three-dimensional quantum problems

The one-dimensional problems we've been examining can can carry us a long way — some of these are directly applicable to many nanoelectronics problems — but there are some important problems that are inherently three-dimensional. We need to know how to handle those. Fortunately, the approach is not significantly different from the 1-D approach. Not surprisingly, the math can become more involved.

The extension to 3 dimensions requires a modification of the kinetic energy term, since momentum is, in general, a vector.

$$\hat{p_x} \rightarrow -i\hbar\frac{\partial}{\partial x} \qquad\qquad \hat{\vec{p}} \rightarrow -i\hbar\vec{\nabla}$$

$$\vec{\nabla} = \frac{\partial}{\partial x}\vec{a_x} + \frac{\partial}{\partial y}\vec{a_y} + \frac{\partial}{\partial z}\vec{a_z}$$

With that change, the time-independent Schrödinger equation in 3-D is

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x,y,z) + U(x,y,z)\,\psi(x,y,z) = E\psi(x,y,z)$$

$$\nabla^2\psi(x,y,z) = \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}$$

(For time-independent potentials, the time dependence can be separated out in the 3-D case just as it was in the 1-D case, and the time-dependence will be of the form exp(-$i\omega t$).)

In 3-D, the free-electron S.E. is

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x,y,z) = E\psi(x,y,z)$$

The simplest solution is still a plane wave, but the form is slightly more complex:

$$\psi(\vec{r}) = A\exp\left(i\vec{k}\cdot\vec{r}\right)$$

$$\vec{k} = k_x\vec{a_x} + k_y\vec{a_y} + k_z\vec{a_z}$$ <u>wave vector</u>

$$\vec{r} = x\vec{a_x} + y\vec{a_y} + z\vec{a_z}$$ <u>position vector</u>

The above solution represents a plane wave traveling in the direction of the wave vector.

The energy still has a familiar form

$$E = \frac{\hbar^2k^2}{2m} \quad \text{where} \quad k^2 = k_x^2 + k_y^2 + k_z^2$$

Exercise: Check that the wave function above is a solution to the 3-D free-electron S.E. with the energy as given. Also, show that the 3-D result reduces to the 1-D if $k_y = k_z = 0$.

As we increase dimensions, there will be a corresponding increase in the "quantum numbers" for a given problem.

For instance, for a 1-D plane wave or a 1-D quantum well, there was only one parameter to characterize a state: k in the case in the wave or n for the well. A 3-D plane wave requires three wave-numbers, k_x, k_y, and k_z. Even though we have yet to see it, you might guess that a 3-D quantum well will need three quantum numbers. (n_x, n_y, n_z ?) The hydrogen atom will also need three parameters (n, l, m_l). There is a direct correspondence between the number of dimensions and the number of quantum indices required.

Solving the 3-D Schroedinger equation looks daunting, but often can be approached using the old separation of variables trick.

If the potential function depends on only one dimension, or can be written as a sum of 3 one-dimensional potentials, then separation of variables will work.

$$U(x,y,z) = U(x) + U(y) + U(z)$$

In that case, you would start by writing the full wave-function as the product of three wave-functions, each of which depends on only one variable.

$$\psi(x,y,z) = \psi_x(x)\,\psi_y(y)\,\psi_z(z)$$

Inserting into the 3-D Schroedinger equation:

$$-\frac{\hbar^2}{2m}\nabla^2\left[\psi_x(x)\,\psi_y(y)\,\psi_z(z)\right]$$

$$+\left[U_x(x)+U_y(y)+U_z(z)\right]\left[\psi_x(x)\,\psi_y(y)\,\psi_z(z)\right]$$

$$=E\left[\psi_x(x)\,\psi_y(y)\,\psi_z(z)\right]$$

Nasty.

Work through the derivatives, and then divide everything by

$\psi_x(x)\,\psi_y(y)\,\psi_z(z)$

$$-\frac{\hbar^2}{2m}\frac{1}{\psi_x(x)}\frac{\partial^2\psi_x(x)}{\partial x^2}+U_x(x)$$

$$-\frac{\hbar^2}{2m}\frac{1}{\psi_y(y)}\frac{\partial^2\psi_y(y)}{\partial y^2}+U_y(y)$$

$$-\frac{\hbar^2}{2m}\frac{1}{\psi_z(z)}\frac{\partial^2\psi_z(z)}{\partial z^2}+U_z(z)=E$$

The long equation divides into three pieces. Each piece is a function of only one variable. The 3 pieces together sum to a constant.

$$f(x) + f(y) + f(z) = E$$

The only way that this can be true for all values of x, y, z is if each piece is individually equal to a constant.

$$f(x) = E_x \qquad f(y) = E_y \qquad f(z) = E_z \qquad E = E_x + E_y + E_z$$

OK, now we're getting somewhere. Through separation of variables, we turned one 3-D problem into three 1-D problems. And we know a little bit about solving some 1-D problems.

in x: $$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi_x(x)}{\partial x^2} + U_x(x)\,\psi_x(x) = E_x \psi_x(x)$$

and similar for the other dimensions.

Example: quantum dot

As an example, consider the situation of an electron confined in all three dimensions by infinitely high barriers. The barriers are located at planes defined by $x = 0$, $x = L_x$, $y = 0$, $y = L_y$, $z = 0$, and $z = L_z$. The potential can be viewed as three 1-D barrier problems – one for each dimension – added together.

As we've seen, the analysis is made much easier by the fact that we can break this into three identical and well-known 1-D problems.

Using the previously obtained results for the 1-D infinitely deep well.

$$\psi_x(x) = A_x \sin(k_x x) \qquad \psi_y(y) = A_y \sin(k_y y) \qquad \psi_z(z) = A_z \sin(k_z z)$$

$$k_x = \frac{n_x \pi}{L_x} \qquad k_y = \frac{n_y \pi}{L_y} \qquad k_z = \frac{n_z \pi}{L_z}$$

$$E_x = \frac{n_x^2 \pi^2 \hbar^2}{2mL_x^2} \qquad E_y = \frac{n_y^2 \pi^2 \hbar^2}{2mL_y^2} \qquad E_z = \frac{n_z^2 \pi^2 \hbar^2}{2mL_z^2}$$

Inserting the pieces to form the complete solution:

$$\psi(x, y, z) = A \sin(k_x x) \sin\left(k_y y\right) \sin(k_z z)$$

$$E = \frac{n_x^2 \pi^2 \hbar^2}{2mL_x^2} + \frac{n_y^2 \pi^2 \hbar^2}{2mL_y^2} + \frac{n_z^2 \pi^2 \hbar^2}{2mL_z^2}$$

Each state is characterized by the three quantum numbers, n_x, n_y, n_z. We can denote the different states $(n_x\ n_y\ n_z)$

Note that in some cases, different states will have the same energy. This is known as degeneracy. For example, if the quantum box is a cube ($L_x = L_y = L_z$), then states with quantum numbers (2 1 1), (1 2 1), and (1 1 2) will all have the same energy and so are *degenerate*. There are many other degenerate combinations.