Semiclassical approx for dynamics of electrons in periodic potential

Same idea as we used in Sommerfeld model.

Imagine constructing wave packets of Bloch states to localize electrons. To each electron assign position $\vec{r}$, crystal momentum $\vec{k}$, band index $n$. Semiclassical equations of motion tell how $\vec{r}$, $\vec{k}$, $n$ evolve in time in presence of applied $\vec{E}$ and $\vec{H}$ fields, in between collisions. Then a relaxation approximation will be used to average over effect of collisions, modify semiclassical equations to include average effect of collisions.

*) Wave packet approx good only when applied fields vary slowly over dimensions of size of primitive cell.
   
   *(localize crystal momentum well on scale of 1st BZ
   \Rightarrow wave packet in $k$-space extends over a few
   primitive cells)

*) Quantum effects are handled entirely through the band structure $E_n(\vec{k})$ which we take as given functions.
   
   These describe how include all effects of quantum mechanics on periodic potential (which varies rapidly
   on scale of primitive cell) is taken into account
   
   in fully quantum mechanical way by each of
   the Bloch states $E_n(\vec{k})$. External slowly varying
   fields are treated in semi-classical manner
Collisions can not be with static periodic cons. There effect already included in $\varepsilon_n(\mathbf{k})$.

In the absence of collisions, $\mathbf{N}, \mathbf{\bar{F}}, \mathbf{\bar{F}}$ evolve as

1) Bond index is constant. No interband transitions.
   Good when field strengths are not too large.
   $eE_a \ll \left[ E_{\text{gap}}(\mathbf{k}) \right]^2 / eF$.
   
   *electric breakdown* when fails.

2) $H_\mathbf{w} \ll \left[ E_{\text{gap}}(\mathbf{k}) \right]^2 / eF$.
   
   *magnetic breakdown* when fails.

$i)$ always true in metals, can fail in insulators + semiconductors.

ii) possible in strong $H$ fields.

Also need

\[ H_\mathbf{w} \ll E_{\text{gap}} - \text{photon cannot excite to higher band} \]

\[ \mathbf{N} \gg \mathbf{a} \quad \text{slowly varying fields} \]

2) $\mathbf{N}$ and $\mathbf{\bar{F}}$ evolve just like classical particle.
   
   If we took $\mathbf{\bar{F}}$ as ordinary momentum (which *is not*)

\[
\mathbf{N} = \mathbf{\bar{F}}_n(\mathbf{k}) = \frac{1}{m} \frac{\partial \varepsilon_n(\mathbf{k})}{\partial \mathbf{k}}
\]

\[
\mathbf{\bar{F}} = - e \left[ \mathbf{E}(\mathbf{k}, t) + \frac{1}{c} \mathbf{\bar{F}}_n(\mathbf{k}) \times \mathbf{H}(\mathbf{k}, t) \right]
\]

3) States $\mathbf{k}$ and $\mathbf{k} + \mathbf{R}$ are equivalent when $\mathbf{R}$ is reciprocal lattice vector.

In equilibrium, states occupied with Fermi function

\[
\tilde{f}(\varepsilon_n(\mathbf{k})) = \frac{1}{\exp(\varepsilon_n(\mathbf{k}) - \mu) / kT + 1}
\]

*) $\hbar \mathbf{k}$ is not total momentum. $\mathbf{p}$ is given by total force.
   \[ \mathbf{f} = \mathbf{H} \]
reasons to believe semi-classical equations: For more see references given in text

\[ \overrightarrow{\varepsilon} = \overrightarrow{\nabla} \phi \] is just definition of potential

+ we derived earlier that \( \overrightarrow{\nabla} \phi = \frac{i}{\hbar} \overrightarrow{\nabla} \phi \)

We show that equation for \( \overrightarrow{\varepsilon} \) is consistent with energy conservation for motion in electric field, \( \overrightarrow{\varepsilon} = -\overrightarrow{\nabla} \phi \) electrostatic expectation \( \varepsilon_n(\overrightarrow{\varepsilon}(t)) = -e \phi(\overrightarrow{\varepsilon}(t)) \) to be constant: bond energy + electrostatic energy = constant

\[ \frac{d}{dt} \left[ \varepsilon_n(\overrightarrow{\varepsilon}(t)) - e \phi(\overrightarrow{\varepsilon}(t)) \right] = 0 \]

\[ \frac{d\varepsilon_n}{dt} + \frac{d\overrightarrow{\varepsilon}}{dt} = 0 \]

or \( \frac{d\vec{\varepsilon}}{dt} = -\varepsilon \cdot \frac{d\vec{E}}{dt} \) consistent *classic* equation

true when \( \frac{d\vec{\varepsilon}}{dt} = -\varepsilon \frac{d\vec{E}}{dt} \) though when \( \frac{d}{dt} = 0 \)

