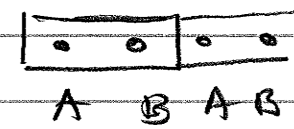
Using our 2nd quantized approach we saw

how a periodic potential $\epsilon_A, \epsilon_B = \epsilon + \Delta(-1)^\ell = \epsilon + \Delta e^{i\pi\ell}$

ℓ odd $\quad$ ℓ even

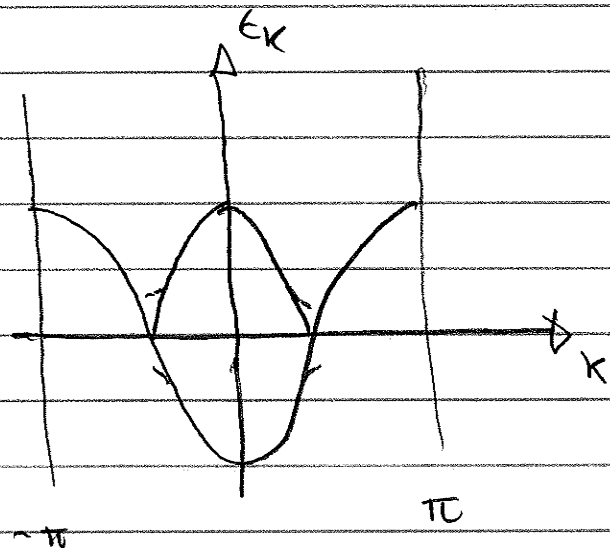
$\epsilon - \Delta \quad \epsilon + \Delta$



coupled k to $k+\pi$ only, leading to a

simple 2x2 matrix $\begin{pmatrix} \epsilon_k & \Delta \\ \Delta & \epsilon_{k+\pi} \end{pmatrix}$

whose eigenvalues are $\frac{1}{2}\left[\epsilon_k \pm \sqrt{\epsilon_k^2 + \Delta^2}\,\right]$

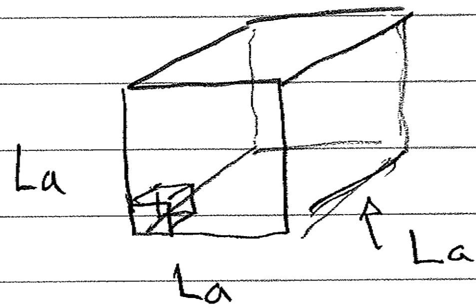


We will now see how this "restricted coupling" of k only to a "small #" of other k values arises in Sch Eqn "first quantized QM"

K7-8 Expand soln $\psi(\vec{r})$ to Sch Eqn in plane waves

$$\psi(\vec{r}) = \sum_k C_k e^{i\vec{k}\cdot\vec{r}}$$

$\psi(\vec{r})$ will be ~~periodic~~ chosen to obey periodic bc over whole crystal:



$N = L^3$ atoms

L atoms in each direction

La = size of crystal side

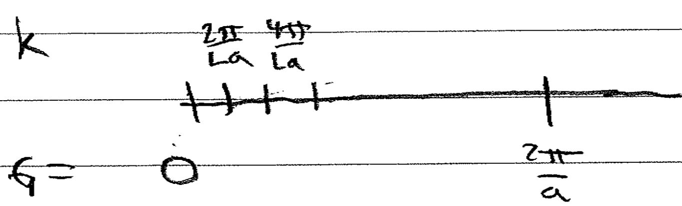
$$\psi(\vec{r} + La\hat{x}) = \psi(\vec{r})$$

This means $k = \frac{2\pi}{La}\{1, 2, \ldots L\}$

Meanwhile the potential $U(\vec{r})$ is periodic when we move from cell to cell inside the big crystal

$$U(\vec{r}) = \sum_{\vec{G}} U_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} \qquad \vec{G} = \frac{2\pi}{a}\{\text{integer}\}$$

