Central ideas of 1 particle band theory (28 Aug 2015)

1. Bloch Hamiltonian
2. Bloch theorem
3. Solution of Bloch Hamiltonian
4. Decomposition of a general state
5. Idea of an effective Hamiltonian
6. Meaning of momentum and crystal momentum
7. The tight binding approximation
8. Many body wave functions.

Upto (6) is available in labelled notes.

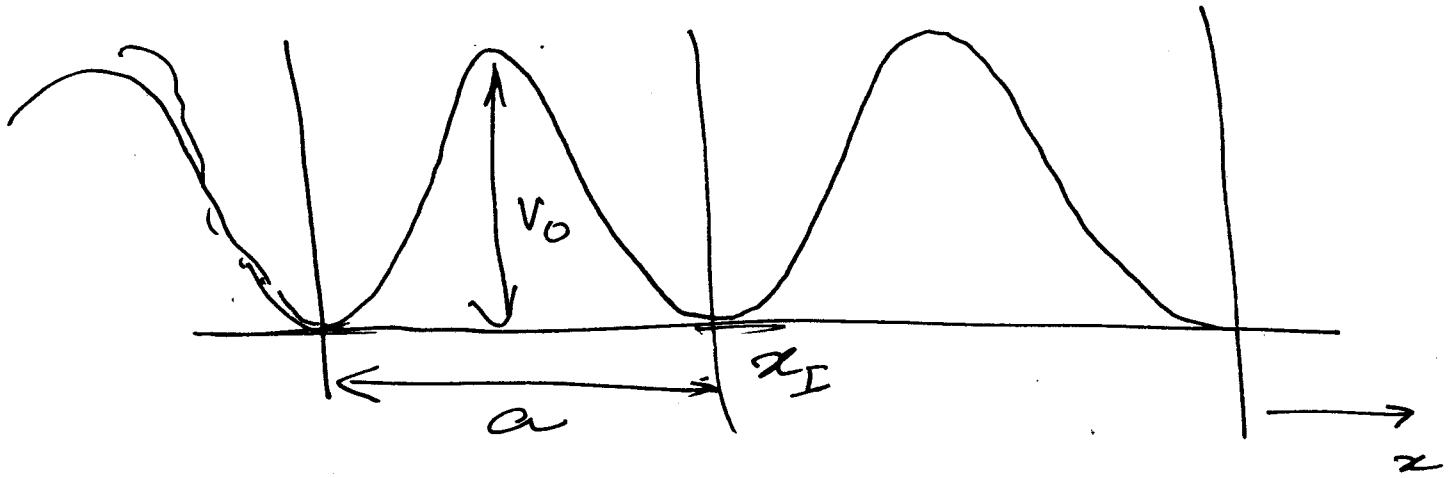
The tight binding approximation

We have seen how to solve the bloch hamiltonian, and seen also how to arrive at the effective hamiltonian. Now will we push this idea further so that we can obtain "simple forms" of the effective hamiltonian. I will motivate this ida with an example from cold atoms.

Consider two lasers (phase coherent) that ~~Bosden~~ interfere in a repeat to produce the following intensity pattern

$$I(x) = V_0\left(1-\cos\left(\frac{2\pi x}{a}\right)\right) + (\text{const})$$

$$V_0\left(1-\cos\left(\frac{2\pi x}{a}\right)\right) +$$



Look at the scales involved in

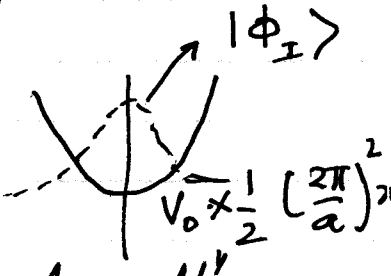
~~V_0 given~~ $\mathcal{H}_B = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_0\left(1-\cos\left(\frac{2\pi x}{a}\right)\right)$

potential energy scale $= V_0$

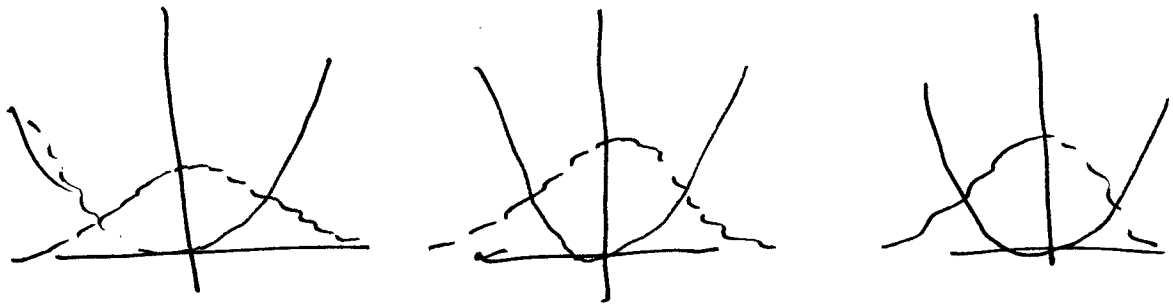
kinetic energy scale $= \frac{\hbar^2}{2ma^2}$

