Understanding Band Structures in Solids via solving Schrödinger equation for Dirac comb

Saravanan Rajendran (I-Ph.D., Physics DI 1505)
IIT Mandi

February 15, 2016

Abstract: The Understanding of the band structure of the solids begins with the solving of Schrödinger equation for the electron which is subjected to a series of potentials arised due to the presence of lattice sites. The periodicity is assumed to the potential series such that the mathematics looks even simpler! To understand the band structure of solids, we begin with solving of Schrödinger equation for a simplistic model i.e., Dirac barrier in 1-D and even with this simple model, we could realise band gaps in solids which are manifestation of translational invariance. Although, Dirac barrier admits only scattering states.Then, we inverted barrier to well i.e.,Dirac well, which admits both scattering and bound states and again we are able to see band gaps with bound state, hence closer to the real picture. Finally, we worked out the classic model for rectangular periodic potential in a solid i.e., K-P model and we showed in certain limit (i.e., when the barrier width is zero), it can be a reduced Dirac barrier.

1 Introduction

The free electron theory was successful in explaining the behaviour of valence electrons in the crystal structure but not the band gaps which are manifestation of periodic potential in a crystalline solid. As a result of periodicity in a crystalline solids,our present understanding of crystalline solids is much more advanced than amorphous solids.To understand the origin of band gaps in

crystalline solids via Schrödinger equation, basic challenge is in the form of potential. The first order approximation towards assuming form of $V(r)$ in crystalline solids begins with assuming a periodic potential with the periodicity of lattice parameter. In order to understand the origin of band gaps, we begin by assuming a simple form for periodic potential (i.e., Dirac Comb).As a realisation of potential influence by the lattice sites, an one dimensional potential spike comb is considered. Of course, there going to be 10^{23} potentials to be solved which is going to be a diificult task. Hence, the solving of one spike and approximating it to N-th spike is done by assuming periodicity and the relation between the solution of spikes is given by Bloch's theorem. The solving of periodic potential spikes (*Although, real case are wells!*) leads us to a mathematical formulation that shows the arisal of energy band gaps in a solid.
This paper is concerned in solving the Dirac comb with both cases barrier and well in 1D and the Kronig Penny potential so that the origin of band gaps in solids is realised.

2 General Formalism, Discussion of results

Case A. The electron is subjected to a Dirac comb potential given as,

$$V(x) = \alpha \sum_{j=0}^{N-1} \delta(x - ja)$$

Where α is delta potential strength.
The Schrodinger equation is solved in the region $0 < x < a$,
where $V(x) = 0$(Figure 1),

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \tag{1}$$

The solution for the differential equation is,

$$\psi(x) = A\sin(kx) + B\cos(kx) \tag{2}$$

where 'k' is the wave vector given as,

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

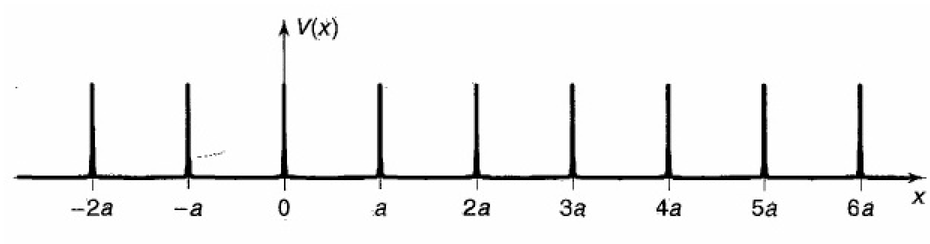


Figure 1: Dirac comb

Using Bloch's theorem (discussed in details below),

$$\psi(x+a) = e^{iKa}\psi(x)$$

where "K' is some constant to be found out later.

