<u>Semi classical approx</u> 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, <u>inbetween collisions</u>. 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 1^{st} BZ
⇒ wave packet in r-space extends over a few primitive cells)

*) Quantum effects are handled entirely through the band structure $\varepsilon_n(\vec{k})$ which we take as given functions. ~~[illegible] describes [illegible] includes all effects of quantum mechanics or~~ Periodic potential (which varies rapidly on scale of primitive cell) is taken into account in fully quantum mechanical way by use of the Bloch states $\varepsilon_n(\vec{k})$. External slowly varying fields are treated in semi classical way.

* Collisions can not be with static periodic ions. Their effect all ready included in $\varepsilon_n(\vec{k})$.

In the absence of collisions, n, $\vec{k}$, $\vec{r}$ evolve as

1) band index is constant. No interband transitions
Good when field strengths are not too large

see Apendix J) i) $eEa \ll [\varepsilon_{gap}(\vec{k})]^2/\varepsilon_F$ "electric breakdown" when fails

ii) $\hbar\omega_c \ll [\varepsilon_{gap}(\vec{k})]^2/\varepsilon_F$ "magnetic breakthrough" when fails

i) ~~usually~~ always true in metals, can fail in insulators + semiconductors

ii) possible in strong $\vec{H}$ fields

Also need $\begin{cases} \hbar\omega \ll \varepsilon_{gap} & \text{— photon cannot excite to higher band} \\ \lambda \gg a & \text{slowly varying fields} \end{cases}$

2) $\vec{r}$ and $\vec{k}$ evolve just like classical particle if we took $\hbar\vec{k}$ as ordinary momentum (which it is not)

$$\dot{\vec{r}} = \vec{v}_n(\vec{k}) = \frac{1}{\hbar}\frac{\partial\varepsilon_n(\vec{k})}{\partial\vec{k}}$$

$$\hbar\dot{\vec{k}} = -e\left[\vec{E}(\vec{r},t) + \frac{1}{c}\vec{v}_n(\vec{k}) \times \vec{H}(\vec{r},t)\right]$$

3) States $\vec{k}$ and $\vec{k}+\vec{K}$ are equivalent when $\vec{K}$ is reciprocal lattice vector.
In equilibrium, states occupied with fermi function $f(\varepsilon_n(\vec{k})) = \dfrac{1}{e^{(\varepsilon_n(\vec{k})-\mu)/kT}+1}$

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*) $\hbar\vec{k}$ is not total momentum. $\dot{\vec{p}}$ is given by total force (includes ion potential) $\hbar\dot{\vec{k}}$ is given by applied force only.

<u>Reasons to</u> believe Semi classical equations: For more see references given in text

$\dot{\vec{r}} = \vec{v}_n(k)$ is just definition of velocity + we derived earlier that $\vec{v}_n(\vec{k}) = \frac{1}{\hbar}\frac{\partial \mathcal{E}_n}{\partial \vec{k}}$

We show that equ for $\dot{\vec{k}}$ is consistent with energy conservation
For motion in ~~the~~ electric field $\vec{E} = -\vec{\nabla}\phi$ ~ electrostatic potential
expect $\mathcal{E}_n(\vec{k}(t)) - e\phi(\vec{r}(t))$ to be constant : band energy + electrostatic energy = constant

$$\Rightarrow \quad \frac{d}{dt}\left[\mathcal{E}_n(\vec{k}(t)) - e\phi(\vec{r}(t))\right] = 0$$

$$\Rightarrow \quad \frac{d\mathcal{E}_n}{d\vec{k}} \cdot \frac{d\vec{k}}{dt} - e\vec{\nabla}\phi \cdot \frac{d\vec{r}}{dt} = 0$$

or $\hbar\vec{v}\cdot\dot{\vec{k}} = -\vec{v}\cdot e\vec{E}$ plug in $\hbar\dot{\vec{k}}$ = semi class equation $\Rightarrow$ consistent

~~cons~~ true when $\hbar\dot{\vec{k}} = -e\vec{E}$ ~~although~~ when $\vec{H}=0$
Could also have piece $\perp$ to ~~$\frac{e}{c}\vec{v}_n(k)\times\vec{H}$~~ $\vec{v}$
although we haven't shown that only possible such piece is $-\frac{e}{c}\vec{v}_n \times \vec{H}$

<u>Consequences</u>: Filled bands do not contribute to transport properties.

electric current $\vec{j} = -e\int_{BZ}\frac{d^3k}{4\pi^3}\frac{1}{\hbar}\frac{\partial \mathcal{E}}{\partial \vec{k}}$

thermal current $j_{\mathcal{E}} = \int_{BZ}\frac{d^3k}{4\pi^3}\frac{\mathcal{E}}{\hbar}\frac{\partial\mathcal{E}}{\partial\vec{k}} = \frac{1}{2}\int\frac{d^3k}{4\pi^3}\frac{1}{\hbar}\frac{\partial}{\partial\vec{k}}(\mathcal{E}^2$

$\vec{j} = \vec{j}_\varepsilon = 0$ for filled bands

Proof:

If crystal has inversion symmetry $\varepsilon(k) = \varepsilon(-k)$,
$\varepsilon^2(k) = \varepsilon^2(-k) \Rightarrow \frac{d}{dk}\varepsilon(k) = -\frac{d}{dk}\varepsilon(-k)$
$\frac{d}{dk}\varepsilon^2(k) = -\frac{d}{dk}\varepsilon^2(-k)$ so these are odd functions

so $\int$ over 1st BZ vanishes.

Actually ~~proof~~ this is true more generally, even if no inversion symmetry. Gradient of <u>any</u> periodic function always integrates to zero over unit cell. See text
$\varepsilon(k)$ is periodic in translation by $\vec{K}$

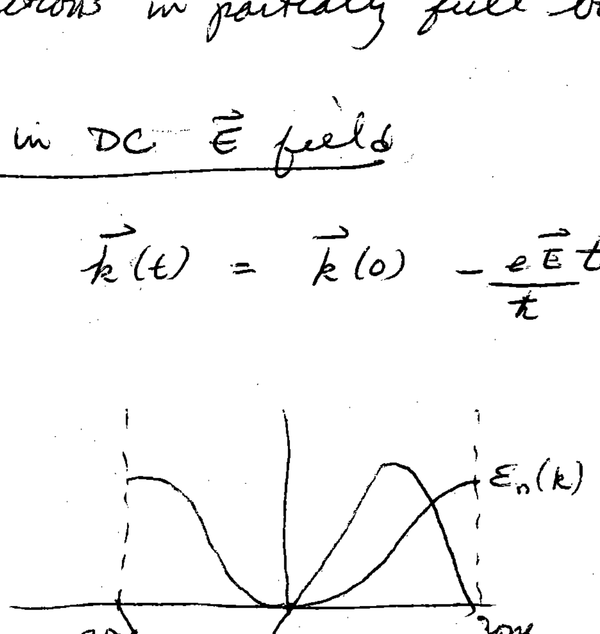
Therefore current is carried only by <u>partially</u> full bands. ~~density of~~ Conduction electrons in Drude model should be just electrons in partially full bands.

<u>Motion in DC $\vec{E}$ field</u>

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

in general $\dot{\vec{v}} \not\propto \dot{\vec{k}}$

Since



so only when $\vec{k}$ is ~~in center of~~ near band ~~to~~ minimum is $\dot{\vec{v}} \propto \dot{\vec{k}}$. Near band max (near zone edge) $\dot{\vec{v}} \propto -\dot{\vec{k}}$
As electron approaches zone edge, it slows down and goes in reverse
due to scattering at Bragg plane