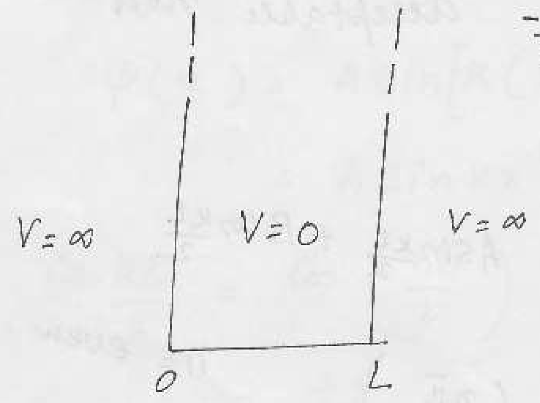
PH-101

Course material for one Week (18.10.04 – 24.10.04)

Particle in a box.



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

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi$$

$$= -K^2\psi$$

$$\psi = A\sin Kx + B\cos Kx$$

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

Boundary Conditions.

1. $\psi(0) = 0 = \psi(L)$

2. $\frac{d\psi(0)}{dx} = \frac{d\psi(L)}{dx}$

Cosine solution is unacceptable because of (1)

$\psi = A\sin Kx$, using (1) $A\sin KL = 0$

$$KL = n\pi \qquad n = 1, 2, 3 \ldots$$

$$K = \frac{n\pi}{L}$$

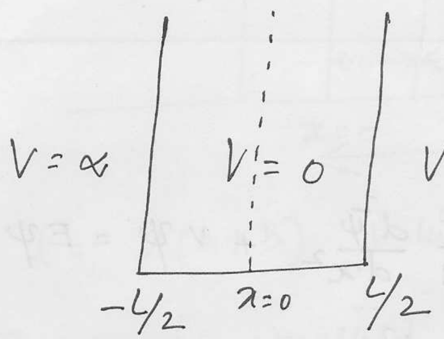
$\psi = A\sin\frac{n\pi}{L}x$ using normalisation

$\int_0^L \psi^*\psi\, dx = 1$ yields, $A = \sqrt{\frac{2}{L}}$

$$\psi(x) = \sqrt{\frac{2}{L}}\sin\frac{n\pi}{L}x\ ; \quad E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

> Ask students to calculate $\frac{\Delta E_n}{E_n}$ for large n (correspondence principle)

Particle in a symmetric box.



$\psi(x) = A\sin kx + B\cos kx$

Both solutions are acceptable now

$\psi\left(-\frac{L}{2}\right) = \psi\left(\frac{L}{2}\right)$

$-A\sin\frac{kL}{2} + B\cos\frac{kL}{2} = A\sin\frac{kL}{2} + B\cos\frac{kL}{2}$

$n =$ even.

$2A\sin\frac{kL}{2} = 0 = \sin\left(\frac{n\pi}{2}\right)$

the solution is

$k = \frac{n\pi}{L}$. for $n =$ even,

$\psi(x) = A\sin kx$

$\psi'\left(-\frac{L}{2}\right) = \psi'\left(\frac{L}{2}\right)$

$AK\cos\frac{kL}{2} + BK\sin\frac{kL}{2} = AK\cos\frac{kL}{2} - BK\sin\frac{kL}{2}$

$2BK\sin\frac{kL}{2} = 0$.

the solution is

$K = \frac{n\pi}{L}$ $n =$ odd,

$\psi(x) = B\cos kx$.

Alternative Solution for particle in a Symmetric box.

Consider the Solution,

$$\psi(x) = A\sin kx$$

Change $x \to x - \frac{L}{2}$

$$\psi(x) = A\sin\left[k\left(x-\frac{L}{2}\right)\right]$$

$$= A\sin kx \cos\left(\frac{kL}{2}\right) - A\cos kx \sin\left(\frac{kL}{2}\right)$$

$$\cos\frac{kL}{2} = \cos\left(\frac{n\pi}{2}\right) = 0 \quad \text{for } n = \text{odd } (1,3\cdots)$$

$$= \pm 1 \quad \text{for } n = \text{even } (2,4\cdots)$$

$$\sin\frac{kL}{2} = \sin\left(\frac{n\pi}{2}\right) = 0 \quad \text{for } n = \text{even } (2,4\cdots)$$

