Solutions

PHY 481/581 - HOMEWORK SET 5

Northern Arizona University | Due: 11/19/2018

Problem 1. Describe the difference between the free electron and nearly free electron models. Draw the dispersion curves for both models using the extended and reduced zone schemes. What is the origin of the band gap opening at the Brillouin zone boundaries? Be sure to label your drawings clearly.

Problem 2. Consider electrons of mass m moving in a one-dimensional "Dirac comb" potential defined as

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

where α is a "strength parameter" with units of energy, N is the number of lattice points, and a is the spacing between points in the direct lattice.

(a) Show that $\psi(x + a) = e^{ika}\psi(x)$ given that $\psi(x) = e^{ikx}u(x)$, where $u(x) = u(x + a)$ has periodicity matching the lattice.

(b) Show that the solution to the Schrödinger equation is $\psi(x) = A\sin(qx) + B\cos(qx)$, where q is the wavenumber of the electron, for regions with $V(x) = 0$, in particular $0 < x < a$.

(c) Using the continuity of the wave function at $x = 0$, derive

$$B = e^{-ika}\big[A\sin(qa) + B\cos(qa)\big]. \tag{2}$$

(d) Using the discontinuity of the derivative at $x = 0$ given by

$$\left.\frac{d\psi}{dx}\right|_{x=0^+} - \left.\frac{d\psi}{dx}\right|_{x=0^-} = \frac{-2m\alpha}{\hbar^2}\psi(0) \tag{3}$$

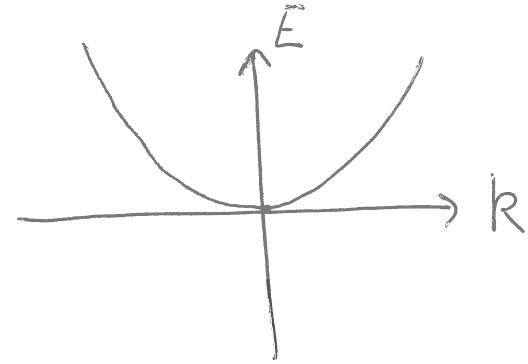
derive the following relation:

$$qA - e^{-ika}q\big[A\cos(qa) - B\sin(qa)\big] = \frac{2m\alpha}{\hbar^2}B. \tag{4}$$

(e) Use Eqs. (2) & (4) to derive the relationship for allowed values of q that we discussed in class (see notes from Nov. 09). Draw the resulting curve and indicate the locations of the allowed and disallowed bands. Make sure to mark your axes clearly.

(1) "Free" in the free electron model means the potential $V=0$ everywhere within the solid + energy of the electron is given by

$$E = \frac{\hbar^2 k^2}{2m}$$



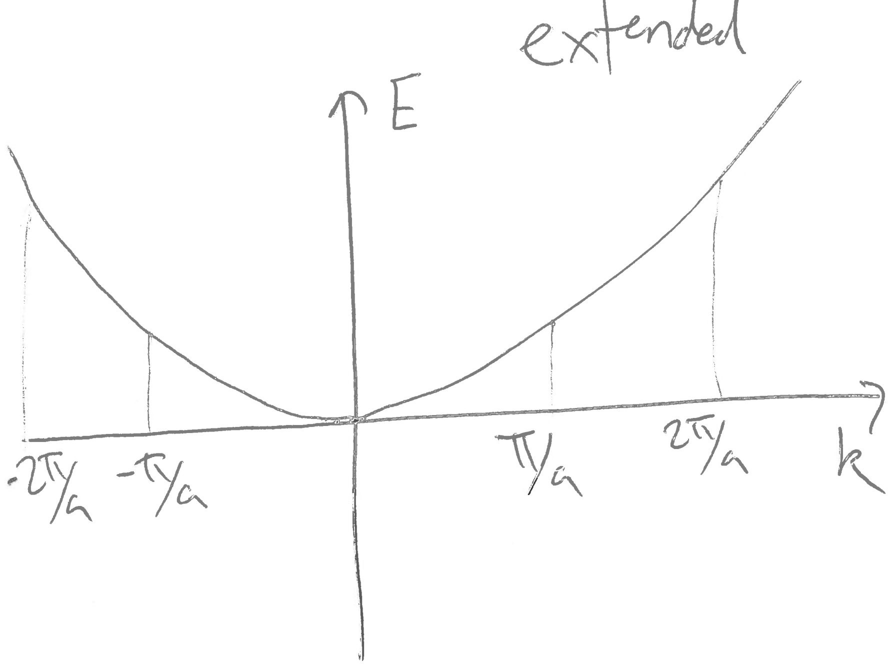
- because no two electrons can be in the same state, the energies are progressively higher with additional electrons until the Fermi level

