HW-3

①

$E\text{-}K \Rightarrow \quad E(K) = C(1 - \cos Ka)$

a) $K \approx 0$

$$E(K) \approx C\left(1 - \left(1 - \frac{K^2a^2}{2}\right)\right)$$

$$E(K) \approx \frac{CK^2a^2}{2}$$

$$m^* = \frac{\hbar^2}{\partial^2 E / \partial K^2}$$

$$\boxed{m^* = \frac{\hbar^2}{Ca^2}}$$

b) $$\partial E / \partial K = C\,a \sin Ka$$

$$\partial^2 E / \partial K^2 = Ca^2 \cos Ka$$

$$\boxed{m^* = \frac{\hbar^2}{Ca^2 \cos Ka}}$$

c) Constant Force = F

$$F = m a = m^* \partial v/\partial t = \text{constant}$$

$$\gamma = \frac{\hbar^2}{Ca^2 \cos Ka} \partial v/\partial t$$

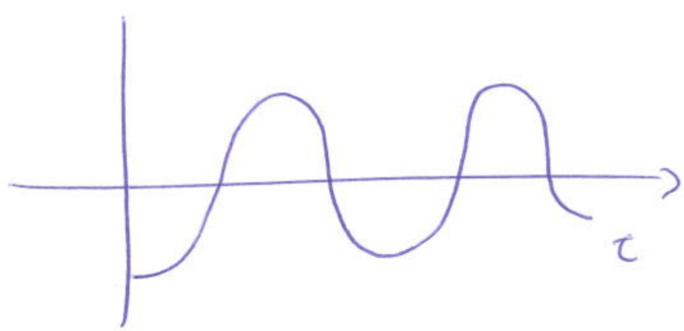
$$\alpha \cos Ka = \partial v/\partial t$$

$$\hbar \, \partial K/\partial t = qF$$

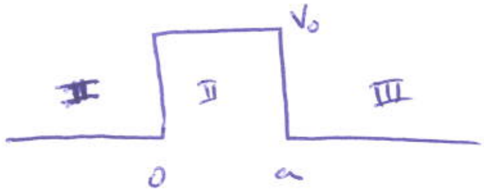
$$K(t) = \frac{q}{\hbar} F t$$

$$\partial v/\partial t = \alpha \cos \frac{qFa}{\hbar} t$$

$$X(t) = -\alpha \frac{\hbar^2}{Fa} \cos \frac{Fa t}{\hbar}$$



Shift barrier



$$K_1 = \sqrt{\frac{2mE}{\hbar^2}} \qquad K_2 = i\sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

$$\psi_I = e^{iK_1 x} + re^{-iK_1 x}$$

$$\psi_{II} = Ae^{iK_2 x} + Be^{-iK_2 x}$$

$$\psi_{III} = te^{iK_1 x}$$

$$\psi_1(0) = \psi_2(0) \qquad \psi_2(a) = \psi_3(a)$$

$$\psi_1'(0) = \psi_2'(0) \qquad \psi_2'(a) = \psi_3'(a)$$

$$1 + r = A + B$$

$$iK_1 - riK_1 = AiK_2 - BiK_2$$

$$Ae^{iK_2 a} + Be^{-iK_2 a} = te^{iK_1 a}$$

$$AiK_2 e^{iK_2 a} - BiK_2 e^{-iK_2 a} = tiK_1 e^{iK_1 a}$$

$$A = 1 + r - B$$

$$\cancel{B_1} \qquad ik_2(1+r) + ik_1 - r\,ik_1 = 2ik_2 A$$

$$\boxed{ik_2(1+r) + ik_1(1-r) = 2ik_2 A}$$

$$A e^{ik_2 a} + B e^{-ik_2 a} = t e^{ik_1 a}$$

$$A i k_2 e^{ik_2 a} + B i k_2 e^{-ik_2 a} = i k_2 t e^{ik_1 a}$$

$$+ \quad A i k_2 e^{ik_2 a} - B i k_2 e^{-ik_2 a} = i k_1 t e^{ik_1 a}$$

$$\boxed{2 A i k_2 e^{ik_2 a} = t(ik_1 + ik_2) e^{ik_1 a}}$$

$$e^{-ik_2 a} + r e^{-ik_2 a} = A e^{-ik_2 a} + B e^{-ik_2 a}$$

$$t e^{ik_1 a} = A e^{ik_2 a} + B e^{-ik_2 a}$$

$$\boxed{e^{-ik_2 a} + r e^{-ik_2 a} - t e^{ik_1 a} = A\left(e^{-ik_2 a} - e^{ik_2 a}\right)}$$