That leads to

$$\psi(x) = e^{-iKa}[A\sin(k(x+a)) + B\cos(k(x+a))] \tag{3}$$

Using boundary conditions:-

1.$\psi(x)$ is continuous at x=0,

$$B = e^{-iKa}[A\sin(ka) + B\cos(ka)] \tag{4}$$

2.The derivative of $\psi(x)$ at is discontinuous where $V = \infty$ $(x = 0)$, Discontinuity is proportional to the strength of the delta function (α)

$$kA - e^{-iKa}k[A\cos(ka) - B\sin(ka)] = \frac{2m\alpha}{\hbar^2}B \tag{5}$$

Equation (4) gives,

$$A = \frac{B[e^{iKa} - \cos(ka)]}{\sin(ka)} \tag{6}$$

putting (6) in (4) gives,

$$kB[e^{iKa} - \cos(ka)] - e^{-iKa}k[B(e^{iKa} - \cos(ka))\cos(ka) + B\sin^2(ka)] = \frac{2m\alpha}{\hbar^2}B\sin(ka) \tag{7}$$

$$[e^{iKa} - \cos(ka)][1 - e^{-iKa}\cos(ka)] + e^{-iKa}\sin^2(ka) = \frac{2m\alpha}{\hbar^2 k}\sin(ka)$$

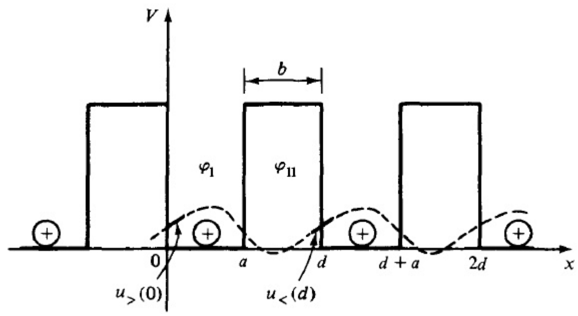


Figure 2: Kronig-Penny Model

simplifies to,

$$\cos(Ka) = \cos(ka) + \frac{m\alpha}{\hbar^2 k}\sin(ka)$$

Let, $z = ka$ and $\beta = \frac{ma\alpha}{\hbar^2}$

$$f(z) = \cos(z) + \beta\frac{\sin(z)}{z} \tag{8}$$

Case B. Then the actual case of attractive potentials (Dirac well) is solved,

$$V(x) = -\alpha\sum_{j=0}^{N-1}\delta(x - ja)$$

The delta function strength(α) is negative (for wells),

$$f(z) = \cos(z) - \beta\frac{\sin(z)}{z} \tag{9}$$

Case C. The Kronig Penny approximation to the potential is rectangular periodic pattern (as shown in figure 2),

$$V(x) = \begin{cases} 0, & 0 < x < a \\ V_0, & a < x < d \end{cases}$$

The similar treatment of boundary conditions to the rectangular potential gives a more complicated transcedental equation,

$$\cos Kd = \cos k_1 a \cos k_2 b - \frac{k_1^2 + k_2^2}{2k_1 k_2}\sin k_1 a \sin k_2 b \tag{10}$$

$$k_1^2 - k_2^2 = \frac{2mV}{\hbar^2} \tag{11}$$

2.1 Bloch theorem: Derivation

Statement: The eigen states ψ of the one-electron hamiltonian $\hat{H} = \frac{-\hbar^2}{2m}\Delta^2 + U(r)$, where $U(\vec{r}) = U(\vec{R} + \vec{r})$ for all $\mathbf{R}$ in a Bravais lattice, can be choosen to have the form of plane wave times a function with the periodicity of the Bravais lattice.i.e.,

$$\psi(x) = e^{iKx}u(x)$$

$$\psi(x+a) = e^{iKa}\psi(x)$$

Proof 1. Let 'D' be some transational operator such that,

$$\hat{D}\psi(x) = \psi(x+a)$$

The Hamiltonian is periodic i.e.,

$$H(x+a) = H(x)$$

The commutation between D and H (Hamiltonian Operator),

$$[\hat{D}, \hat{H}]\psi = (\hat{D}\hat{H} - \hat{H}\hat{D})\psi = E\psi(x+a) - E\psi(x+a) = 0$$

$$[\hat{D}, \hat{H}] = 0$$

means $\hat{D}$ and $\hat{H}$ can have simultaneous eigenfunctions.

$$\hat{D}\psi = \lambda\psi$$

with an eigenvalueλ.
In three dimensions,

$$\hat{D}\psi(\mathbf{r}) = \psi(\mathbf{r} + \mathbf{R}) = \lambda\psi(\mathbf{r})$$

