Semiclassical dynamics of electrons or in Bloch states

Velocity of a Bloch electron is
\[ \vec{V}_{nk} = \frac{1}{\hbar} \hat{\nabla}_k E_n(\vec{k}) \]
(already proved)

Equation

"Semiclassical equation of motion"
\[ \hbar \dot{\vec{r}} = \vec{F}_{\text{field}} = -e \left( \vec{E} + \frac{\vec{V}_{nk} \times \vec{B}}{c} \right) \]

\[ \vec{E} = \text{electric field} \]

Justification of second equation: Basically, it often works.

Plausibility argument in presence of weak electric field \( \vec{E} = -\vec{\nabla} \phi \)

Then let us consider a "wave packet" built out of states near the Bloch vector \( \vec{k} \). Since this is a group of states, we can say that this packet is near the position \( \Delta r \), provided we don't violate the uncertainty principle \( \Delta k \Delta r \gtrsim 1 \).

At time \( t \), the energy of this packet is
\[ E_n(\vec{k}(t)) - e \Phi(\vec{r}(t)) \]
But we expect this to have no energy to be a constant of the motion, since the Hamiltonian is time-independent. Thus

\[ \frac{d}{dt} \left[ E_0 \left( \mathbf{r}(t) \right) - e \Phi(\mathbf{r}(t)) \right] = 0 \]

\[ = \frac{\partial}{\partial \mathbf{r}} E_0 \left( \mathbf{r} \right) - e \hat{\mathbf{r}} \cdot \nabla \Phi \]

\[ = \frac{\partial}{\partial \mathbf{r}} \mathbf{v} \left( \mathbf{r} \right) + e \hat{\mathbf{r}} \cdot \mathbf{E} \]

\[ = \frac{\partial}{\partial \mathbf{r}} \mathbf{v} \left( \mathbf{r} \right) + e \mathbf{v} \left( \mathbf{r} \right) \cdot \mathbf{E} = 0 \]

Thus, \( \frac{\partial}{\partial \mathbf{r}} \mathbf{r} = -e \mathbf{E} \) as claimed.

Also, we can say that this would be the natural form of Newton's second law, provided we interpret \( \frac{\partial}{\partial \mathbf{r}} \mathbf{r} \) as the momentum, which it is not.

Limitations:

- Selective field not too big - charge
- \( \mathbf{E}, \mathbf{H} \) not too big.

Discuss more later.

Consequences: quite simple and elegant, however.
First consequence: filled bands are inert.

We will not discuss detailed argument, except to say that, in presence of fields, \( k \) changes but electrons just move to different places in same band, so no current is produced.

Total electric current from a filled band is

\[
\bar{J} = \frac{1}{4\pi^3} \int \alpha^3 k \left( \frac{1}{\hbar} \right) \nabla_k E_k(r)
\]

1st zone

But \( E_k(r) \) is periodic in \( \bar{k} \)-space

so this integral vanishes.

Proof: If \( E_k(r) \) is periodic in the reciprocal lattice, it has a Fourier transform of the form

\[
E_n(\bar{k}) = \sum_{\bar{R}} a_{\bar{R}} e^{ik \cdot \bar{R}}
\]

where \( \bar{R} = \) vectors of the direct (Bravais) lattice (since recip. of the reciprocal lattice is the direct lattice).

Thus,

\[
\bar{J} = \frac{1}{4\pi^3} \int \alpha^3 k \sum_{\text{b.z.}} \frac{1}{\hbar} \nabla_k \sum_{\bar{R}} a_{\bar{R}} e^{ik \cdot \bar{R}}
\]

\[
= -\frac{e}{4\pi^3} \int \alpha^3 k \sum_{\text{b.z.}} \sum_{\bar{R}} \hat{n}_{\bar{R}} e^{ik \cdot \bar{R}}
\]

\[
= -\frac{e}{4\pi^3} \int \alpha^3 k \sum_{\text{b.z.}} \sum_{\bar{R}} \hat{n}_{\bar{R}} e^{ik \cdot \bar{R}}
\]
But \( \int d^3k e^{i \mathbf{k} \cdot \mathbf{R}} = 0 \) if \( \mathbf{R} \neq 0 \).

Proof

\[
\int_{B.Z.} d^3k e^{i \mathbf{k} \cdot \mathbf{R}} = \frac{1}{N} \sum_{\mathbf{R}} \int d^3k e^{i \mathbf{k} \cdot \mathbf{R}} = 0
\]

since this prim. cells in k-space is oscillating

Q.E.D.

