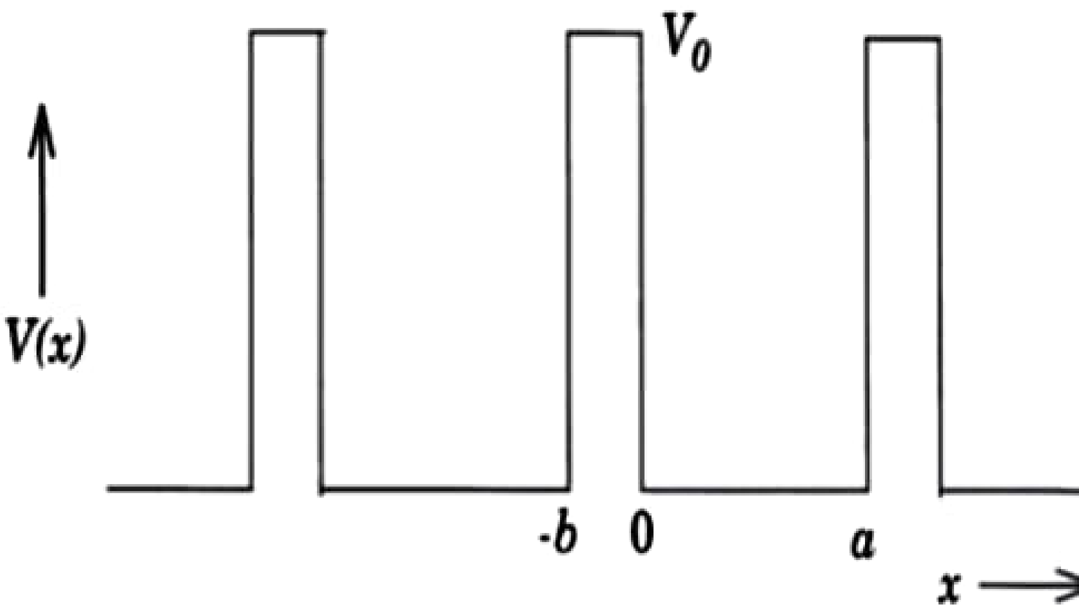
Kronig Penney model

- The essential behaviour of electron may be studied periodic rectangular well in one dimensional which was first discussed by Kronig Penney in 1931.
- It is assumed that when an electron is near the positive ion site, potential energy is taken as zero. Where as outside the well, that is in between two positive ions potential energy is assumed to be Vo.



The wave function associated with electron when it is in firs state is derived as follows

According to Schrodinger time independent equation,

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}(E - V_0)\psi = 0$$

According to Bloch theorem the potential V=0 then,

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Let us consider

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

Then the equation transforms to

$$\frac{\partial^2 \psi}{\partial x^2} + \alpha^2 \psi = 0$$

----- Eq - (1)

The wave function associated with the electron when it is in second state is derived as follows. Here the conditions are

$$V = V_0 \quad Since \quad -b < x < 0$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2}(E - V_0)\psi = 0$$

Let us consider

$$\beta^2 = \frac{2m}{\hbar^2}(V_0 - E)$$

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$$Since\ always\ V_0 > E$$

Hence the equation transforms as

$$\frac{\partial^2\psi}{\partial x^2} - \beta^2\psi = 0$$

----------- Eq - (2)

Bloch has given the solution for Schrodinger equation as

$$\psi(x) = e^{\pm ikx}\, U_k(r)$$

Partially differentiating the above equation, we get

$$\frac{\partial\psi}{\partial x} = ike^{ikx}\, U_k(x) + e^{ikx}\,\frac{\partial U_k}{\partial x}$$

Again differentiating we get,

$$\frac{\partial^2\psi}{\partial x^2} = -k^2e^{ikx}\, U_k(x) + ik\, e^{ikx}\,\frac{\partial U_k}{\partial x} + ik\, e^{ikx}\,\frac{\partial U_k}{\partial x} + e^{ikx}\frac{\partial^2 U_k}{\partial x^2}$$

