Problem set 5

1. Hybridization allows us to understand the properties of chemical bonds and plays a central role in polymers and other organic materials. Specifically the carbon atom can undergo sp, sp\(^2\) and sp\(^3\) hybridization, which explains the richness of bonding configurations associated with the carbon atom. A hybridized orbital is a wavefunction made up of a linear combination of energy eigenfunctions. Hybridized orbitals occur when the atom is subjected to an additional potential provided by a nearby atom. Assume that the second shell of the carbon atom orbital has “hydrogen-like” eigenfunctions and calculate the following hybridization orbitals, plot the radial and angular part and comment on it (e.g. average particle distance from the origin, new angular dependence etc.):
   a) linear hybridization sp:
   \[
   \psi_+ = u_{2s} + u_{2p_0}, \\
   \psi_- = u_{2s} - u_{2p_0}
   \]
   b) planar hybridization sp\(^2\):
   \[
   \psi_1 = \frac{1}{2\sqrt{3}} \left( 2\psi_s + \sqrt{2} \psi_{p_0} + \sqrt{2} \psi_{p,1} \right) \\
   \psi_2 = \frac{1}{2\sqrt{3}} \left( 2\psi_s + \sqrt{3} - 1 \psi_{p_0} - \sqrt{3} + 1 \psi_{p,1} \right) \\
   \psi_3 = \frac{1}{2\sqrt{3}} \left( 2\psi_s - \sqrt{3} + 1 \psi_{p_0} + \sqrt{3} - 1 \psi_{p,1} \right)
   \]
   c) tetragonal hybridization sp\(^3\):
   \[
   \psi_1 = \frac{1}{2} (\psi_s + \psi_{p_0} + 2\psi_{p_1}) \\
   \psi_2 = \frac{1}{2} (\psi_s - \psi_{p_0} + 2\psi_{p,1}) \\
   \psi_3 = \frac{1}{2} (\psi_s - \psi_{p_0} - 2\psi_{p_1}) \\
   \psi_4 = \frac{1}{2} (\psi_s + \psi_{p_0} - 2\psi_{p,1})
   \]

2. Nanoparticles are being developed for a variety of interesting applications ranging from energy conversion in solar cells to non-linear optical devices for telecommunications. And obviously a multitude of electronic devices such as FET’s (Field Effect Transistors). Consider a particle in a 3D potential:
\[
V(r, \theta, \phi) = \begin{cases} 
0 & r < R \\
\infty & r > R
\end{cases}
\]
this problem (the best approximation of a real quantum dot) can be solved exactly using spherical Bessel functions. We will find estimates for the ground state energy using the variational method.
a) we start with a trial function of the form \( \psi(r, \theta, \varphi) = A(\theta, \varphi)r^\lambda + B(\theta, \varphi)r^\mu \), with A,B complex and \( \lambda, \mu \) real and \( \lambda > \mu \)
Assuming that the ground state has angular momentum \( l=0 \) and using the boundary conditions, show that the normalized \( \psi(r, \theta, \varphi) \) must be:

\[
\psi(r, \theta, \varphi) = \begin{cases} 
N(R^2 - r^2), \lambda > 1 \text{with} |N|^2 = \frac{3(2\lambda + 3)(\lambda + 3)}{8\pi \lambda^2 R^{2\lambda + 3}} & r < R \\
0 & r > R
\end{cases}
\]

b) using the latter expression for \( \psi(r, \theta, \varphi) \), calculate the approximate ground state energy as a function of \( \lambda \) and minimize its energy.

3. Consider a one dimensional square potential \( V(x) = V_0 \) with a width \( d \), exactly like the one in the last problem set. Assume that a wave-packet is traveling in space from minus infinity to plus infinity. We can always write the mathematical expression for this wave

\[
\psi(x) = \int c(k)\psi_k(x)dk
\]
packet as follows:

\[
k = \frac{\sqrt{2mE}}{h} \\
\psi_k = Ae^{ikx}
\]
Each single wavefunction interacts with the barrier independently so we can safely assume that the transmission coefficient that was calculated in the last problem set for a single k was correct.

a) Use that transmission coefficient and plot is in function of k. Note that to do that you have to express the wave-vector \( k' \) of the waves in the barrier region of space a function of k first. (show that \( k' = \sqrt{k^2 - \frac{2mV_0}{h^2}} \))

b) Now assume that \( c(k) = e^{-k^2} \). Write the transmitted curve as

\[
\psi(x) = \int c'(k)e^{i\varphi(k)}\psi_k(x)dk
\]
and plot \( c(k) \), \( c'(k) \) and \( \varphi(k) \) as a function of k

c) Comment on the shape of the function before and after the barrier and discuss the difference with the same problem in classical mechanics.

d) (30 extra points) In today’s science presenting the resulting visually is very important. Visit the following website

http://www.kfunigraz.ac.at/imawww/thaller/ and try to write a mathematical code that does a movie of this wavepacket going through the barrier using the color code seen in class.

This part of the exercise will help you with your carriers.

4. One of the major, if not the major, challenge in modern electronics is shrinking device sizes. One piece of the problem is putting metallic conductor close together. Discuss as a function of possible conductive metals the localization/delocalization of the electrons that run through the wires. Further discuss the effect of the size (width and/or cross section) of the wires, is there an absolute minimum or is that minimum material dependent.

Modern CPU are shifting from silver to copper, can you explain why, is there a reason why people are not using/considering alloys?