Thus current from filled band vanishes.

Same is true for energy current (see A+M).

Thus filled bands are insulators

( Check periodic table to see that all insulators have even # of electrons per prim. cell.)

Holes \( \mathbf{J} = -\frac{e}{4\pi^2} \int d^3k \nabla_n f_n^0(k) \)

\[
= -\frac{e}{4\pi^2} \int d^3k \nabla_n f_n^0(k) + \frac{e}{4\pi^2} \int d^3k \nabla_n f_n^0(k)
\]

apparent charge \( +e \).
Semiclassical eqs. of motion:

\[ \frac{\mathbf{v}_k}{\hbar} = \frac{1}{\hbar} \mathbf{\nabla}_k E_n(\mathbf{r}) \]

\[ \hbar \mathbf{a}^2 = (-e) \left( \frac{\mathbf{v}_k}{\hbar} \times \mathbf{B} \right) \]

Gross current due to nearly full band

\[ \mathbf{J} = \frac{e}{\hbar 4 \pi^2} \int \frac{d^3 k}{\text{occ.}} \mathbf{V}_k E_n(\mathbf{r}) = \frac{e}{4 \pi^2 \hbar} \int d^3 k \nabla_k E_n(\mathbf{r}) \]

\[ \mathbf{E} = \frac{e}{4 \pi^2 \hbar} \int d^3 k \nabla_k E_n(\mathbf{r}) \]

Pure electric field: (dc elec. field)

\[ \frac{\mathbf{v}_k}{\hbar} = -e \mathbf{E} \]

\[ \mathbf{k}(t) = \mathbf{k}(0) - \frac{e \mathbf{E} t}{\hbar} \quad \mathbf{V}(t) = \mathbf{V} (\mathbf{k}(t)) \]

A couple of examples:

Behavior near band minimum: (say near \( k = 0 \))

\[ E(k) = E(0) + C k^2 \]

\[ \sqrt{E} = \frac{1}{\hbar} \mathbf{V}_k E = 2 C \mathbf{k}^2 \]

\[ \frac{\mathbf{k}}{\hbar} = \mathbf{k}(0) - \frac{e \mathbf{E} t}{\hbar} \]
"effective mass" $m_c$ by

$$C = \frac{\hbar^2}{2mc}.$$  

Then $\vec{V}_k = \frac{\hbar \vec{k}}{m_v c}$

$$\hbar \vec{k} = m_v \vec{V}_k = -e\vec{E},$$ just like classical

electron of mass $m_v$, charge $-e$.

Now consider an electron near the top of the

band.

Assume again that band maximum is isotropic

and located at $\vec{k}=0$. We write

$$E(\vec{k}) = E_0 - \frac{\hbar^2 \vec{k}^2}{2 m_v} \quad m_v = \text{another effective mass}.$$

$$\vec{V}_k = \frac{1}{\hbar} \frac{\hbar \vec{k} E(\vec{k})}{m_v} = -\frac{\hbar \vec{k}}{m_v}$$

Electrons behaves like particle of charge $-e$, mass $-m_v$.

since velocity in opposite direction to $\vec{k}$.

And in the presence of an electric field

$$\hbar \vec{k} = -e \vec{E} \quad \text{so we still have}$$

$$\vec{k}(t) = \vec{k}(0) - \frac{e \vec{E} t}{\hbar}.$$
holes at time $t=0$

\[ \vec{x} \]

Electrons go to left

$\leftarrow$ \[ \vec{e} \] \[ \rightarrow \] \[ \vec{v} \]

Holes also go to left.

In presence of field, holes go the same direction as
the electrons would have gone, had they occupied
the hole states.

So electrons acquire acceleration

Equation of motion for electron velocity is

\[
\vec{v}(t) = \vec{v}(0) - \frac{e}{m} \frac{\vec{E}}{t} \\
\vec{v}_R(t) = \vec{v}(0) + \left( -\frac{e}{m} \frac{\vec{E}}{t} \right) \left( -\frac{m}{e} \right) = \frac{e \vec{E}}{m v} + v_R(0)
\]

Finally, the current of the hole in this
state is just \( \left( \frac{e \vec{E}}{m v} \right) \cdot \vec{e} \)

Thus, to summarize, we can treat holes in
every respect as particles of charge \( e \)
mass \( m + m_v \).
Tensor effective mass:
\[ E(k) = E_0 + \frac{\hbar}{2} \sum_{i=1}^{3} \sum_{j=1}^{3} (k - k_0)_i (k - k_0)_j (M^{-1})_{ij} \]

for electrons
\[ = E_0 - \frac{\hbar}{2} \sum_{i=1}^{3} (k - k_0)_i (M^{-1})_{ii} \]

for hole bands.

