Effective mass approximation

and its application for understanding “hydrogen-like” impurities in semiconductors

July 1, 2021

Effective mass

- The behavior of an electron in a lattice is slightly different from a free electron, because it feels a periodic potential in the lattice (A good model is the kronig-penney model).
- Hence, the electron is subjected to internal forces from the lattice (ions and core electrons), and if we apply an external force such as electric fields in a crystal lattice, and the net force may be opposite to the external force.
- If we consider the second newton law: $a = \frac{1}{m_e}(F_{ext} + F_{int}) = \frac{F_{ext}}{m_e^*}$ where m_e^* is the effective mass.
- This new mass take into account the interaction of the electron with the lattice and the equation reduces to the simpler newton second law with only one force acting $F_{ext} = m_e^* a$.
- Once adopting the effective mass approach we can treat the electron in a crystal as a free electron with mass m^*

Effective mass

- However, we don't know the exact form of F_{int}, but we can get around it considering the energy that follows from the solution of the shoedinger equation in a periodic potential, and we get allowed and forbidden energy levels from the equation.
- The solution of the shoedinger equation as a consequence provide also the relationships between the total energy of the electron and its momentum (or wave-number) and their dependence on the shape and magnitude of the potential.
- So we linked the energy of an electron with its wave-length, this is called dispersion relationship. (Note that the electron can be represented as a wave packet that moves in the lattice)
- We can now derive the expression of this effective mass using a semi-classical approach, knowing that electrons lie on the possible levels, and the effect of the crystals on the electron are contained in the dispersion relation $E(k)$

Effective mass derivation

- We start from the second newton law $m_e^* a = F$
- By definition the group velocity of an electron is : $v_g = \frac{d\omega(k)}{dk}$, and the energy associated to the wave-packet is: $E(k) = \hbar\omega(k)$.
  This yields to:

$$v_g = \frac{d\omega(k)}{dk} = \frac{1}{\hbar}\frac{dE(k)}{dk}$$

- Hence the acceleration is:

$$a = \frac{d}{dt}v_g = \frac{1}{\hbar}\frac{d}{dt}\frac{dE(k)}{dk} = \frac{1}{\hbar}\frac{dk}{dt}\frac{d^2E(k)}{d^2k}$$

- The momentum of the wave-packet is $p = \hbar k$, knowing from classical mechanics that $\frac{dp}{dt} = F$, we yield with:

$$F = \frac{dp}{dt} = \hbar\frac{dk}{dt}$$

Effective mass

- Putting everything in the second newton law and we get:

$$m_e^* = \hbar^2 \left(\frac{d^2 E(k)}{dk^2} \right)^{-1} \tag{1}$$

This is the expression for the effective mass. Once adopting the effective mass approach we can treat the electron in a crystal as a free electron with mass m^*, this approximation however is valid only around of a stationary point of a band gap.

Effective mass in the minimum of a band gap

Effective mass more dimension

- The effective mass is not a constant and can change with the lattice structure. For example, looking at the figure the effective mass of the electron that moves along the x axis is different from that one which moves along the y axis, because the lattice constant is different, so the potential is different, the shape of the energy bands is different, the effective mass is different.

Hidrogen atom impurities

- At equilibrium we have some vacancies or impurity
- We have to take into account these in the potential when we solve the Shroedinger equation. However, sometimes these impurities are difficult to schematise.
- Nevertheless, a P-doped silicon crystal can be modeled as an Hydrogen-like atom, because it has one unpaired electron in the outer orbital
- So approximately we can use the Bohr model for an idrogenoid atoms:

$$\begin{aligned} r &= 4\pi\varepsilon_0 \frac{n^2\hbar^2}{mZe^2} \\ v &= \frac{n\hbar}{mr} = \frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{n\hbar} \end{aligned} \tag{2}$$

- The total energy is given by the sum of the kinetc and the potential (coulomb):

$$E = K + V = -\frac{Ze^2}{(4\pi\varepsilon_0)^2\, 2r} = -K \Rightarrow E = -\frac{mZ^2e^4}{(4\pi\varepsilon_0)^2\, 2\hbar^2}\frac{1}{n^2} \tag{3}$$

Hidrogen atom impurities

- Instead of m_0 we have to use m_n^* and instead of ϵ_0, we have to use $K_s\epsilon_0$ where K_s is the dielectric constant of the material where in this case is the silicon
- If we look at the formula is more evident:

$$E_{\mathrm{H}} = -\frac{m_0 q^4}{2(4\pi\varepsilon_0\hbar)^2} = -13.6\mathrm{eV}$$
$$E_{\mathrm{d}} = -\frac{m_{\mathrm{n}}^* \mathrm{q}^4}{2(4\pi K_{\mathrm{s}}\varepsilon_0\hbar)^2} = -13.6\mathrm{eV}\,\frac{m_{\mathrm{n}}^*}{m_0}\left(\frac{\varepsilon_0}{K_{\mathrm{s}}\varepsilon_0}\right)^2 \approx -0.05\mathrm{eV} \tag{4}$$