Semiclassical Model of Electron Dynamics

I.

$$\frac{-\hbar^2}{2m}\left\{\left(\frac{\nabla}{i}+k\right)^2+U(x)\right\}u_{nk}(x)=\mathcal{E}_{nk}u_{nk}(x)$$

$$\frac{-\hbar^2}{2m}\left\{\left(\frac{\nabla}{i}+k+q\right)^2+U(x)\right\}u_{nk+q}(x)=\mathcal{E}_{nk+q}\,u_{nk+q}(x)$$

$$H_{k+q}=H_k+\underbrace{\frac{\hbar^2}{m}q\cdot\left(\frac{\nabla}{i}+k\right)}_{\text{linear order term}}+\frac{\hbar^2q^2}{2m}$$

$$\rightarrow \sum_i \frac{\partial \mathcal{E}_n}{\partial k_i}q_i=\sum_i\int d^3r\, u^*_{nk}(r)\frac{\hbar^2}{m}\left(\frac{\nabla}{i}+k\right)_i q_i\, u_{nk}(r)$$

$$\rightarrow \vec{\nabla}_k\mathcal{E}_n=\int d^3r\, u^*_{nk}(r)\frac{\hbar^2}{m}\left(\frac{\vec{\nabla}}{i}+k\right)u_{nk}(r)$$

$$=\int d^3r\,\psi^*_{nk}(r)\frac{\hbar^2}{m}\left(\frac{\vec{\nabla}}{i}\right)\psi_{nk}(r)$$

But
$$\frac{dr}{dt}=\frac{1}{i\hbar}[r,H]=\frac{1}{i\hbar}\left[r,\frac{-\nabla^2\hbar^2}{2m}\right]$$

$$=\frac{1}{i\hbar}\left(\frac{-\hbar^2}{2m}\right)\left\{\left(x\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial x^2}x\right)\hat{x}+\cdots\right\}$$

$$=\frac{1}{i\hbar}\left(\frac{-\hbar^2}{2m}\right)\left\{\left(x\frac{\partial^2}{\partial x^2}-\frac{\partial}{\partial x}x\frac{\partial}{\partial x}+\frac{\partial}{\partial x}x\frac{\partial}{\partial x}-\frac{\partial^2}{\partial x^2}x\right)\hat{x}+\cdots\right.$$

$$=\frac{1}{i\hbar}\left(\frac{-\hbar^2}{2m}\right)\left\{\left(\frac{-\partial}{\partial x}-\frac{\partial}{\partial x}\right)\hat{x}+\cdots\right\}$$

$$=\frac{\hbar}{m}\frac{\vec{\nabla}}{i}$$

$$\rightarrow \boxed{v_n=\frac{1}{\hbar}\nabla_k\mathcal{E}_n}$$

	Sommerfeld	Bloch
Quantum Numbers	$\vec{k}$	$n, \vec{k}$
Range	$\vec{k}$ consistent w/ P.B.C.	$\vec{k} \in 1^{st}$ B.Z.
Energy	$\mathcal{E}(\vec{k})$	$\mathcal{E}_n(\vec{k}) = \mathcal{E}_n(\vec{k}+\vec{K})$
Velocity	$v = \frac{\hbar k}{m} = \frac{1}{\hbar}\frac{\partial \mathcal{E}}{\partial k}$	$v_n(k) = \frac{1}{\hbar}\frac{\partial \mathcal{E}_n}{\partial k}$
Wave Fnt.	$\psi_k(r) = \frac{e^{ik\cdot r}}{\sqrt{V}}$	$\psi_{nk}(r) = e^{ik\cdot r} u_{nk}(r)$ $u_{nk}(r+R) = u_{nk}(r)$
Eqs. of Motion	$\dot{r} = v$ $\hbar\dot{k} = -e(E + \frac{v}{c} \times H)$	$\dot{r} = v_n$ $\hbar\dot{k} = -e(E + \frac{v_n}{c} \times H)$

II. $\vec{j} = (-e)\int \frac{d^3k}{4\pi^3} \frac{1}{\hbar} \vec{\nabla}_k \varepsilon$

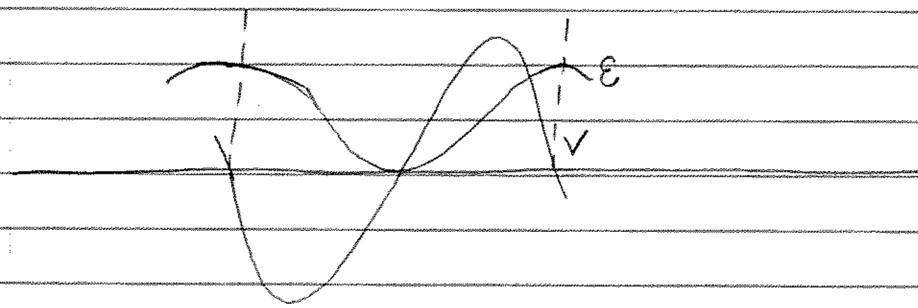
$$\vec{j}_\varepsilon = \int \frac{d^3k}{4\pi^3} \varepsilon(k) \frac{1}{\hbar} \vec{\nabla}_k \varepsilon = \frac{1}{2}\int \frac{d^3k}{4\pi^3} \frac{1}{\hbar} \vec{\nabla}_k (\varepsilon)^2$$