$$= \pm 1 \quad \text{for } n = \text{odd}.$$

$$\psi(x) = A\sin kx \quad \text{for } n = \text{even} \quad (1)$$

$$= B\cos kx \quad \text{for } n = \text{odd}. \quad (2)$$

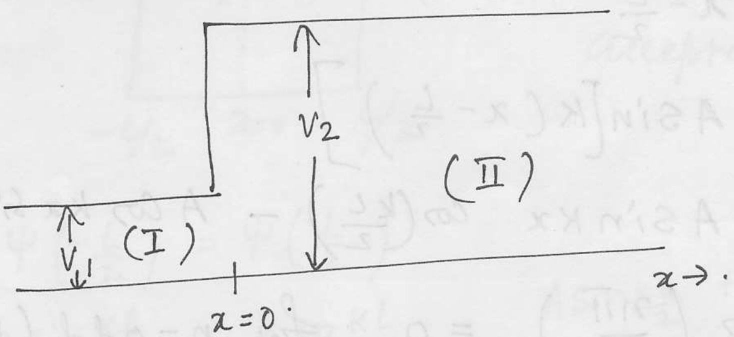
(1) has odd parity, (2) has even parity.

$\boxed{\text{Discuss briefly Parity Violation}}$.

Barrier transmission problems.

Transfer Matrix approach

Example 1 (Potential Discontinuity at $x = 0$).



$$V(x) = V_1 \qquad -\infty < x \leq 0$$
$$= V_2 \qquad x > 0$$
$$E > V_2 > V_1$$

In regions (I) $\quad \psi_{I}(x) = A_1 e^{ik_1 x} + B_1 e^{-ik_2 x} \quad (1)$

(II) $\quad \psi_{II}(x) = A_2 e^{ik_2 x} + B_2 e^{-ik_2 x} \quad (2)$

The boundary conditions are –

$$\psi_I(0) = \psi_{II}(0) \Rightarrow A_1 + B_1 = A_2 + B_2 \quad (3)$$

$$\frac{d\psi_I(0)}{dx} = \frac{d\psi_{II}(0)}{dx} \Rightarrow ik_1(A_1 - B_1) = ik_2(A_2 - B_2) \quad (4)$$

The above eqns. (3) and (4) can be represented as –

$$\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \frac{1}{2k_2} \begin{pmatrix} k_1 + k_2 & k_2 - k_1 \\ k_2 - k_1 & k_1 + k_2 \end{pmatrix} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}$$

$$= \frac{1}{2} \begin{pmatrix} 1 + \frac{k_1}{k_2} & 1 - \frac{k_1}{k_2} \\ 1 - \frac{k_1}{k_2} & 1 + \frac{k_1}{k_2} \end{pmatrix} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}$$

$$= M(k_1, k_2) \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}$$

Properties of the M-matrix

1. $M(k_1, k_2)\, M(k_2, k_3) = M(k_2, k_3)\, M(k_1, k_2)$
   — self commuting.

2. $M(k_1, k_2)\, M(k_2, k_3) = M(k_1, k_3)$.

3. $M(k_1, k_2)\, M(k_2, k_1) = \mathbb{1}$.

Reflection & Transmission Coefficients.

We have,

$$\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = M(k_1, k_2) \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}$$

So,

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = M(k_2, k_1) \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}$$

$$= \frac{1}{2} \begin{pmatrix} 1 + \frac{k_2}{k_1} & 1 - \frac{k_2}{k_1} \\ 1 - \frac{k_2}{k_1} & 1 + \frac{k_2}{k_1} \end{pmatrix} \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}$$

Now to calculate ~~transmission~~ ~~to~~ reflection coefficient, we can assume $B_2 = 0$ (no -ive moving wave)
In addition take $A_2 = 1$. With this we have made the normalisation arbitrary.

