

10 Quantum Confinement in “Quantum dots”, Thomas Fermi Functional

We will now concern ourselves with the application of this concept to a current “niche” area called quantum dots.

1. A quantum dot is a very small chunk of semiconductor material with quantum-like properties. These are any effects that the bulk form of the same material does not possess. This phenomenon is called quantum confinement.
2. Since these particles are confined in small spatial domains, **boundary conditions of confinement apply as we learnt earlier** and this leads these substances to have quantum mechanical properties and discrete energy levels.
3. As a first approximation these materials can be understood from a particle in a box perspective.
4. We note from the previous section that as the box size reduces the energy spacing changes. Hence you may expect that the extent of confinement changes the spectroscopic properties of quantum dots.

5. This is indeed true and has been noted experimentally.

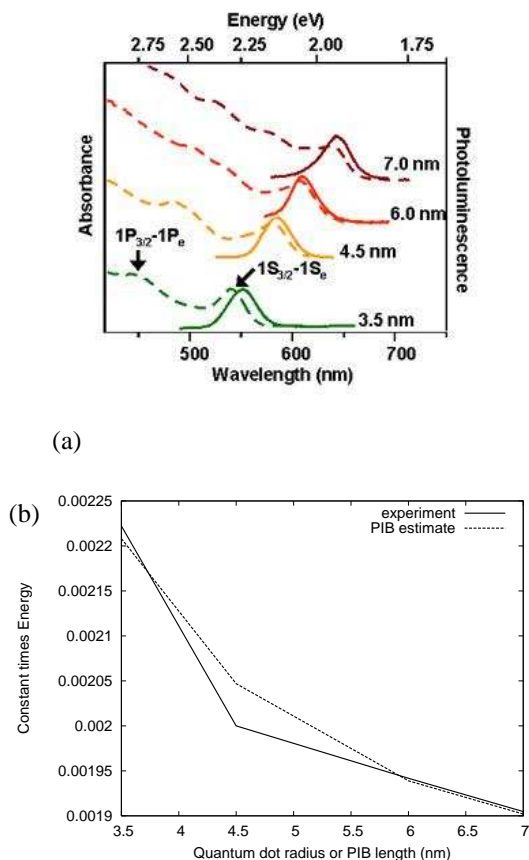


Figure 14: Figure (a): The experimental absorption peak in Cadmium Selenide quantum dots shifts with size of the CdSe nano crystal. This is quantum confinement. Figure (b): Comparison of the experimental wavelength (converted to energy) and the PIB energy which depends on $1/L^2$ where L is the box length of radius of quantum dot. The quadratic dependence of the experimental energy is clearly seen and hence these quantum dots are well described by the PIB model.

6. The excitation energy shifts with change in the size of the nano-crystal. You could interpret this as a change in box length and we know from the 3D PIB case that as the box length reduces the energy spacing increases and vice versa. This is consistent with the experimental result we see above.

7. Thus the PIB does provide a conceptually correct picture of what

happens to optical transitions in quantum dots. As a result this picture is used to understand many experiments. However, beware, this conceptual picture is in no way complete. Two other factors involved that we will discuss in class. These two factors become more clear as we proceed further in the semester.

10.1 PIB: Density of states

Consider the following picture?

This question is relevant in two regards:

1. People are interested in knowing how many electrons are accommodated in a given quantum dot if a certain “biasing voltage” is applied. (The term “biasing voltage” essentially means fixed total energy, that is fixed maximum radius of the Fermi sphere.)
2. The density of states we obtain is in fact what is used in density functional theory for the Thomas Fermi expression.

So we will derive the DOS in class.