Physics 222 CID ____________

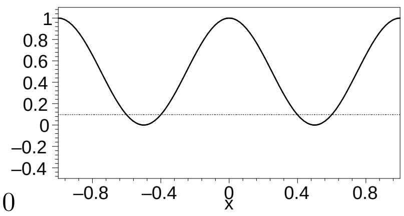
Lab 7 - Band Theory

Score ________ / 10

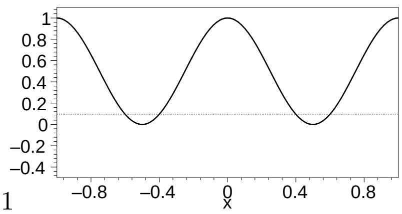
We saw in the last lab that when I had a double well potential I ended up with energy eigenstates that came in pairs. For example, the ground state and the first excited state differed only by a zero crossing between the two wells. This zero crossing occurred where the wave function was small and therefore didn't change the energy of the state much, resulting in a ground and first excited state which were nearly the same energy. Likewise the second and third excited states had nearly the same energy, differing again only by a zero crossing between the wells.

So what happens when I have many wells which are regularly spaced? This turns out to be of significant importance, because that's exactly what crystalline solids are. Each ion in the crystal generates a potential well for the valance electrons. Since the ions are regularly spaced, the electrons see a periodic potential of regularly spaced potential wells. As you might expect, if we have N such potential wells in a row, we get energy eigenstates which come in clusters of N!

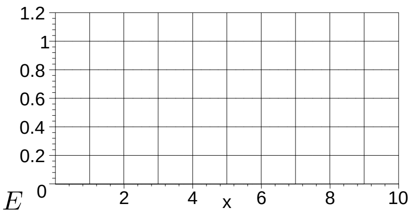
Open the program (if it is not already open), and lets generate a periodic potential with 2 wells. Enter the potential `1-sin(pi*x)^2`, set "mass/hbar^2" to 500, and click "recalculate." Sketch the $n = 0$ and $n = 1$ wave functions and the energies of the first 10 eigenstates below.



$n = 0$



$n = 1$



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Now lets see what happens when we increase the number of wells. Change the potential to `1-sin(a*pi*x)^2`, where *a* is an integer, with the values of *a* in the table below. After entering each value of *a*, click on "recalculate" and fill in the number wells and the number of energy levels per energy "band" in the table below each value of `a`.

a =	2	3	4	5
# of wells	______	______	______	______
levels per band	______	______	______	______

Now set *a* to 20 and take a look at the wave functions for various values of n. It should look an awful lot like the stationary states for a particle in an infinite square well. In other words, an electron moving around in the periodic potential of a piece of metal has energy eigenstate wave functions which look almost like the wave functions for a free particle in a box the same size as the piece of metal! So is there any effect of having the metal there at all? Yes! Although the wave functions have the same shape as a free particle, the energies of the different states are not the same as they would be for a particle in a box. In the following part of this lab we will see what effect this has.

While you look at these wave functions, answer the following questions. Remember that in the program everything is in S.I. units. For example, the x axis of the upper plot runs from -1 to 1 *meters*.

What is the wavelength and wavenumber of the $n = 0$ state?

What is the wavelength and wavenumber of the $n = 2$ state?

What is the wavelength and wavenumber of an arbitrary state as a function of n?

With this relation we can see an interesting effect of the periodic potential. Look at the plot of energy vs. n. If this were a free particle, the total energy would just be the potential in the well (which depends on what we define zero potential to be) plus the kinetic energy, which ought to increase as $p^2/2m = \hbar^2 k^2/2m$. In a periodic potential, it turns out that the energy does go as $U + A \cdot p^2$ (where U and A are a constants) as long as we are close to the top or bottom of a band. But A is not equal to $1/2m$. As such we often define an "effective" mass m^* for the particle which is equal to $1/2A$. To find the effective mass, simply take the energy and wavenumber for two different states, write down the relation $E_n = U + \hbar^2 k_n^2/2m^*$ for the two states, and solve the two equation for the two unknowns (U and m^*). Do this in the space below using the $n = 0$ and $n = 5$ states. Instead of solving for m^*, however, solve for $m^*/\hbar^2$, since that is what we entered into the computer simulation.

$m^*/\hbar^2 =$____________

$U =$____________

Now to ensure that the particle's dispersion relation ($\omega(k)$ which is really the same thing as $E(p)$) really looks like a free particle by doing the same calculation but using the energy and wavenumber for the $n = 5$ and $n = 10$ states. Enter the values you get below:

$m^*/\hbar^2 =$____________

$U =$____________

Because the zero-point energy is fairly high compared to the top of the periodic potential, you should get an effective mass which is close to the real mass. For this problem we were near the bottom of the lowest band. If you are near the top of the band, the dispersion relation has the opposite curvature, and you actually get a negative effective mass!.

If you are curious, you could enter a square well potential (`1-squarepulse(x)`) and see that the energy levels appear to be quadratic in n which is just proportional to k.