(band maxima)

Acceleration equation near tensor band min
\[ \dot{\mathbf{k}} = -e \mathbf{E} \]

and \[ (\mathbf{\Omega}) = \frac{1}{\hbar} \left( \frac{\partial}{\partial k} \mathbf{E} \right) \]
\[ = \frac{1}{\hbar} \left( \frac{\hbar}{3} \sum_{j=1}^{3} (k - k_0)_j (M^{-1})_{ij} \right) \]
\[ = \frac{1}{\hbar} \sum_{j=1}^{3} (k - k_0)_j (M^{-1})_{ij} \quad \text{or} \quad \frac{1}{\hbar} \mathbf{\Omega} = \mathbf{\Omega} (k - k_0) \]

Rewrite in matrix notation as
\[ \frac{3}{\hbar} \mathbf{\Omega} = (M^{-1}) (k - k_0) \frac{\mathbf{E}}{\hbar} \]

or \( (k - k_0) = M \mathbf{\nu}/\hbar \)
\[ \mathbf{k} = \frac{M \mathbf{\nu}}{\hbar} = -e \left( \frac{\mathbf{E}}{\hbar} + \frac{\mathbf{v} \times \mathbf{B}}{c} \right) \]

if \( k_0 = \) band min. \( = 0 \)
or in general
\[ M \overset{\partial}{\nu} = -e \left( \overset{\partial}{E} + \frac{\overset{\partial}{\nu} \times \overset{\partial}{B}}{c} \right) \] (for elec)

For holes it is
\[ M \overset{\partial}{\nu} = +e \left( \overset{\partial}{E} + \frac{\overset{\partial}{\nu} \times \overset{\partial}{B}}{c} \right) \]

Very handy.

Semiclassical motion in a uniform dc magnetic field

Here we have
\[ \overset{\partial}{p} = \overset{\partial}{\nu} = \frac{1}{\hbar} \nabla_{\nu} E(\nu) \]
\[ \overset{\partial}{p} = -e \frac{\overset{\partial}{\nu} \times \overset{\partial}{B}}{c} \] (for electron)

Corresponding

General features:

In \( \nu \) space
\[ \frac{d\nu}{dt} \perp \overset{\partial}{H} \]
and\[ \frac{d\overset{\partial}{\nu}}{dt} \perp \overset{\partial}{\nu} \]

Thus velocity in \( \nu \) space \( \perp \) to \( \overset{\partial}{H} \)
and \( \perp \) to \( \overset{\partial}{\nu} = \text{velocity in real space} \)

Let the orbit be as shown on next page.
Since \( \mathbf{r} \perp \mathbf{\hat{H}} \), the motion lies in the plane \( \perp \mathbf{\hat{H}} \). \( \mathbf{j}_k \cdot \mathbf{\hat{H}} = 0 \).

Also \( \frac{d\mathbf{j}_k}{dt} \perp \mathbf{\hat{v}}_k \)

But \( \mathbf{\hat{v}}_k = \frac{1}{\hbar} \mathbf{\hat{E}}_n(k) \)

So \( \mathbf{\hat{v}}_k \) is normal to surface of const. energy.

Therefore, \( \mathbf{j}_k \) lies in the plane of const. energy (just as in classical physics).

 Orbit lies in intersection of plane \( \mathbf{j}_k \mathbf{\hat{H}} = \text{const} \) with surfaces of const. energy.

Simple example: band minimum:

\[
E = E_0 + \frac{\hbar^2 k^2}{2m_c}
\]
\[ \hat{t} \hat{z} = -\frac{e}{c} \vec{J}_k \times \hat{H} \]
\[ = -\frac{e}{c} \frac{\hat{t} \hat{z} \hat{k}}{m_0} \times \hat{H} \]
\[ or \ \hat{k} = -\frac{e}{m_0} \hat{t} \hat{z} \hat{k} = -\frac{e}{m_0} \left[ \begin{array}{c} \hat{x} \\ \hat{y} \\ \hat{z} \end{array} \right] \]

