Phys 472 Assignment 5 Due Oct. 9, 2020, before 9:00 am Marsiglio, Fall 2020

***** Please show your work, and include a copy of all programs used!*****

1. (a) For the Kronig-Penney model, with $V(x) = V_0$, for $0 < x < w$, and $V(x) = V_1$, for $w < x < \ell$, and this repeated indefinitely with period $\ell = w + b$, we derived the equation, in class,

$$\cos(k\ell) = \cos(k_1 w)\cosh(\kappa_2 b) + \frac{\kappa_2^2 - k_1^2}{2\kappa_2 k_1}\sin(k_1 w)\sinh(\kappa_2 b), \qquad [1]$$

which gives energies for $E < V_1$, where k is a quantum number with $-\pi/\ell < k \leq \pi/\ell$, and

$$\frac{\hbar^2 k_1^2}{2m} \equiv E - V_0, \qquad \text{and} \qquad \frac{\hbar^2 \kappa_2^2}{2m} \equiv V_1 - E.$$

Derive the equation that applies for $E > V_1$. You are allowed (encouraged!) to use Mathematica, or any other software, but if you do be certain to include the program with your assignment, with clear instructions (i.e. comments) on what you are doing. How is this equation related to the previous one (i.e. how could you have done this simply without recalculating the determinant) ?

(b) Plot the right-hand-side of this equation as a function of E (from $E = 0$ to $E = 700$ eV), and illustrate the regions in which solutions exist. Use $V_0 = 0$ and $V_1 = 360$ eV, $w = 1.5a_B$, and $b = 0.5a_B$ for definiteness, where a_B is the Bohr radius. Comment on the characteristics of the solutions.

(c) (i) Solve for the first few energy bands, i.e. E vs. k, and plot these for the case above. Use $k\ell/\pi$ for the x-axis, with domain $-1 < k\ell/\pi < 1$, and E (eV) for the y-axis with range $0 < E < 1400$ eV. *Hint: there is nothing to "solve" here! You might choose a value of $k\ell$ and then iterate on the right-hand-side (RHS) of Eq. [1] to figure out the E, but this would require work. Instead, pretend for a moment that you want to plot $k\ell$ vs. E. You would then choose a range of values of E, and for every E, simply take the arc-cosine of the RHS,* **provided it had magnitude less than unity**. *If it doesn't have magnitude less than unity, then there is no solution and you move on. Once you have done this you have two columns of numbers, one for E and the second for the corresponding value of $k\ell$ (if a solution to Eq. [1] exists). So now you just plot the result (not column 2 vs column 1, but column 1 vs column 2!*

This should illustrate the first 6 energy bands (and part of the 7th). On the same plot (use a different colour) plot the bands that correspond to $V_0 = 0$ and $V_1 = 0$ (or use 0.00001 eV if your program complains) with the same well and barrier widths. This choice of parameters corresponds to an "empty lattice" (this problem has no wells and/or barriers!), but doing it this way allows us to carry out the thought experiment of reducing the barriers to essentially zero height for a (still!) periodic potential.

What do the curves for the empty lattice correspond to? *Hint: students of PHYS 415 have an advantage here, because they have learned or will learn about the "folding" of* *energy bands into the first Brillouin zone, and reduced, repeated and periodic zone schemes. If you allow k to vary over all space, and translate the folded bands in your figure to other "Brillouin zones" (i.e. beyond $-\pi/\ell < k < \pi/\ell$) then it will become clear that these empty lattice curves form a parabola. That's a big hint...in fact it is the answer!*

One of the take-away messages here is the energy gaps that are now present. This allows a simple delineation of metals vs insulators. Notice in particular that gaps exist for energies well above the top of the barriers (airplanes flying above a periodic terrain are not allowed to travel at certain speeds!).

(ii) Lets now focus on the lowest band of energies. It looks pretty flat, right? Choose a range of energies $34 < E < 40$ eV, and plot the energy (in eV) vs. $k\ell/\pi$ with $-1 < k\ell/\pi < 1$, as before. Just for fun plot $E = E_0 - 2t\cos(k\ell)$ on the same plot, with $E_0 \approx 37.31$ eV and $t \approx 2.52$ eV. Not too bad a fit, right? For this assignment I figured this out "by hand" (iterated a bit) but see the Scientific Reports paper for a systematic procedure that provides an actual formula for figuring out these numbers in terms of more "microscopic" parameters. This tells us that a simple description (dispersion given by a cosine curve) is reasonably accurate.

(iii) Note how at the $k = 0$ and $k = \pi/\ell$ points the dispersion looks parabolic (it is!). This means you can write the dispersion in either of these regions as $\hbar^2 k^2/2m_e^{\text{eff}}$ for k values near $k = 0$ and $\hbar^2(k - \pi/\ell)^2/2m_h^{\text{eff}}$ for k values near $k = \pi$. This defines an *effective* mass for "electrons" as m_e^{eff} and an *effective* mass for "holes" as m_h^{eff} (this one is negative!). They are called holes because when this band is nearly filled with electrons (so we are focussing on $k = \pm\pi/\ell$), it is simpler to keep track of the empty states (holes). Can you tell at a glance whether the magnitude of the effective mass is different for electrons (at $k = 0$) than it is for holes (at $k = \pm\pi/\ell$). If so, which is larger, and why is this so, physically? *Hint: The effective mass is connected to the curvature (2nd derivative of the dispersion) and if the equation $E = E_0 - 2t\cos(k\ell)$ fit the Kronig-Penney result perfectly, then the magnitudes of the two effective masses would be the same.*