XII. Electron Dynamics

- We are concerned with <u>electron dynamics</u>.
- So far, we have solved (in principle) the Schrödinger equation for an electron in a periodic $V(\vec{r})$:

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi_{\vec{k}}(\vec{r}) = \mathcal{E}(\vec{k})\psi_{\vec{k}}(\vec{r})$$

<u>Key results</u>: $\psi_{\vec{k}}(\vec{r})$ takes on the Bloch form

eigenvalues $\mathcal{E}(\vec{k})$ form energy bands

<u>Important Points</u>

- The Bloch functions $\psi_{\vec{k}}(\vec{r})$ are <u>extended</u> wavefunctions. (as opposed to localized wave-functions)
- $\psi_{\vec{k}}(\vec{r})$ are <u>eigenstates</u> of the Hamiltonian that <u>includes</u> $V(\vec{r})$
  ⇒ they have <u>infinite lifetime</u>

  <u>Meaning</u>: an electron in state $\psi_{\vec{k}}(\vec{r})$ will stay in the state <u>forever</u> (<u>if $V(\vec{r})$ is the only influence around</u>)

More explicitly,

- for an electron in $\psi_{\vec{k}}(\vec{r})$

  if we have <u>perfect periodicity</u>

  <u>Note</u>: the atoms/ions actually form a <u>dense array</u> of lattice constant $\sim$ Å

  the dense ordered array of atoms/ions <u>CANNOT</u> cause a change from state $\psi_{\vec{k}}$ to $\psi_{\vec{k}'}$.

∴ Resistance is <u>not</u> caused by the <u>perfectly ordered array!</u> (Hard to imagine without quantum mechanics!)

Thus, resistance is <u>caused by deviations from perfect periodicity</u>

$\sigma = \frac{ne^2\tau}{m}$; τ is governed by { e.g. lattice vibrations (phonons), sample size (boundary), impurities, defects, other excitations }

An electron in Bloch state $\psi_{\vec{k}}(\vec{r})$ does not "see" the complicated things that give rise to $V(\vec{r})$ any more, as $V(\vec{r})$ has been fully considered in band theory!

A. Velocity $\vec{v}_n(\vec{k})$ of a Bloch electron

Q: For an electron in $\psi_{n\vec{k}}(\vec{r})$ with eigenenergy $\varepsilon_n(\vec{k})$, what is its velocity?

Key result[+]:

$$\vec{v}_n(\vec{k}) = \frac{1}{\hbar}\vec{\nabla}_{\vec{k}}\varepsilon_n(\vec{k}) \equiv \frac{\langle\vec{p}\rangle}{m}$$

where $\vec{\nabla}_{\vec{k}}$ = gradient with respect to $\vec{k}$

$\langle\vec{p}\rangle$ = expectation value of momentum in the state $\psi_{n\vec{k}}(\vec{r})$

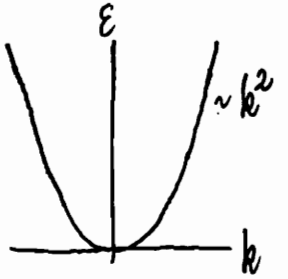
Remark:

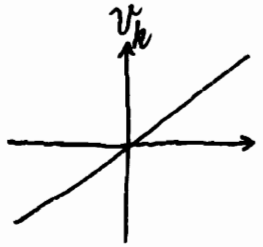
Since $\psi_{n\vec{k}}(\vec{r})$ is an eigenstate, an electron in state $\psi_{n\vec{k}}(\vec{r})$ will move forever with $\vec{v}_n(\vec{k})$.

[+] The result, though non-trivial, is not surprising. $\frac{\varepsilon_n(\vec{k})}{\hbar} \equiv \omega_n(\vec{k})$ and $\vec{\nabla}_{\vec{k}}\omega_n(\vec{k})$ is the group velocity.

- Let's first consider the trivial case of free particle ($V=0$).
  - The wave function is $\psi \sim e^{i\vec{k}\cdot\vec{r}}$
  - $\varepsilon(\vec{k}) = \frac{\hbar^2k^2}{2m}$
  - The momentum $\vec{p} = \hbar\vec{k} \Rightarrow$ velocity $= \frac{\hbar\vec{k}}{m}$
  - $\frac{1}{\hbar}\nabla_{\vec{k}}\varepsilon(\vec{k}) = \frac{\hbar k}{m}$

  $\therefore \vec{v} = \frac{1}{\hbar}\nabla_{\vec{k}}\varepsilon(\vec{k})$ works for free particles

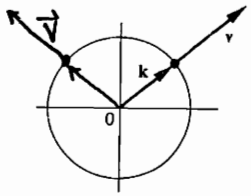




Note: $\vec{v}(-\vec{k}) = -\vec{v}(\vec{k})$ free electrons

or indicating, the result in $\vec{k}$-space

$\begin{cases} \vec{v} \text{ in direction of } \vec{k} \\ |\vec{v}| \propto |\vec{k}| \end{cases}$



How does the electron move in real space?

$$\vec{r}(t) = \vec{r}_0 + \vec{v}t$$

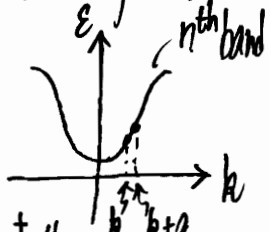
But, in solids $V(\vec{r}) \neq 0 \Rightarrow$ Bloch functions (not plane waves!)