If \( \hat{H} = H \hat{z} \)
\[ \hat{k} = -\frac{eH}{m_0} \hat{k}_y \]
\[ \hat{k}_y = +\frac{eH}{m_0} \hat{k}_x \]

\[ \hat{k}_x \hat{y} + \hat{k}_y \hat{k}_x = 0 \]
\[ \hat{k}_z = \text{const.} \]
\[ \hat{k}_x = -\omega_0^2 \hat{k}_x \] where \( \omega_0 = \frac{eH}{m_0} \)
\[ \hat{k}_x = k_0 \cos(\omega_0 t + \phi_0) \]
\[ \hat{k}_y = -\frac{i}{\omega_0} \hat{k}_x = k_0 \sin(\omega_0 t + \phi_0) \]

Circular orbit in \( k \) space.
Open and closed orbits:

Sometimes, orbits don't close ⇒ takes an infinite amount of time for orbit to return home.

Depends on energy surface.

E.g. motion on cylindrical energy surface.

Suppose

\[ E(k) = \frac{k_y^2 + k_x^2}{2m^*} \]

Surfaces of const. energy are cylinders

Now consider.

\[ \dot{\mathbf{p}}_k = -\frac{\mathbf{E}}{m^*} \times \mathbf{H} \]

\[ \dot{\mathbf{v}}_k = \frac{1}{\hbar} \frac{\partial}{\partial k} E(k) = \frac{\hbar}{m^*} \left( k_x \hat{y} + k_y \hat{z} \right) \]

Let \( \mathbf{H} = H \hat{z} \cos \theta + H \hat{x} \sin \theta \)

\[ \dot{v}_k \times \mathbf{H} = \begin{bmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{\hbar k_x}{m^*} & \frac{\hbar k_y}{m^*} & 0 \\ H \sin \theta & 0 & H \cos \theta \end{bmatrix} = \begin{bmatrix} \frac{\hbar k_x}{m^*} H \cos \theta \\ \frac{\hbar k_y}{m^*} H \cos \theta \\ -\frac{\hbar k_y}{m^*} \sin \theta \end{bmatrix} \]
Thus we have:

\[ \dot{k}_x = -\frac{eH}{m*c} \cos \theta \]  
\[ \dot{k}_y = +\frac{eH}{m*c} \cos \theta \]  
\[ \dot{k}_z = -\frac{eH}{m*c} \sin \theta H \]  

(1) and (2) can be combined to give

\[ \dot{k}_x = -\left(\frac{eH}{m*c} \cos \theta \right) k_x \]  
\[ \dot{k}_y = -\left(\frac{eH}{m*c} \cos \theta \right) k_y \]  

**Quickly Solution:**

\[ k_x(t) = k_0 \cos (\omega c t + \phi_0) \]  
\[ k_y(t) = k_0 \sin (\omega c t + \phi_0) \]

where \( \omega c = \frac{eH \cos \theta}{m*c} \)

Electro cyclotron freq \( \omega \) to \( H_z \).

\[ \dot{k}_z = -\frac{eH}{m*c} \sin \theta k_y \]  
\[ = -\frac{eH}{m*c} \sin \theta k_0 \sin (\omega c t + \phi_0) \]
So \( k_2 = \frac{eH}{m^2c} \sin \theta k_0 \frac{\cos(\omega_c t + \phi_0)}{\omega_c} \) 

\[ = k_0 + eH \cos(\frac{eH}{mc} \cos \theta) \] using \( \omega_c = \frac{eH}{mc} \cos \theta \)

**Solution:** elliptical orbit.

**Geometrically**

**Special case:** \( \theta = \frac{\pi}{2} \) then \( k_x = k_y = 0 \)

\( k_y = \text{const.} \)

\( k_z = -\frac{e k_y}{m^2 c} \) \( \text{(radial)} \)

\( k_z = \frac{e k_y}{m^2 c} Ht \) (open orbit)

Orbit when \( H \) has is

oriented \( \parallel \) to const.-energy surface is a circle
Motion in real space (for cylindrical orbit)

we have \( v_x = \frac{\hbar k_x}{mc} \) \( v_y = \frac{\hbar k_y}{mc} \)

\( v_z = 0 \)

So for elliptical orbits

\[ v_x = \frac{\hbar k_0}{mc} \cos(w_c t + \phi_0) \]

\[ v_y = \frac{\hbar k_0}{mc} \sin(w_c t + \phi_0) \]

\[ x = \frac{\hbar k_0}{mc w_c} \sin(w_c t + \phi_0) + x_0 \]

\[ y = -\frac{\hbar k_0}{mc w_c} \cos(w_c t + \phi_0) + y_0 \]

\[ z = z_0 \]