Where $\hat{D}$ is an Unitary operator.

$$\hat{D} = e^{i\hat{p}.\vec{R}/\hbar}$$

$$\hat{D}^\dagger = e^{-i\hat{p}.\vec{R}/\hbar}$$

$$\hat{D}^\dagger\hat{D} = I$$

For such an operator the eigenvalue is complex with modulus 1 and of the form given as,

$$\lambda = e^{2(\pi)ix_i}$$

where x_i is an integer.
R in a bravais lattice is equivalent to

$$\mathbf{R} = n_1\hat{\mathbf{a_1}} + n_2\hat{\mathbf{a_2}} + n_3\hat{\mathbf{a_3}}$$

where $\mathbf{K} = x_1\hat{\mathbf{b_1}} + x_2\hat{\mathbf{b_2}} + x_3\hat{\mathbf{b_3}}$ and $\mathbf{b_i}.\mathbf{a_j} = 2\pi\delta_i j$

$$\mathbf{K}.\mathbf{R} = 2\pi(integer)$$

$$\lambda = e^{iK.\mathbf{R}}$$

$$\psi(\mathbf{r} + \mathbf{R}) = e^{iK.\mathbf{R}}\psi(\mathbf{r})$$

In one dimension,

$$\psi(x + a) = e^{iKa}\psi(x)$$

Proof 2. By Statement,

$$\psi(x) = e^{iKx}u(x)$$

where $u(x + a) = u(x)$

$$\psi(x + a) = e^{iK(x+a)}u(x + a)$$

$$= e^{iKa}e^{iKx}u(x) = e^{iKa}\psi(x)$$

$$\boxed{\psi(x + a) = e^{iKa}\psi(x)}$$

Proof 3. Expanding $\psi(x + a)$ as a series

$$\psi(x + a) = \sum_{n=0} a^n(\frac{d}{dx})^n\psi$$

$$\hat{\mathbf{p_x}} = -i\hbar\frac{d}{dx}$$

$$\frac{d}{dx} = i\hat{\mathbf{p_x}}/\hbar$$

$$\psi(x + a) = \sum_{n=0} a^n(i\hat{\mathbf{p_x}}/\hbar)^n\psi$$

we get,

$$\psi(x+a) = e^{iP_x a/\hbar}\psi = \hat{\mathbf{D}}\psi$$
$$\hat{\mathbf{D}}\,|\psi\rangle = e^{i\hat{\mathbf{p}}.\mathbf{R}/\hbar} = \lambda\,|\psi\rangle \tag{12}$$

Projecting (12)in $|\mathbf{r}\rangle$ basis,

$$\langle r|\,\hat{\mathbf{D}}\,|\psi\rangle = \lambda\,|\psi\rangle$$

$$\psi(\mathbf{r}+\mathbf{R}) = \lambda\psi(\mathbf{r})$$

Projecting (12) in $|\mathbf{K}\rangle$-basis,

$$\langle K|\,\hat{\mathbf{D}}\,|\psi\rangle = \langle K|\,e^{i\hat{\mathbf{p}}.\mathbf{R}/\hbar}\,|\psi\rangle = \lambda\,\langle K|\,|\psi\rangle \tag{13}$$

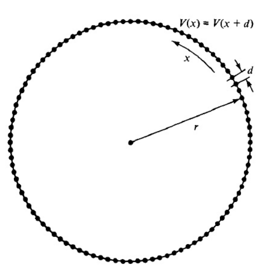
$$\langle K|\,e^{i\hat{\mathbf{p}}.\mathbf{R}} = e^{-i\hat{\mathbf{p}}.\mathbf{R}}\,|K\rangle$$
$$= (1 - iK.\mathbf{R} + ..)\,|K\rangle$$
$$e^{iK.\mathbf{R}}\,\langle K|\,|\psi\rangle = \lambda\,\langle K|\,|\psi\rangle$$
$$e^{-i\hat{\mathbf{K}}.\mathbf{R}}\,|K\rangle = \langle K|\,e^{i\hat{\mathbf{K}}.\mathbf{R}} \tag{14}$$

Putting equation (14) in (13),
$\lambda = e^{iK.\mathbf{R}}$ (Or) $\langle K|\,|\psi\rangle = 0$ is not feasible.

$$\boxed{\hat{\mathbf{D}}\,|\psi\rangle = e^{iK.\mathbf{R}}\,|\psi\rangle}$$

Determine of 'K' values from periodic boundary condition :

The edges of the solid (10^{23}-th site) will spoil the periodicity. hence, the x-axis is assumed to be wrapped around as a circle.(i.e., Periodic boundary condition)



.

