Problem set 10

Problem 1.

Remember three length scale $a \ll \Delta R \ll L$

It means $\Delta R$ is so large (equivalenely $\Delta k$ is $\ll \frac{2\pi}{a}$), that locally ($\sim a$), the wave packet is still a Bloch electron. But at the same time, $\Delta R \ll L$ the sale of the solid and the scale of external field. Therefore, this wave packet is microscopically a Bloch electron and meanwhile, macroscopieally a "point".

Starting from electric static force with potential $U(R)$

Consider translation operator $\hat{T}_{\vec{a}} = e^{\frac{i}{\hbar}\hat{p}\cdot a} = e^{\nabla\cdot\vec{a}}$

The operation of $\hat{T}_{\vec{a}}$ one function $f(\vec{x})$ is $T_{\vec{a}}f(\vec{x}) = f(\vec{x}+\vec{a})$

Remember a Bloch wave $\psi_{\vec{k}}(\vec{r}) = e^{ik\cdot r}u_{\vec{k}}(\vec{r})$ is eigenstate of $T_{\vec{a}}$

$\hat{T}_{\vec{a}}\psi_{\vec{k}}(\vec{r}) = e^{ik\cdot a}\psi_{\vec{k}}(\vec{r})$

So, $\langle\hat{T}_{\vec{a}}\rangle = \langle\psi_{\vec{k}}|\hat{T}_{\vec{a}}|\psi_{\vec{k}}\rangle = e^{i\vec{k}\cdot\vec{a}}$

For wave packet, we similarly define $\langle\hat{T}_{\vec{a}}(t)\rangle = e^{i\vec{k}(t)\cdot\vec{a}}$

Consider Hamiltonian $\hat{H} = \hat{H}_0 + U(R)$

Heisenberg equation of motion is

$$\frac{d}{dt}\hat{T}_{\vec{a}}(t) = \frac{i}{\hbar}[\hat{H}, \hat{T}_{\vec{a}}] + \frac{\partial}{\partial t}\hat{T}_{\vec{a}}$$

$$= \frac{i}{\hbar}[\hat{H}_0 + U(R), \hat{T}_{\vec{a}}]$$

By definition, $[\hat{H}_0, \hat{T}_{\vec{a}}] = 0$, the only non-vanishing term is $[U(R), \hat{T}_{\vec{a}}]$

$$[U(\vec{R}), T_{\vec{a}}]f(\vec{R}) = U(\vec{R})T_{\vec{a}}f(\vec{R}) - T_{\vec{a}}U(R)f(R) = [U(\vec{R}) - U(R+a)]\cdot T_{\vec{a}}f(R).$$

Since external field varies slowly respect to $a$, it is reasonable to approximate

$$[U(R+a) - U(R)] = \vec{\nabla}_R U(R)\cdot\vec{a}$$

Calculating the expectation gives

$$\frac{d}{dt}\langle T_{\vec{a}}(t)\rangle = \frac{i}{\hbar}\langle -\vec{\nabla}_R U(R)\cdot\vec{a}\, T_{\vec{a}}\rangle$$

Remember $\langle\cdots\rangle$ is calculated w.r.t. a wave packet, which is localized comparing to field.

$$\frac{d}{dt}\langle T_{\vec{a}}(t)\rangle = \frac{i}{\hbar}(-\vec{\nabla}_R U\cdot\vec{a})\langle T_{\vec{a}}\rangle = \frac{i}{\hbar}\vec{F}\cdot\vec{a}\langle T_{\vec{a}}(t)\rangle$$

By definition $e^{i\vec{k}(t)\cdot\vec{a}} = \langle T_{\vec{a}}(t)\rangle$

$$\frac{d}{dt}\langle T_{\vec{a}}(t)\rangle = \frac{d}{dt}e^{i\vec{k}(t)\cdot\vec{a}} = i\frac{d\vec{k}}{dt}\cdot\vec{a}\langle T_{\vec{a}}(t)\rangle$$

Compare two equation and noctice $\vec{a}$ can be chosen arbitrarily

$$\frac{1}{\hbar}\vec{F} = \frac{d\vec{k}}{dt} \iff \hbar\frac{d\vec{k}}{dt} = \vec{F}$$

Now we study the equation of motion of the center of wave packet $\vec{R}$

$$\frac{d}{dt}\vec{R} = \frac{i}{\hbar}[H,\vec{R}] = \frac{i}{\hbar}\left[\frac{\hat{p}^2}{2m_e} + V(\vec{R}) + U(\vec{R}), \vec{R}\right] = \frac{i}{2\hbar m_e}[p^2, \vec{R}]$$

Using $[R, p^2] = 2\hbar i \vec{p}$

$$\frac{d}{dt}\vec{R} = \frac{\vec{P}}{m_e} \mapsto \frac{d}{dt}\langle\vec{R}\rangle = \frac{\langle\vec{P}\rangle}{m_e}$$

For Bloch wave $\psi_{\vec{k}}(\vec{r}) = e^{ik\cdot r}u_k(\vec{r})$ , $\hat{H}_0\psi_{\vec{k}}(\vec{r}) = \varepsilon(\vec{k})\,\psi_{\vec{k}}(\vec{r})$

$$\nabla_{\vec{k}}\varepsilon(\vec{k}) = \nabla_k\langle\psi_{\vec{k}}|\hat{H}_0|\psi_{\vec{k}}\rangle = \nabla_{\vec{k}}\langle u_{\vec{k}}|e^{-ikr}\hat{H}_0 e^{ikr}|u_{\vec{k}}\rangle = \nabla_{\vec{k}}\langle u_k|e^{-ikr}\frac{p^2}{2m_e}e^{ikr}|u_k\rangle$$

$$= \frac{-i}{2m_e}\langle\psi_k|[\vec{r},\hat{p}^2]|\psi_{\vec{k}}\rangle = -\frac{i}{2m_e}\cdot 2\hbar i\langle\psi_k|\vec{p}|\psi_k\rangle = \frac{\hbar}{m_e}\langle\psi_k|\vec{p}|\psi_k\rangle$$

Comparing two equations gives $\frac{d}{dt}\langle\vec{R}\rangle = \frac{1}{\hbar}\nabla_{\vec{k}}\varepsilon = v_g$

For generalization to Lorentz force, we can only provide a heuristic derivation.