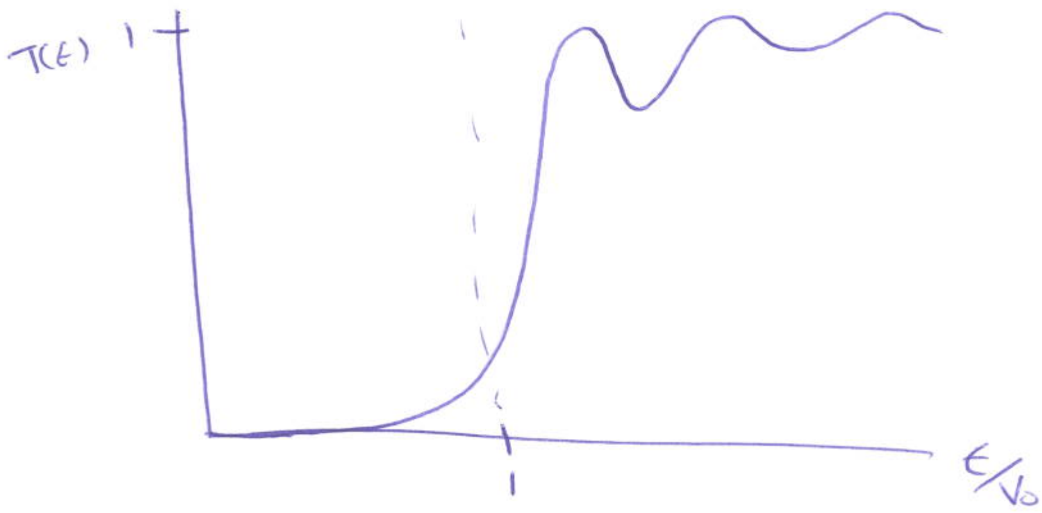
(1) $$A = \frac{1}{2ik_2}\left[ik_2(1+r) + ik_1(1-r)\right]$$

$$A = \frac{t e^{ik_2 a}}{2ik_2}(ik_1 + ik_2)$$

$$\boxed{t e^{ik_2 a}(ik_1 + ik_2) = ik_2(1+r) + ik_1(1-r)}$$

t vs r

$$\boxed{e^{-ik_2 a} + r e^{-ik_2 a} - t e^{ik_1 a} = \frac{t e^{ik_2 a}}{2ik_2}(ik_1 + ik_2)} \quad t \text{ vs } r$$



T(E)
1
E/V0

3)

N-atom x-tal

a) $\vec{k} = \dfrac{2\pi n}{N(a+b)} \qquad n = 0, \pm 1, \pm 2 \ldots \pm N/2$

b) Each band holds ~N electrons

so if each atom has 4 electrons,

there are a total of 4N electrons

in the x-tal

$\boxed{\text{4 bands are filled}}$

c) $\boxed{\text{2 bands}}$

4)

$a = b = 3\mathring{A} \qquad V_0 = V_0 = 1eV$

$$f(\zeta) = \frac{1-2\zeta}{2\sqrt{\zeta(1-\zeta)}} \sin \alpha_0 a\sqrt{\zeta} \sinh \alpha_0 b\sqrt{1-\zeta} + \cos \alpha_0 a\sqrt{\zeta} \cosh \alpha_0 b\sqrt{1-\zeta}$$

