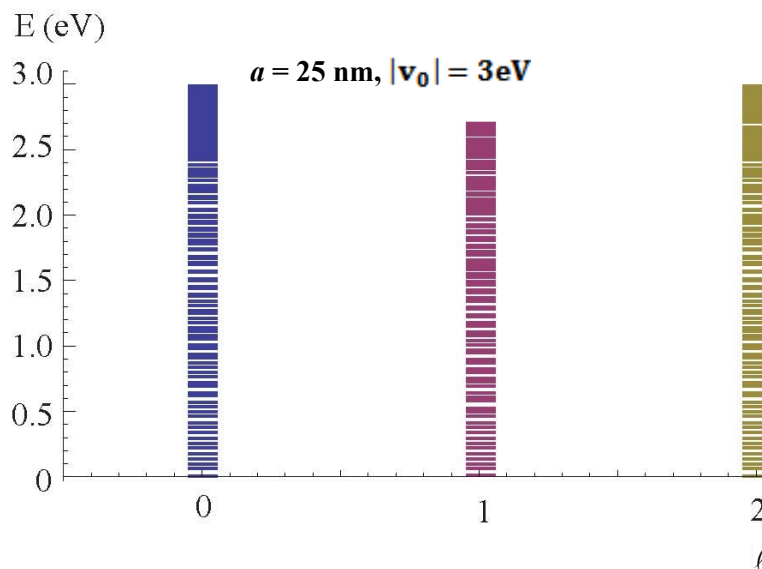


Figure 4: Variation of energy levels with the angular momentum quantum number l (for $2a = 50 \text{ nm}$, $|v_0| = 3 \text{ eV}$)

Figure 3 and figure 4 show the variation of the energy levels of nano particles of sizes 5 nm and 25 nm with an attractive potential $v_0 = -3 \text{ eV}$ for different angular momentum quantum numbers.

As in the one dimensional case, again the results shown in figure 3 and figure 4 show that the energy levels are very sensitive to the size of the particle.

Thus our study gives the possibility of determining the optimum parameters of nano particles for practical applications.

4. CONCLUSION

The obtained results are in good agreement with reported experimental observations. The most interesting size dependent property related to the semiconducting nano particles is that, we can obtain every colour of the visible spectrum by changing the size within the nano range, while the composition is unchanged. This study reveals that the material property can be accommodated in v_0 while the nano particle size can be optimized to yield the required electronic properties of the nano particle.

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