The result $\vec{v}_n(\vec{k}) = \frac{1}{\hbar}\vec{\nabla}_{\vec{k}}\varepsilon_n(\vec{k})$ is non-trivial.

Derivation)

We want to calculate $\langle \vec{p} \rangle = \int_V d^3r\, \psi^*_{n\vec{k}}(\vec{r})\, \vec{p}\, \psi_{n\vec{k}}(\vec{r})$

Technique: Consider the mathematical relation between two "neighboring states in k-space", i.e. $\psi_{n\vec{k}}(\vec{r})$ and $\psi_{n\vec{k}+\vec{q}}(\vec{r})$



($|\vec{q}|$ is small)

and invoke first order perturbation[+] theory.

Let's do it!

Bloch's theorem ⇒ $\psi_{n\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, u_n(\vec{k},\vec{r})$ ← periodic in r-space

$$\psi_{n\vec{k}+\vec{q}}(\vec{r}) = e^{i(\vec{k}+\vec{q})\cdot\vec{r}}\, u_n(\vec{k}+\vec{q},\vec{r})$$

We have shown that $u_n(\vec{k},\vec{r})$ satisfies the equation:

$$\left[\frac{1}{2m}(\vec{p}+\hbar\vec{k})^2 + V(\vec{r})\right] u_n(\vec{k},\vec{r}) \equiv \hat{H}(\vec{k},\vec{r})\, u_n(\vec{k},\vec{r}) = \mathcal{E}_n(\vec{k})\, u_n(\vec{k},\vec{r})$$

(see p. IX-⑯)

[+] See supplementary pages for a review.

Similarly, the periodic function $u_n(\vec{k}+\vec{q},r)$ satisfies:

$$\hat{H}(\vec{k}+\vec{q},r)\, u_n(\vec{k}+\vec{q},\vec{r}) = \mathcal{E}_n(\vec{k}+\vec{q})\, u_n(\vec{k}+\vec{q},\vec{r})$$

where

$$\hat{H}(\vec{k}+\vec{q},\vec{r}) = \frac{1}{2m}(\vec{p}+\hbar\vec{k}+\hbar\vec{q})^2 + V(\vec{r})$$

• Expand $\hat{H}(\vec{k}+\vec{q},\vec{r})$: ($|\vec{q}|$ is small)

$$\hat{H}(\vec{k}+\vec{q},\vec{r}) = \underbrace{\left[\frac{(\vec{p}+\hbar\vec{k})^2}{2m} + V(\vec{r})\right]}_{\hat{H}(\vec{k},\vec{r})} + \frac{\hbar\vec{q}}{m}\cdot(\vec{p}+\hbar\vec{k}) + \frac{\hbar^2 q^2}{2m}$$

$$= \hat{H}(\vec{k},\vec{r}) + \frac{\hbar\vec{q}}{m}\cdot(\vec{p}+\hbar\vec{k}) + \frac{\hbar^2 q^2}{2m} \quad \text{(exact up to here)}$$

$$\approx \hat{H}(\vec{k},\vec{r}) + \frac{\hbar\vec{q}}{m}\cdot(\vec{p}+\hbar\vec{k})$$

($|\vec{q}|$ is infinitesimal ($\vec{k}+\vec{q}$ is very close to $\vec{k}$)
⇒ ignore q^2 term in $\hat{H}(\vec{k}+\vec{q},\vec{r})$)

$$\therefore\ \hat{H}(\vec{k}+\vec{q},\vec{r}) = \hat{H}(\vec{k},\vec{r}) + \underbrace{\frac{\hbar}{m}\vec{q}\cdot(\vec{p}+\hbar\vec{k})}_{\text{perturbation}}$$

↑ "perturbed Hamiltonian"

↑ unperturbed Hamiltonian ($u_n(\vec{k},\vec{r})$ known)

Consistency: 1st order perturbation theory (order q^1)

Thus, to first order in $\vec{q}$:

$$\mathcal{E}_n(\hbar\vec{k}+\vec{q}) = \mathcal{E}_n(\hbar\vec{k}) + \frac{\hbar}{m}\vec{q}\cdot\int_V d^3r\, u^*_{n\hbar\vec{k}}(\vec{r})(\vec{p}+\hbar\vec{k})\,u_{n\hbar\vec{k}}(\vec{r})$$

Consider $\hat{p}\,\psi_{n\hbar\vec{k}}(\vec{r}) = \frac{\hbar}{i}\vec{\nabla}\left(e^{i\vec{k}\cdot\vec{r}}u_{n\hbar\vec{k}}(\vec{r})\right)$

$$= e^{i\vec{k}\cdot\vec{r}}(\vec{p}+\hbar\vec{k})\,u_{n\hbar\vec{k}}(\vec{r})$$

$$\therefore\ \psi^*_{n\hbar\vec{k}}(\vec{r})\,\hat{p}\,\psi_{n\hbar\vec{k}}(\vec{r}) = e^{-i\vec{k}\cdot\vec{r}}u^*_{n\hbar\vec{k}}(\vec{r})\,e^{i\vec{k}\cdot\vec{r}}(\vec{p}+\hbar\vec{k})\,u_{n\hbar\vec{k}}(\vec{r})$$

$$= u^*_{n\hbar\vec{k}}(\vec{r})(\vec{p}+\hbar\vec{k})\,u_{n\hbar\vec{k}}(\vec{r})$$

Thus,

$$\mathcal{E}_n(\hbar\vec{k}+\vec{q}) = \mathcal{E}_n(\hbar\vec{k}) + \frac{\hbar}{m}\vec{q}\cdot\int_V \psi^*_{n\hbar\vec{k}}(\vec{r})\,\vec{p}\,\psi_{n\hbar\vec{k}}(\vec{r})$$

$$= \mathcal{E}_n(\hbar\vec{k}) + \frac{\hbar}{m}\vec{q}\cdot\underbrace{\langle\vec{p}\rangle}_{\text{expectation value of momentum w.r.t. Bloch state } \psi_{n\hbar\vec{k}}}$$

Note: $\hbar\vec{k}$ = crystal momentum (appears in conservation rules when electron is scattered) but it is not the physical momentum.

