RECAP - 1

We have developed 2 pictures of electronic structure:

(A) "Tight Binding" or "2nd quantized"

In $d=1$ $\epsilon_k = -2t\cos k$ were free particle levels (no periodic potential)

When we added $\mathcal{U}_\ell = \Delta(-1)^\ell = \Delta e^{i\pi\ell}$ $\epsilon_A = \epsilon + \Delta$, $\epsilon_B = \epsilon - \Delta$

↗ Fourier transform $\mathcal{U}_q$ has component only for $q = \pi$, $\mathcal{U}_\pi = \Delta$

$k = \frac{2\pi}{N}\{\text{integer}\}$ k mixed only with $k+\pi$

$\epsilon_k \rightarrow E_k = \pm\sqrt{\epsilon_k^2 + \Delta^2}$

Nicely pictured by taking $-\pi/a < k < +\pi/a$

to First BZ $-\frac{\pi}{2a} \leq k \leq +\frac{\pi}{2a}$

and then turning on Δ

NB: 1) gaps open at $k = \pm q/2$ (identical to "Bragg condition" (k lie on $\perp$ bisector)

2) For Δ small as long as $k \neq \pm q/2$ $\epsilon_k \neq 0$ and

$$E_k = (\epsilon_k^2 + \Delta^2)^{1/2} = \epsilon_k\left(1 + \Delta^2/\epsilon_k^2\right)^{1/2}$$
$$= \epsilon_k\left(1 + \Delta^2/2\epsilon_k^2\right)$$

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That is, for $k \neq \pm G/2$ the E_k are corrected from ϵ_k to 2nd order in the potential $U(\Delta)$

Meanwhile, when $k = \pm G/2$ the shift is first order $\epsilon_k = 0 \rightarrow \epsilon_k = \pm \Delta$, Gap is $2\Delta = 2U_G = \pi$

1st order vs 2nd order

Kittel has an argument for this in a more "traditional" setting. Indeed

(B) Traditional Approach to band structure:

[HW problem: general calculation showing bands appear for any $U(r)$ and relate bands to scattering problem of single instance of repeated potential]

Started $d=3$ $\quad \epsilon_k = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2)$

Simple cubic $\quad U(r) = \sum U_G e^{iG\cdot r}$

$$\vec{G} = \left(\frac{2\pi}{a} n_x \hat{x} + \frac{2\pi}{a} n_y \hat{y} + \frac{2\pi}{a} n_z \hat{z}\right)$$

Very dense set of allowed k values

$$k_x = \frac{2\pi}{La} m_x \hat{x} + \ldots \qquad L \sim 10^8$$

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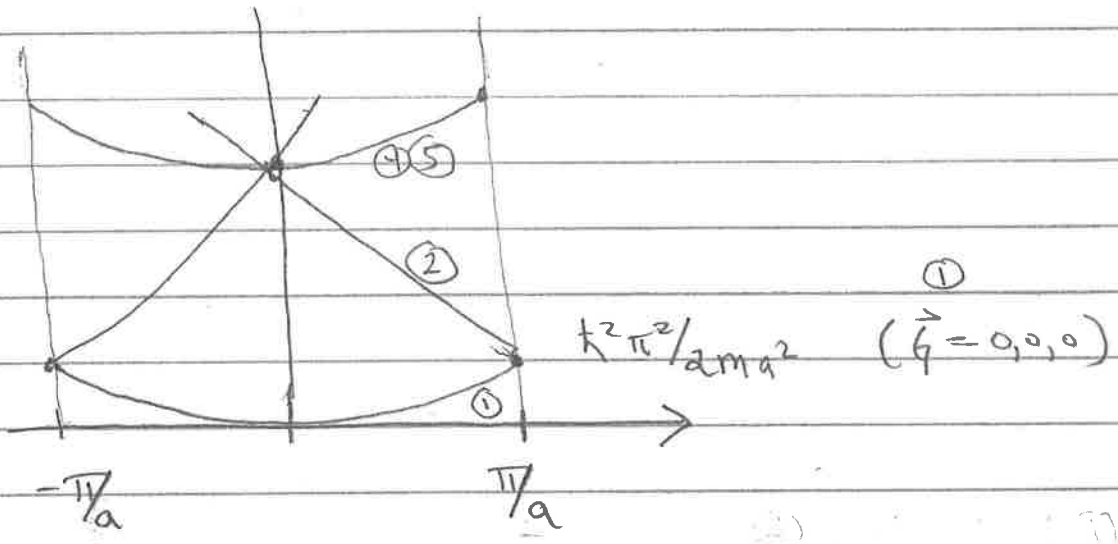
$\vec{k}$ coupled only to $\vec{k} + \vec{G}$