Could also have piece \( \frac{d\overrightarrow{\varepsilon}}{dt} = -\varepsilon \overrightarrow{\nabla} \times \overrightarrow{B} \)

although we haven't shown that only possible such piece is \( -\frac{e}{c} \overrightarrow{\nabla} \times \overrightarrow{B} \)

**Consequences:** Filled bands do not contribute to transport properties.

electric current \( \overrightarrow{j} = -e \int \frac{d^3 k}{4\pi^3} \frac{1}{i} \frac{2\varepsilon}{\hbar} \)

thermal current \( \overrightarrow{j}_T = \frac{\hbar}{2e} \int \frac{d^3 k}{4\pi^3} \frac{\varepsilon}{\hbar} \frac{2\varepsilon}{\hbar} \overrightarrow{B} \)
\( \int = \int_0^\infty \) for filled bands

Proof:

If crystal has inversion symmetry \( \varepsilon(k) = \varepsilon(-k) \),

\[ \varepsilon^2(k) = \varepsilon^2(-k) \Rightarrow \frac{d}{dk} \varepsilon(k) = -\frac{d}{dk} \varepsilon(-k) \]

so there are odd functions

so \( \int \) over 1st BZ vanishes.

Actually this is true more generally, even if no inversion symmetry. Gradient of any periodic function always integrates to zero over unit cell. See text

\( \varepsilon(k) \) is periodic in transition by \( \hat{k} \)

Therefore current is carried only by partially full bands.

Conduction electrons in Drude model should be just electrons in partially full bands.

Motion in DC \( \vec{E} \) field:

\[ \vec{r}(t) = \vec{r}(0) - \vec{E} t \]

in general \( \vec{v} \neq \vec{r} \)

So only when \( \vec{r} \) is near band minimum \( \vec{v} \approx \vec{r} \).

Near band max (near zone edge) \( \vec{v} \approx -\vec{r} \).

As electron approaches zone edge, it slows down and rods in reverse.
If electrons could travel distances in k-space larger than BZ size n between collisions, then a DC \( \mathbf{E} \) field would produce oscillating current! However, collisions will spoil this effect. Electron in general will have only small changes in \( \mathbf{k} \) before it gets scattered and its \( \mathbf{k} \) randomized.

However the fact that \( \mathbf{k} \approx \mathbf{k}_0 \) near band max, produces the phenomenon of holes — metal can behave as if it had positive carriers.

Consider 1-d example. Near band minimum at \( \mathbf{k}_0 \), we can expand \( \mathcal{E}(\mathbf{k}) = \mathcal{E}(\mathbf{k}_0) + \frac{\mathcal{E}''(\mathbf{k}_0)}{2} (\mathbf{k} - \mathbf{k}_0)^2 \)

where \( \mathcal{E}''(\mathbf{k}_0) \equiv \frac{\hbar^2}{2m^*} > 0 \)

we call \( m^* \) the effective mass of electrons at band minimum.

Then semiclassical equations are:

\[
\frac{\hbar^2}{2m^*} \frac{d^2 \mathbf{k}}{dt^2} = \mathbf{\nabla}_\mathbf{k} \mathcal{E}(\mathbf{k}) = \frac{1}{\hbar} \frac{d\mathcal{E}}{d\mathbf{k}} \approx \frac{1}{\hbar} \frac{d}{d\mathbf{k}} \left( \frac{\hbar^2}{2m^*} (\mathbf{k} - \mathbf{k}_0)^2 \right) \\
\Rightarrow \mathbf{v} = \frac{\mathbf{k}}{m^*} \text{ so just like classical particles of mass } m^*, \text{ charge } e
\]

\[
\frac{\hbar}{m^*} \frac{d}{dt} \mathbf{k} = -e [\mathbf{E} + \frac{1}{c} \mathbf{v} \times \mathbf{H}] \\
\Rightarrow m^* \mathbf{v} = -e \left[ \mathbf{E} + \frac{1}{c} \mathbf{v} \times \mathbf{H} \right]
\]

So electrons near band minimum behave like classical electron of charge \(-e\) and mass \( m^* = \frac{\hbar^2}{d^2 \mathcal{E}} \).
But for an electron near top of band, we expand

$$\varepsilon(k) = \varepsilon(k_1) + \frac{\hbar^2}{2m^*} (k_1 \cdot \nabla_k)(k - k_1)^2$$

where we define $\frac{\hbar^2}{2m^*} = -\frac{\hbar^2}{m_h}$, where $m_h^* > 0$.