On the other hand, we can expand the function $\mathcal{E}_n(\hbar\vec{k}+\vec{q})$ for small $\vec{q}$:

$$\mathcal{E}_n(\hbar\vec{k}+\vec{q}) \approx \mathcal{E}_n(\hbar\vec{k}) + \vec{q}\cdot\vec{\nabla}_{\hbar\vec{k}}\mathcal{E}_n(\hbar\vec{k}) + \underbrace{\cdots}_{O(q^2)\text{ or higher}}$$

Comparing with

$$\mathcal{E}_n(\hbar\vec{k}+\vec{q}) = \mathcal{E}_n(\hbar\vec{k}) + \vec{q}\cdot\frac{\hbar}{m}\langle\vec{p}\rangle,$$

we get

$$\frac{\hbar}{m}\langle\vec{p}\rangle = \vec{\nabla}_{\hbar\vec{k}}\mathcal{E}_n(\hbar\vec{k})$$

$$\therefore\ \boxed{\vec{v}_n(\hbar\vec{k}) \equiv \frac{\langle\vec{p}\rangle_{n\hbar\vec{k}}}{m} = \frac{1}{\hbar}\vec{\nabla}_{\hbar\vec{k}}\mathcal{E}_n(\hbar\vec{k})}\ {}^{\dagger}$$

$\vec{v}_n(\hbar\vec{k})$: velocity of an electron in state $\psi_{n\hbar\vec{k}}(\vec{r})$ gives motion in r-space!

$\vec{\nabla}_{\hbar\vec{k}}\mathcal{E}_n(\hbar\vec{k})$: gradient of band structure at $\hbar\vec{k}$

$\therefore$ Direction of $\vec{v}_n(\hbar\vec{k})$ = direction of $\vec{\nabla}_{\hbar\vec{k}}\mathcal{E}_n(\hbar\vec{k})$

$\perp$ constant energy surface

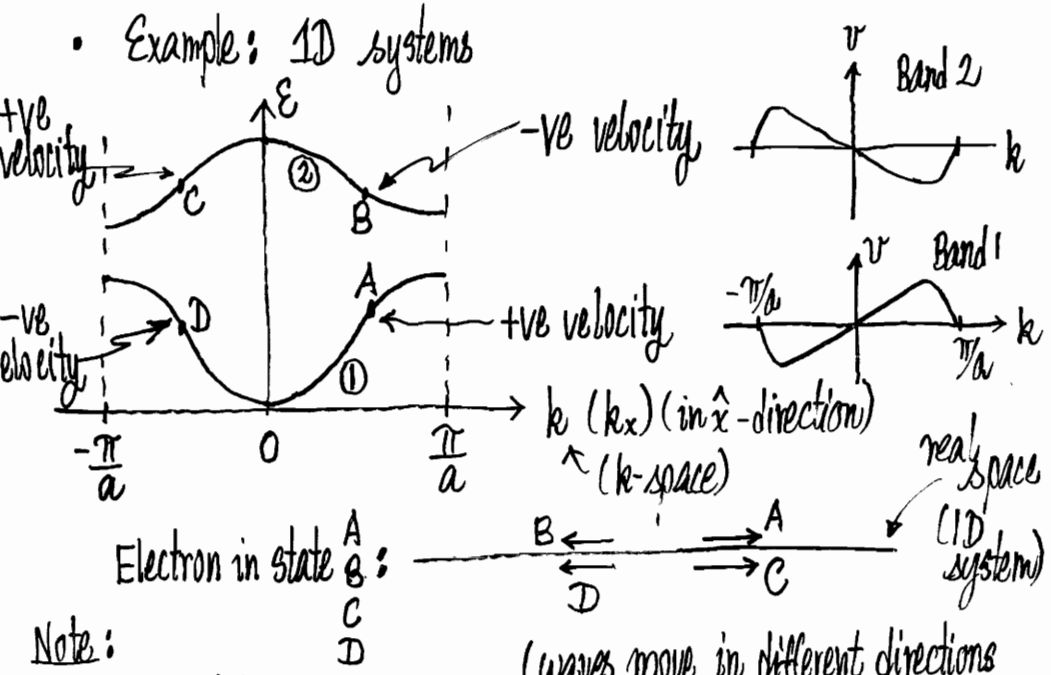
$\therefore$ Direction of $\vec{v}_n(\hbar\vec{k})$ is perpendicular to constant energy surface.

† Following the proof, the mass m is the bare electron mass. It is NOT the effective mass m^*. The band structure effects come in through $\mathcal{E}_n(\hbar\vec{k})$.

