Semiclassical model of electron dynamics

How does the electron move in a lattice + weak external field?

so that interband transition can be ignored

✓ Electric field → Bloch oscillation

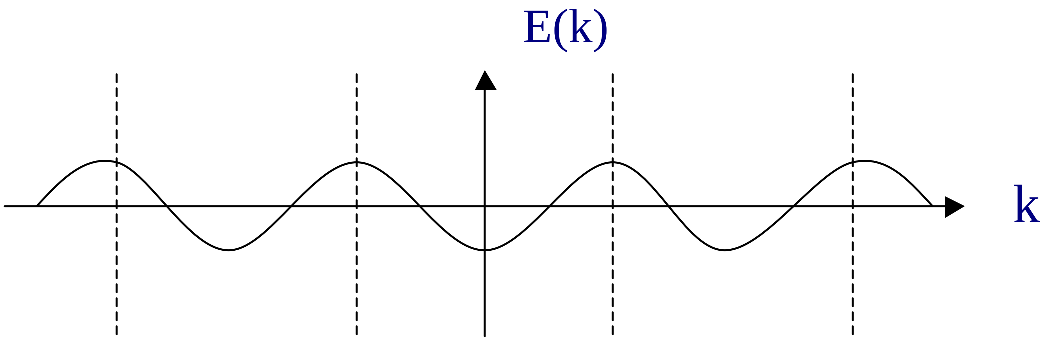
✓ Magnetic field → cyclotron motion

✓ Electric+magnetic field → Hall effect

Table 12.1
COMPARISON OF SOMMERFELD AND BLOCH ONE-ELECTRON EQUILIBRIUM LEVELS

	SOMMERFELD	BLOCH
QUANTUM NUMBERS (EXCLUDING SPIN)	$\mathbf{k}$ ($\hbar\mathbf{k}$ is the momentum.)	$\mathbf{k}$, n ($\hbar\mathbf{k}$ is the crystal momentum and n is the band index.)
RANGE OF QUANTUM NUMBERS	$\mathbf{k}$ runs through all of k-space consistent with the Born-von Karman periodic boundary condition.	For each n, $\mathbf{k}$ runs through all wave vectors in a single primitive cell of the reciprocal lattice consistent with the Born-von Karman periodic boundary condition; n runs through an infinite set of discrete values.
ENERGY	$\mathcal{E}(\mathbf{k}) = \frac{\hbar^2 k^2}{2m}$.	For a given band index n, $\mathcal{E}_n(\mathbf{k})$ has no simple explicit form. The only general property is periodicity in the reciprocal lattice: $\mathcal{E}_n(\mathbf{k}+\mathbf{K}) = \mathcal{E}_n(\mathbf{k})$.
VELOCITY	The mean velocity of an electron in a level with wave vector $\mathbf{k}$ is: $\mathbf{v} = \frac{\hbar\mathbf{k}}{m} = \frac{1}{\hbar}\frac{\partial\mathcal{E}}{\partial\mathbf{k}}$.	The mean velocity of an electron in a level with band index n and wave vector $\mathbf{k}$ is: $\mathbf{v}_n(\mathbf{k}) = \frac{1}{\hbar}\frac{\partial\mathcal{E}_n(\mathbf{k})}{\partial\mathbf{k}}$.
WAVE FUNCTION	The wave function of an electron with wave vector $\mathbf{k}$ is: $\psi_{\mathbf{k}}(\mathbf{r}) = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{V^{1/2}}$.	The wave function of an electron with band index n and wave vector $\mathbf{k}$ is: $\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{n\mathbf{k}}(\mathbf{r})$ where the function $u_{n\mathbf{k}}$ has no simple explicit form. The only general property is periodicity in the direct lattice: $u_{n\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r})$.

- Energy dispersion (periodic zone scheme)



- Electron velocity

$$\vec{v}(\vec{k}) = \frac{1}{\hbar}\frac{\partial E_n(\vec{k})}{\partial \vec{k}}$$

- Electric current

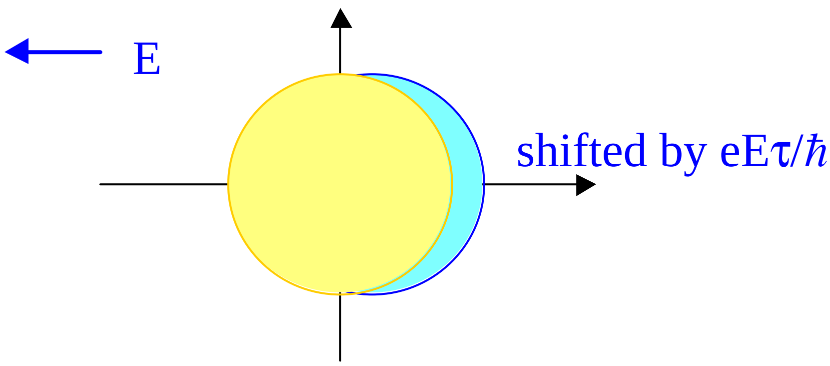
$$\vec{j} = -\frac{e}{V}\sum_k \vec{v} = -e\int \frac{d^3k}{(2p)^3}\frac{1}{\hbar}\frac{\partial E_n(\vec{k})}{\partial \vec{k}}$$

- For crystals with inversion symmetry,

$$E_n(k)=E_n(-k)$$

→ electrons with momenta hk and -hk have opposite velocities

→ no net current in equilibrium

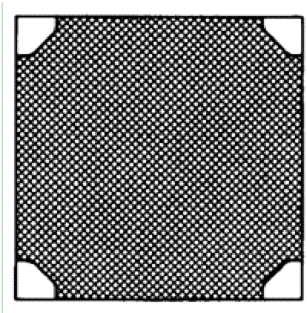


Note: The relaxation time of a perfect crystal is infinite.

