Density of states

Let's consider a three dimensional quantum well, with equal lengths of each side. If we try to calculate the energy levels that are allowed, we start by breaking the problem up via separation of variables. Recall, that Schrödinger's equation is the wave version of a Hamiltonian… This means that it is essentially a description of the total energy of the system. A three dimensional potential, so long as it is conservative can be easily separated according to the axes of space (x,y,z for example). If you have not heard of the idea of a conservative potential, the concept is simply this: any path between two points should end up with the same change in kinetic energy. For example, if you walk from a valley to a hilltop, it does not technically matter if you went straight up the hill or went on a long winding path, even if that path took you over a mountain. It only matters that any energy spent climbing an extraneous hill is reclaimed when going back down. A non-conservative potential landscape could be imagined if one of the paths involved walking through a muddy swamp. We are not going to worry about such issues here, so in the case of our 3-D quantum well, we can readily state that the potential can be treated with separation of variables.

Kinetic energy is always separable. If you want proof of that, imagine walking on the side of the road when you are just barely brushed by a car driving at high speed. Assuming there are no mirrors or other protrusions to hit you, the worse you would experience is some friction. Far better than if the car hit you head on! If the kinetic energy could not be separated according to the orthogonal directions, you would have been in a world of hurt no matter how it hit you!

What does this mean for us? It makes this problem much simpler to solve… all we have to do is solve three unrelated 1-D quantum wells, just like we did the first week of class! In that case, then recall that the energy levels are described as follows:

$$E = \frac{\hbar^2 \pi^2}{2mL^2} n_?^2$$

Note that I added a subscript to the quantum number n. The reason for this is that we will end up with three distinct quantum numbers, which can then be labeled as $? = x,\ y,\ or\ z$, for each axis. The energy, E, as listed then is not the total energy, we have to sum of the energies for each axis to get the total energy:

$$E = \frac{\hbar^2 \pi^2}{2mL^2} \left(n_x^2 + n_y^2 + n_z^2 \right)$$

Now let's try an exercise: Ignore the term before the quantum numbers and calculate the energies of the following unique quantum states:

n_x	n_y	n_z	Energy
1	1	1	
1	1	2	
1	2	1	
2	1	1	

Notice anything? The last three quantum states have the same energy. Big deal? Yes it is because we have a limited number of ways to probe a quantum system experimentally to find out any information about it. Energy is the most common and most useful way. So here we have a situation where we would not be able to tell which state the system is in. Moreover, assuming we are working with electrons, the Pauli exclusion principle states that any fermion, such as an electron, must have a unique set of quantum numbers. So, if we imagine filling this quantum well with electrons, we would observe the following; As we raise the energy of the electrons we are pushing into the system (increase the voltage applied to the terminals feeding the electrons in) we first see that two electrons enter the system at one energy. As we raise the energy more, we notice that six electrons entered at a slightly higher energy. This continues, with the numbers always being even, but varying in value from level to level. If one didn't know about the "degeneracy" of the energy levels, as it is called, this would probably be very confusing.

The same thing happens for continuum states as well. Understanding this is not really that difficult: If you could only probe energy, a car travelling east and a car travelling north at the same speed would be considered to be in degenerate states. Of course the math for this is a bit more involved than that, but not by much. However, since there are only a select few dimensionalities in which we can consider a quantum system (3-D, 2-D, 1-D, and 0-D), I will simply state what the formulas are. By the way, the key to all of this is that we care about energy, but the quantum system cares about the momentum, since that is directly related to the wavelength.

3-D

$$D(E) = \frac{8\pi\sqrt{2}}{h^3} m^{3/2} \sqrt{E - E_{min}}$$

Note that E_{min} here refers to the minimum energy that an electron or hole could possibly have (The edge of the band in a 3-D material).

