acceleration of Bloch electrons

$$\frac{d\vec{v}}{dt} = \frac{1}{\hbar}\frac{d}{dt}\underbrace{\nabla_{\vec{k}}\,\varepsilon(\vec{k})}_{\equiv \frac{\partial \varepsilon}{\partial \vec{k}}} = \frac{1}{\hbar}\frac{\partial^2 \varepsilon(\vec{k})}{\partial \vec{k}\,\partial \vec{k}} \cdot \frac{d\vec{k}}{dt} \qquad (++)$$

switch on weak electric field $\vec{E}$ (sufficiently weak that electron cannot overcome band gap)

rate with which electron absorbs energy from electric field $\vec{E}$

$$\underbrace{\frac{d\,\varepsilon(\vec{k})}{dt}}_{=\nabla_{\vec{k}}\varepsilon(\vec{k})\cdot\frac{d\vec{k}}{dt}} = \underbrace{e\,\vec{E}}_{=\vec{F}\text{ force}}\cdot\vec{v} = \vec{F}\cdot\frac{1}{\hbar}\nabla_{\vec{k}}\,\varepsilon(\vec{k})$$

$$\Rightarrow \vec{F} = \frac{d\hbar\vec{k}}{dt}$$

$\hbar\vec{k}$ in general <u>not</u> momentum of Bloch electron

in $(++)$ $\Rightarrow$

$$\frac{d\vec{v}}{dt} = \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon(\vec{k})}{\partial \vec{k}\,\partial \vec{k}} \cdot \vec{F}$$

components $$\left(\frac{d\vec{v}}{dt}\right)_\alpha = \underbrace{\frac{1}{\hbar^2}\frac{\partial^2 \varepsilon(\vec{k})}{\partial k_\alpha\,\partial k_\beta}}_{=\left(\frac{1}{m^*}\right)_{\alpha\beta}} F_\beta$$

$\left(\frac{1}{m^*}\right)_{\alpha\beta}$ → tensor of inverse effective mass
→ symmetrical 3×3 matrix

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(B) (5)

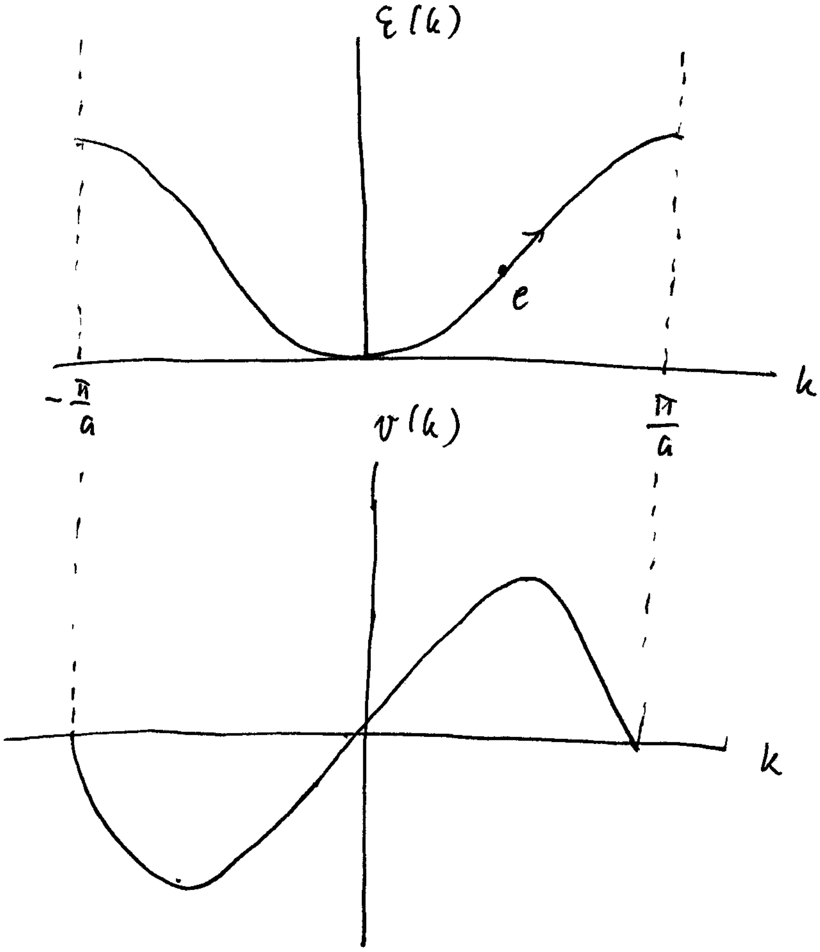
examples:

(i) free electrons $\varepsilon(\vec{k}) = \frac{\hbar^2 k^2}{2 m_e} \Rightarrow \frac{\partial^2 \varepsilon(\vec{k})}{\partial k_\alpha \partial k_\beta} = \frac{\hbar^2}{m_e} \delta_{\alpha\beta} \Rightarrow m_e = m^*$

(ii) tight binding model for cubic lattice at small $\vec{k}$

$$\varepsilon(\vec{k}) = \varepsilon_0 - 6t - a^2 t k^2 \Rightarrow m^* = \frac{\hbar^2}{2a^2 t}$$

(iii) Bloch electrons



example: $\underline{d = 1}$

velocity
$$\vec{v}(\vec{k}) = \frac{1}{\hbar} \nabla_{\vec{k}} \varepsilon(\vec{k})$$

<u>remarks:</u>

- weak electric field $\vec{E}$ → convention: electron jumps at $k = \frac{\pi}{a}$ back to $-\frac{\pi}{a}$
- oscillating velocity → AC current induced by constant field $\vec{E}$

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(A) (6)

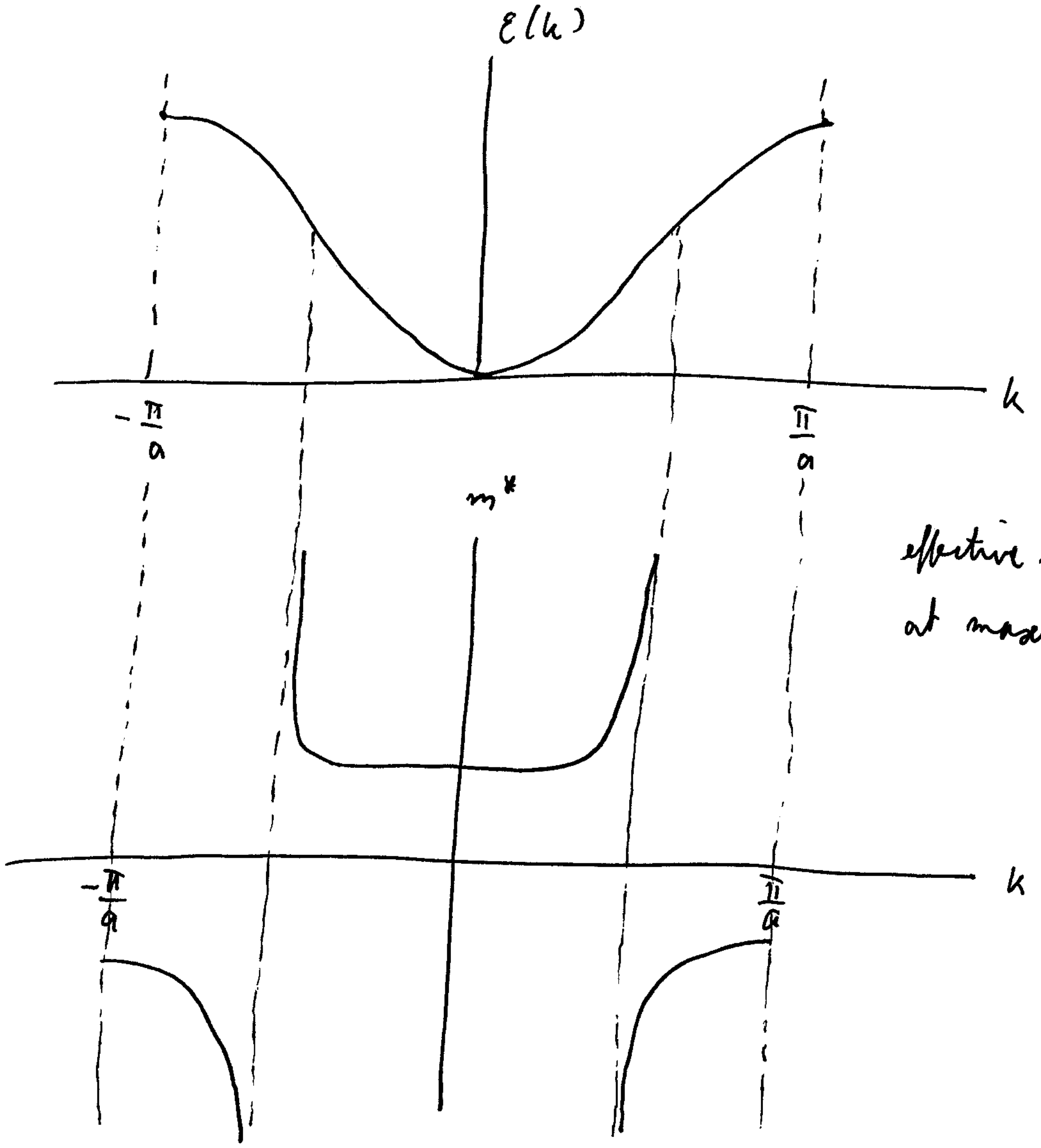
- real electrons interact with phonons and defects
  → short "k paths"

