The Physics of Low-Dimensional Systems and Quantum Devices; Fall 2012

Computer lab: Density of States

Bring the book (Davies) to the lab. You will work in pairs during the lab.

In this lab you explore the concept of Density of States (DOS). Low-dimensional structures have a density of states that differ from that of bulk structures. Transport and optics properties of low-dimensional structures that we will discuss in the course depend heavily on the DOS of the systems.

We will consider infinite square quantum wells of different dimensionality. Dimensionality refers to the number of spatial dimensions in which particles can move freely, or at least less restricted, compared to the dimensions in which they cannot (see fig. 1). A two-dimensional system is thus a system in which electrons/holes can move (almost) freely in two dimensions while they are confined in the third.

The DOS $n(E)$ (following the notation of Davies) tells us how many electronic states there are in a small energy interval ΔE at energy E. To find $n(E)$ for a particular system, we can compute the eigen-energies E and then count how many states we have in each small energy interval ΔE. The eigen-energies we find from the Schrödinger equation

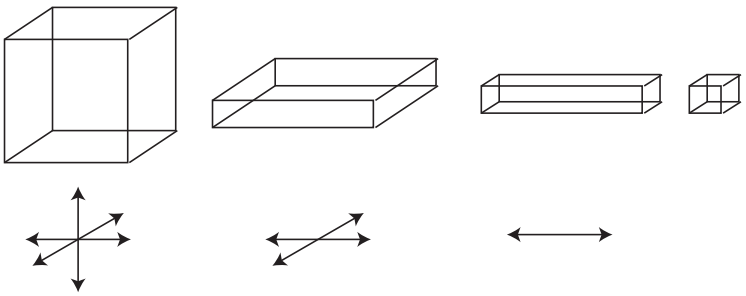
$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(x,y,z)\right)\Psi(x,y,z) = E\Psi(x,y,z)$$

The potential $V(x,y,z)$ is zero inside the quantum well, and infinite outside it. The eigenenergies E are

$$E = \frac{\hbar^2\pi^2}{2m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right)$$

To model a 3D system, we would for instance set $L_x = L_y = L_z$, or at least have the lengths with the same order of magnitude. To model a 2D system, we would set one of them considerably shorter than the other two.

In this lab, we will approach the Density of States from a brute force perspective. We will simply calculate very many eigenvalues and study how they are distributed with respect to energy. As an introduction to this, complete the following preparation problem which is intended to have you start thinking about quantum numbers of states in infinite quantum wells.



Figur 1: From left to right: 3D system, 2D system, 1D system and 0D system. Whether a specific system would be referred to as 3D or 0D really depend on the energy resolution. If we can resolve individual quantum states, that is, if the spacing between energy eigenvalues is non-negligible compared to other energy scales in the system (often thermal energy kT), then it may be relevant to think of it as a 0D system.

Preparation problem: Set $L_x = L_y = 10L_z$ (is this a 1D or 2D system?), so that the energies are given by

$$E = \frac{\hbar^2\pi^2}{2m100L_z^2}(n_x^2 + n_y^2 + 100n_z^2) = A(n_x^2 + n_y^2 + 100n_z^2)$$

where we will set $A = 1$. Now, write down the combinations (n_x,n_y,n_z) which gives us the 10 lowest energy eigenvalues. Repeat the exercise fo a 3D system ($L_x = L_y = L_z$).

At the lab: Start MatLab and download the m-files `dos.m` and `perm.m` from the course homepage.

In the m-file `dos.m` you specify the dimensions of your quantum well (`dx`, `dy`, `dz`) and also set the range of quantum numbers associated with each dimension. The subroutine `perm.m` returns all possible combinations of the quantum numbers you enter (in the variable `N`). `dos.m` then calculates the energy eigenvalue for each permutation of (`nx`, `ny`, `nz`) and stores it in `E`.

Lab task 1: Make sure that you understand what `perm.m` does. Set

```
dx=dy=dz=100
nx=1:5; ny=1:5; nz=1:2
```

Print the resulting matrix `N` which contains all the permutations to the screen and check that it agrees with your expectations.

Lab task 2: We start with a 3D system, that is $L_x = L_y = L_z$. Keep `dx=dy=dz=100` and let `nx, ny` and `nz` run from 1 to 200.

Use the command `hist` to plot a histogram of the energies. You can set the number of bins into which the values of `E` are distributed by using `hist(E,M)`. Try some different values `M` for the number of bins until you think your plot looks nice, and at least partly what you expected for a 3D system. It will exhibit a tail at high energies that we hope you find odd - why do you think this tail appeared?

Lab task 3: Now we change the settings in `dos.m` to those of a 2D system. In `dos.m`, set `dz=1` and `nz=1:10` and run it again (why do we reduce `nz`?). This probably looks nothing like you expected (what did you expect?). We need to make some more changes. Let `nx` and `ny` run up to 1000, and reduce `nz` so that it only runs to 10. Does it look any better now? Do you have any idea why?

Lab task 4: Now for the 1D system. Try to figure out settings which gives you what you want (and what is that?), but if you cannot seem to find good settings you can use these, which should give you a nice 1D system.

```
nx=1:20000; ny=1:8; nz=1:8;
dx=3000; dy=1; dz=1;
```

Now, there is a series of peaks in the histogram. Can you calculate, by hand, from the dimensions of your 1D system, the energies at which the first five peaks should appear? Compare to your plot!

If you want to: go back to, or replot, your 2D plot and redo the exercise - that is, find the energies where the first 3 or so steps occur.