- From QM, $\psi_{n\vec{k}}(\vec{r})$ has time dependence $e^{-iE_n(\vec{k})t/\hbar} \sim e^{-i\omega_n(\vec{k})t}$

$$\vec{\nabla}_{\vec{k}}\left(\frac{1}{\hbar}E_n(\vec{k})\right) = \vec{v}_n(\vec{k}) \sim \vec{\nabla}_{\vec{k}}\omega_n(\vec{k}) \sim \text{group velocity}$$

- Example: 1D systems



Note:
$\vec{v}(-\vec{k}) = -\vec{v}(\vec{k})$

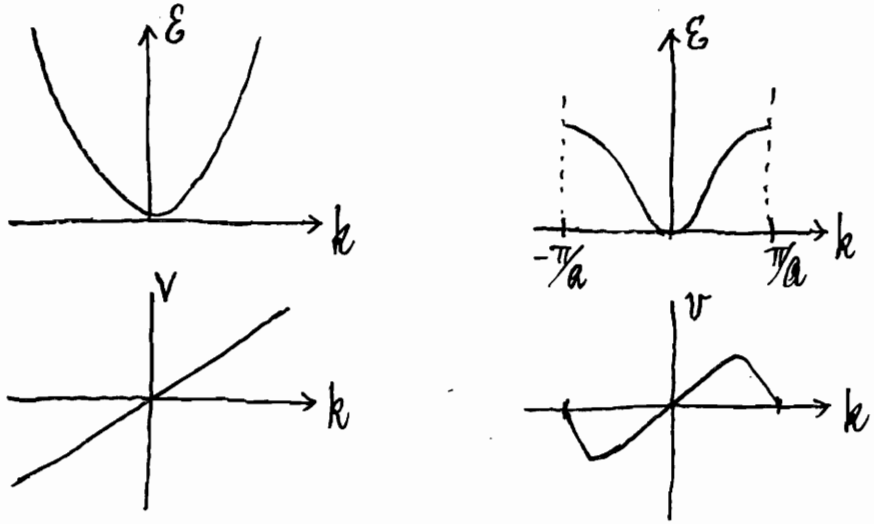
(waves move in different directions and different magnitudes depending on $\vec{\nabla}_{\vec{k}}E_n(\vec{k})$)

- No deviations from perfect periodicity, an electron in $\psi_{n\vec{k}}(\vec{r})$ will move forever with $\vec{v}_n(\vec{k})$

- How to induce transitions from $\psi_{n\vec{k}}$ to $\psi_{n'\vec{k}'}$?
  - Things not included in $V(\vec{r})$!
    e.g. external forces, deviations from perfect periodicity.

Thus, $V(\vec{r})$ (or band structure) does have a significant effect on $\vec{v}(\vec{k})$!

Constrast free electron case with band structure:



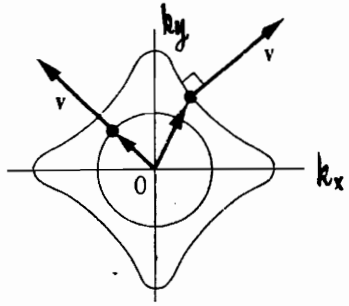
free electron $V=0$
(plane waves)

periodic $V(\vec{r})$
band structure effect
(Bloch functions)

Physically, the effect comes from the scattering of plane waves by the periodic $V(\vec{r})$, when $V(\vec{r})$ is present.

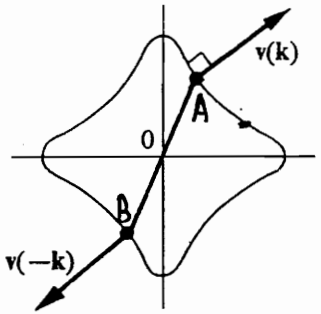
- With periodic $V(\vec{r})$, constant-energy surfaces are not always spherical surfaces.

  But $\vec{v}_n(\vec{k}) = \frac{\hbar}{m}\vec{\nabla}_{\vec{k}}\mathcal{E}_n(\vec{k})$ implies $\vec{v}_n(\vec{k}) \perp$ constant energy surface.



contours show constant energy surfaces

- Band structure has the property $\mathcal{E}_n(\vec{k}) = \mathcal{E}_n(-\vec{k})$.
  It follows that $\vec{v}_n(-\vec{k}) = -\vec{v}_n(\vec{k})$.



pt. A: state $\vec{k}$ } they lie on the same constant energy surface
pt. B: state $-\vec{k}$ }

$\vec{v}(-\vec{k}) = -\vec{v}(\vec{k})$

- If both states $\vec{k}$ and $-\vec{k}$ in a band are occupied, the net electron velocity is zero.

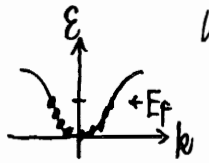
B. A completely filled band has zero total electron velocity

Full band $\Rightarrow$ All $\vec{k}$'s in 1st B.Z. are occupied

Total electron velocity $= \sum_{\substack{\text{all } \vec{k}\text{'s} \\ \text{in 1st B.Z.}}} \vec{v}_n(\vec{k})$ for the band concerned

- For every $\vec{k}$, there is a $-\vec{k}$ in the 1st B.Z.
  But $\vec{v}(-\vec{k}) = -\vec{v}(\vec{k})$
  thus, pair by pair the velocities cancel!
  $\therefore$ Total electron velocity for full band $= 0$

Remark: The argument also works for partially filled band with no external field (e.g. electric field) applied.



All states up to E_f are occupied.
Since $\mathcal{E}(\vec{k}) = \mathcal{E}(-\vec{k})$
$\Rightarrow$ when state $\vec{k}$ is occupied, state $-\vec{k}$ is also occupied.

$\therefore \sum_{\text{occupied } \vec{k}\text{'s}} \vec{v}(\vec{k}) = 0$ (no external field)

Consequence: No current in metal when no voltage is applied, which is our daily experience!