Took simple cubic and $(k_x, k_y, k_z) = (k, 0, 0)$

Folded bands into First BZ just as in tight binding

and drew bands



② $\vec{G} = \pm\frac{2\pi}{a}\hat{x}$ $\quad \epsilon_k = \frac{\hbar^2}{2m}\left(k + \frac{2\pi}{a}\right)^2$

④, ⑤, ⑥, ⑦ $\vec{G} = \pm\frac{2\pi}{a}\hat{y}, \pm\frac{2\pi}{a}\hat{z}$ $\quad \epsilon_k = \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2$

HW: fcc allowed $\vec{G}$ values = ...

look along $(k_x\, k_y\, k_z) = k, k, k$

RECAP-4 second step after "folding" is effect of

$$U(\bar{r}) = \sum U_G e^{iG\cdot r}$$

It opens gaps at all the $G/2$ Bragg planes

Summarizing traditional approach to electronic structure

at its simplest level 1) take lattice structure; SC, BCC, FCC, ... and fold $\epsilon_k = \hbar^2 k^2/2m$ into First BZ

2) gaps open up at edges. Size of gap is $2|U_G|$

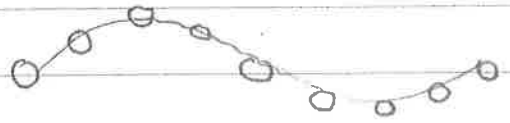
Puzzle in connecting these views: why only 2 bands in tight binding picture but many in "traditional"?

One answer is: $d=1$ vs $d=3$, but that's not whole story. The other answer is our very simple choice of

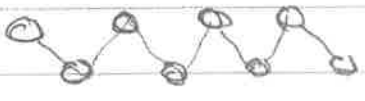
$$U(r) = \Delta(-1)^\ell = \Delta e^{i\pi\ell}.$$

On a lattice have λ (shortest λ) $\geq$ a (maximum K) that can exist:

$K = \frac{\pi}{a}$



longish $\lambda \sim 10a$



shortest $\lambda = 2a$

$k = \frac{2\pi}{\lambda} = \frac{\pi}{a}$

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If we had chosen $\epsilon_A \epsilon_B \epsilon_C \epsilon_D \epsilon_A \epsilon_B \epsilon_C \epsilon_D$

(Four species of atoms/sites)

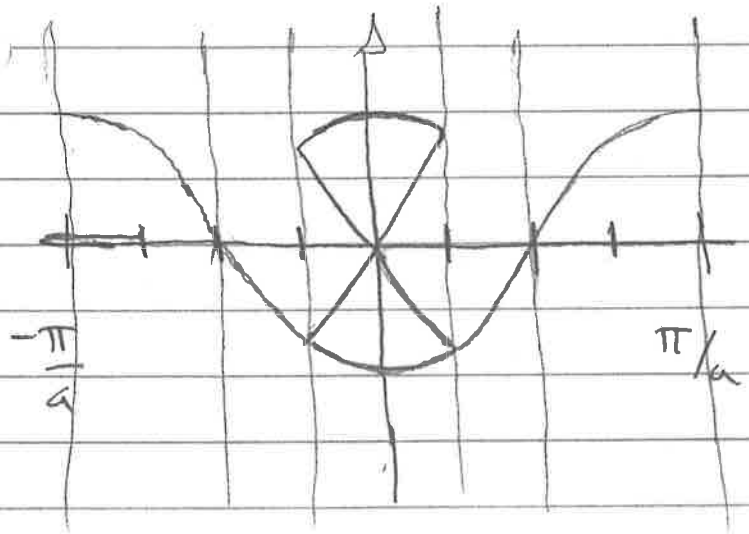
2 species $u_{\ell+2} = u_\ell$ $\Big\}$ $e^{i2q} = 1$

$u_\ell = \sum e^{iq\ell} u_q$ $\qquad 2q = 2\pi n$

$q = \pi n$

4 species $u_{\ell+4} = u_\ell$ $\qquad e^{i4q} = 1$

$4q = 2\pi n \qquad q = \frac{\pi}{2} n$



4 bands

So our tight binding picture with just 2 bands was not the most general case