Suppose $V_0 \gtrsim \frac{\hbar}{2ma^2}$, then we can obtain a simple model describing the lowest band.

idea. if $V_0 \gg \frac{\hbar^2}{2ma^2}$, then the particle will be as if in one of the "wells" its wave function looks like the ground state and like $\langle x|\Phi_1\rangle \approx \pi e^{-\#(x-x_I)^2}$ looks like the ground states of the "local well".



picture



Idea; Translate the Hilbert space

① Take $|\Phi_I\rangle$, there one N of these

② Approximate $\langle \Phi_I | \Phi_J \rangle = \delta_{IJ}$

(not essential) ~~[illegible]~~

③ any state is linear combination

$$|\Psi\rangle = \sum_I C_I |\Phi_I\rangle.$$

④ ~~what is the~~ Hamiltonian ← hopping amplitude

$$H = -\sum_{\langle IJ \rangle} t_{IJ} |\Phi_I\rangle\langle\Phi_J|.$$

t_{IJ} ~~[illegible]~~ $= \langle \Phi_I | \partial H_B | \Phi_J \rangle$.

⑤ t_{IJ} in most physical systems

depends only on the "nearest neighbors" or a "few" neighbors

⑥ Note t_{IJ} must be a function of only I, J

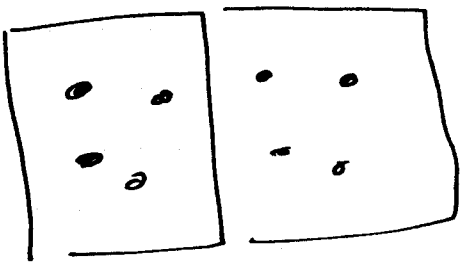
⑦ suppose I have a bravais lattice

$\sqrt{2}$

with 1 i on per site then $\vec{\delta}$ one etc "new neighbor relations

$$\mathcal{H}_{TB} = -\sum_{\delta}^{'}\sum_{I}^{'} t(\vec{\delta})\, |\Phi_{I+\vec{\delta}}\rangle\langle\Phi_I|$$

If there are more atoms per unit cell, (non Bravais lattice) then



$$H_{TB} = -\sum_{I}^{'}\sum_{\delta}^{'}\sum_{\alpha\beta} t_{\alpha\beta}(\vec{\delta})\, |\Phi_{I+\vec{\delta},\alpha}\rangle\langle\Phi_{\beta,I}|$$

General solution

Define $|\vec{k}\alpha\rangle = \frac{1}{\sqrt{N}}\sum_{I}^{'} e^{i\vec{k}\cdot\vec{R}_I}|\Phi_{I\alpha}\rangle$

↑ crystal momentum (Abuse of notation)

$$|\Phi_{I\alpha}\rangle = \frac{1}{\sqrt{N}}\sum_{k}^{'} e^{-i\vec{k}\cdot\vec{R}_I}|k\alpha\rangle$$

$$\langle\vec{k}\alpha|\mathcal{H}_{TB} = -\sum_{I}^{'}\sum_{\delta}^{'}\sum_{\alpha\beta}^{'} t_{\alpha\beta}(\vec{\delta})\, e^{-i\vec{k}(\vec{R}_I+\vec{\delta}-\vec{R}_I-\vec{r}_\alpha+\vec{r}_\beta)}$$

etc.

$$= \sum_{\vec{k}}^{'} \varepsilon_{\alpha\beta}(\vec{k})\, |\vec{k}\alpha\rangle\langle\vec{k}\beta|$$

where $\varepsilon_{\alpha\beta}(\vec{k}) = -\sum_{\delta}^{'} t_{\alpha\beta}(\vec{\delta})\, e^{-i\vec{k}\cdot\vec{\delta}}$.