Circular motion in real space

For open orbit \( (H \perp \hat{z}) \)

\[ k_y = -\text{const.} \quad \text{so} \quad v_y = \frac{\hbar k_y}{mc} = \text{const.} \]

\[ k_x = \text{const.} \quad \text{so} \quad v_x = \text{const.} \]

\[ k_2 = -\frac{\epsilon k_y H}{mc} \quad \text{But} \quad v_2 = \frac{\hbar}{c} \nabla_k E \]

\( = 0 \)

Period of the orbit (if orbit is closed)

\( = \text{time for an electron to traverse the orbit} \)

There is a formula for the period in terms of the area of the orbit [See A+M, eq. (12.42)]
Electrons in combined electric and magnetic fields

Let \( \hbar k^2 = -e\left( \vec{E} + \frac{\vec{v} \times \vec{H}}{c} \right) \) (for electrons; neglecting any scattering).

Then we have

\[
\vec{V}_k = \frac{1}{\hbar} \vec{V}_k E(k)
\]

Suppose \( E(k) = \frac{\hbar^2}{2} \sum_{ij} k_i (M^{-1})_{ij} k_j \).

\[
(\vec{V}_k)_i = \frac{1}{\hbar} \frac{\partial E(k)}{\partial k^*_i} = \hbar \sum_j (M^{-1})_{ij} k_j
\]

Thus \( k_j = \frac{1}{\hbar} \sum_j M_{ij} v_j \) and we have

\[
\sum_j M_{ij} v_j = -e\left( \vec{E} + \frac{\vec{v} \times \vec{H}}{c} \right)_i
\]

or \( \vec{M} \vec{v} = -e\left( \vec{E} + \frac{\vec{v} \times \vec{H}}{c} \right) \).

Now add electronic damping of the form

\[
-\frac{\vec{M} \vec{v}}{\tau}
\]

Then in steady state, we get \( \vec{M} \vec{v} = -e \tau \left( \vec{E} + \frac{\vec{v} \times \vec{H}}{c} \right) \).
\[ \alpha \bar{v} = -(M^{-1})e \tau \left( \bar{E} + \frac{\nabla \times \bar{H}}{c} \right) \]

\[ \bar{J} = -ne \bar{v} = \frac{1}{4} (M^{-1}) ne^2 \tau \left( \bar{E} + \frac{\nabla \times \bar{H}}{c} \right) \]

\[ \sigma = (M^{-1}) ne^2 \tau \quad \text{if} \quad \bar{H} = 0 \]

**Tensile (anisotropic) conductivity.**

If we have a magnetic field as well as an electric field we get

\[ \bar{J} = (M^{-1}) ne^2 \tau \left( \bar{E} + \frac{\nabla \times \bar{H}}{c} \right) \]

But \( \bar{v} = -\frac{\bar{J}}{ne} \) so

\[ \bar{J} = (M^{-1}) ne^2 \tau \left( \bar{E} - \frac{\bar{J}}{ne} \frac{\nabla \times \bar{H}}{c} \right) \]

or \( \bar{E} = -\frac{\bar{J} \times \bar{H}}{ne c} = \frac{M \bar{J}}{ne^2 \tau} \quad M = \text{matrix} \)

\[ \bar{E} = \frac{M \bar{J}}{ne^2 \tau} + \frac{1}{ne c} \frac{\bar{J} \times \bar{H}}{c} \]

or \( \bar{E} = \frac{\bar{J} \times \bar{H}}{ne c} + \frac{1}{ne c} \bar{J} \times \bar{H} \)
Special case: isotropic band:

\[ \mathbf{E} = \frac{mc}{ne^2c} \mathbf{p} + \frac{1}{2} \mathbf{J} \times \mathbf{H} \]

If \( \mathbf{H} \parallel \mathbf{\hat{z}} \), we get

\[
\begin{pmatrix}
\varepsilon_x \\
\varepsilon_y \\
\varepsilon_z 
\end{pmatrix} = \begin{pmatrix}
\mathbf{p} & -R_H & 0 \\
+R_H & \mathbf{p} & 0 \\
0 & 0 & \mathbf{p}
\end{pmatrix}
\begin{pmatrix}
J_x \\
J_y \\
J_z
\end{pmatrix}
\]

where

\[ p = \frac{\mu m c}{ne^2c} \]

\[ R_H = -\frac{1}{nec} \]

For hole bands, \( R_H = \frac{1}{nec} \)