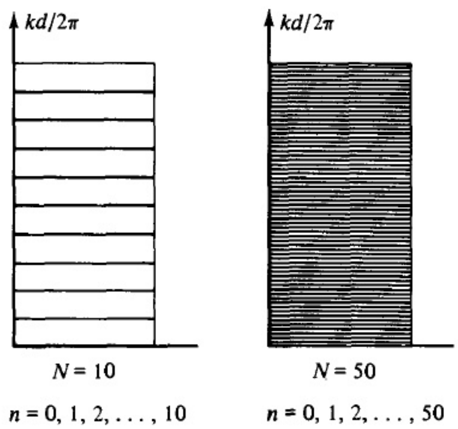
Such that the Nth spike appears at $x = -a$

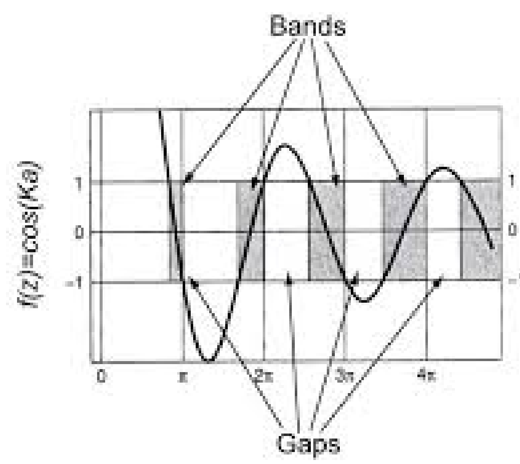
$$\psi(x + Na) = \psi(x)$$
$$e^{iNKa}\psi(x) = \psi(x)$$
$$e^{iNKa} = 1 \implies \frac{2n\pi}{Na} = K$$

where $n = 0, \pm1, \pm2...$

2.2 Results

To Understand the origin of band gaps,one need to understand solution of equation (9) qualitatively, for that we plotted equation (9) for different strength of potential, see figure(3, 4, 5)