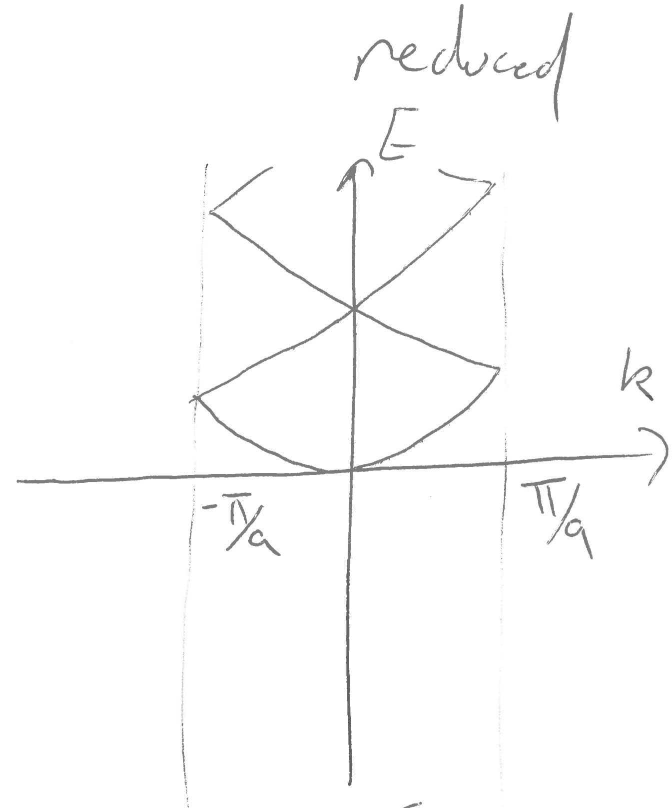
- the nearly free electron model assumes a weak periodic potential is felt by the electrons e.g. in 1D $V(x) = V(x+a)$, where 'a' is the lattice spacing. The potential causes band gaps to open near the Brillouin zone boundaries. The physical origin of this effect arises from the electrons near the boundary satisfying the Bragg condition

#1 continued

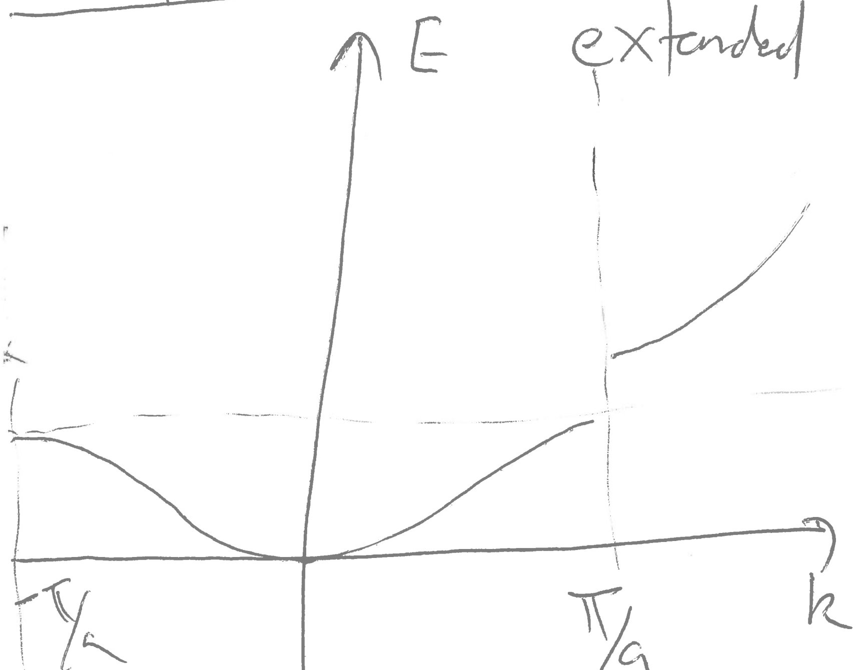
Dispersion curves:

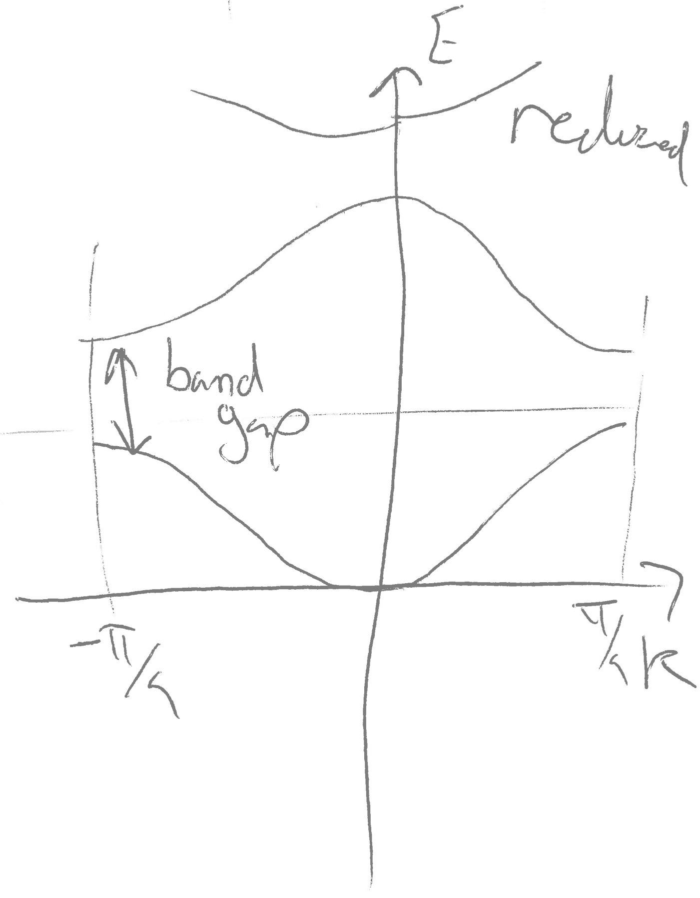
Free electron:



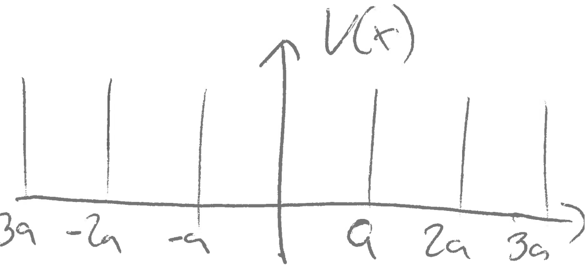


Nearly Free electron:





② $V(x) = \alpha \sum_{j=1}^{N-1} \delta(x - ja)$



Dirac "comb"

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

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

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

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

$= \psi(x) e^{ika}$ ✓

- no need to know form of $V(x)$ for this problem

(b) for $V = 0$, the Schrödinger eq.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \underbrace{\cancel{V(x)\psi(x)}}_{0} = E\psi(x)$$

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

$q \equiv \sqrt{2mE}/\hbar$

#2 continued

(c) immediately to the left of the origin at $x=0$, Bloch's theorem gives

$$\psi(x) = e^{-ika}\left[A\sin(x+a)q + B\cos(x+a)q\right]$$

for $(-a<x<0)$

@ $x=0$, ψ is continuous

$$\psi(0)\Big|_{(-a<x<0)} = \psi(0)\Big|_{(0<x<a)}$$

$$\Rightarrow e^{-ika}\left[A\sin(qa) + B\cos(ka)\right]$$

$$= B \quad \checkmark$$

$\rightarrow$

#2 Continued

(d) $$\left.\frac{d\psi}{dx}\right|_{x=0^+} - \left.\frac{d\psi}{dx}\right|_{x=0^-} = \frac{-2m\alpha}{\hbar^2}\psi(0)$$