The resistivity comes not from periodic ions, but from impurities, defects, thermal vibrations… etc

The concept of holes

The current in a filled band is zero even if E ≠ 0



$$\vec{j} = -e \int_{occupied} \frac{d^3k}{(2p)^3} \frac{1}{\hbar} \frac{\partial E_n(\vec{k})}{\partial \vec{k}} = +e \int_{unoccupied} \frac{d^3k}{(2p)^3} \frac{1}{\hbar} \frac{\partial E_n(\vec{k})}{\partial \vec{k}}$$

∴unoccupied states behave as +e charge carriers

The concept of effective mass

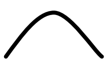
Near the bottom of a conduction band,

$$E(\vec{k}) = E_0 + \frac{1}{2}\sum_{i,j} \frac{\partial^2 E(\vec{k})}{\partial k_i \partial k_j} k_i k_j + O(k^3) \approx E_0 + \frac{1}{2}\sum_{i,j}\left(\frac{1}{m^*}\right)_{ij} p_i p_j$$

Reciprocal effective mass matrix

$$\left(\frac{1}{m^*}\right)_{ij} \equiv \frac{1}{\hbar^2} \frac{\partial^2 E(\vec{k})}{\partial k_i \partial k_j}$$

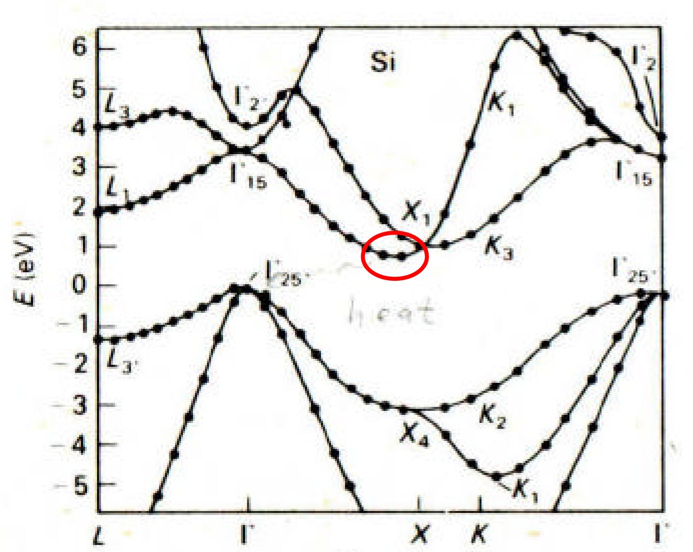
- ➢ In general, electron in a flatter band has a larger m*
- ➢ Negative effective mass:

  If E(k) is  (e.g. near zone boundary) then $m^*<0$

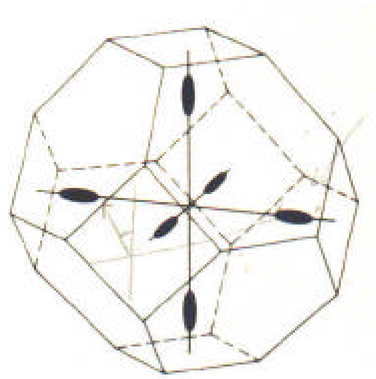
→ electron (-e) with negative m* = hole (+e) with positive m*

- For a spherical FS, $m^*_{ij} = m^* \delta_{ij}$, one m* is enough.
- For ellipsoidal FS, there can be at most three different m^*s

  Eg. the FS of Si is made of six identical ellipsoidal pockets

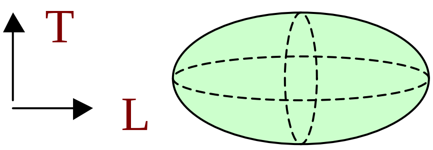


Band structure of Si



Near the conduction band bottom,

$$E(\vec{k}) = E_g + \frac{\hbar^2 k_x^{\;2}}{2m_L} + \frac{\hbar^2 k_y^{\;2}}{2m_T} + \frac{\hbar^2 k_z^{\;2}}{2m_T}$$



For Si,

$E_g = 1.1$ eV, $m_L = 0.9$ m, $m_T = 0.2$ m

(it's more difficult for the electron to move along the L direction because the band is flatter along that direction)

Electron dynamics in an external field

Consider a wave packet centered at k in k-space, then

$$\hbar \frac{d\vec{k}}{dt} = q(\vec{E}(\vec{r},t) + \frac{\vec{v}(\vec{k})}{c} \times \vec{H}(\vec{r},t))$$

where $$\vec{v}(\vec{k}) = \frac{1}{\hbar} \frac{\partial E_n(\vec{k})}{\partial \vec{k}}$$