By substituting this value is equations 1 we get,

$$-k^2e^{ikx}\, U_1 + 2ik\, e^{ikx}\,\frac{\partial U_1}{\partial x} + e^{ikx}\frac{\partial^2 U_1}{\partial x^2} + e^{ikx}\,\alpha^2\, U_1(x) = 0$$

$$e^{ikx}[\frac{\partial^2 U_1}{\partial x^2} + 2ik\,\frac{\partial U_1}{\partial x} + (\alpha^2 - k^2)\, U_1(x)] = 0$$

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$$e^{ikx}\left[\frac{\partial^2 U_1}{\partial x^2} + 2ik\,\frac{\partial U_1}{\partial x} + (\alpha^2 - k^2)\, U_1(x)\right] = 0$$

---------- Eq - (3)

Similarly by substituting this in equation 2

$$e^{-i\omega t}\left[\frac{\partial {U_2}^2}{\partial x^2} + 2ik\,\frac{\partial U_2}{\partial x} - (\beta^2 + k^2)U_2\right] = 0$$

---------- Eq - (4)

By writing the general solutions for equations 3 and 4 we get four constants A,B,C,D. To know the values of these constants we apply the boundary conditions, as x=0, x=a, x=-b. In evaluation the constants A,B,C,D are vanished and the

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$$\frac{\beta^2 - \alpha^2}{2\alpha\beta} sinhb\beta\ sina\alpha + coshb\beta\ cosa\alpha = cosk(a+b)$$

---------- Eq - (5)

This equation can not describe motion of electron with periodic motion. In order to express the relation in more simplified form.

So let us consider Vo tends to infinity then, b=0 and

$$sinhb\beta = b\beta$$
$$cosb\beta = 1$$

Then the initial conditions of the constants α^2 and β^2

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

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and

$$\beta^2 = \frac{2m(V_0 - E)}{\hbar^2}$$

$$\beta^2 - \alpha^2 = \frac{2m(V_0 - E - E)}{\hbar^2}$$

$$\beta^2 - \alpha^2 = \frac{2m(V_0 - 2E)}{\hbar^2}$$

$$P\frac{\sin\alpha a}{\alpha a} + \cos\alpha a = \cos ak$$

This equation satisfies only for those values of αa between -1 to 1

<u>Conclusions from graph:</u>

1. The substance contains a number of allowed and forbidden energy gaps.
2. Width of the allowed band increase with increase of αa.
3. If P tends to infinity,

$$\sin\alpha a = 0$$

then

$$\alpha a = n\pi$$

$$\alpha = \frac{n\pi}{a}$$

$$\alpha^2 = \frac{n^2\pi^2}{a^2}$$

We also know that

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

$$\alpha^2 = \frac{8\pi^2 mE}{h^2}$$

$$\alpha^2 = \frac{4\pi^2}{h^2} p^2$$

$$since\ \lambda = \frac{h}{p}$$

Equating both the equations we get,

$$\frac{2mE}{\hbar^2} = \frac{4\pi^2}{h^2} \times p^2$$

$$\frac{8\pi^2 mE}{h^2} = \frac{4\pi^2}{h^2} \times p^2$$

$$[\ \hbar = \frac{h}{2\pi}\ ]$$

after a simple calculation, we get

$$E = \frac{p^2}{2m}$$

$$[\frac{p^2}{2m} = \frac{1}{2} m v^2\ ]$$

This expression shows all the electrons are free to move without any constrains. This supports classical free electron theory.

$$\beta^2 = \frac{2m(V_0 - E)}{\hbar^2}$$

$$\beta^2 - \alpha^2 = \frac{2m(V_0 - E - E)}{\hbar^2}$$

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$$\frac{2mV_0}{\hbar^2(2\alpha\beta)} \times \beta b\, sin a\alpha + 1 \times cos a\alpha = cos k(a)$$

$$\frac{maV_0}{\hbar^2 \alpha a} \times sin a\alpha + cos a\alpha = cos ka$$

Let us consider

$$P = \frac{maV_0 b}{\hbar^2}$$

Where P is the measure of potential barrier between the two potential wells.