There are many, many more $\vec{k}$ values than $\vec{G}$



$\mathcal{U}(\vec{r})$ is real $\qquad \mathcal{U}_{-G} = \mathcal{U}_G^*$

Choose $\mathcal{U}_{G=0} = 0$ as origin of energy

$$\frac{\hat{p}^2}{2m}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi = \sum_k \frac{\hbar^2 k^2}{2m} C_k e^{i\vec{k}\cdot\vec{r}}$$

$$\mathcal{U}\psi = \sum_G \mathcal{U}_G e^{i\vec{G}\cdot\vec{r}} \sum_k C_k e^{i\vec{k}\cdot\vec{r}}$$

$$= \sum_{Gk} \mathcal{U}_G C_k e^{i(G+k)\cdot r} = \sum_{Gk'} \mathcal{U}_G C_{k'-G} e^{ik'\cdot r}$$

$$k' = G + k$$
$$k = k' - G$$

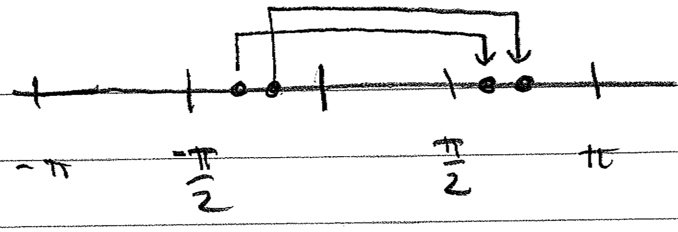
(Rename k' to k) $\rightarrow$ $\displaystyle = \sum_{Gk} \mathcal{U}_G C_{k-G} e^{ik\cdot r}$

The "Central Eq n"

$$\boxed{\left(\frac{\hbar^2 k^2}{2m} - \varepsilon\right) C_k + \sum_G \mathcal{U}_G C(k-G) = 0}$$

NOTE: Just as in second quantized approach Each $\vec{k}$ value (very dense) coupled only to $k+G$ ← sparse

K7-10



dense set of $\vec{k}$ values $\longrightarrow$ 2×2 problem

100 Eqns in 100 unknowns

$$\begin{aligned} x_1 + x_2 &= 7 \\ x_1 - 3x_2 &= 9 \\ x_3 - x_4 &= 2 \\ 2x_3 + x_4 &= 1 \end{aligned}$$

Realspace looks like all 100 coupled

$\hookrightarrow$ k space realize only coupled in pairs $\longleftarrow$ our $\epsilon_A \epsilon_B$ problem

only coupled $k, k+G$ $\longleftarrow$ our Sch Eqn picture

NOW SOLN IS NUMERICAL

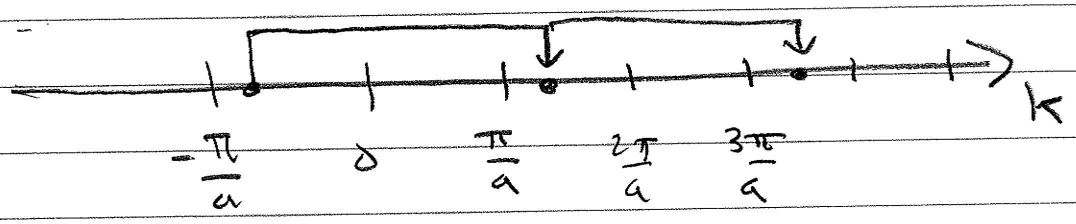
So if you look inside electronic structure (DFT) code.

(Kittel gives an example)

So we need to look at k on $\left(\frac{-\pi}{a}, \frac{\pi}{a}\right)$

and then these k get coupled by $\vec{G}$ to all other $\vec{k}$

values:



First step in process is then to "fold" all

free energy bands back to $(-\pi/a, \pi/a)$ and then

consider what U_G does to them.

Let's describe that process for simple cubic lattice

(your HW is fcc)

K7-12

$$\epsilon(k_x\, k_y\, k_z) = \frac{\hbar^2}{2m}(\vec{k}+\vec{G})^2$$

$$= \frac{\hbar^2}{2m}\left[(k_x+G_x)^2+(k_y+G_y)^2+(k_z+G_z)^2\right]$$

Consider $\vec{G}=0$ and examine ϵ along $(k_x,0,0)$

$\vec{G}=0$: $\epsilon(k_x,0,0) = \frac{\hbar^2}{2m}k_x^2$ "band 1"

$\vec{G}=\pm\frac{2\pi}{a}\hat{x}$: $\epsilon(k_x,0,0) = \frac{\hbar^2}{2m}\left(k_x \pm \frac{2\pi}{a}\right)^2$ "bands 2,3" (+ → 2, − → 3)

$\vec{G}=\pm\frac{2\pi}{a}\hat{y}$ or $\pm\frac{2\pi}{a}\hat{z}$: $\epsilon(k_x,0,0) = \frac{\hbar^2}{2m}\left[k_x^2+\left(\frac{2\pi}{a}\right)^2\right]$ "bands 4,5,6,7"