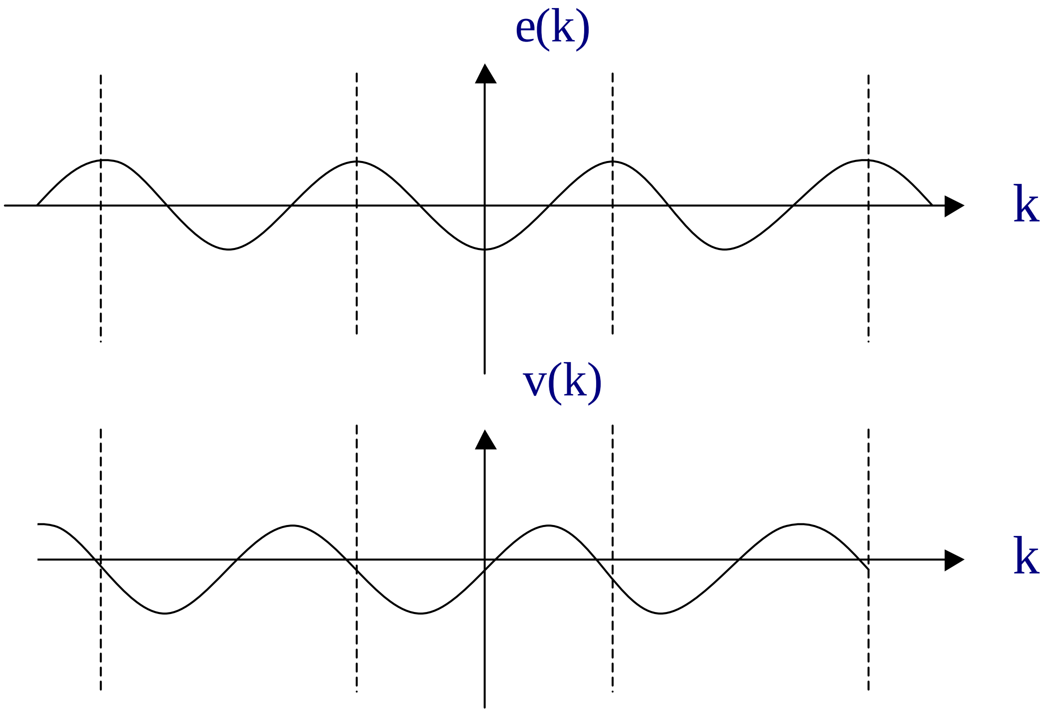
(The derivation is nontrivial and is neglected here)

- Notice that E is the external field, whcih does not include the lattice field. The effect of lattice is hidden in $E_n(k)$!
- This looks like the usual Lorentz force eq. But the validity of this equation is more limited. It is good only if
  1. Interband transition can be neglected (not valid if there is electric or magnetic breakdown due to a strong field).
  2. E and H can be non-uniform in space, but they have to be much smoother than the lattice potential.
  3. E and H can be oscillating in time, but with the condition

$$\hbar w << E_g$$

Bloch electron in a uniform electric field

$$\hbar\frac{dk}{dt} = -eE \quad \rightarrow \quad \hbar k(t) = -eEt$$



In a DC electric field, the electrons decelerate and reverse its motion at the BZ boundary!

A DC bias produces an AC current!! (Bloch oscillation)

- Why the oscillation is not observed in ordinary crystals?

  To complete a cycle (a is the lattice constant),

  $$eET / \hbar = 2\pi / a \rightarrow T = h / eEa$$

  For $E = 10^4$ V/cm, and a=1 A, $T = 10^{-10}$ sec

  But electron collisions take only about 10^{-14} sec.

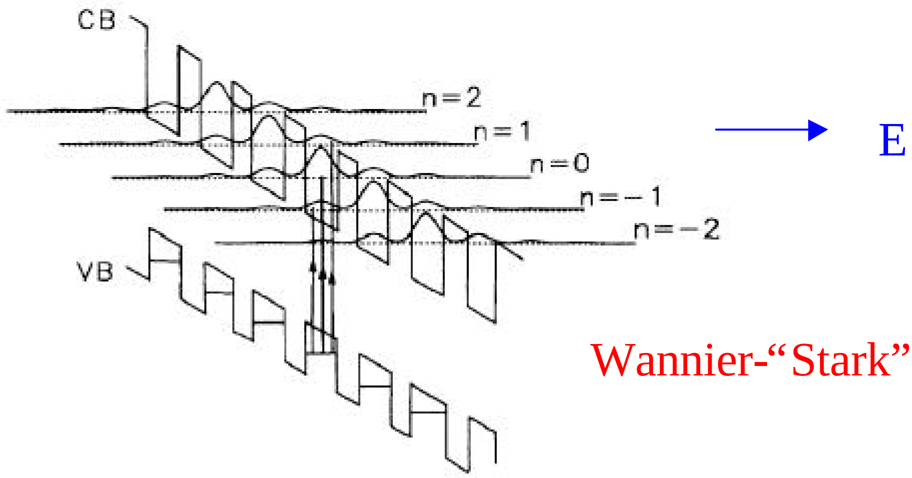
  ∴ the Bloch electron cannot get to the zone boundary