$$\left.\frac{d\psi}{dx}\right|_{x=0^-} = e^{-ika}\left[qA\cos(qa) - qB\sin(qa)\right]$$

$$\left.\frac{d\psi}{dx}\right|_{x=0^+} = qA\cos(0) - \cancel{Bq\sin(0)}$$

$$qA - e^{-ika}\left[qA\cos(qa) - qB\sin(qa)\right]$$

$$= -\frac{2m\alpha}{\hbar^2}\psi(0) = \frac{-2m\alpha}{\hbar^2}B \checkmark$$

#2 continued

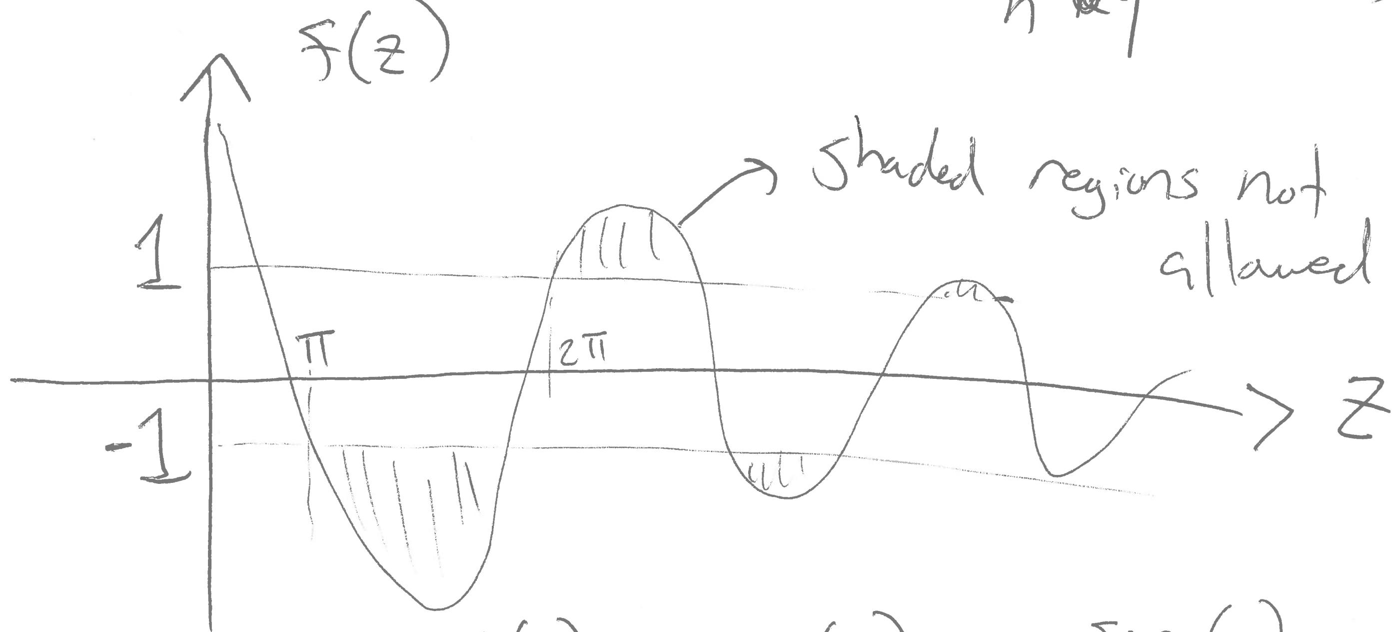
(e) Solving Eq. (2) for $A\sin(qa)$

$$A\sin(qa) = \left[e^{ika} - \cos(qa)\right]B$$

- put this into Eq. (4)

$$\left[e^{ika} - \cos(qa)\right]\left[1 - e^{-ika}\cos(qa)\right] + e^{-ika}\sin^2(qa) = \frac{2m\alpha}{\hbar^2 q}\sin(qa)$$

$$\Rightarrow \cos(ka) = \cos(qa) + \frac{m\alpha}{\hbar^2 q}\sin(qa)$$



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