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ANALYSIS OF KRONIG-PENNEY MODEL IN ONE DIMENSION

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We consider a wave function of an electron in a periodic potential of metal. The wave function of electron for a periodic potential are the product of plane wave and a periodic function. In this paper we shall discuss the Dirac delta function, Bloch theorem, discontinuity and continuity conditions. The solution of time independent Schrödinger wave equation involves periodic potential in one-dimension. The potential is zero near the nucleus and is maximum at the point half way between two neighbouring atoms. We also assume that the product of the potential height (V_0) and the width is a constant value, Even in the limiting case of large potential the product remains a finite quantity.

INTRODUCTION :

In the Kronig Penney model, the discret energy level scheme of isolated atoms, the energy bands would be infinitely continuous. In generally is observed a region of forbidden energies between the two successive bands. An energy bands is almost cantered around its parent level. Kronig and Penney[2,3](1930) demonstrated after the Bloch theorem[1to7] (1928) came in to existence. That regions of forbidden energies intervene the regions of allowed energies. They accomplished that using a one-dimension square-well crystal potential as depicted. By Fourier analysis I found that the wave differed from the plane wave of free electrons only by a periodic modulation. F-Bloch prove theorem that the solutions of time independent Schrödinger equation for a periodic potential is given by

$$\Phi_k(x) = u_k(x) \exp (ikx)$$

where $u_k(x)$ is a periodic function on the crystal lattice, that is,

$$u_k(x+a) = u_k(x)$$

Proof of the Bloch Theorem[6]:-

Let us consider the motion of an electron in a periodic potential. The system is one-dimensional crystal and consist of *N* atoms in a length *Na* with inter atomic spacing *a*. The potential energy is a periodic with $V(x) = V(x+1a)$, where l is an integer.

We are imposed by the symmetry of the solution of the wave function such that

$$\Phi(x+a) = T\Phi(x) \tag{1}$$

where *T* is a constant number.

Let us determine the number *T* appearing in equation (1) for this purpose. We write the relation on going once in a length *Na*

$$\Phi(x+Na) = T^N \Phi(x) = \Phi(x) \tag{2}$$

Because Φ(x) must be single value. Consequently,

$$T^N = 1$$

$$T = \exp\,(i2\pi n/N) \qquad ...(3)$$

where $n = 0,1,2.......,N-1$

We see that

$$\Phi_k(x) = u_k(x)\exp[i2\pi nx/(Na)] \qquad ...(4)$$

where $u_k(x) = u_k(x+a)$ is a arbitrary periodic function with lattice constant a with $k=2\pi n/Na$.

Dirac Delta function :

This is the most important function $\delta(t)$. This function is define to be 0, if $t\neq 0$ and to be ∞ at $t = 0$ such that,

$$\int_{-\infty}^{+\infty} \delta(t)dt = 1 \qquad ...(5)$$

This is very large and very small region and 0, outside this region and has a unit integral. Suppose that the function $\delta(t)$ has following values:

$$d(t) = \begin{cases} 0 & t \le 0 \\ 1/\varepsilon & 0 < t < \varepsilon \\ 0 & t > \varepsilon \end{cases} \qquad ...(6)$$

where ε may be made as small as we require.

Periodic potential Kronig-Penney model :

Electrons in a lattice represent in a periodic potential due to the presence of the atoms in fig 1.

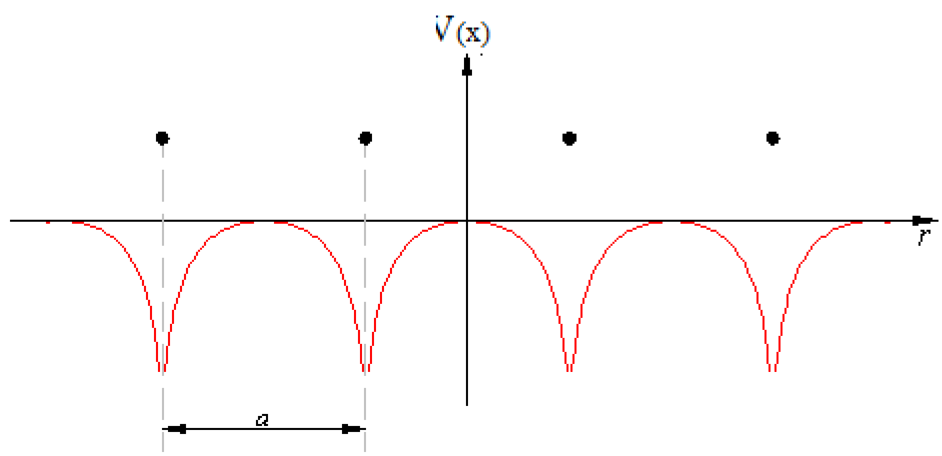

Figure 1. Periodic potential in a one-dimensional lattice.