- To observe it, need

  1. stronger E field → but only up to about 10^6 V/cm
  2. larger a → use superlattice (eg. a = 100 A)
  3. reduce collision time → use high quality sample

  (Mendez et al, PRL, 1988)

- Discrete spectrum due to oscillation:



Wannier-“Stark” ladders

- Bloch oscillator generates THz microwave:

  frequency ≈ $10^{12\sim13}$, wave length $\lambda \approx$ 0.01 mm - 0.1mm

  (Waschke et al, PRL, 1993)

Bloch electron in a uniform magnetic field

$$\hbar \frac{d\vec{k}}{dt} = q\frac{\vec{v}}{c} \times \vec{H}, \quad \vec{v}_k = \frac{1}{\hbar}\frac{\partial E(\vec{k})}{\partial \vec{k}}$$

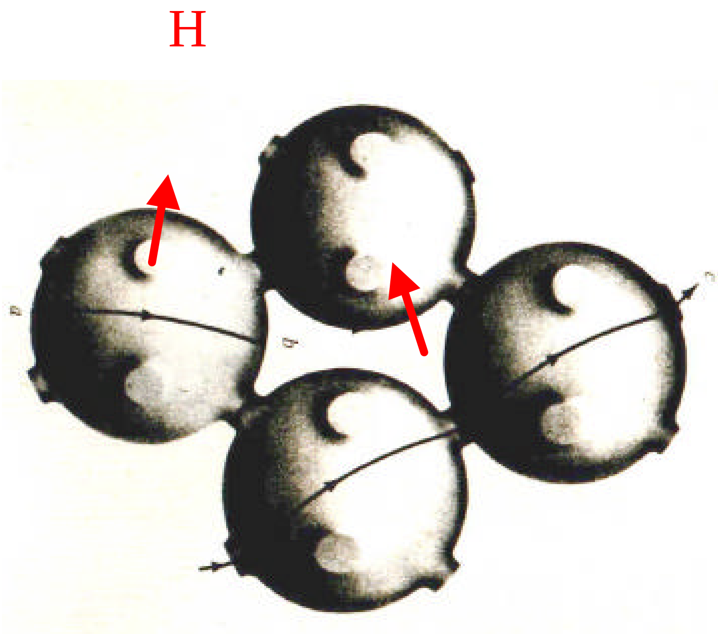
$$\longrightarrow \quad \dot{\vec{k}} \cdot \vec{H} = 0, \qquad \dot{\vec{k}} \cdot \vec{v}_k = \frac{1}{\hbar}\frac{dE(\vec{k})}{dt} = 0$$

Therefore, 1. Change of k is perpendicular to the H field,

→ $k_{||}$ does not change

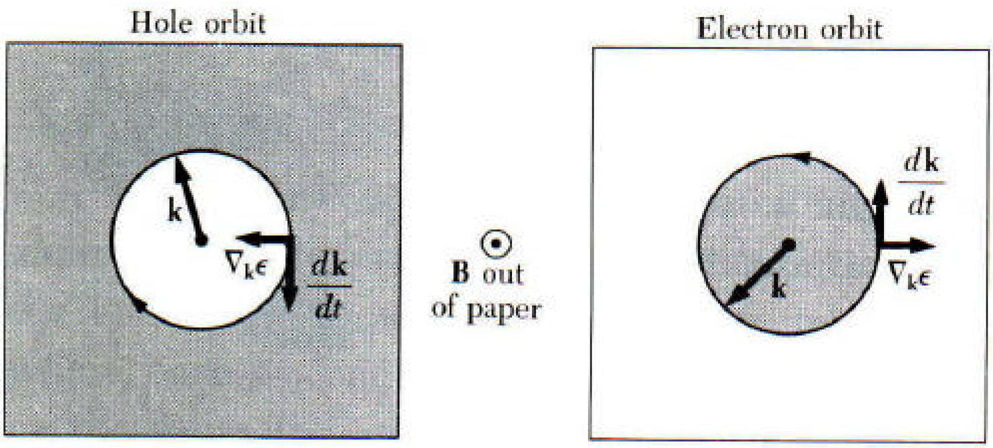
and 2. E(k) is a constant of motion

This determines uniquely the electron orbit on the FS



- For spherical FS, it is just the usual cyclotron orbit,
- For connected FS, there might be open orbits

- Orientation of the orbit



smaller k	smaller k
higher energy	lower energy

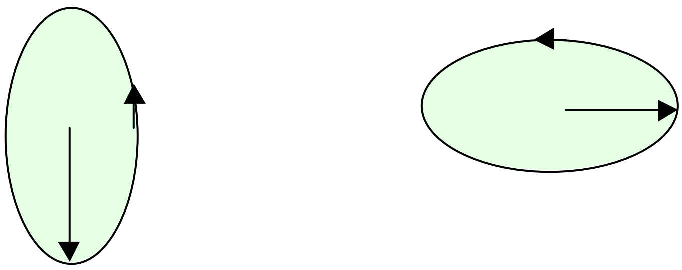
→ The "hill" is always on one's right hand side