$\cos^2 - \sin^2 = \cos 2$

① Questions

② Idea of RG $\quad \frac{1}{m^*} \sim t a^2$ $\quad m^*$ dimensionless

$t \Lambda^{-2}$ $\quad t$ energy $\tilde{t}(\Lambda)\Lambda^{-2}$

$\frac{1}{m^*} = \tilde{t}(\Lambda)\Lambda^{-4}$ $\quad \Lambda \frac{\partial}{\partial \Lambda}(\tilde{t}(\Lambda))\Lambda^{-4} - 4\tilde{t}(\Lambda)\Lambda^{-4} = 0$

$= \beta(\tilde{t}) = 4\tilde{t}(\Lambda)$

③ Back to tight binding 2-band model

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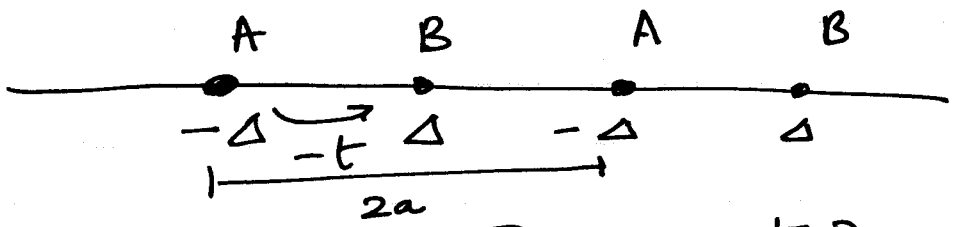
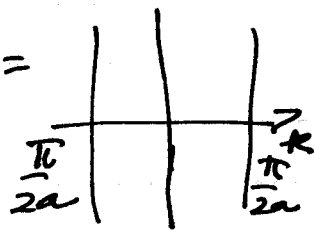


$$t_{\alpha\beta}(0) = \begin{bmatrix} -\Delta & -t \\ -t & \Delta \end{bmatrix}$$

B_2
B_2



$$t_{\alpha\beta}(2a) = \begin{bmatrix} 0 & -t \\ 0 & 0 \end{bmatrix}$$

$$t_{\alpha\beta}(-2a) = \begin{bmatrix} 0 & 0 \\ -t & 0 \end{bmatrix}$$

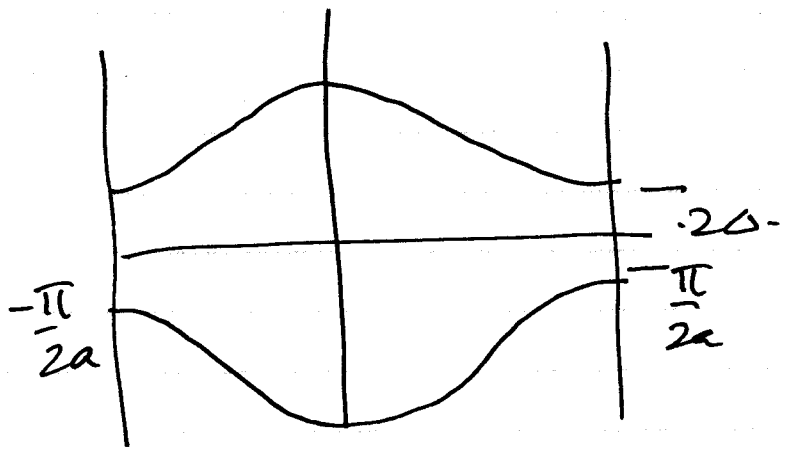
$$\varepsilon_{\alpha\beta}(k) = \begin{bmatrix} -\Delta & -t - te^{-ik2a} \\ -t - te^{ika} & \Delta \end{bmatrix}$$

$$\mathcal{E}_{\alpha\beta}(k) = \begin{bmatrix} -\Delta & -t - t\cos(2ka) + it\sin 2ka \\ \end{bmatrix}$$

$$= -\Delta\,\sigma_x - t(1+\cos 2ka)\,\sigma_x - t\sin 2ka\,\sigma_y$$

$$\mathcal{E}_1 = \mp\sqrt{\Delta^2 + 4t^2\cos^4 ka + 4t^2\cos^2 ka\sin^2 ka}$$

$$= \mp\sqrt{\Delta^2 + 4t^2\cos^2 ka}.$$

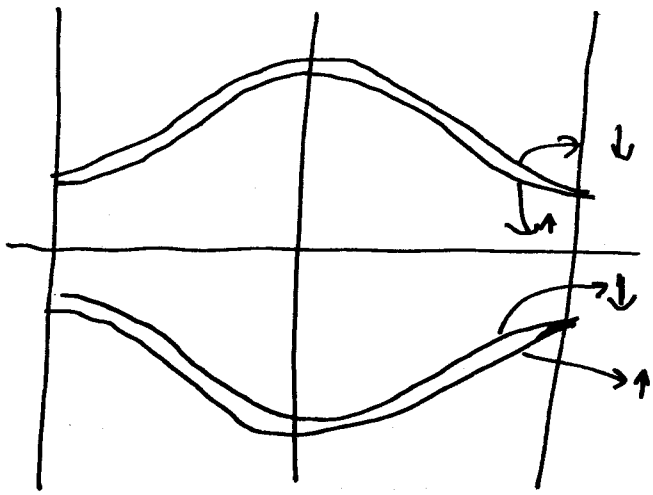


gap = 2Δ

We thus see that we can obtain a band structure with a gap.