Consider the potential energy $V(x)$ of an electron shown in the illustration with an infinite sequence of potential wells of depth $-V_0$ and width a, arranged with a spacing. The width and the curvatures of the allowed bands increase with energy. This periodic potential will open gaps in the dispersion relation, To solve this problem we will assume that the width of the potential energy term goes to zero, we represent them as δ-functions fig 2

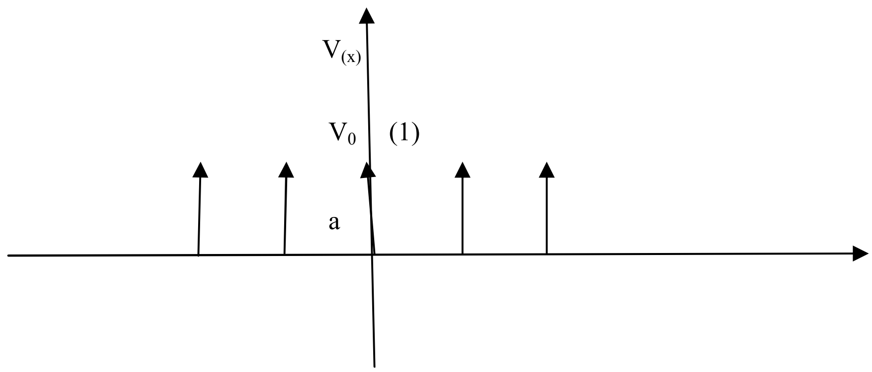

Figure 2. Periodic δ-function potentials

For this system potential energy is given by,

$$V(x) = V_0 \sum_{-\infty}^{\infty} (x + Na) \qquad ...(7)$$

Which represents a series of delta function, Now we solve the one dimension Schrödinger wave equation for the kronig-penney model,

$$\frac{d^2\phi(x)}{dx^2} + \frac{2m}{\hbar^2}(E - V(x))\Phi(x) = 0 \qquad ...(8)$$

For periodic potential given by

$$V(x+a) = V(x) \qquad ...(9)$$

Now $u(x)$ has the periodicity of the lattice i.e.

$$u(x+a) = u(x) \qquad ...(10)$$

Thus,

$$\Phi_k(x+a) = e^{ik(x+a)}u(x+a)$$

$$= e^{ika}(e^{ikx}u(x))$$

$$= e^{ika}\Phi(x) \qquad ...(11)$$

Now derivative of $\Phi(x)$ is

$$\frac{d\Phi(x)}{dx} = ike^{ik(x+a)}u(x) + e^{ikx}\frac{du(x)}{dx} \qquad (12)$$

Similarly

$$\frac{d\Phi(x)}{dx}\Big|_{x+a} = e^{ika}\frac{d\Phi(x)}{dx} \qquad (13)$$

$$\frac{d\Phi(x)}{dx}\Big|_{x} = e^{-ika}\frac{d\Phi(x)}{dx} \qquad (14)$$

In general

$$\frac{d\Phi(x)}{dx}\Big|_{x=-\varepsilon} = e^{-ika}\frac{d\Phi(x)}{dx}\Big|_{x=a-\varepsilon} \qquad ...(15)$$

where ε is infinitesimal quantity

Now we calculate the discontinuities of $\frac{d\Phi(x)}{dx}$ at a point where $V_{(x)}$ is a Delta function.

Integrating the equation (8) from $x = -\varepsilon$ to $x = +\varepsilon$ then,

$$\sum_{-\in}^{+\in} \frac{d^2\Phi(x)}{dx^2}\, dx = -\frac{2m}{\hbar^2} E\int_{-\in}^{+\in} dx\Phi(x) + \frac{2mv0}{\hbar^2}\int_{-\in}^{+\in} \delta(x)\Phi(x)\, dx$$

$$\frac{d\Phi(x)}{dx}\Big|_{x=+\varepsilon} - \frac{d\Phi(x)}{dx}\Big|_{x=-\varepsilon} = \frac{2mv0}{\hbar^2}\Phi(0)$$

$$\frac{d\Phi(x)}{dx}\Big|_{x=+\varepsilon} = \frac{d\Phi(x)}{dx}\Big|_{x=-\varepsilon} - \frac{2mv0}{\hbar^2}\Phi(0) \qquad ...(16)$$

Hence, from equation (15) we get

$$e^{-ika}\frac{d\phi(x)}{dx}\Big|_{x=a-\varepsilon} = \frac{d\phi(x)}{dx}\Big|_{x=+\varepsilon} - \frac{2mV0}{\hbar^2} \qquad ...(17)$$