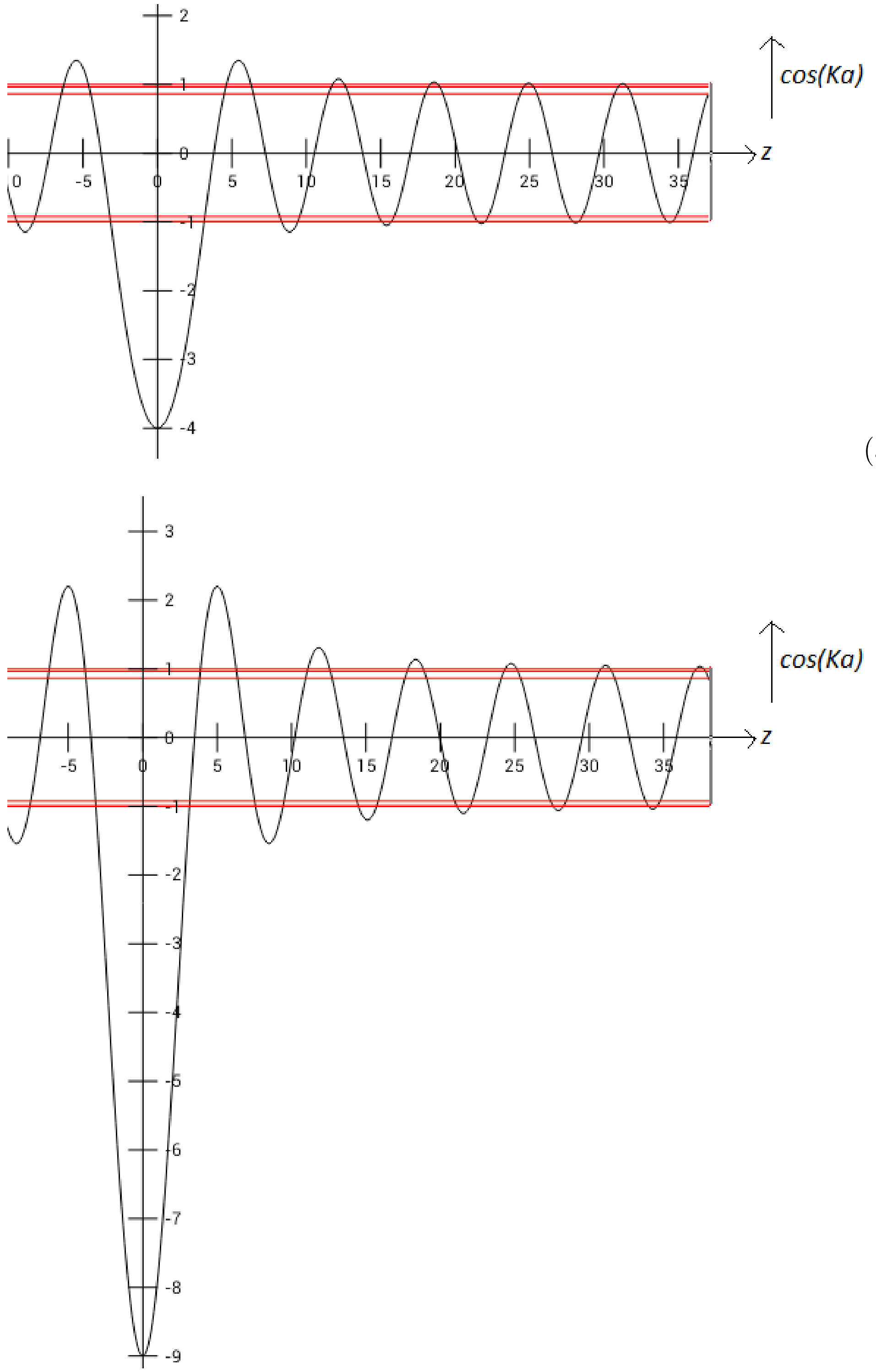




2.3 Summary

1. The treatment of one dimensional periodic potential in a crystalline solid helps us to figure how exactly the band gaps arise in a crystalline solid.