C. Semi-classical Dynamics for Bloch Electrons

- Up to now, perfectly periodic crystal with no external forces, no imperfections

  For an electron in the Bloch state $(n, \vec{k})$, it will remain in that state forever! [eigenstate]

- Only when we have something more than perfect periodicity, there are some mechanisms causing a change in the Bloch state (from $\vec{k}$ to $\vec{k}'$, say).

  These mechanisms can be:
  - some applied external fields ($\vec{\mathcal{E}}$, $\vec{B}$ fields)
  - shining a light
  - phonons, impurities, sample boundaries

[They may counteract each other so as to achieve steady state.]

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† Deriving the Bloch electron dynamical equations is highly non-trivial. We will state the key results here. Interested readers will find the review by G. Wannier, Rev. Mod. Phys. (1962) useful.

Question: T=0, perfectly periodic

A weak external force $\vec{F}_{ext}$ (e.g. $-e\vec{\mathcal{E}}$)

How does $\vec{F}_{ext}$ alter the state $\vec{k}$ of Bloch electron?

Key result:

$$\frac{d}{dt}(\hbar\vec{k}) = \vec{F}_{ext}$$

Semiclassical equation of motion or the "acceleration theorem"

An argument†: "Weak": no inter-band transitions

$\Rightarrow$ same band index n throughout

Rate of work done (power) by $\vec{F}_{ext}$ on electron in state $\vec{k}$

$= \vec{F}_{ext} \cdot \vec{v}_n(\vec{k})$

= rate of change of energy $= \frac{d}{dt}\mathcal{E}_n(\vec{k})$

$$\therefore \vec{v}_n(\vec{k}) \cdot \vec{F}_{ext} = \frac{d}{dt}\mathcal{E}_n(\vec{k}) = \nabla_{\vec{k}}\mathcal{E}_n(\vec{k}) \cdot \frac{d\vec{k}}{dt}$$

$$= \frac{1}{\hbar}\nabla_{\vec{k}}\mathcal{E}_n(\vec{k}) \cdot \frac{d}{dt}(\hbar\vec{k}) = \vec{v}_n(\vec{k}) \cdot \frac{d}{dt}(\hbar\vec{k})$$

$$\therefore \frac{d}{dt}(\hbar\vec{k}) = \vec{F}_{ext}$$

$\frac{d}{dt}$(crystal momentum) $= \vec{F}_{ext}$.

[Note: crystal momentum $\neq$ physical momentum]

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† This is not a rigorous proof.

$\boxed{\frac{d}{dt}(\hbar\vec{k}) = \vec{F}_{ext}}$ gives how $\vec{k}$ changes in the presence of $\vec{F}_{ext}$.

- Note that $\vec{F}_{ext}$ refers to forces acting on the electrons in a <u>crystalline solid</u>
- $\vec{F}_{ext}$ does <u>not</u> refer to the force due to the periodic potential $V(\vec{r})$ ($\because$ <u>included</u> in band theory)
- Effects of $V(\vec{r})$ are included in the band structure $\mathcal{E}_n(\vec{k})$
- Here $\frac{d}{dt}(\hbar\vec{k}) = \vec{F}_{ext}$ gives the rate of change of $\vec{k}$ (labelling the Bloch states which already included effects of $V(\vec{r})$) in the presence of $\vec{F}_{ext}$

$\therefore$ If only $V(\vec{r})$ is present, $\frac{d}{dt}(\hbar\vec{k}) = 0$ and an electron in $\psi_{n\vec{k}}$ will remain in $\psi_{n\vec{k}}$ forever

$\Rightarrow$ <u>no scattering</u> of electron <u>due to $V(\vec{r})$</u> to take it out of $\vec{k}$

[In early 1900's, scientists thought that electrons would undergo frequent scatterings in a solid due to the densely packed array of ions.]

<u>Example</u>: A uniform static electric field

$$\hbar\frac{d\vec{k}}{dt} = -e\vec{\mathcal{E}}$$

$\vec{\mathcal{E}}$ = electric field

$-e$ = electron charge

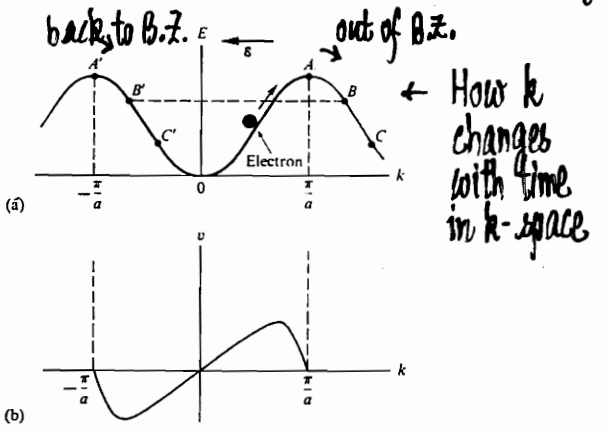
$$\therefore \vec{k}(t) = \vec{k}(t=0) - \frac{e\vec{\mathcal{E}}}{\hbar}t$$

<u>1D case</u>

$$\vec{\mathcal{E}} = -\mathcal{E}\hat{x} \Rightarrow \vec{F}_{ext} = +e\mathcal{E}\hat{x}$$

$$\Rightarrow k = k_0 + \frac{e\mathcal{E}}{\hbar}t$$

$\Rightarrow$ k changes with time uniformly (in k-space)



← How k changes with time in k-space

(a) The motion of an electron in k-space in the presence of an electric field (directed to the left). (b) The corresponding velocity.