Cyclotron orbit in real space

$$\hbar\dot{\vec{k}} = -\frac{e}{c}\dot{\vec{r}}\times\vec{H} \quad\rightarrow\quad \dot{\vec{r}} = -\frac{\hbar c}{eH^2}\vec{H}\times\dot{\vec{k}}$$

$$\rightarrow\quad \vec{r}(t)-\vec{r}(0) = -\frac{\hbar c}{eH}\hat{H}\times[\vec{k}(t)-\vec{k}(0)]$$

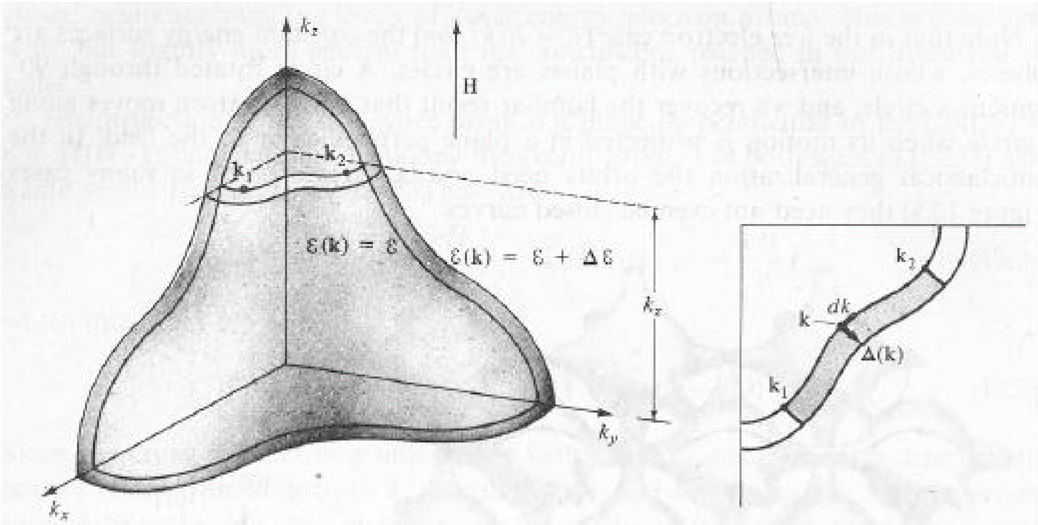
r-orbit k-orbit



rotated by 90 degrees and scaled by $\hbar c/eH = \lambda_B^2$

λ_B = 256 A at H= 1 Tesla (magnetic length)

Temporal period of the orbit



$$dt = dk/|\dot{\vec{k}}| = \frac{\hbar^2 c}{eH}\frac{dk}{|(\partial E/\partial \vec{k})_\perp|}$$

$$\Delta E(\vec{k}) = \frac{\partial E(\vec{k})}{\partial \vec{k}} \cdot \Delta \vec{k} = \left| \left(\frac{\partial E}{\partial \vec{k}} \right)_\perp \right| \Delta(\vec{k})$$

Therefore,

$$t_2 - t_1 = \frac{\hbar^2 c}{eH}\frac{1}{\Delta E}\int_{k_1}^{k_2} dk\Delta(\vec{k}) = \frac{\hbar^2 c}{eH}\frac{\partial A_{1,2}}{\partial E}$$

$$\rightarrow \quad T(E, k_z) = \frac{\hbar^2 c}{eH}\frac{\partial A(E, k_z)}{\partial E}$$

Compare with the period of a cyclotron orbit, we have $\omega_c = eH/m^* c$, where the cyclotron effective mass is

$$m_c^* \equiv \frac{\hbar^2}{2p}\frac{\partial A(E, k_z)}{\partial E}$$

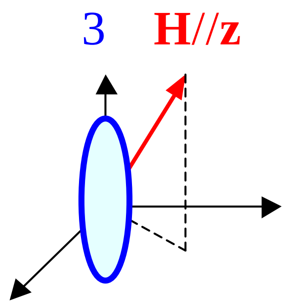
More on the cyclotron effective mass

Near a band minimum

$$E(\vec{k}) = E_0 + \frac{\hbar^2}{2}\left(\vec{k}-\vec{k}_0\right)\cdot M^{-1}\cdot\left(\vec{k}-\vec{k}_0\right)$$

where M is the effective mass matrix.

It can be shown that (Prob. 12.2 (a))



$$m_c{*} = \left(\frac{|M|}{M_{zz}}\right)^{1/2}$$

$$= \left(\frac{m_1 m_2 m_3}{\hat{H}_1^2 m_1 + \hat{H}_2^2 m_2 + \hat{H}_3^2 m_3}\right)^{1/2},$$

where m_1, m_2, m_3 are the eigenvalues of M,

and $\vec{H} = H\left(\hat{H}_1, \hat{H}_2, \hat{H}_3\right)$ along the principal axis

Pf: From the theory of matrix diagonalization, we have

$$M = R\, M_D\, R^T$$

where M_D is the diagonalized matrix, and

$$R = \begin{pmatrix} e_1^1 & e_1^2 & e_1^3 \\ e_2^1 & e_2^2 & e_2^3 \\ e_3^1 & e_3^2 & e_3^3 \end{pmatrix}, \quad \vec{e}^{\,l} = \begin{pmatrix} e_1^l \\ e_2^l \\ e_3^l \end{pmatrix} \text{ is the } l\text{-th eigenvector of } M$$

Note that $\mathbf{e}^3$ is the vector along 3-axis on the (x,y,z)-coord;

$(e^1{}_3 . e^2{}_3 . e^3{}_3)$ are the components of **z** on the (1,2,3)-coord.

