Project A: Quantum dots

(Andrea Idini) ***andrea.idini@matfys.lth.se***

A quantum dot is a quasi two-dimensional semiconductor device build on clumps of atoms of with size between few and few hundreds nanometers. It has uses in solar cells, biomedicine, and nowadays some TV are made with a layer of nanodots particles. The reason for its versatile uses relies in the fact that it has has a shell structure. That means that the properties, e.g. energy, have complex features in functions of the number electrons present in the quantum dot. These features are effects from quantum mechanics.

In this project you will study the structure of a quantum dot. The quantum dot has a height that is much smaller than its radius. We can therefore study a 2D model of the quantum dot and see how it compares with experiments.

Set up a simple quantum mechanical model of a circular quantum dot with the radius R (choose a suitable value of R). Study two cases, namely *a* a circular 2D Harmonic Oscillator and *b)* a circular billiard. The potential energy for the two cases is:

$$V_a = \frac{1}{2}m\omega^2$$

$$V_b = \begin{cases} 0 & \text{if } r < R, \\ \infty & \text{if } r > R \end{cases}$$

Solve these two models and calculate the energy (single-particle energies) of the ground state both for (several) excited states.

Construct a single-particle diagram: that is, draw the 10-20 lowest the energy levels with the energy value in the y-axis as horizontal lines, for the two cases. Now fill the quantum dot filling the states from the lowest energy with N electrons and calculate how the total energy of the system, $E(N)$, varies by N. Keep in mind that some states can be degenerate (i.e. can hold several electrons) and consider the angular momentum and spin to find out how much. Note that the electron has an internal spin $s = 1/2$, i.e. it is one Fermion and thus follows the Pauli principle. Because the spin can assume two values in each quantum state (spin up and spin down), each calculated state can be occupied by two electrons. Furthermore, coinsidering the angular momentum you can find several states with the same energy and different angular momentum projections. For simplicity, we neglect the interaction between the electrons (note a complete account for a system of 1000 particle, will take more the age of the universe to calculate with all the computers on Earth, ask yourself why). Therefore, we can write the total energy as the sum of the N single-particle energies that we filled with the electrons. Can you calculate $E(N)$ from $N = 0$ up to $N \approx 1000$ for the two models?

In order to better see the scale structure of the harmonic oscillator, we can fit a soft function (e.g. a low degree polynomial) to $E(N)$, which we can call $\tilde{E}(N)$. The difference between the two functions, can be called the shell energy $E_{shell}(N)$. Study the scale energy of the two models and draw it as a function of electron number, N. Compare minima of the function with how the one-particle energies filled for different N (single particle diagram). Do this for the two models. How do they differ? Note that while for the Harmonic Oscillator the potential has a soft profile, the edge of the billiards is sharp, i.e. the potential energy has a discontinuity at the edge of the quantum dot.

Experimentally, one can via electron transport through the quantum dot extract the so-called addition energy,

$$\Delta_2(N) = E(N + 1) - 2E(N) + E(N - 1),$$

that is the average energy gained by adding or removing a particle (note: not $\tilde{E}$).

Calculate the addition energy for the two models for particle numbers between 2-40 and draw how the addition energy depends on the particle number. In 1996, before all the new applications, a measurement of the addition energy was made in a quantum dot with the following results:

Compare your calculations with the two models with Tarucha's experimental data.

Some more advanced theory and computational tools:

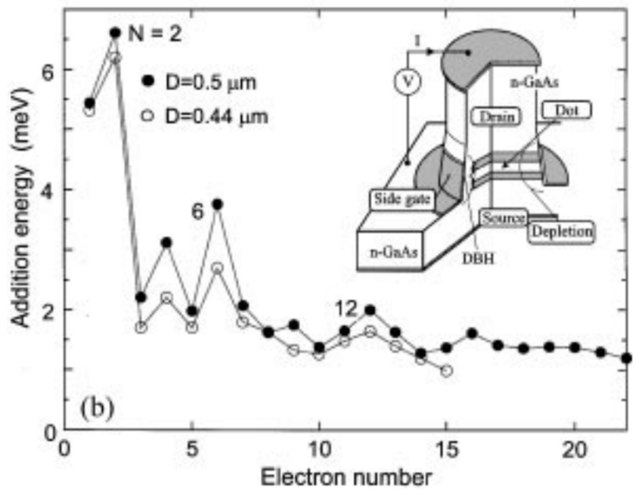

Figure 1: Tarucha et al., Phys. Rev.Lett. 77, 3613 (1996)

- S. Tarucha et al., "Shell filling and spin effects in a few electron quantum dot" Phys. Rev.Lett. 77, 3613 (1996)
- S. M. Reimann and M. Manninen. "Electronic structure of quantum dots." Reviews of modern physics 74, 1283 (2002).
- https://github.com/Scienza/Schroedinger