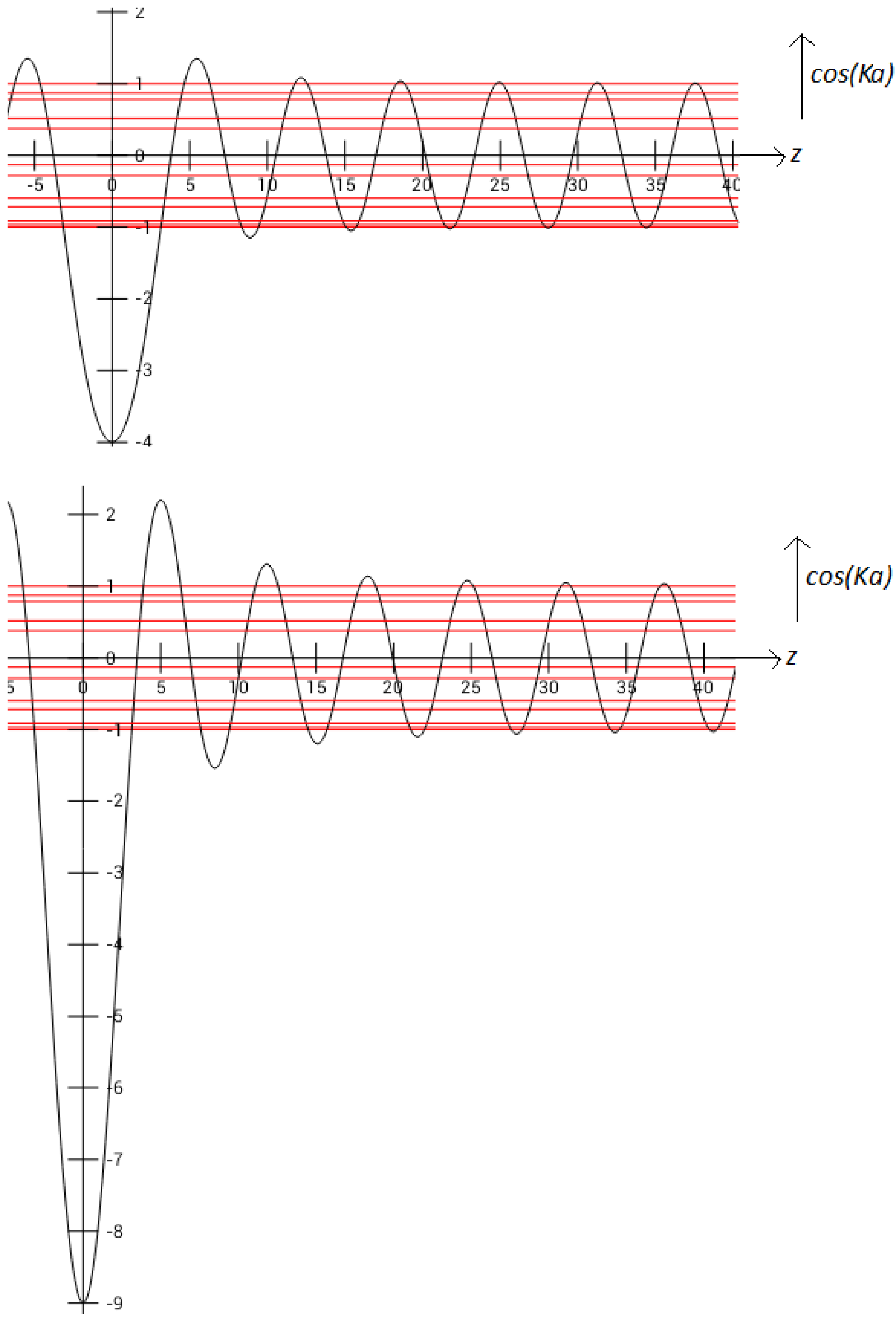
2. The Dirac comb solution can be easily obtained from K-P model solution under certain criterion as:



(a)

(b)

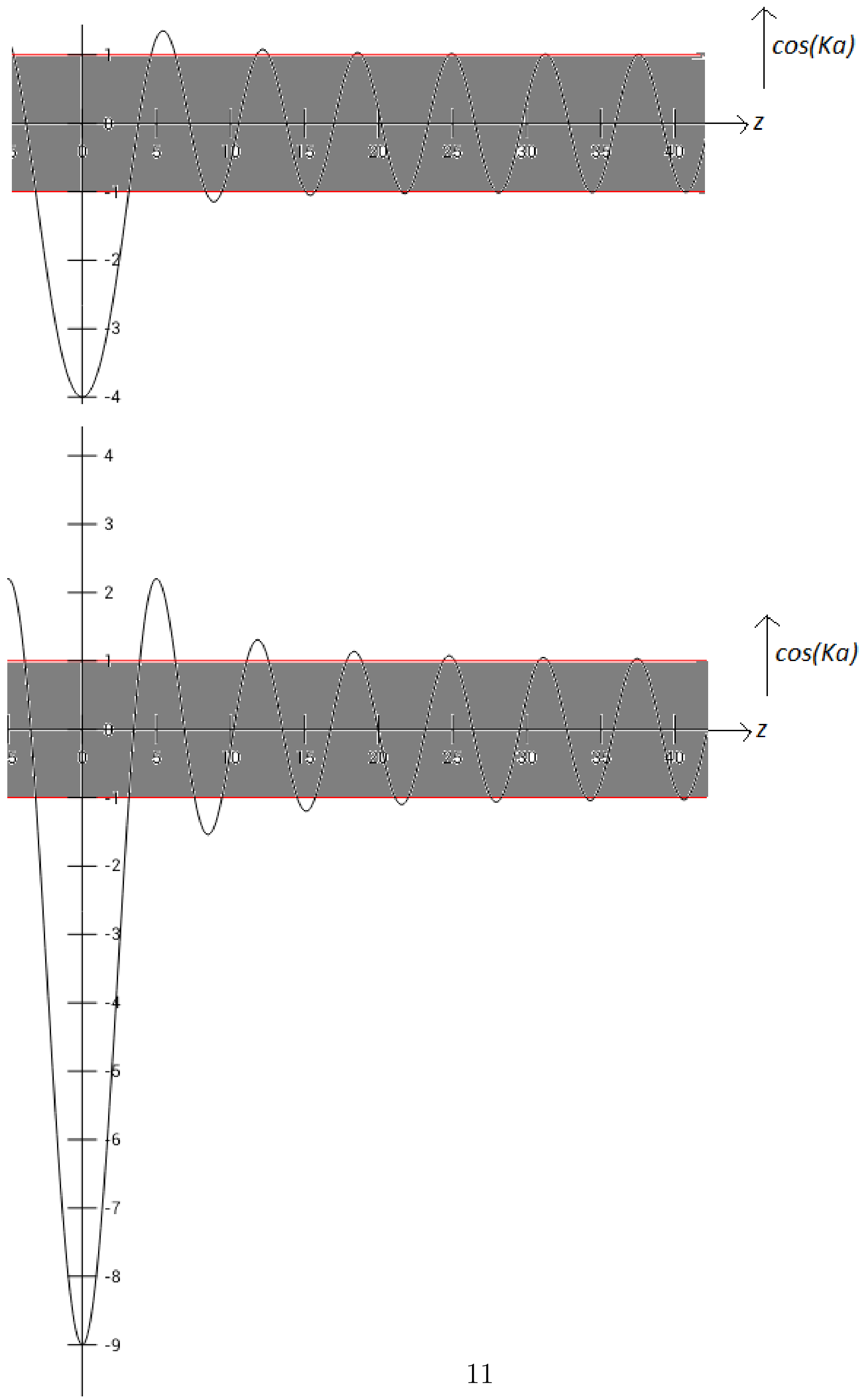
Figure 3: Plot of equation (9) for $N = 5$ and $\beta = 5$(a) and$\beta = 10$(b)
For higher β, the bands exists even for larger 'z' (i.e) the strength of the delta function makes the band gaps arise.