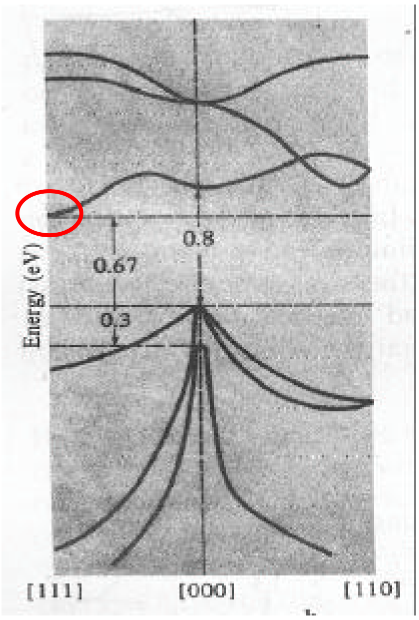
$$M_{zz} = \left(e_3^1\right)^2 m_1 + \left(e_3^2\right)^2 m_2 + \left(e_3^3\right)^2 m_3$$

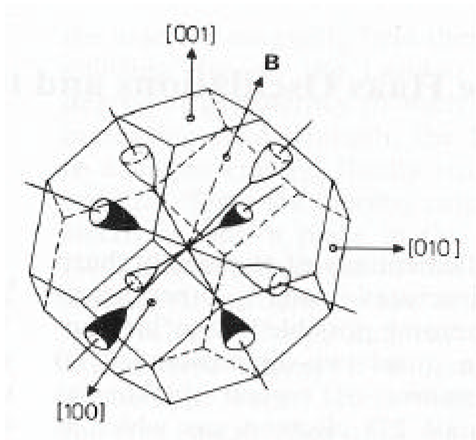
$$= \hat{H}_1^2 m_1 + \hat{H}_2^2 m_2 + \hat{H}_3^2 m_3$$

Also, $|M| = m_1 m_2 m_3$ $\qquad Q.E.D.$

Band structure of Ge

FS has eight ellipsoids





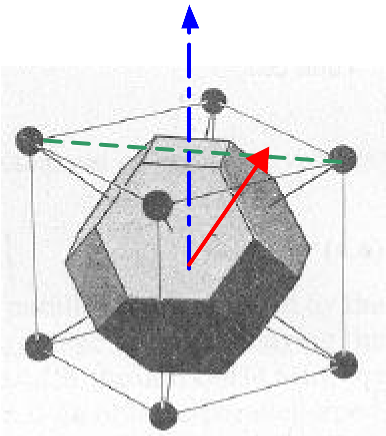
$(e^1_3.e^2_3.e^3_3)=(\sin\theta \cos\phi, \sin\theta \sin\phi, \cos\theta)$

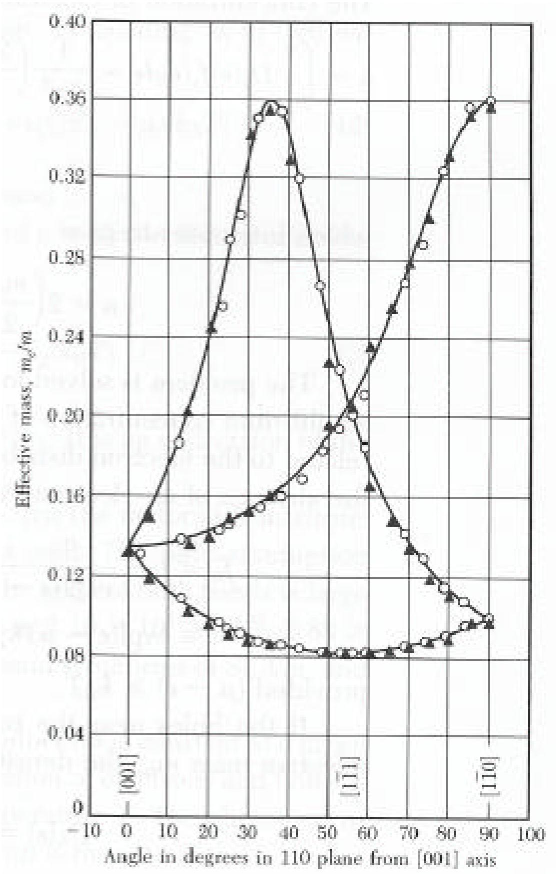
For a symmetric ellipsoid, $m_1=m_2=m_T$, $m_3=m_L$

→ $M_{zz} = \sin^2\theta\, m_T + \cos^2\theta\, m_L$

$$\rightarrow \quad m_c* = \left(\frac{\sin^2 q}{m_T m_L} + \frac{\cos^2 q}{m_T^2}\right)^{-1/2}$$

