"Traditional" Approach to Energy Bands in Solids

In P140A we discussed two pictures of energy bands in solids:

(1) Evolution from highly degenerate discrete atomic levels as nuclei pushed closer

(2) Second quantized approach $H = -t\sum(c_\ell^\dagger c_{\ell+1} + c_{\ell+1}^\dagger c_\ell)$

$\rightarrow \epsilon(k) = -2t\cos k$

we now follow Kittel ch 7 by considering what periodic potential might do to change $\psi = e^{i\vec{k}\cdot\vec{r}}$ $E = \hbar^2k^2/2m$ of free particles.

* Great quote by Felix Bloch from Kittel $\longrightarrow$

How can e^- sneak by all the ions?

$\psi(r)$ differs from $e^{i\vec{k}\cdot\vec{r}}$ by only a periodic modulation!

Key point: For some k the effect is stronger than others, so strong that the associated $\epsilon(k)$ are no longer allowed $\rightarrow$ Energy gaps

metals vs insulators

Hall coefficient $\gtrless 0$

explain host of phenomena

K7-2 **PHYSICAL PICTURE**

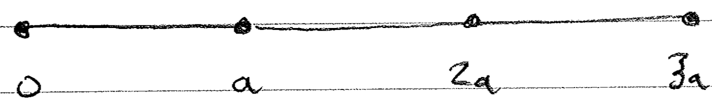
Bragg condition.

X rays scattering off nuclei $\vec{k}' = \vec{k} + \vec{G}$

$\in n_1\vec{b}_1 + n_2\vec{b}_2 + n_3\vec{b}_3$

likewise e^- are scattered off nuclei

$d=1$:



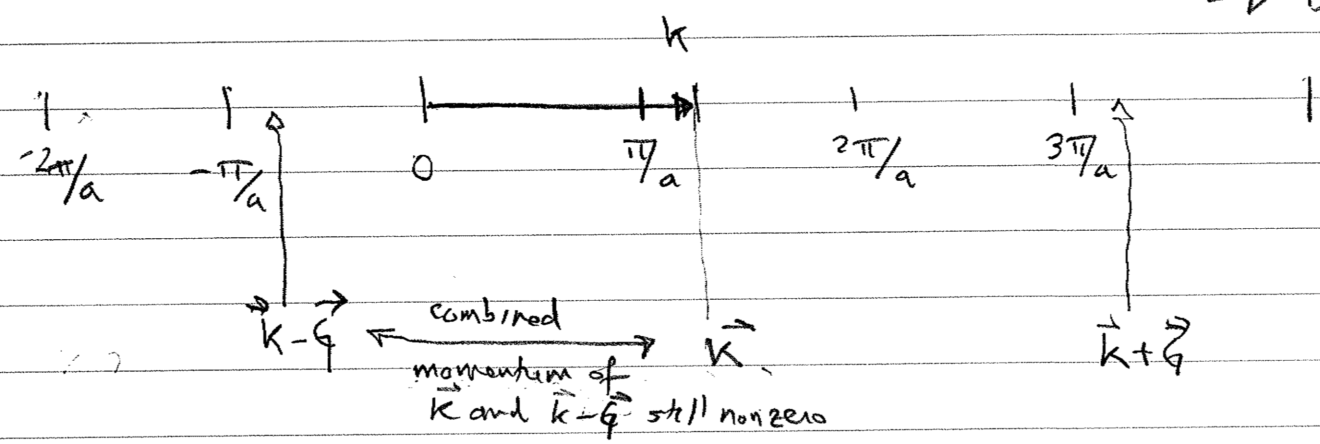
$\vec{R}_n = n\vec{a}$

$\vec{G} = \frac{2\pi}{a} m$

$\Big\} \; e^{i\vec{G}\cdot\vec{R}_n} = 1$

x rays — constructive interference of all scatterings $\Rightarrow$ Bragg peak

Suppose $\vec{k} = \frac{\pi}{a} 1.2$



Something special might happen when $k = \pi/a$

because then $\vec{k} - \vec{G} = -\vec{k}$ and combined momenta

of $\vec{k}$ and $\vec{k}-\vec{G}$ is zero $\Rightarrow$ no flow of e^-

Really looks a lot like x-ray problem $\vec{K}$ lies on $\perp$ bisector of $\vec{G}$ vector!

$n \leftarrow$ "band" (orbital) index

BLOCH'S THM

The eigenstates of $-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})$

where $U(\vec{r}) = U(\vec{r} + \vec{R}) \quad \forall \vec{R} \in$ Bravais lattice

have the form $\psi_{nk}(r) = e^{i\vec{k}\cdot\vec{r}} u_{nk}(\vec{r})$

where $u_{nk}(\vec{r} + \vec{R}) = u_{nk}(\vec{r})$

$\rightarrow$ K7-3'

proof #1 Define the translation operator $T_{\vec{R}} f(r) = f(r+R)$

T_R commutes with $\mathcal{H}$ since

$$T_R H \psi = H(r+R)\psi(r+R) = H(r)\psi(r+R) = H T_R \psi(r)$$

T_R also commute with each other

$$T_R T_{R'} \psi(r) = T_R \psi(r+R') = \psi(r+R'+R) = T_{R'} \psi(r+R)$$

$$= T_{R'} T_R \psi(r)$$

So can choose eigenstates of $\mathcal{H}$ to be eigenstates of T_R

$$H\psi(r) = \varepsilon\psi(r)$$
$$T_R\psi(r) = c(R)\,\psi(r)$$

K7-3'

$$\psi_{nk}(r+R) = e^{ik(\vec{r}+\vec{R})} u_{nk}(r+R)$$

$$= e^{ik\cdot R} \underbrace{e^{ikr} u_{nk}(r)}$$

$$= e^{ik\cdot R} \psi_{nk}(r)$$

$$\boxed{\psi_{nk}(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot\vec{R}} \psi_{nk}(r)}$$