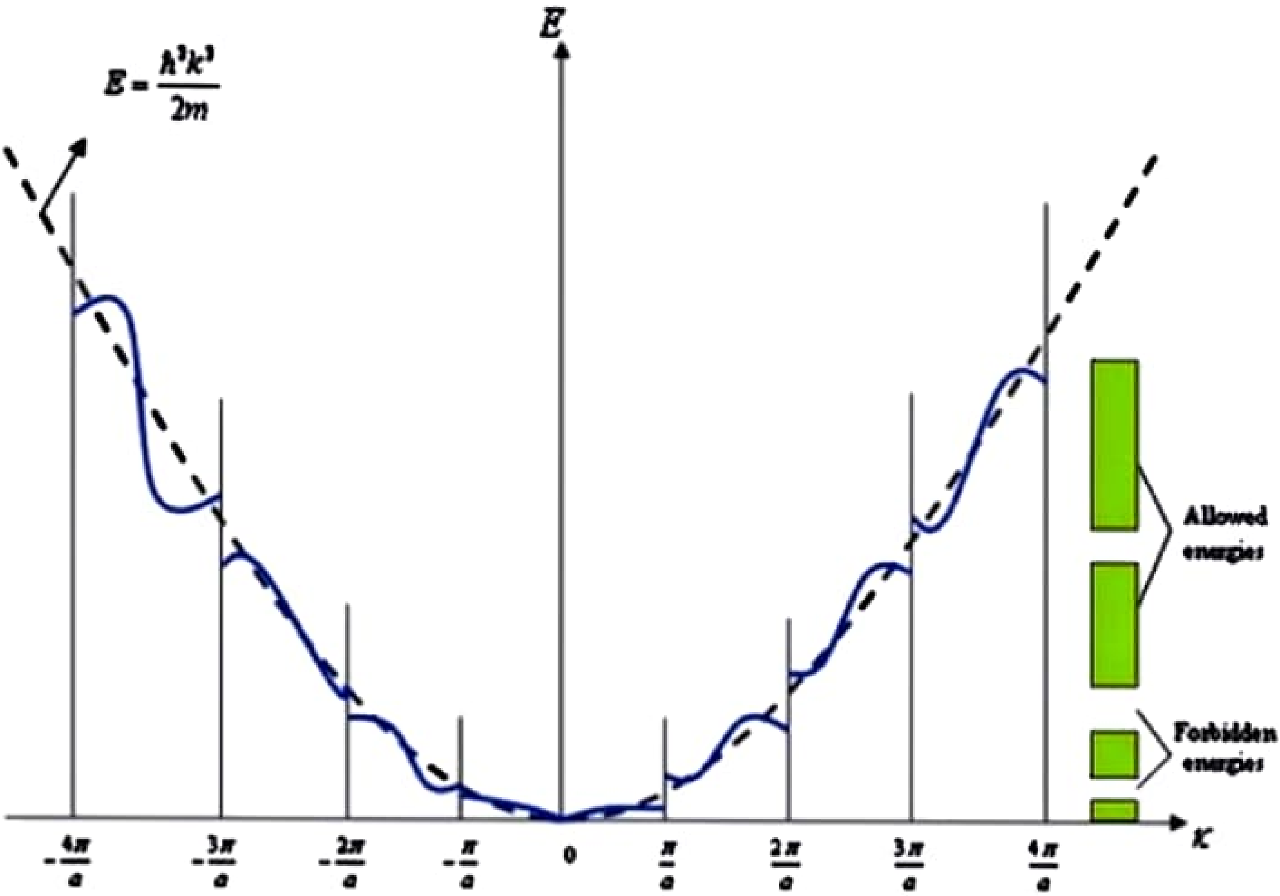
$$P\frac{sin \alpha a}{\alpha a} + cos a\alpha = cos ak$$

When we plot graph between by taking

$$\alpha a \text{ on } x - axis$$

$$\frac{P}{\alpha a} sin \alpha a + cos a\alpha = cos ak \text{ on } y - axis$$

Brillouin zones



- If we brought a graph between energy & propagation K, it is clear from the figure that the energy of the electron is increasing from K = 0 to $-\pi/a$
- The allowed region or zone which is from π/a to π/a is called 1st brillouin zone.
- After discontinuity another allowed zone extented from $-2\pi/a$ to $-\pi/a$ & π/a to $2\pi/a$. This is known as 2nd brillouin zone.
- In the same way further Brillouin zones are continued......