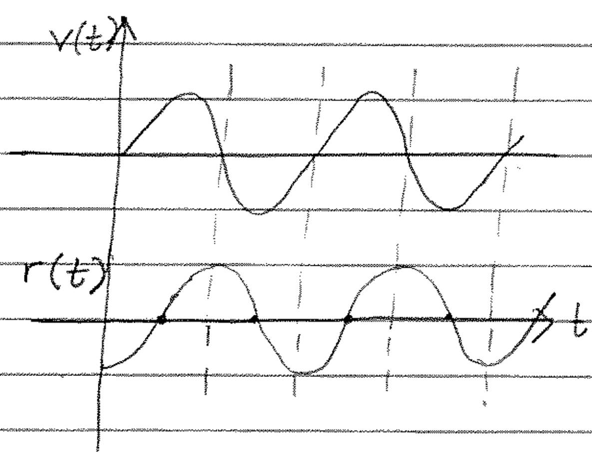
"Liouville's Thm." – Take a filled band. The "phase space" density, $d^3r\, d^3k = 1/4\pi^3$. The time evolution of ρ is determined by $\rho(r(t), k(t))$, which is first order in time: $v \cdot \nabla_r \rho + F/\hbar \cdot \nabla_k \rho$. Since both $\nabla_r \rho$ & $\nabla_k \rho$ are zero at $t=0$, ρ remains constant.

III. Motion is an applied DC field

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

$$v(k(t)) = v\left(k(0) - \frac{eEt}{\hbar}\right)$$





$\int \sin(t)\, dt = -\cos(t)$

IV. Holes:

A. $$j = (-e)\int_{occ.} \frac{d^3k}{4\pi^3}\, v(k)$$

$$0 = \int \frac{d^3k}{4\pi^3}\, v(k) = \int_{occ.} \frac{d^3k}{4\pi^3}\, v(k) + \int_{unocc.} \frac{d^3k}{4\pi^3}\, v(k)$$

$$\Longrightarrow j = (+e)\int_{unocc.} \frac{d^3k}{4\pi^3}\, v(k)$$

B. $$\mathcal{E}(k) \approx \mathcal{E}(k_0) - A(k-k_0)^2 \qquad A = \frac{\hbar^2}{2m^*}$$

$$v(k) \approx \frac{-2A}{\hbar}(k-k_0) \qquad \frac{-2A}{\hbar} = \frac{-\hbar}{m^*}$$

$$\left.\begin{aligned} a &= \frac{dv}{dt} = \frac{-\hbar}{m^*}\dot{k} \\ \hbar\dot{k} &= (-e)\left(E + \frac{1}{c} v \times H\right) \end{aligned}\right\} \rightarrow m^* a = (+e)\left(E + \frac{1}{c} v \times H\right)$$

C. Motion in a uniform B-field:

$$\dot{r} = v(k) = \frac{1}{\hbar}\nabla_k \mathcal{E}$$

$$\hbar\dot{k} = (-e)\frac{1}{c} v(k) \times H$$

1. $\dot{k}(t) \cdot \hat{H} = 0 \rightarrow$ Component $\parallel H$ = const.
2. In const. energy surface:

$$\frac{d\,\mathcal{E}(k)}{dt} = \dot{k} \cdot \vec{\nabla}_k \mathcal{E} = 0$$

3. $r_\perp = r - \hat{H}(\hat{H}\cdot r)$

$\dot{r}_\perp = \dot{r} - \hat{H}(\hat{H}\cdot\dot{r})$

$$\hat{H}\times\hbar\dot{k} = (-e)\frac{1}{c}\,\hat{H}\times(\vec{v}\times\vec{H})$$

$A\times(B\times C) = (A\cdot C)B - (A\cdot B)C$

$$= (-e)\frac{1}{c}\left(H\vec{v} - (\hat{H}\cdot\vec{v})\vec{H}\right)$$

$$= (-e)\frac{H}{c}\left(\vec{v} - \hat{H}(\hat{H}\cdot\vec{v})\right)$$

$$\hat{H}\times\hbar\dot{k} = -\frac{eH}{c}\dot{r}_\perp$$

$$\rightarrow \hat{H}\times\hbar(k(t)-k(0)) = -\frac{eH}{c}(r_\perp(t)-r_\perp(0))$$

$$r_\perp(t)-r_\perp(0) = -\frac{\hbar c}{eH}\hat{H}\times(k(t)-k(0))$$

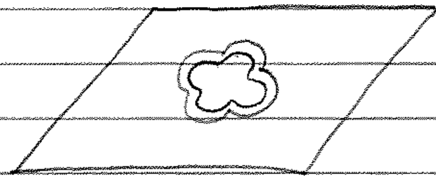
$\Rightarrow$ Real space path rotated through $90°$ relative to k-space path.