This concludes our discussion of tight binding model.

Some frills: We know that electrons have spin, thus there is a band for each spin



four bands in total.

We now need to construct a many body state

The idea of filling.

We have N sites (or unit cells).

Number of electrons per unit cell = Ne

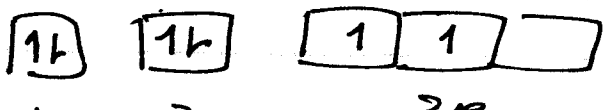
$$f = \frac{Ne}{N}$$ (usually called as filling (aka x)

Now we will use

How do we construct a many body wavefunction?

Revise when we have constructed a many body wave function:

Carbon



what does this mean?

Let us label the configuration of the electron

$\vec{r}_i = (\vec{x}_i, \sigma_i)$

↑ orbital ↳ spin

Wave function is

$$\Psi(r_1, r_2 \ldots r_{N_e})$$

Simplify to just two particles

$$\psi(r_1, r_2).$$

Key <u>experimental</u> fact: identical particles are indistinguishable:

$$P\{\psi(r_1, r_2) = \psi(r_2, r_1) = e^{i\alpha}\psi(r_1, r_2)$$

$$P^2\psi = e^{i2\alpha}\psi(r_1, r_2) = \psi(r_1, r_2)$$

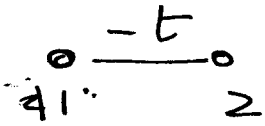
$$\Rightarrow e^{i2\alpha} = 1 = e^{i\alpha} = \pm 1$$

+1 bosons, −1 fermions!

In distinguishable forces us to have certain symmetry properties of wavefunctions of many particles, for fermions

For $\psi(Pr) = (-1)^P\psi(r)$ P is the permutation

Now let us look at a simple example



$$-t\sum_{\sigma}^{\downarrow}\left(|1\sigma\rangle\langle 2\sigma| + |2\sigma\rangle\langle 1\sigma|\right)$$

$$= -t\sum_{\sigma}^{\downarrow} |b_\sigma\rangle\langle b_\sigma| + t\sum_{\sigma}^{\downarrow} |b_\sigma\rangle\langle a_\sigma|$$

Suppose filling is $\frac{1}{2}$ i.e. $\frac{N_e}{N} = 1$ $(N_c = 2)$

we need to put 2 electrons

$\boxed{\uparrow\downarrow}$ $\boxed{\quad}$ this would
b a

be our picture of the ground state

$$\left(b_\sigma(r_i) = \langle r_i | b_\sigma\rangle\right) \begin{vmatrix} b_\uparrow(r_1) & b_\uparrow(r_2) \\ b_\downarrow(r_1) & b_\downarrow(r_2) \end{vmatrix} := |b_\uparrow b_\downarrow|$$

Note that ① $\psi(r_1, r_2) = -\psi(r_2, r_1)$

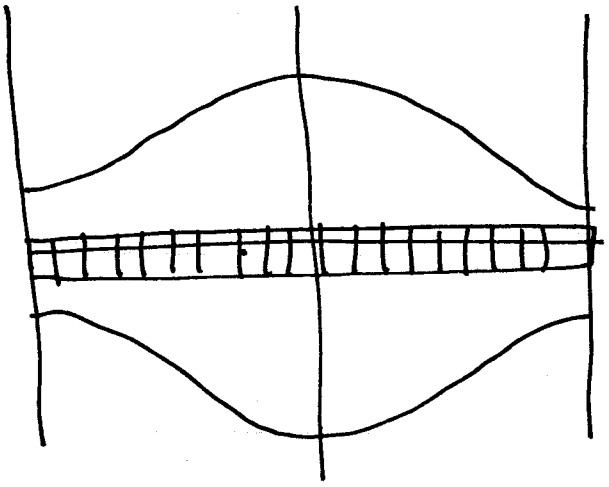
② Pauli Exclusion principle.

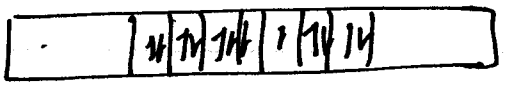
Main idea. ③ The basis of many particle Hilbert space is the antisymmetrized product of 1-particle states.

For ~~bosons~~ we get such states are called a slater determinant..

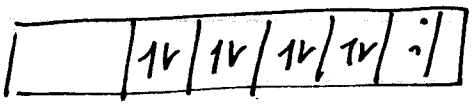
(For bosons we get something which are called as permanents).

With this in mind we can now write the ground state of our fermionic system





what is an excited state?



what is the ground state when $\sum_i l_i = 2$?

(each band can take 1 electron per unit cell)

- Gapped vs Gapless.