Now $\nabla_k \varepsilon = \frac{\hbar^2}{m_h^*} \Rightarrow m_h^* \nabla = -\frac{\hbar^2}{m_h} k$

Thus, $\nabla k = -e \left[ \mathbf{E} + \frac{2}{c} \mathbf{v} \times \mathbf{H} \right] \Rightarrow m_h^* \nabla_\mathbf{v} = +e \left[ \mathbf{E} + \frac{2}{c} \mathbf{v} \times \mathbf{H} \right]$

electron near top of band behaves like classical particle of mass $m_h^* = -\frac{\hbar^2}{(\hbar^2/2m^*)}$ and charge $+e - e$ like a positive charge.

This is referred to as a hole.

In three dimensions, if max and min of band occur at point of cubic symmetry, we still can expand

$$\varepsilon(\mathbf{k}) = \varepsilon(\mathbf{k}_0) + \frac{\hbar^2}{2m^*} (\mathbf{k} - \mathbf{k}_0)^2$$

to define effective mass. However if no symmetry, then we need to define effective mass tensor

$$\mathbf{M}^{-1}_{ij} = 0$$

$$\mathbf{M}^{-1}_{ij} = \pm \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon(k)}{\partial k_i \partial k_j} \bigg|_{\mathbf{k} = \mathbf{k}_0}$$

Equation of motion will be

$$\mathbf{M} \cdot \mathbf{\dot{v}} = -e \left[ \mathbf{E} + \frac{2}{c} \mathbf{v} \times \mathbf{H} \right]$$
in most generality, away from max or min, can write

\[ \frac{\partial \mathbf{r}}{\partial t} = \frac{1}{\hbar} \left( \frac{\partial}{\partial \mathbf{k}} \mathbf{E}(\mathbf{k}) \right) = \frac{1}{\hbar} \frac{\partial \mathbf{E}(\mathbf{k})}{\partial \mathbf{k}} \frac{d\mathbf{k}}{dt} \]

define

\[ M^{-1}(k) = \pm \frac{1}{\hbar^2} \frac{\partial \mathbf{E}(\mathbf{k})}{\partial \mathbf{k}} \]

\[ M^{\ast}(k) \mathbf{\hat{r}} = \pm e \left[ \mathbf{E} + \frac{\mathbf{v}(k) \times \mathbf{H}}{e} \right] \]

\[ \text{taken only if \mathbf{E} \cdot \mathbf{k} = 0} \]

So states at near top of band

behave like \((+)\) particles of mass \(m^*\)

To compute current in a partially full band, note

\[ \mathbf{j} = -e \int \frac{d^3k}{4\pi^3} \mathbf{v}_n(k) = -e \begin{bmatrix} \int \frac{d^3k}{4\pi^3} v_n(k) \\ \int \frac{d^3k}{4\pi^3} \mathbf{v}_n(k) \end{bmatrix} \]

occupied states

\[ = +e \int \frac{d^3k}{4\pi^3} \mathbf{v}_n(k) \quad \text{since} \quad \int \mathbf{v} + \int \mathbf{v} = 0 \]

occupied unoccupied

So we can regard electric current as due to either the

occupied electric states (with

So current due to selections in occupied states is the same

as current that would be if these levels were

empty and the unoccupied states were filled

with particles of charge \(+e\).
Note: unoccupied states evolve under same equations of motion as occupied states - as if they were filled with electrons of charge $-e$.

But unoccupied states generally lie near top of band, so they evolve in time like classical particles of charge $+e$!

For a given band, we can choose to describe it in either the electron or hole picture, but not both.

For a band mostly empty

For a band mostly full

convenient to describe as classical particles (holes) of charge $+e$ and mass

$\text{mass } m^* = -\frac{\hbar^2}{(d^2E/dk^2)_{	ext{min}}}$