4. Period of orbit:

$$t_2 - t_1 = \int_{t_1}^{t_2} dt = \int_{k_1}^{k_2}\frac{dk}{|\dot{k}|}$$

$$\dot{k} = \frac{-e}{c\hbar}\vec{v}\times\vec{H} = \frac{-e}{c\hbar^2}\vec{\nabla}_k\varepsilon\times\vec{H} = -\frac{eH}{\hbar^2 c}\nabla_{k_\perp}\varepsilon$$

$$\Longrightarrow t_2 - t_1 = \frac{\hbar^2 c}{eH}\int_{k_1}^{k_2}\frac{dk}{|\nabla_{k_\perp}\varepsilon|}$$



$$\Delta\varepsilon = (\vec{\nabla}_{k_\perp}\varepsilon)\cdot\vec{\Delta}(k)$$

$$\Delta\varepsilon = |\nabla_{k_\perp}\varepsilon|\,|\Delta(k)|$$

$$\Rightarrow t_2 - t_1 = \frac{\hbar^2 c}{eH}\frac{1}{\Delta\varepsilon}\int_{k_1}^{k_2}\Delta k\,dk = \frac{\hbar^2 c}{eH}\frac{\partial A}{\partial\varepsilon}$$

$$T = \frac{\hbar^2 c}{eH}\frac{\partial A}{\partial\varepsilon} = \frac{\hbar^2 c}{eH}\frac{d\pi k^2}{d\frac{\hbar^2 k^2}{2m^*}} = \frac{2\pi m^* c}{eH}$$

<u>check:</u> $\frac{mv^2}{r} = \frac{qvB}{c} \Rightarrow \frac{v}{r} = \frac{2\pi}{T} = \frac{eB}{cm}$

$$\Rightarrow T = \frac{2\pi mc}{eB}.$$

5. Motion w/perpendicular E & B fields:

$$\hat{H}\times\hbar\dot{k} = -\frac{eH}{c}\left(\vec{v} - \hat{H}(\hat{H}\cdot\vec{v})\right) - e\hat{H}\times\vec{E}$$

$$= -\frac{eH}{c}\left(\dot{r}_\perp + \frac{cE}{H}(\hat{H}\times\hat{E})\right)$$

$$-\frac{\hbar c}{eH}\hat{H}\times(k(t)-k(0)) \underbrace{-\frac{cE}{H}(\hat{H}\times\hat{E})t}_{wt} = r_\perp(t) - r_\perp(0)$$

uniform drift

$$\hbar\dot{k} = -\frac{e}{c}\frac{1}{\hbar}\nabla_k(\varepsilon - \hbar k\cdot w)\times H$$

const. $\bar{\varepsilon} = \varepsilon - \hbar k\cdot w$ surface

$$= -\frac{e}{c}\frac{1}{\hbar}\nabla_k\varepsilon\times H + \frac{e}{c}w\times H$$

$$-\frac{e}{c}\left(\frac{cE}{H}\right)(\hat{H}\times\hat{E})\times H$$

$$= +eE\,\hat{H}\times(\hat{H}\times\hat{E}) = -e\vec{E}$$

Explicit example: $\dot{r} = v$

$$\hbar\dot{k} = -e\left(E + \frac{v}{c}\times H\right)$$

$$v = \hbar k/m$$

$\left.\begin{array}{l}\hat{H} = \hat{z}\\ \hat{E} = \hat{x}\end{array}\right\} \rightarrow$ $\hbar\dot{k} = -e\left(E\hat{x} + \frac{\hbar k}{m}\times H\hat{z}\right)$

$$\hbar\dot{k}_z = 0 \rightarrow k_z = \text{const.}$$

$$\hbar\dot{k}_x = -eE - e\frac{\hbar k_y}{m}H = \frac{-e\hbar H}{m}\left(k_y + \frac{m}{\hbar}\frac{E}{H}\right)$$

$$\hbar\dot{k}_y = +e\frac{\hbar k_x}{m}H$$

Thus, the circle followed by $\vec{k}_\perp$ is just shifted in the y-direction.

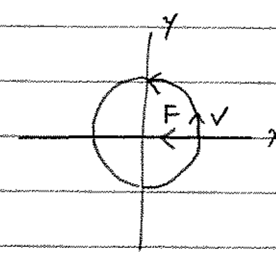
$$\dot{k}_x = -\frac{eH}{m}\tilde{k}_y \qquad \tilde{k}_y = k_y + \frac{mE}{\hbar H}$$

$$\dot{\tilde{k}}_y = +\frac{eH}{m}k_x$$

A solution: $k_x(t) = A\cos(\omega t)$, $\omega = \frac{eH}{m}$

$$\tilde{k}_y(t) = A\sin(\omega t)$$

$$k_y(t) = A\sin(\omega t) - \frac{mE}{\hbar H}$$



$$\Rightarrow v_x(t) = v_0\cos(\omega t)$$

$$v_y(t) = v_0\sin(\omega t) - \frac{E}{H}$$