Equivalent way of expressing Bloch's Thm

K7 - 4

The eigenvalues $c(R)$ must obey $c(R)c(R') = c(R+R')$

$R = n_1 a_1 + n_2 a_2 + n_3 a_3$

$$c(a_1) = e^{2\pi i x_1}$$
$$c(a_2) = e^{2\pi i x_2}$$
$$c(a_3) = e^{2\pi i x_3}$$

Because $\langle \psi | \psi \rangle = 1 = \int d^3r \, \psi^*(r)\psi(r)$

$$= \int d^3r \, \psi^*(r+a_i)\psi(r+a_i)$$

$$= \int d^3r \, c^*(a_i)\psi^*(r)\, c(a_i)\psi(r)$$

$$= c^*(a_i)c(a_i) \underbrace{\int d^3r \, \psi^*(r)\psi(r)}_{1}$$

$$\Rightarrow |c|^2 = 1$$

$$c(R) = c(a_1)^{n_1} c(a_2)^{n_2} c(a_3)^{n_3}$$

$$= e^{2\pi i(x_1 n_1 + x_2 n_2 + x_3 n_3)}$$

But this is the same as saying

$$C(R) = e^{i\vec{k}\cdot\vec{R}}$$

with $\vec{k} = x_1 \vec{b}_1 + x_2 \vec{b}_2 + x_3 \vec{b}_3$ and $\vec{b}_i \cdot \vec{a}_j = 2\pi \delta_{ij}$

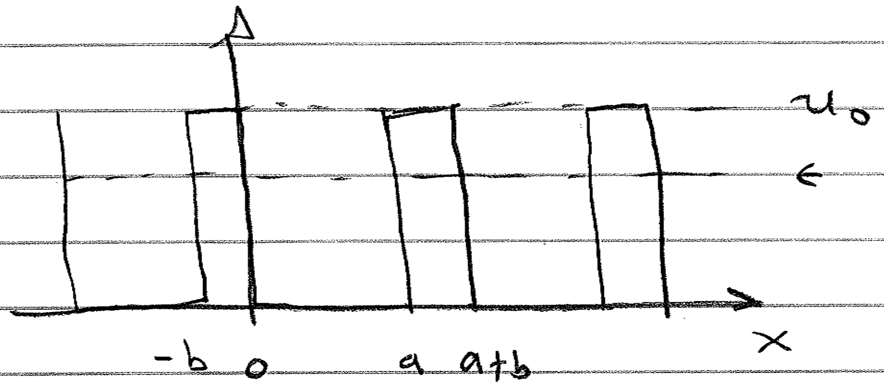
$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$

$$\therefore T_R \psi(\vec{r}) = \psi(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot\vec{R}}\psi(\vec{r})$$

Review δ function first

Kronig-Penney Model

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)\psi(x) = \epsilon\,\psi(x)$$



$0<x<a \qquad \psi(x) = Ae^{iKx} + Be^{-iKx} \qquad \epsilon = \frac{\hbar^2 K^2}{2m}$

$-b<x<0 \qquad \psi(x) = Ce^{Qx} + De^{-Qx}$

$$U_0 - \epsilon = \frac{\hbar^2 Q^2}{2m} \qquad \left(-\frac{\hbar^2}{2m}Q^2 + U_0 = \epsilon\right)$$

A, B, C, D determined by ψ and $\frac{d\psi}{dx}$ continuous at $x=0$, $x=a$

Bloch theorem ψ $a<x<a+b$ related to ψ $-b<x<0$

$$\psi(\quad) = e^{ik(a+b)}\,\psi(\quad)$$

little k

$x=0$: $\quad A+B = C+D$

$\qquad iK(A-B) = Q(C-D)$

$x=a \qquad Ae^{i\bar{K}a} + Be^{-i\bar{K}a} = C\left(e^{-Qb} + De^{-Qb}\right)e^{ik(a+b)}$

$$i\bar{K}\left(Ae^{i\bar{K}a} - Be^{-i\bar{K}a}\right) = Q\left(ce^{-Qb} - De^{Qb}\right)e^{ik(a+b)}$$

Four eqns in four unknowns A B C D

if nonzero sol'n det = 0

$\Rightarrow$ quantization condition on energy

$$\frac{Q^2 - \bar{K}^2}{2Q\bar{K}} \sinh Qb \sin \bar{K}a + \cosh Qb \cos \bar{K}a = \cos k(a+b)$$

Analog of $\bar{K} \tan \bar{K}a = Q$ but obviously a lot messier

Instead of discrete intersections (just one well)

there are ranges of $\bar{K}$ values that work,

Hence ranges of energies and energy bands.

Actually quite messy to work out details. $\Rightarrow$ HW.!

Easiest to understand gaps

Consider x ray, Bragg peak p K7-2

analogy here to e^-