- Starts from k_0, changes to k-value to the right
  - → eventually takes on A (edge of 1st B.Z.)
    - → takes on B (equivalent to B') → C (equivalent to C')
      - → keeps on changing in k-space and goes through the whole zone periodicity

So, describing the electron dynamics (change in $\vec{k}$) in k-space is easy.

How about the motion in real space?

Recall: $V(k)$ depends on k

$k_0 \to$ towards A $\to$ pt. A $\to$ B(B') $\to$ C(C') $\to k=0 \to k_0 \to$

- k_0: V is +ve
- towards A: V is +ve but decreasing (deceleration)
- pt. A: $V=0$ (turn around)
- B(B'): V is -ve
- C(C'): V is -ve (less-ve than B)
- $k=0$: $V=0$ (turn around)
- k_0: V is +ve

as k changes periodically in k-space, there is an oscillatory motion in real space (1D problem)!

↑ "Bloch oscillations"

This is highly unusual! ($\vec{F}_{ext}$ is a constant (always points to +ve $\hat{x}$-direction))

- $\vec{E}$ is a static field, but it leads to an oscillatory response!

This comes from band structure effect!

(No such effect for free electrons)

Is "Bloch oscillations" real? Is it observable exp'tally?

Not in bulk (big piece) samples!

Criteria: need $\vec{k}$ to go through the whole B.Z. without suffering a collision with imperfections

In bulk metal, ~1 collision in 10^{-14} s

↑ scattered electron off the track in moving in k-space periodically

Ways out?

- clean samples, low temperatures
- artifical materials with very small B.Z.
  - ↳ semiconductor superlattices
  - ↳ Bloch oscillations are observed in early 1990's.

Example: $\vec{F}_{ext}$ due to $\vec{B}$ field

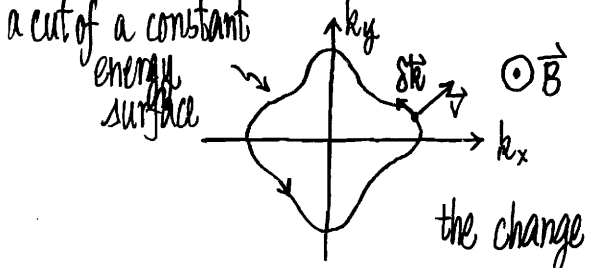
$$\frac{d}{dt}(\hbar\vec{k}) = -e\vec{v}\times\vec{B} = -\frac{e}{\hbar}\vec{\nabla}_{\vec{k}}\mathcal{E}_n(\vec{k})\times\vec{B}$$

Q: How does $\vec{k}$ change?

$\delta\vec{k} \perp \vec{v}$ or $\delta\vec{k} \perp \nabla_{\vec{k}} \varepsilon_n(\vec{k})$

$\delta\vec{k} \perp \vec{B}$

$\therefore$ $\vec{k}$ changes along a contour of constant energy



the change in $\vec{k}$-space is cyclic

How long does it take for $\vec{k}$ to complete a cycle in $\vec{k}$-space?

In a time interval δt,

$$\delta k = -\frac{e}{\hbar}(\vec{v}(\vec{k}) \times \vec{B})\,\delta t$$

$$T = \oint \delta t = \frac{\hbar}{eB} \oint \frac{dk}{v(\vec{k})}$$

T: time to complete a cycle; $\oint$: along orbit

$v(\vec{k}) = |\vec{v}(\vec{k})|$ = magnitude of $\vec{v}(\vec{k})$ along the orbit

$$\omega_c = \frac{2\pi}{T} = \frac{2\pi eB}{\hbar} \frac{1}{\oint \frac{dk}{v(\vec{k})}}$$

ω_c: cyclotron frequency of Bloch electron

- ω_c can be probed exp'tally if $\omega_c > \frac{1}{\tau}$ (basis of mapping out Fermi surface)

  $\frac{1}{\tau}$: can complete cycles before collisions

If we have parabolic band, $\varepsilon(\vec{k}) = \frac{\hbar^2 k^2}{2m}$

$$v(\vec{k}) = \frac{\hbar k}{m^*}$$

$$\oint \frac{dk}{v(\vec{k})} = \frac{2\pi k}{\frac{\hbar k}{m^*}} = \frac{2\pi m^*}{\hbar}$$

$$\therefore \omega_c = \frac{eB}{m^*}$$ ← this is what one would expect for a particle of mass m^* and charge e in a B-field

To achieve $\omega_c > \frac{1}{\tau}$ so that ω_c can be probed, we need high B-field (increase ω_c), clean sample, low temperature (increase τ)

Measuring ω_c in the case of parabolic band gives a measurement on m^*.

