# Quantum Physics, Preparation for Friday, Mar. 22

## Study Q11.6 and Q12.1 to Q12.3

You're finishing Q11 and starting Q12, but we are not going to dive into the numerical approaches in Q12.4 and Q12.5.

In Q11.6, the fermion gas ideas that you learned about in Rebecca's presentation will be applied to conductors and semiconductors.

In Q12.1 to Q12.3, Moore introduces Schrodinger's equation, but then in Q12.4, the first thing he says is, "we will not attempt to solve Schrodinger's equation mathematically in this course," and then he launches into numerical methods.

Numerical solutions are great, but actually there are several problems that are within your reach mathematically, so after you finish Q12.3, but before you start Q12.4, I am going to introduce you to some of these problems. Also, guessing a solution and then showing that it works is a perfectly fine way of "solving" Schrodinger's equation, and a lot of the time, that will be our strategy.

## Presentation

Emma: Applying the ideas of Example 11.1 to other molecules (caffeine?!)

## For Problem Set 13

### Properties of semiconductors

1. Q11B.10 p. 179.

2. Q11B.12 p. 179.

### An application of Example 11.1

3. Q11M.11 p. 180, Moore is helping us reason about the oxacarbocyanine family of molecules.

### A new type of particle-in-a-box problem

4. We have put quantons in boxes and demanded that they cannot go outside the box. Now we are going to start investigating a more realistic case, where it is just very unlikely — but not impossible! —

for them to be outside the box. Consider the following potential: the potential will be $V_0$ high for $x > L/2$ and $x < -L/2$. In between the potential is 0. Consider a quanton that is stuck in this box and that it has an energy $E_n$ (or, actually, one of various energies labeled by an integer $n$), **and that $E_n < V_0$ but also $E_n > 0$.** Because of the assumptions in the description above, classically the particle can bounce between the walls, but never penetrate them (because it doesn't have sufficient total energy to get into the region where the potential is $V_0$).
(a) Graph the potential. Make a nice graph, because you will be adding to it later.
(b) Classically, we know the particle's momentum in the region where the potential is 0. Solve $E_n = \frac{p_n^2}{2m}$ to get $p_n$. Quantum-mechanically, the momentum corresponds to a wavelength. Write down the wavelength too.
(c) In the region between $-L/2$ and $L/2$ does $\psi_n(x) = c\cos\frac{p_n x}{\hbar}$ solve $E_n\,\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}$ the Schrodinger equation? How about $\psi_n(x) = d\sin\frac{p_n x}{\hbar}$? How about the linear combination $\psi_n(x) = c\cos\frac{p_n x}{\hbar} + d\sin\frac{p_n x}{\hbar}$?
NOTE: There is no need to find the constants $c$ and $d$. That would be txhe job of normalization at some later stage of doing a complete solution.

5. In the regions $x > L/2$ and $x < -L/2$, the potential is $V_0$ — not 0 — so there we need $E_n\,\psi_n(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi_n}{dx^2} + V_0\,\psi_n(x)$.
(a) Our function $\psi(x) = c\cos\frac{p_n x}{\hbar} + d\sin\frac{p_n x}{\hbar}$ cannot work in these regions, no matter what (real number) we change $p_n$ to be. Demonstrate this.
(b) In these new regions try the function $\psi(x) = a e^{-\kappa_n x/\hbar} + b\, e^{\kappa_n x/\hbar}$ (the new Greek letter I am using is "kappa"). What is the formula for $\kappa_n$ in terms of the givens $E_n$, $V_0$, and $m$ that makes this work?
(c) In the region $x > L/2$, the function $e^{\kappa_n x/\hbar}$ has a big problem. What is it? Why is $e^{-\kappa_n x/\hbar}$ ok in this region?
(d) In the region $x < -L/2$, the function $e^{-\kappa_n x/\hbar}$ has a big problem. What is it? Why is $e^{\kappa_n x/\hbar}$ ok in this region?

6. Go back to the nice graph you in 4(a) and now we will embellish it.
(a) Knowing what you just discovered in 5(c) add to your graph what the wave function must look like in the region $x > L/2$. Don't worry about normalization.
(b) Knowing what you learned in 5(d), you also have an idea what the wave function look must look like in the region $x < -L/2$? Although I have said you don't have to worry about normalization, choose the constant multipliers so that the regions of the wave function you have drawn so far is even.
(c) In 4(c) you discovered the linear combinations that work in the region $-L/2 < x < L/2$. What does being an even function demand about this linear combination?
NOTE: You could of course be considering the odd case, but in 6(b), you already went down the path of doing the even case, and we are staying on that path.
(d) Given what you learned in 6(c) add to the graph a possibility that can complete the wave function.
NB: Wave functions must be continuous and they cannot even have kinks! The reason is that a second derivative of a kink is infinite and $p^2/2m$ is represented as a second derivative. There is actually an exception to the no-kinks rule, when the potential also is infinite, but in this problem $V_0$ is finite.