2-D

$$D(E) = \frac{4\pi m}{h^2}$$

I need to stress that now that we have discrete energy levels here, this density of state is for *each* state! When the energy is high enough to access the next state, a new density of state function is added to the ones for the lower states, which are still accessible. If that does not make sense, think about it this way: At the lowest energy where the next state is accessible, the momentum of the electron in that state will be zero. But a 2-D well has two axes where the electron can have any momentum value because there is no quantum confinement and thus no restriction on wavelength/momentum. So, it is still possible at that same energy to add an electron to a lower quantum level, it just will have to have non-zero momentum. This results in a staircase effect in the density of states for the 2-D system as you will see in the figure below.
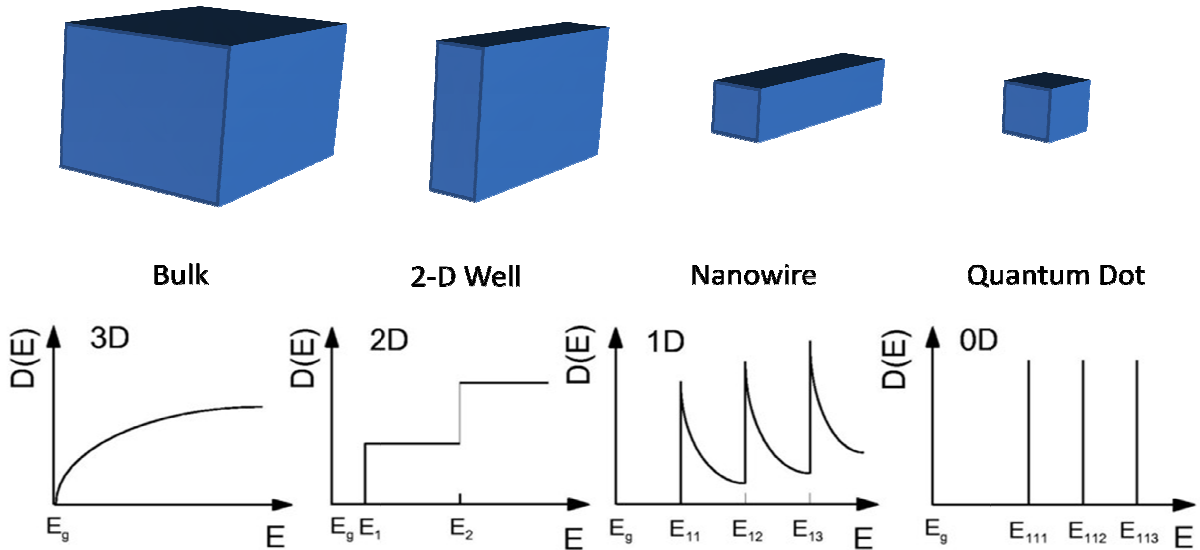
1-D

$$D(E) = \sqrt{\frac{2\pi m}{h^2}} \frac{1}{\sqrt{E - E_{min}}}$$

0-D

This is a trivial case, there are no axes that have a continuum of allowed momenta, so the rule is simply, there are two states for each unique set of quantum numbers (this accounts for electron spin).

Summed up in a chart:

You will note that there are clear trends in the density of states, *D(E)*, as a function of dimensionality. To determine the number of electrons at any energy, we would take the density of states and multiply by the Fermi distribution:

D(E) N(E)

E E
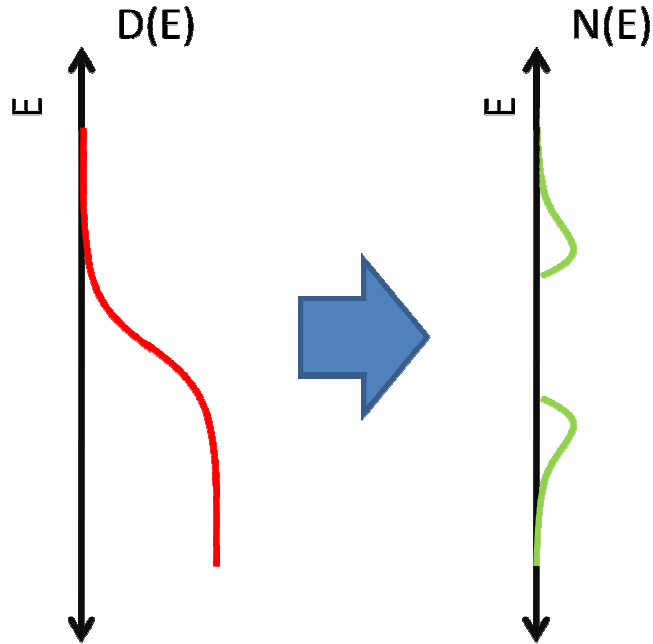
There are two things to note from this: The first being that the only electrons and holes that are available are clustered near the band edges. The second being a little trick I did on the valence band. If I was interested in electrons for that band (I am not), then I would actually have a large number of electrons. But I am not interested in the electrons because they do not contribute to conductivity if they are in the valence band. Rather, I am interested in the holes. The Fermi function for the holes is simply

$$F_h(E) = 1 - F_e(E)$$

Thus the available holes are also few in number.