D. The Dynamical Effective Mass

Recall: $\vec{v}(\vec{k})$ depends on $\vec{k}$

With $\vec{F}_{ext} \rightarrow \vec{k}$ changes $\rightarrow \vec{v}$ changes $\rightarrow$ thus acceleration

(may be useful to introduce a mass)

$\vec{a} = (a_x, a_y, a_z)$ $\quad a_i$ $(i = x, y, z)$ components

$$a_i = \frac{d}{dt}(v_n(\vec{k}))_i = \frac{1}{\hbar}\frac{d}{dt}\left(\vec{\nabla}_{\vec{k}}\mathcal{E}_n(\vec{k})\right)_i \leftarrow i^{th} \text{ component of } \vec{\nabla}_{\vec{k}}\mathcal{E}_n(\vec{k})$$

$$= \frac{1}{\hbar}\frac{d}{dt}\left(\frac{\partial}{\partial k_i}\mathcal{E}_n(\vec{k})\right)$$

$$= \frac{1}{\hbar}\sum_j \frac{\partial^2 \mathcal{E}_n(\vec{k})}{\partial k_i \partial k_j}\frac{dk_j}{dt} = \frac{1}{\hbar^2}\sum_j \frac{\partial^2 \mathcal{E}_n(\vec{k})}{\partial k_i \partial k_j}\left(\hbar\frac{dk_j}{dt}\right)$$

$$= \sum_j \frac{1}{\hbar^2}\frac{\partial^2 \mathcal{E}_n(\vec{k})}{\partial k_i \partial k_j} F_{ext,j}$$

$$\equiv \sum_j \left(\frac{1}{m_n^*}\right)_{ij} F_{ext,j} \qquad \left(\text{defines } \left(\frac{1}{m_n^*}\right)_{ij}\right)$$

For a band $\mathcal{E}_n(\vec{k})$:

$$\left(\frac{1}{m_n^*}\right)_{ij} \equiv \frac{1}{\hbar^2}\frac{\partial^2 \mathcal{E}_n(\vec{k})}{\partial k_i \partial k_j} = \text{Reciprocal effective mass tensor of the } n^{th} \text{ band}$$

Example:

3D nearest-neighbor TBM (SC)

$$\mathcal{E}(\vec{k}) = \mathcal{E}_0 - 2t\,(\cos k_x a + \cos k_y a + \cos k_z a)$$

$$\left(\frac{1}{m^*}\right)_{ij} = \frac{2ta^2}{\hbar^2}\cos(k_i a)\,\delta_{ij}$$

In matrix form:

$$\left(\overleftrightarrow{\frac{1}{m^*}}\right) = \frac{2ta^2}{\hbar^2}\begin{pmatrix} \cos k_x a & 0 & 0 \\ 0 & \cos k_y a & 0 \\ 0 & 0 & \cos k_z a \end{pmatrix}$$

matrix elements are $\vec{k}$-dependent

At $\vec{k}=0$, $\left(\frac{1}{m^*}\right)_{ii} = \frac{2ta^2}{\hbar^2} > 0$ (and near bottom of band)

At $\vec{k} = \left(\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a}\right)$ (corner of 1st B.Z.)

$$\left(\frac{1}{m^*}\right)_{ii} = -\frac{2ta^2}{\hbar^2} < 0 \quad \text{(and near top of band)}$$

$\therefore$ Near bottom of band: $m^* = \frac{\hbar^2}{2ta^2}$

Near top of band: $m^* = -\frac{\hbar^2}{2ta^2}$

(m^* is a simple way to include band structure effects)

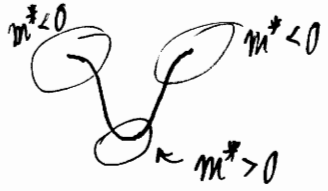
- The dynamical equations look a lot simpler <u>in 1D</u> or <u>for isotropic mass</u>
  - $v_n(k) = \frac{1}{\hbar}\frac{d}{dk}\mathcal{E}_n(k)$
  - $\sum_{\text{all } k\in B.Z} v_n(k) = 0 \Rightarrow$ Total electron velocity in <u>full</u> band $= 0$
  - $\frac{d}{dt}(\hbar k) = F_{ext}$ gives how k changes under F_{ext}
  - $a = \frac{d}{dt}v_n(k) = \frac{1}{dt}\left(\frac{1}{\hbar}\frac{d}{dk}\mathcal{E}_n(k)\right) = \frac{1}{\hbar}\frac{d^2}{dk^2}\mathcal{E}_n(k)\frac{dk}{dt}$

$$= \left(\frac{1}{\hbar^2}\frac{d^2}{dk^2}\mathcal{E}_n(k)\right)\left(\frac{d}{dt}\hbar k\right) = \left(\frac{1}{\hbar^2}\frac{d^2}{dk^2}\mathcal{E}_n(k)\right)F_{ext}$$

$$\equiv \left(\frac{1}{m_n^*}\right)F_{ext}$$

($\mathcal{E}(k)$: isotropic or 1D; n^{th} band)

$$\therefore \frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2}{dk^2}\mathcal{E}(k)$$



<u>Note:</u>
Even in 1D, a is <u>not</u> necessarily in the same direction of F_{ext}. It depends on k, as m^* can be +ve or -ve.

In general, $\vec{a} = \left(\frac{1}{m_n^*}\right)\cdot\vec{F}_{ext}$

($\vec{a}$: vector (acceleration); $\frac{1}{m_n^*}$: 3×3 matrix; $\vec{F}_{ext}$: external force (vector))

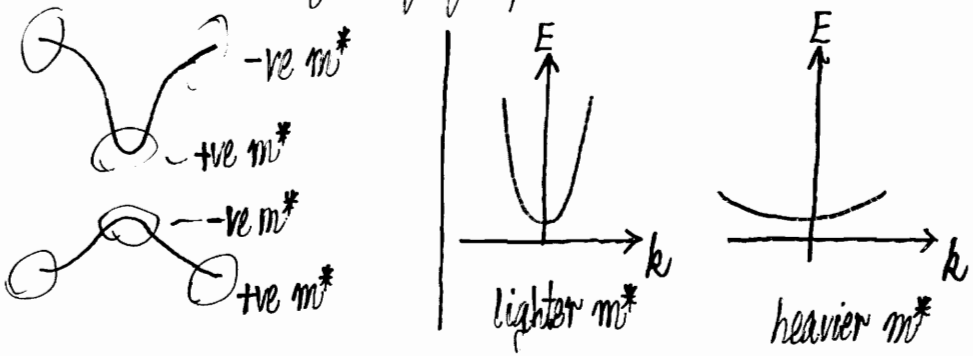
$\therefore \vec{a}$ is <u>not</u> necessarily in the direction of $\vec{F}_{ext}$, due to band structure effect.

