Aghia Paraskevi, 9 Feb 2024

QY2 – Quantum Devices
HOMEWORK

Guidelines:

- *Use the slides from the lectures*
- *Use suggested bibliography*
- *Use tables of physical constants values, if numerical results are asked*
- *Use your favorite software to generate plots (e.g., Excel, Python, Matlab)*

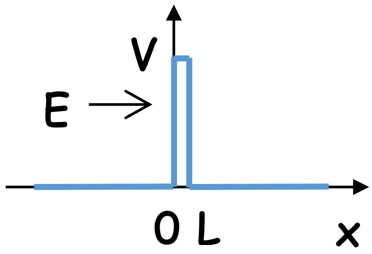
Submission by e-mail, deadline Feb, 26 2024.

Good luck!

Tutor
P. Dimitrakis

Exercises

1. Electron is moving towards an energy a square energy barrier as shown in the picture. If the energy of the electron is E_0 and the barrier height V, which of the following will increase the likelihood of tunneling?
   a) decrease the height of the barrier
   b) decrease the width of the barrier
   c) decrease the mass of the particle
   (*explain briefly*)



2. What is the energy of the electron in (1) that has successfully tunnel through the barrier? (explain briefly)
   a) < initial energy
   b) = initial energy
   c) > initial energy

3. According to the figure above, the electron is approaching the energy barrier height having total energy 8.6eV and the barrier height is 14.2eV. If the width of the barrier is 1.2 nm, what is the probability that the electron will tunnel through the barrier?
   i. What is the probability if the width of the barrier reduced by 50%?
   ii. For the case (i), i.e., barrier's width is 0.6nm, make a plot of the transmission coefficient T considering that the energy of the electron varies from 0.1eV up to 10eV

   Assume that the electron's mass in the barrier remains constant.

4. Graphene is a two-dimensional material, $\boldsymbol{k}=(k_x, k_y)$ with thickness one atom. The energy dispersion relations (band structure) are given by the following equation

$$E_{\pm} = \pm t\sqrt{1 + 4cos\left(\frac{3}{2}k_x a\right) cos\left(\frac{\sqrt{3}}{2}k_y a\right) + 4cos^2\left(\frac{\sqrt{3}}{2}k_x a\right)}$$

   Where (+) stands for the conduction band (E_C), (-) for the valence band (E_V), t is the nearest-neighbor (π orbitals) hopping energy ca. 2.8 eV and a is the lattice constant, ca. 0.246 nm.
   i. Calculate the energy bandgap of a (single layer) graphene. Comment your result.
   ii. Calculate the effective mass for electrons and holes. Comment your result.

Hint: (a) *If you want to plot the E(k), keep in mind that $k_{x,y}=2\pi/a$ and for simplicity plot E/t. Thus, $k_{x,y}=[-1, 1]$ and E/t is dimensionless, i.e., has no units. Finally, no numerical values for t and a are needed.*
(b) Energy gap $E_g=\min\{E_C-E_V\}=\min\{E_+ - |E_-|\}$.
(c) Calculate symbolically (not numerically), if possible, the effective mass in x-direction m_x, and m_y. For numerical calculation, plot m_x vs k_x set k_y=constant (e.g., 0). Similarly, set k_x=constant (e.g., 0) for m_y calculation. Of course (a) should be considered.