Bloch electron in vicinity of local extremum of $\mathcal{E}(\vec{k})$
→ Taylor expansion

$$\mathcal{E}(\vec{k}) = \mathcal{E}_{extr.} + a_1 k_x^2 + a_2 k_y^2 + a_3 k_z^2$$

$$\Rightarrow \quad m^*_{xx} = \frac{\hbar^2}{2a_1} \qquad m^*_{yy} = \frac{\hbar^2}{2a_2} \qquad m^*_{zz} = \frac{\hbar^2}{2a_3}$$

anisotropic effective mass



effective mass negative at maxima of $\mathcal{E}(k)$

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(7)

(iv) dynamics of holes

consider completely occupied energy band

$$\sum_{\vec{k} \in 1.BZ} \vec{v}(\vec{k}) = \frac{1}{\hbar} \sum_{\vec{k} \in 1.BZ} \frac{\partial \varepsilon(\vec{k})}{\partial \vec{k}}$$

$$= 0 \qquad \varepsilon(\vec{k}) = \varepsilon(-\vec{k})$$

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

$\Rightarrow$ no current

now band with one empty state at $\vec{k}_1$

$\Rightarrow$ current

$$\vec{j} = {\sum_{\vec{k} \in 1.BZ}}' \left(-\frac{|e|}{V}\right) \vec{v}(\vec{k})$$

$\sum'$: sum over all $\vec{k} \in 1.BZ$, except for $\vec{k}_1$

$$= -\frac{|e|}{V} \underbrace{\sum_{\vec{k} \in 1.BZ} \vec{v}(\vec{k})}_{=0} + \frac{|e|}{V} \vec{v}(\vec{k}_1)$$

$$= \frac{|e|}{V} \vec{v}(\vec{k}_1)$$

current of "electron" with positive charge

motion of a hole in constant external field $\vec{E}$

$$\frac{d\vec{v}}{dt} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon(\vec{k})}{\partial \vec{k}\, \partial \vec{k}} \cdot \underbrace{\vec{F}}_{= -|e|\vec{E}} = -\frac{1}{\hbar^2} |e| \frac{\partial^2 \varepsilon(\vec{k})}{\partial \vec{k}\, \partial \vec{k}} \cdot \vec{E}$$

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positively charged particle

+ effective mass $\left(\frac{1}{m^*}\right)_{\alpha\beta} = -\frac{1}{\hbar^2} \frac{\partial^2 \mathcal{E}(\vec{k})}{\partial k_\alpha \, \partial k_\beta}$

<u>example</u>: $d = 1$

region around maximum at k_0 in $\mathcal{E}(k)$

$$\mathcal{E}(k) \simeq \mathcal{E}(k_0) - \underbrace{\alpha}_{>0} (k - k_0)^2$$

$$\Rightarrow \quad \frac{1}{m^*} = -\frac{1}{\hbar^2} \frac{\partial^2 \mathcal{E}(k)}{\partial k^2} = \frac{2\alpha}{\hbar^2} > 0 \quad ✓$$