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 + \frac{k_2}{k_1} \\ 1 - \frac{k_2}{k_1} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad R = \frac{|B_1|^2}{|A_1|^2} = \frac{\left(1 - \frac{k_2}{k_1}\right)^2}{\left(1 + \frac{k_2}{k_1}\right)^2}$$

Hence $T = 1 - R = \dfrac{4k_2/k_1}{(1 + k_2/k_1)^2} = \dfrac{4k_1k_2}{(k_1 + k_2)^2}$

Example 2. (Finite potential discontinuity at x

$V_1 < E < V_2$

$k_1 \to k_1$

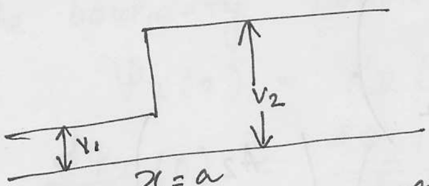
$k_2 \to ik_2$.

$$M(ik_2, k_1) = \frac{1}{2}\begin{pmatrix} 1 + \frac{ik_2}{k_1} & 1 - \frac{ik_2}{k_1} \\ 1 - \frac{ik_2}{k_1} & 1 + \frac{ik_2}{k_1} \end{pmatrix}.$$

$$M(k_1, ik_2) = \frac{1}{2}\begin{pmatrix} 1 + \frac{ik_1}{k_2} & 1 - \frac{ik_1}{k_2} \\ 1 - \frac{ik_1}{k_2} & 1 + \frac{ik_1}{k_2} \end{pmatrix}$$

Example 3. (finite potential discontinuity at $x=a$)

Again consider $E > V_2 > V_1$



The Boundary conditions yield,

$$A_1 e^{ik_1 a} + B_1 e^{-ik_1 a} = A_2 e^{ik_2 a} + B_2 e^{-ik_2 a}$$

$$ik_1\left(A_1 e^{ik_1 a} - B_1 e^{-ik_1 a}\right) = ik_2\left(A_2 e^{ik_2 a} - B_2 e^{-ik_2 a}\right)$$

Define $A' = A e^{ika}$; $B' = B e^{ika}$

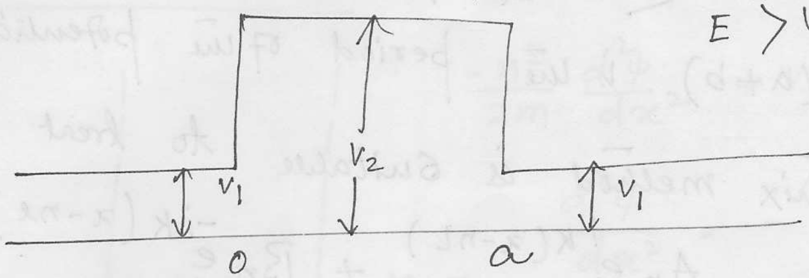
$$\begin{pmatrix} A' \\ B' \end{pmatrix} = \begin{pmatrix} e^{ika} & 0 \\ 0 & e^{-ika} \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix}.$$

Thus we need to displace our earlier calculations by $D(a) = \begin{pmatrix} e^{ika} & 0 \\ 0 & e^{-ika} \end{pmatrix}$.

Example 4. (Usage of the discontinuity matrix M and the propagation matrix D)

Consider a rectangular potential barrier.

$E > V_2 > V_1$



$$\begin{pmatrix} A_3 \\ B_3 \end{pmatrix} = M(K_1, K_2)\, D(a)\, M(k_1, k_2) \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}$$

$$= \begin{pmatrix} 1+\frac{k_1}{k_2} & 1-\frac{k_1}{k_2} \\ 1-\frac{k_1}{k_2} & 1+\frac{k_1}{k_2} \end{pmatrix} \begin{pmatrix} e^{\frac{ika}{2}} & 0 \\ 0 & e^{\frac{ika}{2}} \end{pmatrix} \begin{pmatrix} 1+\frac{k_1}{k_2} & 1-\frac{k_1}{k_2} \\ 1-\frac{k_1}{k_2} & 1+\frac{k_1}{k_2} \end{pmatrix} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}$$

Thus a period structure can be investigated.

$V_2 > E > V_1$

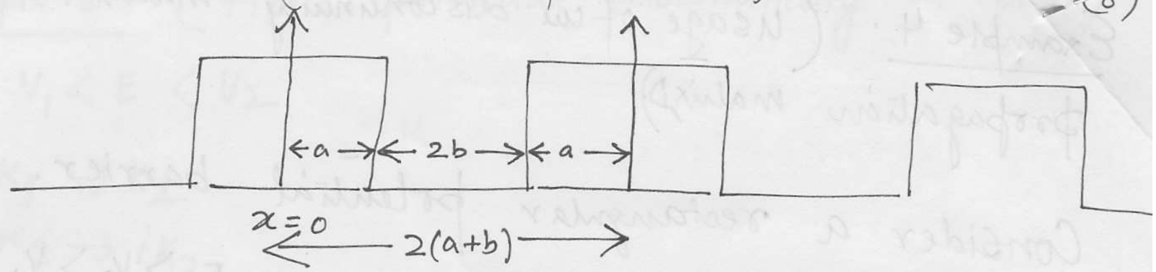
The general structure of the matrix connecting the coefficients between the extreme left and extreme right is