Let us consider the solution of Schrödinger equation in the region $\in < x < a - \in$, But $\in$ tends to 0 for region-1, where $V(x) = 0$ in this region the solution of Schrödinger equation is

$$\Phi(x) = De^{iax} + Be^{-iax} \qquad ...(18)$$

where $$a^2 = 2mE/\hbar^2 \qquad ...(19)$$

By the use of boundary conditions

$$e^{-ika}\Phi(a) = \Phi(0)$$

$$e^{-ika}[De^{i\alpha a} + Be^{-i\alpha a}] = D + B$$

or $$D(1 - e^{-i(\alpha-k)a}) + B(1 - e^{+i(\alpha+k)a}) = 0 \qquad ...(20)$$

Now $$\frac{d\Phi(x)}{dx} = i\alpha[De^{-i\alpha x} - Be^{-i\alpha x}]$$

Hence $$\frac{d\Phi(x)}{dx}\Big|_{x=\varepsilon} - \frac{2mv0}{\hbar^2}\Phi(0) = e^{-ka}\frac{d\Phi(x)}{dx}\Big|_{x=a-\alpha}$$

But ε tends to 0

$$\left[1 - e^{i(\alpha-k)a} + \frac{2iP}{\alpha a}\right]D + \left[1 - e^{-i(\alpha+k)a} - \frac{2iP}{\alpha a}\right]B = 0 \qquad ...(21)$$

Where $$P = \frac{2mv0}{\hbar^2} \qquad ...(22)$$

From equation (20) and (21) we get

$$\left(1-e^{-i(\alpha-k)a}+\frac{2iP}{\alpha a}\right)(1-e^{i(\alpha+k)a})+(1-e^{-i(\alpha-k)a})\left(1-e^{-(\alpha+k)a}-\frac{2iP}{\alpha a}\right)=0$$

$$2\,(1-e^{-i(\alpha-k)a})\,(1-e^{-(\alpha+k)a})=\frac{2iP}{\alpha a}(1-e^{i(a-k)a}-1+e^{-i(\alpha+k)a})$$

$$2\,[1-e^{-i(\alpha-k)a}(e^{i\alpha a}+e^{-i\alpha a})+e^{-2ika}]=\frac{4P}{\alpha a}e^{-ika}\sin\alpha a$$

$$2e^{-ika}[e^{ika}+e^{-ika}-2\cos\alpha a]=\frac{4P}{\alpha a}e^{-ika}\sin\alpha a$$

$$2e^{-ika}[2\cos ka-2\cos\alpha a]=\frac{4P}{\alpha a}e^{-ika}\sin\alpha a$$

$$4e^{-ika}[\cos ka-\cos\alpha a]=\frac{4P}{\alpha a}e^{-ika}\sin\alpha a$$

$$[\cos ka-\cos\alpha a]=\frac{P}{\alpha a}\sin\alpha a$$

$$\frac{P}{\alpha a}\sin\alpha a+\cos\alpha a=\cos ka \qquad ...(23)$$

This is the general solution of the Kronig-penney model. This solution can be obtained by matrix method which is tedious.

Discussion:

In equation (23), the quantity $\cos ka$ can vary only between +1 and –1, If k is real This implies that only some value of α are allowed which means that all values of energy E are not allowed in fig-3. The shaded regions represent the allowed values of $\cos ka$.

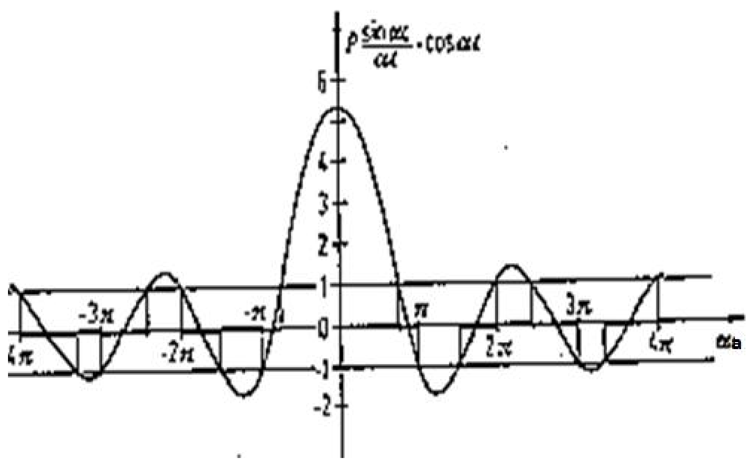

Fig-3

The width of the allowed region is increases as energy increases. The width of the allowed region also depends on P. When P tends to infinity, the allowed region change to discrete levels such that $\alpha a = n\pi$. Where n is positive integer when P tends to 0 the forbidden regions disappear and the electron behave likes a free particle[8to10].

Conclusion:

The equation (23) is derived on the basis of Dirac-Delta function, Bloch function with boundary conditions. This solution of Schrödinger equation simplest as compare to matrix method. The elegance with which the Kronig-Penney model predicates the assurance of band-gapes enhances the significance of the model well beyond its historical value[11to17].

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