$0 < E_0 < V_0$

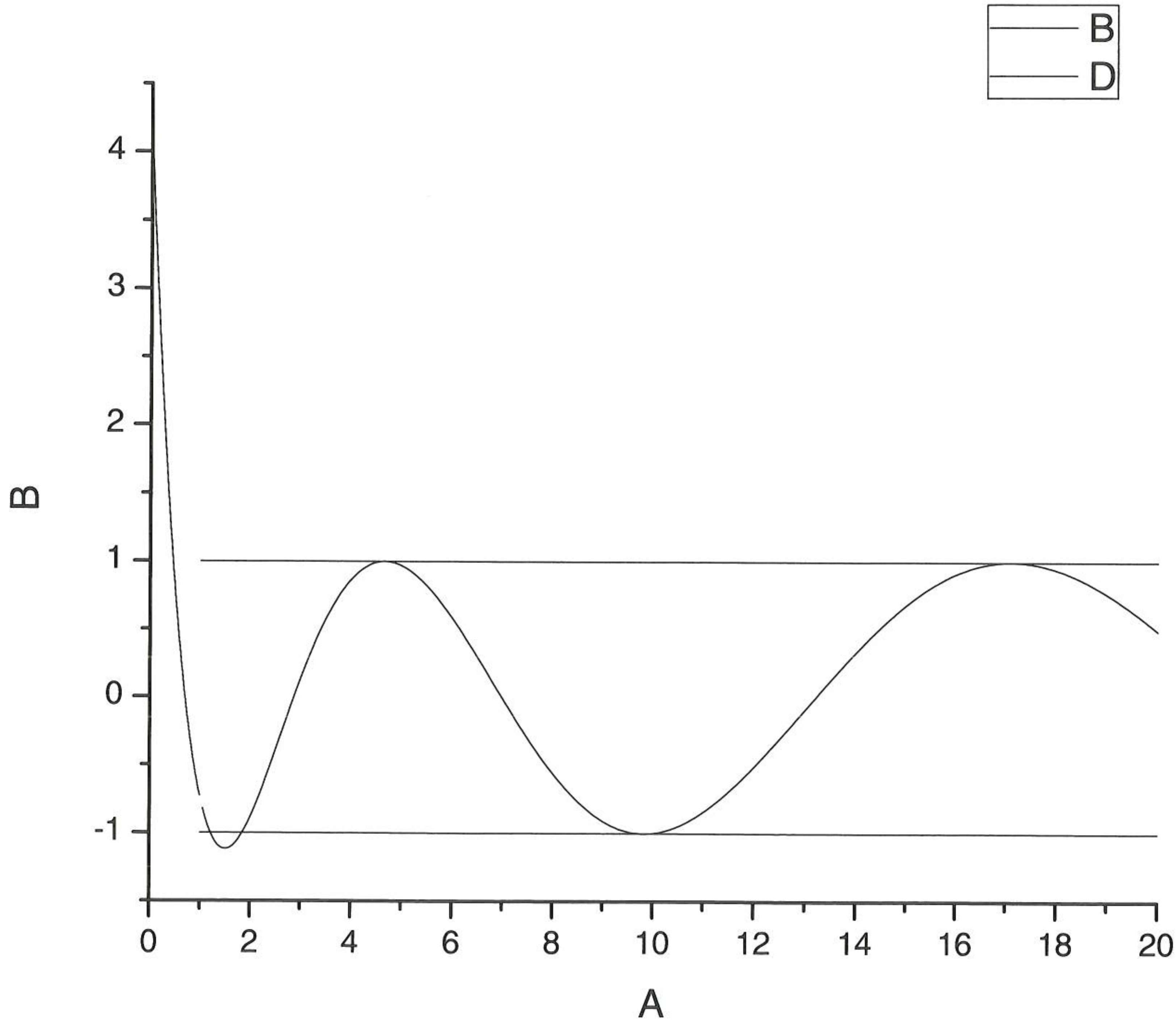
$$f(\zeta) = \frac{1-2\zeta}{2\sqrt{\zeta(\zeta-1)}} \sin \alpha_0 a\sqrt{\zeta} \sin \alpha_0 b\sqrt{\zeta-1} + \cos \alpha_0 a\sqrt{\zeta} \cos \alpha_0 b\sqrt{\zeta-1}$$

$E_0 > V_0$

$$\alpha_0 = \sqrt{\frac{2mV_0}{\hbar^2}} = 5.14 \times 10^9$$

$$a = b = 3 \times 10^{-10}$$

$\zeta_1 = 0.45$	$\zeta_2 = 1.2$	$\zeta_3 = 1.85$	$\zeta_4 = 4.6$
$\zeta_2 = 1.2$	$\zeta_3 = 1.85$	$\zeta_4 = 4.6$	$\zeta_5 = 4.7$
band	gap	band	gap


B
D
4
3
2
1
0
-1
B
0
2
4
6
8
10
12
14
16
18
20
A