- The tensorial nature of m^* comes from $\mathcal{E}(k)$, which may take on different curvatures for different directions of k.
- Let's don't worry too much about the tensorial nature [or consider 1D]

$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k^2} \quad \text{or} \quad m^* = \frac{\hbar^2}{\left(\frac{\partial^2 E}{\partial k^2}\right)}$$

describes how the band curves and therefore includes the effects of ions (band structure effects)

$$m^* \sim \frac{1}{\text{rate of change of slope in band structure}}$$



- The idea of m^* is particularly important for materials in which the key physics comes from the parabolic parts of the energy band structure. An example is <u>semiconductor</u>.

<u>Note:</u> m^* concerns the effective mass of an <u>electron</u> in the state $\mathcal{E}(k)$. Up to here, we have NOT talked about something called <u>hole</u> yet!

For an electron near bottom of band

$\vec{\mathcal{E}} \parallel +\hat{x}$ $\quad \vec{F}_{\text{ext on electrons}} = -e\vec{\mathcal{E}} \parallel -\hat{x}$

$\frac{d}{dt}(\hbar\vec{k}) = \vec{F}_{ext} \Rightarrow$ shift in $-\hat{x}$-direction in k-space

Vel. ~ slope $\frac{dE(k)}{dk}$

$\Rightarrow$ velocity is changing in $-\hat{x}$-direction

(e.g., +ve slope to less +ve slope
+ve slope to -ve slope
-ve slope to more -ve slope)

these give how an electron moves in real space

$\Rightarrow$ acceleration $\parallel -\hat{x}$ direction

Now, $\vec{F}_{\text{ext on electron}} \parallel -\hat{x}$ and acceleration $\parallel -\hat{x}$

→ a positive effective mass for these electrons

$\frac{\partial^2 E}{\partial k_x^2} > 0$

Remark: If we look at $\vec{\mathcal{E}} \parallel +\hat{x}$ and acceleration $\parallel -\hat{x}$, this is just the case one expected for an electron (-ve charge).

∴ All the quantities and concepts tie up fine!

For an electron near top of band

$\vec{\mathcal{E}} \parallel \hat{x}$ $\quad F_{\text{ext on electron}} = -e\vec{\mathcal{E}} \parallel -\hat{x}$

$\Rightarrow$ shift in $-\hat{x}$-direction in k-space

Vel ~ slope of band $\frac{dE(k)}{dk}$

$\Rightarrow$ Velocity is changing in $+\hat{x}$-direction

(e.g. -ve to less -ve
-ve to +ve
+ve to more +ve)

these give how an electron near top of band moves in real space

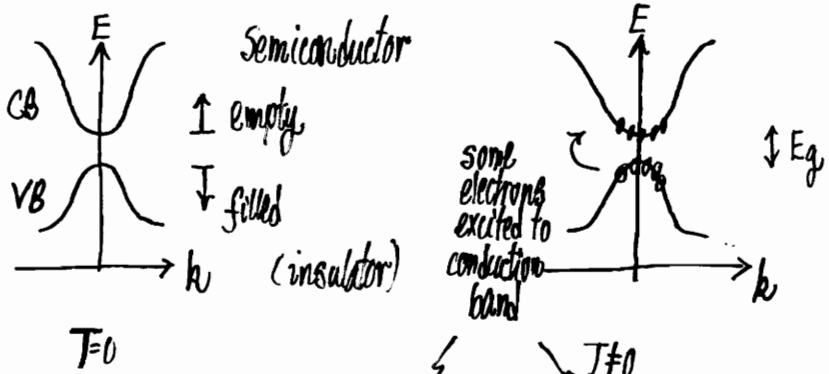
$\Rightarrow$ acceleration $\parallel +\hat{x}$-direction

Now $\vec{F}_{\text{ext on electron}} \parallel -\hat{x}$ and acceleration $\parallel +\hat{x}$

→ a negative effective mass for electron near top of band

∴ All the quantities and concepts tie up fine!

Remark: If we look at $\vec{\mathcal{E}} \parallel +\hat{x}$ and acceleration $\parallel +\hat{x}$, this is the case for a particle of positive charge!



Electrons occupy the <u>bottom part of CB</u>, which is highly parabolic (m_e^* is sufficient to model the band structure effects and then free electron model results can be used)

$$E_c(k) = E_g + \frac{\hbar^2 k^2}{2m_e^*}$$

<u>Missing electrons</u> are those near the top of VB, which is highly parabolic (a parameter m_h^* is sufficient to model the band structure effects)

$$E_v(k) = -\frac{\hbar^2 k^2}{2m_h^*}$$

∴ Semiconductor physics:

≈ free electrons in CB with m_e^*

\+

free <u>missing electrons</u> in top of VB with m_h^*

behave as particles with $m_h^* = -m^* > 0$ and charge (+e)

↑ effective mass is negative near top of bands

Refs. Kittel Ch.8, Ch.9
Christman Sec. 9.1