$$\begin{pmatrix} A_3 \\ B_3 \end{pmatrix} = \begin{pmatrix} \alpha_1 \pm i\beta_1 & i\beta_2 \\ i\beta_2 & \alpha_1 + i\beta_1 \end{pmatrix} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}$$

with $\alpha_1, \beta_1, \beta_2$ satisfying the condition

$$\alpha_1^2 + \beta_1^2 - \beta_2^2 = 1$$

Example V (Periodic potential)



$l = 2(a+b)$ is the period of the potential.

The matrix method is suitable to treat this proble

$$\psi(x) = A_n e^{ik(x-nL)} + B_n e^{-ik(x-nl)} \quad ; \; k = \sqrt{\frac{2mE}{\hbar^2}}$$

The relation between the coefficients can be written as -

$$\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = MD \begin{pmatrix} A_n \\ B_n \end{pmatrix}$$

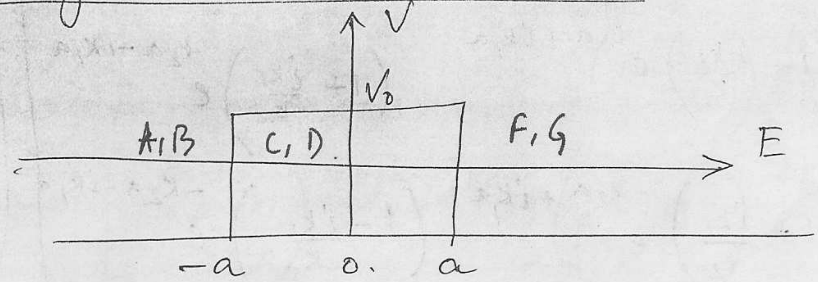
$$= P \begin{pmatrix} A_n \\ B_n \end{pmatrix}$$

$$= \begin{bmatrix} (\alpha_1 - i\beta_1) e^{ikl} & -i\beta_2 e^{ikl} \\ i\beta_2 e^{-ikl} & (\alpha_1 + i\beta_1) e^{ikl} \end{bmatrix} \begin{pmatrix} A_n \\ B_n \end{pmatrix}.$$

Subject to the condition.

$$\alpha_1^2 + \beta_1^2 - \beta_2^2 = 1.$$

Rectangular Potential Barrier



For $E < V_0$

$$\psi(x) = \begin{cases} A e^{ik_1 x} + B e^{-ik_1 x} & \text{for } x < -a \\ C e^{-K_2 x} + D e^{K_2 x} & \text{for } -a < x < a \\ F e^{iK_1 x} + G e^{-ik_1 x} & \text{for } x > a. \end{cases}$$

$$K_1 = \sqrt{\frac{2mE}{\hbar^2}} \; ; \quad K_2 = \sqrt{\frac{2m\cancel{(E-V)}(V_0 - E)}{\hbar^2}}$$

The boundary conditions at $x = \pm a$ ~~to~~ gives

$$A e^{-ik_1 a} + B e^{ik_1 a} = C e^{K_2 a} + D e^{-K_2 a} \qquad (1)$$

and

$$A e^{-ik_1 a} - B e^{ik_1 a} = \frac{ik_2}{k_1}\left(C e^{k_2 a} - D e^{-K_2 a}\right) \qquad (2)$$

This can be represented as

$$\begin{pmatrix} A \\ B \end{pmatrix} = \frac{1}{2} \begin{bmatrix} \left(1 + \frac{ik_2}{k_1}\right) e^{k_2 a + ik_1 a} & \left(1 - \frac{ik_2}{k_1}\right) e^{-k_2 a + ik_1 a} \\ \left(1 - \frac{ik_2}{k_1}\right) e^{k_2 a - ik_1 a} & \left(1 + \frac{ik_2}{k_1}\right) e^{-k_2 a - ik_1 a} \end{bmatrix} \begin{pmatrix} C \\ D \end{pmatrix}$$

(2)

