École Polytechnique Fédérale de Lausanne

SEMICONDUCTOR PROPERTIES AND RELATED NANOSTRUCTURES

MSE-484

Exercise session 1

Teacher:
Dr. Valerio Piazza

Assistants:
Anja Tiede
Ludovica Lunghi
Reyhaneh Ramezani

Laboratory of Semiconductor Materials (LMSC)

February 14, 2025

1 - Electron dispersion in empty regular lattice

Consider a cubic lattice with a lattice parameter of 5.6 Å.

1. Plot the dispersion energy of free electrons (up to 20 eV) for the First Brillouin zone in the (100) direction.

   Hints:

   - Because of the periodicity of the crystal lattice, a periodicity restriction has to be imposed on the wavevector, $\vec{k}$, such that $\vec{k} + \vec{G} = \vec{k}$, where $\vec{G}$ is the reciprocal lattice vector.
   - Remember that G' can be in many directions: $G' = \frac{2\pi}{a}\{i, j, k\}$ so you could check many G's to determine the full band structure of the system.
   - The first Brillouin zone along the (100) direction means that $\vec{k} = \frac{2\pi}{a}\{1, 0, 0\}$.

2. How does the dispersion relationship changes in the case of in a one-dimensional lattice with a periodic delta-function potential (Kronig-Penney Model) with a potential barrier height corresponding to $\beta = 5$ (see the equations below)?

   The Kronig-Penney model describes a crystal as a periodic potential of potential barriers with height U_0, width b and spacing a, as shown in 1.

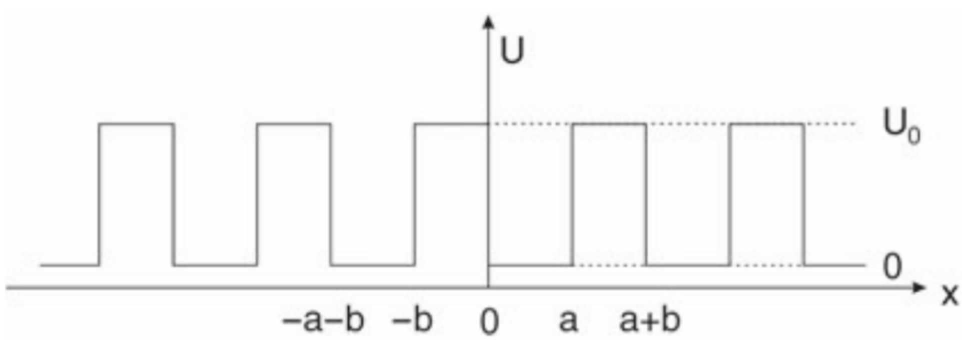

Figure 1: General Kronig-Penney model (source: The Physics of Semiconductors (3rd) - Grundmann, p.866)

The solution to this system yields the equation:

$$cos(k(a+b)) = \left(\frac{(\kappa^2 + K^2)}{2\kappa K}\right) \sinh \kappa b \sin Ka + \cosh \kappa b \cos Ka \tag{1}$$

From this dispersion relation the allowed electron energies can be calculated. If we approximate the barriers with delta functions, then $b = 0$, $\sinh(kb) = kb$, $\cosh(kb) = 1$ and then the dispersion relation can be expressed by:

$$\cos(ka) = \beta \frac{\sin(Ka)}{Ka} + \cos Ka = B(K) \tag{2}$$

2 - Density of states

1. Consider an electron in a finite potential well. Derive an analytical expression for the number of available states as a function of energy E for all the possible **k**-values, i.e., in three dimensions.

   Hints:

   - Schrodinger's equation describes the dynamics of the system using a wave function. Start with writing the time independent Schrodinger equation.
   - De Broglie relation relates the wave-particle duality. It simply says that the momentum of a particle is inversely proportional to his wavelength.
   - Then apply the boundary conditions for finite potential.

2. Consider a particle in a 1D system and derive the analytical expression for the number of available states as a function of E.

3 - Effects of confinement on carriers statistic

Consider the case of a quantum wire (1D):

1. Sketch the E(k) relation in this case.
2. What is the influence of the nanowire's diameter on the energy dispersion relation?
3. Are N_c and N_v higher in a nanowire or in a bulk?
4. How does the bandgap value change when decreasing the dimensionality of the system from 3D to 1D?

Hints:

- Start by looking at the expression for E(k) in the 2D case, what happens if another dimension is confined?
- Compare the energy dependence of the DOS relations for the 3D and 1D case to understand what happens to the carrier densities.
- Think of how you would plot the density of states for the different scenarios to understand what happens to the bandgaps.