Home Problem Set #2 Due: September 24 (Wed), 2014

1. State the two Schrödinger equations for electrons in a periodic potential field (Kronig-Penny model). Use for their solutions, instead of the Bloch function, the trial solution

$$\Psi(x) = Ae^{ikx}$$

Discuss the result. (*Hint*: For free electrons $V_o = 0$)

2. The differential equation for an undamped vibration is $a\frac{d^2u}{dx^2} + bu = 0$ (1)

whose solution is $u = Ae^{ikx} + Be^{-ikx}$ (2)

Where $k = \sqrt{b/a}$

Prove that (2) is indeed a solution of (1)

3. The total electron energy of a hydrogen atom is given by

$$E = \frac{me^4}{2(4\pi\varepsilon_0\hbar)^2}\frac{1}{n^2} = -13.6\cdot\frac{1}{n^2}(eV)$$

where $n = 1, 2, 3, \ldots$.

(a) Derive the above relation in a semiclassical way by assuming that the centripetal force of an electron, $mv^2/r$, is counterbalanced by the Coulombic attraction force, $-e^2/4\pi\varepsilon_0 r^2$, between the nucleus and the orbiting electron. Use Bohr's postulate which states that the angular momentum $L = mvr$ ($v$ = linear electron velocity and $r$ = radius of the orbiting electron) is a multiple integer of Planck's constant (i.e., $n\hbar$). (*Hint*: The kinetic energy of the electron is $E = mv^2/2$)

(b) Derive the above relation by solving the Schrodinger equation for the electron wave of the hydrogen atom.

(Hint, refer to Concepts of Modern Physics, Ed. Arthur Beiser or other books)

4. Consider an electron trapped in a one-dimensional box with infinitely high potential. The box extends from $x = 0$ to $x = a$. The electron has the mass $m$ and the total energy $E$.

(a) Find the energy eigenvalue of the electron by solving Schrödinger equation,

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0$$

(b) If the lowest energy possible for the electron is 10.00 eV, what are the two higher energies the particle can have?

(c) Find the eigenfunction $\psi_n$ corresponding to $E_n$.

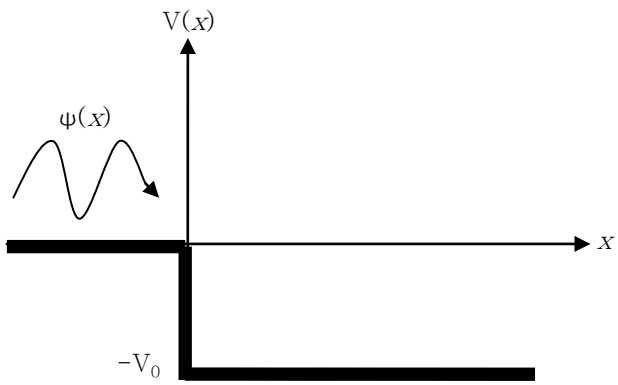
(d) Find the probability density that the electron can be found between $x = 0$ and $a/3$ for the second excited sate ($n$ =3).

5. An electron of mass m and kinetic energy $\boldsymbol{E > 0}$ approaches a potential drop $V_0$

(a) Write down the equations of two regions (x≥0, x≤0) from time-independent Schrödinger equation.

(b) Assume there is no incoming wave to the right, so you can get three amplitude constants. Let A: incident amplitude, B : reflected amplitude, C : transmitted amplitude.

Determine the reflection coefficient $R$. $\left( R = \frac{|B|^2}{|A|^2} \right)$




(c) What is $R$ if $E = V_0 / 3$?

Calculate the transmission coefficient $T$ in this case from $R + T = 1$.

6. For an electron in a one dimensional crystal, assuming it experiences one dimensional periodic potential (Kronig-Penny model) shown below, ($E < V_0$)

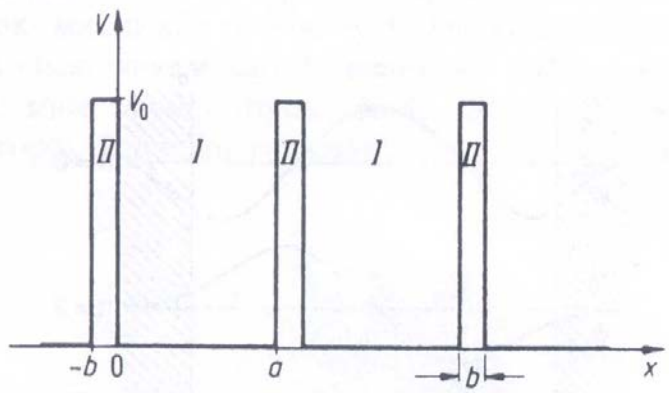



Figure 4.9. One-dimensional periodic potential distribution (simplified) (**Kronig-Penney model**).

(a) Using the Bloch function $\psi(x) = u(x) \cdot e^{ikx}$ as the wave function of the electron, show that solution of the Schrodinger equations in regions I and II leads to

$$\frac{\gamma^2 - \alpha^2}{2\alpha\gamma} \sinh(\gamma b) \cdot \sin(\alpha a) + \cosh(\gamma b) \cdot \cos(\alpha a) = \cos k(a+b)$$

Where, $\alpha^2 = \frac{2m}{\hbar^2} E \qquad \gamma^2 = \frac{2m}{\hbar^2}(V_0 - E)$

(b) Describe in what condition, the above relation becomes

$$P \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka \quad \text{where} \quad P = \frac{maV_0 b}{\hbar^2}$$