Similarly matching the conditions at $x = a$

$$\begin{pmatrix} C \\ D \end{pmatrix} = \frac{1}{2} \begin{bmatrix} \left(1 - \frac{ik_1}{k_2}\right) e^{k_2 a + ik_1 a} & \left(1 + \frac{ik_1}{k_2}\right) e^{k_2 a - ik_1 a} \\ \left(1 + \frac{ik_1}{k_2}\right) e^{-k_2 a + ik_1 a} & \left(1 - \frac{ik_1}{k_2}\right) e^{-k_2 a - ik_1 a} \end{bmatrix} \begin{pmatrix} F \\ G \end{pmatrix}$$

Thus,

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{bmatrix} \alpha_1 + i\beta_1 & \alpha_2 + i\beta_2 \\ \alpha_3 + i\beta_3 & \alpha_4 + i\beta_4 \end{bmatrix} \begin{pmatrix} F \\ G \end{pmatrix}$$

~~check these~~ i's.

$$\alpha_1 = \cosh(2k_2 a)\, e^{2ik_1 a} \; ; \quad \beta_1 = \frac{i}{2}\left(\frac{k_2}{k_1} - \frac{k_1}{k_2}\right) \sinh(2k_2 a)\, e^{2ik_1 a}$$

$$\alpha_2 = 0 \; ; \quad \beta_2 = i\left(\frac{k_2}{k_1} + \frac{k_1}{k_2}\right) \sinh(2k_2 a)$$

$$\beta_3 = -\beta_2$$

$$\alpha_3 = 0$$

$$\alpha_4 = \alpha_1 \qquad \beta_4 = -\beta_1 .$$

They reduce the no. of variables.

Thus: $G=0$
$$\frac{F}{A} = \frac{e^{-2ik_1 a}}{\cosh(2k_2 a) + \frac{i}{2}\left(\frac{k_2}{k_1} - \frac{k_1}{k_2}\right)\sinh(2k_2 a)}$$

If: $V_0 \to \infty$ and $a \to \infty$ (very poor transmission)

$$\cosh(2k_2 a) \approx \sinh(2k_2 a) \approx \frac{e^{2k_2 a}}{2}.$$

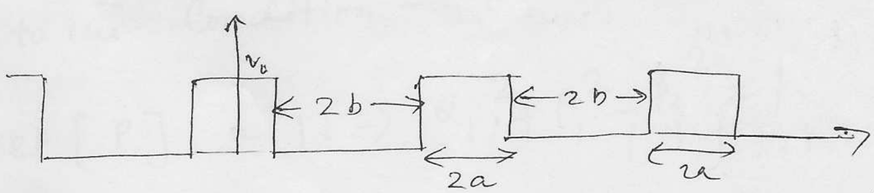
Thus $T = \left|\frac{F}{A}\right|^2 \simeq 16\, e^{-4k_2 a}\left(\frac{k_1 k_2}{k_1^2 + k_2^2}\right)^2$

Check: The determinant of the matrix $\Rightarrow D = 1$

Thus $\alpha_1^2 + \beta_1^2 - \beta_2^2 = 1.$

Because of this relation we are left with 2 independent parameters depending on $k_1 a$ and $k_2 a$.

The periodic Potential (Kronig Penny model)



The periodic potential has period $2(a+b)$

The Sch. Eqn. in the valleys $(V=0)$ and $\hbar k = \sqrt{2mE}$ are

$$\psi(x) = A_n e^{ik(x-nL)} + B_n e^{-ik(x-nl)}.$$

l = period $= 2(a+b)$. ← check this.

and. $(a-l) < (x-nl) < -a$.

where the coefficients belonging to successive values of n can be related by a matrix. The maxima of the wavefn. have coordinates $x = nl$, Thus —

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = \begin{bmatrix} \alpha_1 + i\beta_1 & i\beta_2 \\ -i\beta_2 & \alpha_1 - i\beta_1 \end{bmatrix} \begin{pmatrix} A_{n+1}\, e^{-ikl} \\ B_{n+1}\, e^{ikl} \end{pmatrix}$$

This can also be written as —

$$\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = [P] \begin{pmatrix} A_n \\ B_n \end{pmatrix}$$

Where $[P]$ is defined as —

$$[P] = \begin{bmatrix} (\alpha_1 - i\beta_1)\, e^{ikl} & -i\beta_2\, e^{ikl} \\ i\beta_2\, e^{-ikl} & (\alpha_1 + i\beta_1)\, e^{-ikl} \end{bmatrix}$$