Let $\vec{k}(t) = \frac{1}{\hbar}[\vec{P} - \frac{q}{c}\vec{A}(R,t)]$ and $\hat{T}_{\vec{a}} = e^{i\vec{k}(t)\cdot\vec{a}}$

Again, the Heisenberg EoM

$$\frac{d}{dt}\hat{T}_{\vec{a}} = \frac{i}{\hbar}[H,\hat{T}_{\vec{a}}] + \frac{\partial}{\partial t}\hat{T}_{\vec{a}}$$

The explicit part gives $\frac{\partial}{\partial t}\hat{T}_a = \frac{i}{\hbar}(-\frac{q}{c})\frac{\partial}{\partial t}\vec{A}\cdot\hat{T}_{\vec{a}}$

$$\frac{i}{\hbar}[H,T_{\vec{a}}] = \frac{i}{\hbar}[\varepsilon(\vec{k}),T_{\vec{a}}] + \frac{i}{\hbar}[q\phi(R),T_{\vec{a}}]$$

The second term again gives $\frac{i}{\hbar}[q\phi, T_{\vec{a}}] = \frac{iq}{\hbar}(-\vec{\nabla}_R\phi\cdot\vec{a}\,\hat{T}_{\vec{a}})$

The first term $\frac{i}{\hbar}[\varepsilon(\vec{k}),T_{\vec{a}}] = \frac{i}{\hbar}(-\nabla_{\vec{k}}\varepsilon(\vec{k})\cdot\delta\vec{k})\,T_{\vec{a}}$

$$= \frac{i}{\hbar}(-\hbar\vec{v}_g\cdot\vec{\nabla}_R\vec{A}\cdot\vec{a})(-\frac{q}{\hbar c})\hat{T}_{\vec{a}}$$

$$= \frac{iq}{\hbar c}\vec{v}_g\cdot\vec{\nabla}_R\vec{A}\cdot\vec{a} \overset{?}{=} \frac{iq}{\hbar c}v_g\times(\nabla\times\vec{A})\,\hat{T}_{\vec{a}}$$

All together gives

$$\frac{d}{dt}\hat{T}_{\vec{a}} = \frac{iq}{\hbar}\left\{\frac{1}{c}\vec{v}_g\times(\vec{\nabla}\times\vec{A}) - \vec{\nabla}_R\phi - \frac{1}{c}\frac{\partial}{\partial t}\vec{A}\right\}\cdot\vec{a}\;T_{\vec{a}}$$

Similarly. $\hbar\frac{d\vec{k}}{dt} = q\left\{\frac{1}{c}\vec{v}_g\times(\vec{\nabla}\times\vec{A}) - \nabla\phi - \frac{1}{c}\frac{\partial}{\partial t}\vec{A}\right\}$.

Using $\nabla\times A = \vec{B}$, $-\nabla\phi - \frac{1}{c}\frac{\partial}{\partial t}\phi = \vec{E}$

$$\hbar\frac{d\vec{k}}{dt} = F = q\left\{\frac{1}{c}\vec{v}_g\times\vec{B} + \vec{E}\right\}.$$

Let $q = -e$

Problem 2.

Relation between electrons and holes

$$\vec{K_h} = -\vec{k_e}, \quad \varepsilon_e(\vec{k_e}) = -\varepsilon_h(\vec{K_h})$$

$$v_g = \frac{d}{dt}\vec{R_e} = \frac{1}{\hbar}\nabla_{k_e}\varepsilon_e = \frac{1}{\hbar}\nabla_{k_h}\varepsilon_h = \frac{d}{dt}\vec{R_h}$$

$$\frac{d}{dt}v_g = \frac{d^2}{dt^2}\vec{R} = \frac{d}{\hbar dt}\nabla_{k_e}\varepsilon_e = \frac{1}{\hbar}\sum_{ij}\frac{\partial^2}{\partial k_i \partial k_j}\varepsilon_e \vec{i} \cdot \frac{\partial k_j}{\partial t}$$

Using $\varepsilon(\vec{k}) = \varepsilon(\vec{k_0}) - \frac{\hbar^2}{2m^*}(\vec{k}-\vec{k_0})^2$ and $\hbar\frac{d\vec{k}}{dt} = -e\{\vec{E} + \frac{\vec{v}}{c}\times\vec{B}\}$.

$$\frac{d}{dt}v_g = \frac{e}{m^*}\{\vec{E} + \frac{1}{c}\vec{v}\times\vec{B}\}$$

While hole's EOM gives $\hbar\frac{d\vec{K_h}}{dt} = -\hbar\frac{d\vec{k}}{dt} = +e\{\vec{E} + \frac{\vec{v}}{c}\times\vec{B}\}$.

$$\nabla_{k}\vec{v_g} = -\nabla_{k_h}\vec{v_g} = -\frac{\hbar}{m^*}$$

For holes

$$\frac{d^2}{dt^2}R = \nabla_{k_h}v_g \cdot \frac{dk_h}{dt} = \frac{e}{m^*}\{\vec{E} + \frac{\vec{v}}{c}\times\vec{B}\}$$