$m_T=0.082m$, $m_L=1.59m$ for Ge



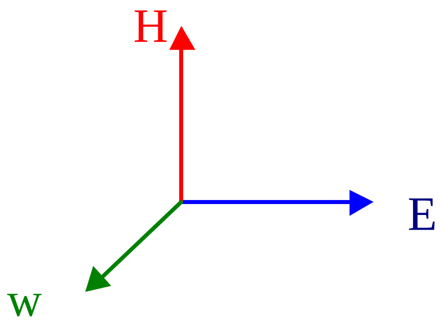


H lies on the (110) plane

Bloch electron in crossed E and H fields (both uniform)

$$\hbar\frac{d\vec{k}}{dt} = -e\vec{E} - e\frac{\dot{\vec{r}}}{c}\times\vec{H}$$

$$= -\frac{e}{c\hbar}\frac{\partial\tilde{e}}{\partial\vec{k}}\times\vec{H}$$



where $\tilde{e}(\vec{k}) = e(\vec{k}) - \hbar\vec{k}\cdot\vec{w},\quad \vec{w}\equiv c\frac{E}{H}\hat{E}\times\hat{H}$

The 2nd term is usually very small compared to ε(k)

So the effect is to tilt the band structure slightly

(max along **w**, min ⊥ **w**), and earlier analysis about the

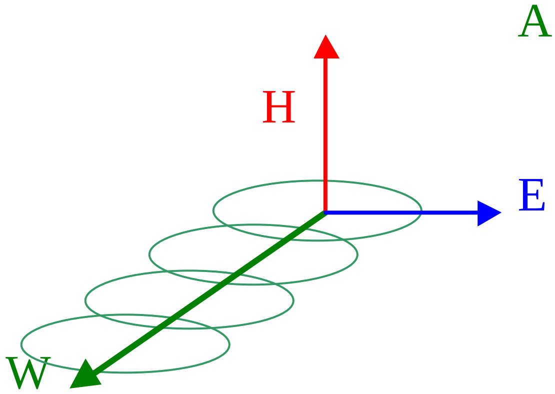
cyclotron orbit still applies (not restricted to closed orbits).

Real space orbit

$$\hbar\frac{d}{dt}\left(\vec{k}+\frac{e}{\hbar}\vec{E}t\right) = -e\frac{\dot{\vec{r}}}{c}\times\vec{H}$$

$$\rightarrow\quad \dot{\vec{r}} = l_B^2\frac{d}{dt}\left(\vec{k}+\frac{e}{\hbar}\vec{E}t\right)\times\hat{H}$$

$$\rightarrow\quad \vec{r}(t)-\vec{r}(0) = l_B^2\left(\vec{k}(t)-\vec{k}(0)\right)\times\hat{H} + \underbrace{c\frac{E}{H}\left(\hat{E}\times\hat{H}\right)t}_{\text{A steady E}\times\text{H drift}}$$



Current density

$$\vec{j}_\perp = qn\langle \dot{\vec{r}}_\perp \rangle$$

If "all" orbits on the FS are closed, then

$$\langle \dot{\vec{r}}_\perp \rangle = e\frac{E}{H}\hat{E}\times\hat{H} \quad \rightarrow \quad \vec{j}_\perp = \frac{qnc}{H}\hat{E}\times\hat{H}$$

This result is valid for different band structures!

Hall coefficient

$$R_e = -\frac{1}{n_e ec}; \quad R_h = \frac{1}{n_h ec}$$

If both electrons and holes are present in a metal, then

$$R = \frac{R_e s_e^2 + R_h s_h^2}{\left(s_e + s_h\right)^2}, \quad s_{e,h} = \frac{n_{e,h} e^2 t_{e,h}}{m_{e,h}*}$$

R>0 or <0 depends on whether e's or h's dominate

(eg. Zn and Cd have positive R)

The analysis is more complicated if there are open orbits

(neglected here)

What happens if the H field is very strong?