Subject to the condition —

$$\det[P] = 1. \Rightarrow \alpha_1^2 + \beta_1^2 - \beta_2^2 = 1$$

Thus by iteration

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = P^n \begin{pmatrix} A_0 \\ B_0 \end{pmatrix}$$

As $n \to \pm\infty$, the limit of P_n should exist. This is most conveniently discussed in terms of the eigenvalue problem of the matrix P. The eigenvalues of p are the roots of the equation.

$$\lambda^2 - \lambda\left[\text{Trace } P\right] + \left[\det P\right] = 0$$

or,
$$\lambda^2 - 2(\alpha_1 \cos kl + \beta_1 \sin kl)\lambda + 1 = 0.$$

$$\lambda_\pm = \frac{1}{2}\left[\text{Trace } P \pm \sqrt{(\text{Trace } P)^2 - 4}\right]$$

If the roots are different, then the eigenvectors are linearly indep. Thus

$$P\begin{pmatrix} A_0^{(\pm)} \\ B_0^{(\pm)} \end{pmatrix} = \lambda_\pm \begin{pmatrix} A_0^{\pm} \\ B_0^{\pm} \end{pmatrix}.$$

Thus the solution at the nth period can be connected with those at the beginning –

$$\begin{pmatrix} A_n^{(\pm)} \\ B_n^{(\pm)} \end{pmatrix} = \lambda_\pm^n \begin{pmatrix} A_0^{(\pm)} \\ B_0^{(\pm)} \end{pmatrix}.$$

If $|\text{Trace } P| > 2$, λ_+ and λ_- are real.

Thus. $\lim_{n\to\infty} |\lambda_\pm^n| \to \infty$ a $\lim_{n\to-\infty} |\lambda_\pm^n| \to$ ..

One can prove that — for $E > V_0$.

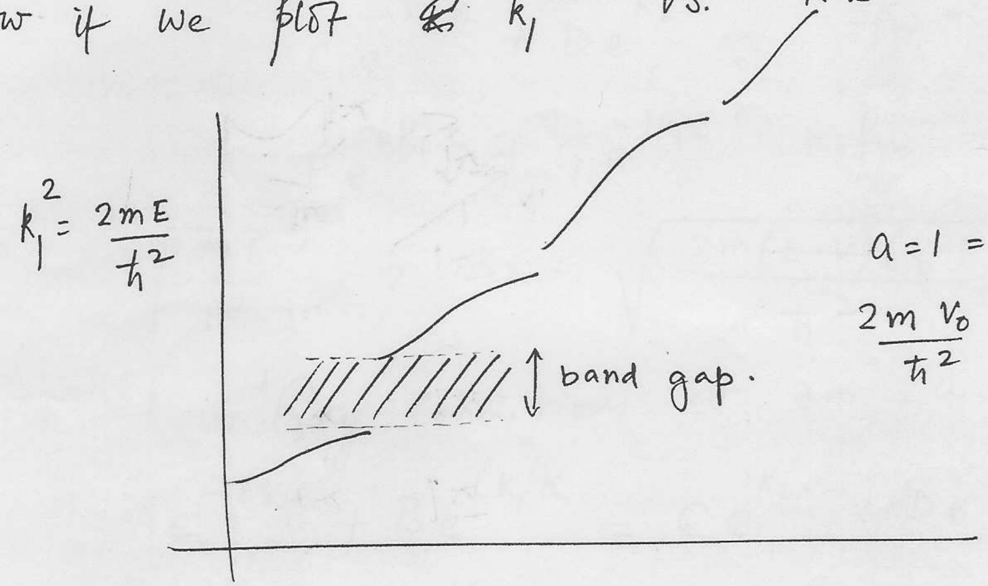
$$\cos K'\ell = \cos(2k_2 a)\cos(2k_1 b) - \frac{k_2'^2 + k_1^2}{2k_1 k_2'}\sin(2k_2' a)\sin(2k_1 b)$$

$$k_2' = \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$$

Now the forbidden bands are

$$2k_2 a + 2k_1 b = N\pi$$

Now if we plot k_1^2 vs. $K'\ell$.



$a = 1 = b$.

$$\frac{2m V_0}{\hbar^2} = \frac{\pi^2}{4}.$$

So the energy spectrum consists of continuous bands separated by forbidden gaps.