Quantum Dots PreLab
Rochester Institute of Technology

PHYS-316 Advanced Lab*

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You will consider a series of sucessively better models for the energy levels of the quantum dots. Complete the algebra here to determine the wavelength λ emitted by the dots for each model, in terms of the dot diameter D. After you collect your data, you will determine the best model based upon your measured wavelengths.

Please note that when you studied square wells in Modern Physics 1 class, the $n = 0$ electron state was not allowed, for it would have energy of zero and wavefunction of zero everywhere. That is the trivial solution to Schrodinger's equation. However, for a semiconductor quantum dot, the ground state $n = 0$ does exist: there simply is no conduction electron. So our lowest energy transition is from $n = 1$ to $n = 0$, unlike what you learned in Modern Physics 1. In each of the following models, assume the flourescence is caused by a transition from the first excited state (lowest in conduction band) back to the n=0 (valence band) state. See Figure 1. This can be thought of as 'exciton recombination' or the electron falling back into the hole it left behind.

1. One-Dimensional Infinite Square Well
   Assume that the formula you derived in Modern Physics for an electron in a one-dimensional square well is appropriate. Given the width D of the well, what is the emitted photon wavelength? Quantum dots aren't one-dimensional, so this is a poor approximation.

2. Three-Dimensional Cube Infinite Square Well
   If our dots were perfect little cubes, a particle would be trapped within a three-dimensional infinite well. Derive or look up (give citation) the energy of an electron in a three-dimensional cube well of side length D, and solve for the emitted photon wavelength. While this is getting closer to the real shape of a quantum dot, it still assumes we obtained the electron for zero energy, and that the electron is in vacuum (which is not realistic) so this is also a poor approximation.

3. Cubical Semiconductor Dots
   Our quantum dots are made of a semiconducting material having a band gap energy E_g, required to move electrons from the valence band ($n = 0$) to the conduction band ($n = 1$); the bands are shown in Figure 1. Thus the photon of flourescent emission that you observe has energy

$$E = E_g + E_n \tag{1}$$

*Prepared by L. Barton and A. McGowan

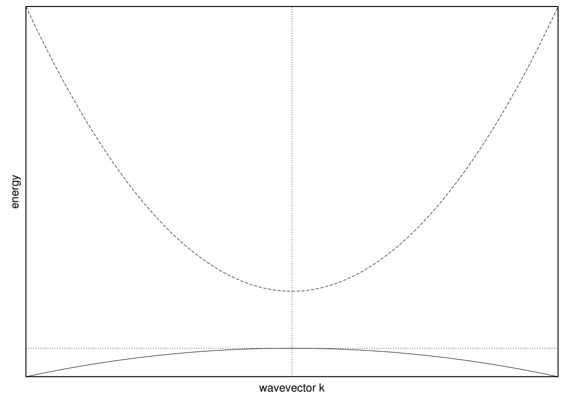

Figure 1: Semiconductors have an upper "conduction" and lower "valence" band for the allowed states. Band structure diagrams show the energy of these allowed states as a function of wavevector k.

where E_n is the particle-in-a-3D-cube energy. What is the emitted photon wavelength in terms of cube side length D and E_g? This should be a decent approximation for our quantum dots.

4. Spherical Semiconductor Dots
Real quantum dots are not perfect cubes. They're probably not perfect spheres, either, but they are much closer to spherical than cubical. Look up (give citation) or derive the energy E_n of a particle in a spherical well. Warning: you will find your self using spherical harmonics and spherical Bessel functions. In terms of E_n, the gap energy E_g, and the diameter D of the particle, what is the emitted photon wavelength?

5. Spherical Semiconductor Dots with Free Electron and Hole
A free particle has energy given by $E = \hbar^2 k^2/2m$, where k is the wavenumber. For a semiconducting material, when an electron is excited from the valence band up into the conduction band, two "quasi-free" particles exist: the electron in the conduction band and the "hole" in the valence band. Each of these "bands" represents allowed states. The degree of curvature in the band (the shape of the parabola) is determined by an "effective mass" which is **not** the rest mass of the electron. Effective masses are typically smaller within a factor of 10-100 of the rest mass of an electron.

   Thus the resulting description of the energy for a free electron-hole pair in a semiconducting spherical well is given by:

$$E = E_g + \frac{h^2}{8m_e^* R^2} + \frac{h^2}{8m_h^* R^2} \tag{2}$$

   where R is the radius of the well, m_e^* is the effective mass of the electron and m_h^* is the effective mass of the hole. In this model, what is the emitted photon wavelength?

6. More Complete Models (Bonus)
Do a literature search, considering that the negative electron and positive hole feel each other, so there will be Coulomb potential energy holding this exciton together. When quantum dots are similar in size to the exciton Bohr radius (about 2.5 nm for CdSe), the effective mass approximation starts to break down. You will find that our measured wavelengths agree with Model 5 better for the larger dots than for the smaller dots.