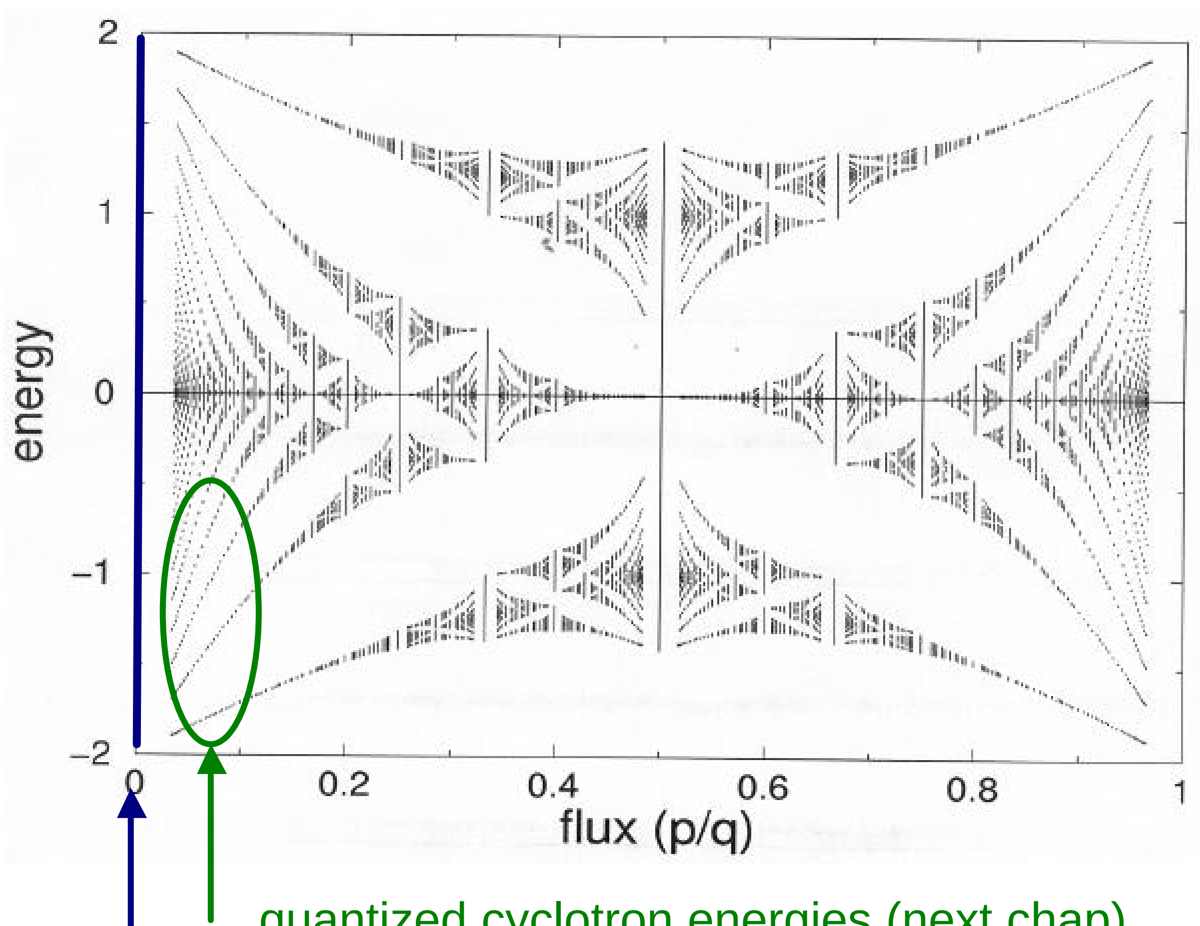
Rigorous calculation using the Schrodinger shows that,

if Ha^2=(p/q)×flux quantum,

where a is the lattice constant, and p.q are co-prime integers,

then one Bloch band splits to q subbands

Hofstadter's butterfly spectrum (PRB, 1976)



quantized cyclotron energies (next chap)

originally only one Bloch band

For a = 0.1 μm, need H = 10 T to get p/q=1/2

Very challenging to observe it experimentally

“Magnetic” Bloch band

(eg., the subbands in the Hofstadter spectrum)

For magnetic Bloch band carrying quantized Hall conductance, the electron obeys slightly different semiclassical dynamical eqs.

TABLE I. Comparison between properties of the usual and magnetic Bloch bands.

	Bloch band	Magnetic Bloch band $[(p/q)\phi_0$ per plaquette$]$
Unperturbed Hamiltonian	$H_0=\frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial\mathbf{r}}\right)^2+V(\mathbf{r})$	$H_0=\frac{1}{2m}\left[-i\hbar\frac{\partial}{\partial\mathbf{r}}+e\mathbf{A}_0(\mathbf{r})\right]^2+V(\mathbf{r})$
Translation operators	$T(\mathbf{R})=e^{\mathbf{R}\cdot\partial/\partial\mathbf{r}}$	$\tilde{T}(\mathbf{R})=e^{ie/\hbar\int_0^{\mathbf{R}}d\mathbf{r}'\cdot\mathbf{A}_0(\mathbf{r}+\mathbf{r}')}e^{\mathbf{R}\cdot\partial/\partial\mathbf{r}}$
Number of plaquettes per unit cell	1 plaquette	q plaquettes
Range of **k** vector	One Brillouin zone	One magnetic Brillouin zone (one Brillouin zone divided by q)
Perturbing fields	$\mathbf{E},\mathbf{B}$	$\mathbf{E},\delta\mathbf{B}$
Velocity of electron	$\dot{\mathbf{r}}=\partial\mathscr{E}_n(\mathbf{k})/\hbar\partial\mathbf{k}$	$\dot{\mathbf{r}}=\partial E_n(\mathbf{k})/\hbar\partial\mathbf{k}-\dot{\mathbf{k}}\times\boldsymbol{\Omega}_n(\mathbf{k})$, $E_n(\mathbf{k})=\mathscr{E}_n^{\mathrm{mag}}(\mathbf{k})+(e/2m)\delta\mathbf{B}\cdot\mathbf{L}_n(\mathbf{k})$
Dynamics for **k**	$\hbar\dot{\mathbf{k}}=-e\mathbf{E}-e\dot{\mathbf{r}}\times\mathbf{B}$	$\hbar\dot{\mathbf{k}}=-e\mathbf{E}-e\dot{\mathbf{r}}\times\delta\mathbf{B}$
Quantization condition for cyclotron orbits	$\mathrm{Area}(C_m)=2\pi(m+\frac{1}{2})eB/\hbar$	$\mathrm{Area}(C_m)=2\pi\left(m+\frac{1}{2}-\frac{\Gamma(C_m)}{2\pi}\right)e\delta B/\hbar$

Chang and Niu, Phys. Rev. B53, 7010 (96)