

Recitation #3

ENEE 313: Introduction to Device Physics

Fall, 2018

1 summary

The notes of this week cover from orbitals to bonds to energy bands. You need to know the conceptual interpretation of quantum numbers, bonding force types, energy bands, and how electronic structure defines device properties.

1. Quantum numbers describe atomic orbitals. It's a region of probability where an electron can be found.
 - (a) n is principal quantum number, describing the orbit and "energy level" of the electron. $n = 1, 2, 3, \dots$
 - (b) l is the polar angle quantum number, describing the suborbital. It tells the type of the orbital. $l = 0, 1, 2, n-1$.
 - (c) m indicates the azimuthal dependence of the wave-function and specifies the orbital. $m = -l, \dots, l$.
 - (d) s is electron "spin", including two possible states, spin up state and spin down state.
2. Pauli principle states that no more than one electrons can occupy the same quantum state.
3. Bonding forces in solid
 - (a) ionic bonding
 - (b) covalent bonding
 - (c) metallic bonding
4. Energy bands: when isolated atoms are brought together to form a solid, energy bands arise.
5. Electronic structure to engineering properties: electrons in the valence band involve in chemical bonding and electrical conductivity. The properties are mostly determined by the arrangement of the exterior shell of electrons. This relates to how readily they accept or donate an electron to surrounding structures. Their bonding with nearby elements relates to physical characteristics and the number of free electrons they donate to the material relates to conductivity.

Exercise 1.

Calculate the expectation value for position and momentum for a particle in the n^{th} energy state of the infinite well.

Solution. The Schrodinger equation of the infinite well problem is,

$$\Psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right), x \text{ in } [0, L]$$

Thus, the expectation value of the position is,

$$\begin{aligned} \langle x \rangle &= \int \Psi^* x \Psi dx \\ &= \frac{2}{L} \int_0^L x \sin^2\left(\frac{n\pi}{L}x\right) dx \\ &= \frac{2}{L} \int_0^L \frac{x}{2} (1 - \cos\left(\frac{2n\pi}{L}x\right)) dx \\ &= \frac{1}{L} \left(\int_0^L x dx - \int_0^L x \cos\left(\frac{2n\pi}{L}x\right) dx \right) \\ &= \frac{L}{2} \end{aligned}$$

the expectation value of the momentum is,

$$\begin{aligned} \langle p \rangle &= \int \Psi^* \frac{h}{j} \frac{\partial}{\partial x} \Psi dx \\ &= \frac{2nh\pi}{jL^2} \int_0^L \sin\left(\frac{n\pi}{L}x\right) \cos\left(\frac{n\pi}{L}x\right) dx \\ &= 0 \end{aligned}$$

□

Exercise 2. Tunneling barrier problem

Find the Schrodinger wave equation for the case that an electron travels in $+x$ direction toward the barrier shown in Figure 1. The barrier has potential higher than the energy of the electron.

Solution. In the region I, the wave function is,

$$\begin{aligned} \Psi_I(x) &= A \exp(j\alpha x) + B \exp(-j\alpha x) \\ \alpha &= \sqrt{\frac{2mE}{\hbar^2}} \end{aligned}$$

In the region II, the wave function is,

$$\begin{aligned} \Psi_{II}(x) &= C \exp(\beta x) + D \exp(-\beta x) \\ \beta &= \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \end{aligned}$$

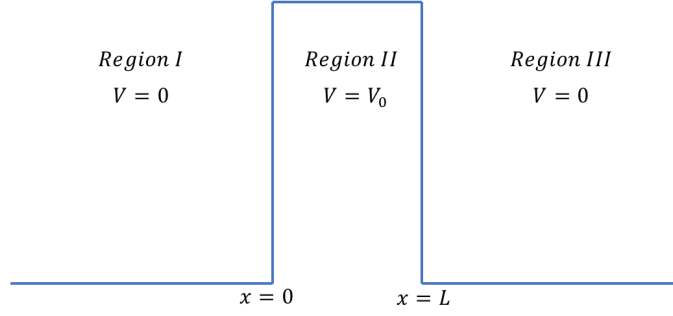


Figure 1: Finite potential well

In the region III, the wave function is,

$$\Psi_{III}(x) = F \exp(j\alpha x) + G \exp(-j\alpha x)$$

$$\alpha = \sqrt{\frac{2mE}{\hbar^2}}$$

Since the wave function represents the electron that has passed through the barrier and is traveling only in the +x direction. $G = 0$. Therefore, we have

$$\begin{aligned}\Psi_I(x) &= A \exp(j\alpha x) + B \exp(-j\alpha x) \\ \Psi_{II}(x) &= C \exp(\beta x) + D \exp(-\beta x) \\ \Psi_{III}(x) &= F \exp(j\alpha x)\end{aligned}$$

The boundary conditions are

$$\begin{aligned}\Psi_I(0) &= \Psi_{II}(0) \\ \Psi_{III}(L) &= \Psi_{II}(L) \\ \frac{\partial \Psi_I(0)}{\partial x} &= \frac{\partial \Psi_{II}(0)}{\partial x} \\ \frac{\partial \Psi_{III}(L)}{\partial x} &= \frac{\partial \Psi_{II}(L)}{\partial x} \\ \int_{-\infty}^{\infty} \Psi^* \Psi dx &= 1\end{aligned}$$

Again, with the suitable conditions, it's still not trivial to solve the equations. However, the physical interpretation under the equation is

1. Ψ_I indicates the incident electrons travels toward +x direction (the A term) and part of them are reflected (the B term)
2. in the barrier, Ψ_{II} decay exponentially. This represents that the electrons can enter and exist.

3. Ψ_{III} indicates the fact that the electrons passed through the barrier.

□

Exercise 3. Band Structure of Solid Crystals

1. Explain how energy bands arise in a crystal by bringing atoms together. How many quantum states are in each energy band?
2. What is the difference between an insulator, a metal and a semiconductor in terms of the bands? Explain this using bandgap and the filling of states by electrons.
3. Why cant a full energy band conduct electricity?
4. What is the difference between a conduction electron and a non-conduction electron?
5. What is a hole?
6. What is the general form of the Schrodinger equation for a crystal?

Solution. 1. When two atoms are far apart, the valence electrons in the atoms do not interact. As they are brought closer, the valence electrons feel the forces of adjacent nucleus and electrons. Therefore, the existing energy levels split into two antibonding (higher energy) and bonding (lower energy). As N atoms are brought together, we get two continuous bands of energies separated by an energy gap and there are 2N quantum states in each band.

2. Please refer to Figure 3.4 in the textbook
3. In a full energy band, electrons do not have energy states to move in when a field is applied. therefore, they dont conduct.
4. Conduction electrons are those that have been promoted to the conduction band or those which have vacant states to moves into in the valence band. Non-conduction electrons are the electrons, which do not have vacant energy states to move into and are still bound to the lattice.
5. Vacancy created by the absence of an electron in the valence band.
6. a periodic function $V(x) = V(x + na)$ can be represented by Fourier series,

$$V(x) = \sum_{n=0}^{\infty} V_n \exp\left(\frac{j2n\pi}{a}x\right)$$

$$-\frac{\hbar^2}{2m} \nabla^2 \Psi(x) + V(x) \Psi(x) = E \Psi(x)$$

□