(a)

(b)

Figure 4: Plot of equation (9) for $N = 10$ and $\beta = 5$(a) and$\beta = 10$(b)



(a)

(b)

Figure 5: Plot of equation (9) for $N = 10^{23}$ and $\beta = 5$(a) and$\beta = 10$(b)
For larger 'N' s even the solutions are quantised in terms of 'n' (is an integer) it forms a band which is continuous.

Putting (10) in (9)

$$\cos Kd = \cos k_1 a \cos k_2 b - \frac{\frac{-2mV}{\hbar^2} + 2k_1^2}{2k_1 k_2} \sin k_1 a \sin k_2 b$$

Now, $V = \alpha\delta(x)$, $b = 0$ and $k_1 = k_2$

$$\cos Ka = \cos k_1 a + \frac{m\alpha}{\hbar^2 k_1^2} \sin k_1 a$$

Hence by applying limits we can get back to Dirac comb from the results of Kronig Penny model.

3. Though the bands are discrete ('n' is an integer) it has 'N' number of solutions that makes the band forming a continuoum (For very large 'N').

4. For higher β, the bands exists even for larger 'z' (i.e) the strength of the delta function makes the band gaps arise.

5. For larger z, bands start vanishing.

3 Acknowledgement

Thanks to my guide Dr. Pradeep Kumar who has been there for useful discussions and for the directions. And IIT Mandi for providing Computer lab facility all time.
Thanks to my friends Rishu and Priyamedha sharma for their support and guidance in Latex.

References

[1] Neil W Ashcroft and N David Mermin. Introduction to solid state physics. *Saunders, Philadelphia*, 1976.

[2] David Jeffery Griffiths. *Introduction to quantum mechanics*. Pearson Education India, 2005.

[3] Charles Kittel. *Introduction to solid state physics*. Wiley, 2005.

[4] R de L Kronig and WG Penney. Quantum mechanics of electrons in crystal lattices. In *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, volume 130, pages 499–513. The Royal Society, 1931.

[5] Richard L Liboff. Introductory quantum mechanics. 1987.

[6] Ramamurti Shankar. *Principles of quantum mechanics*. Springer Science & Business Media, 2012.