

An introduction of semiclassical theory

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Outline

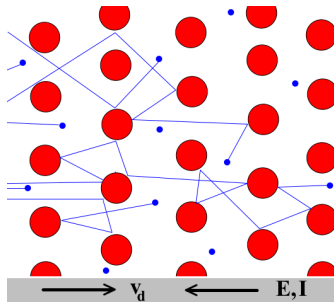
Classical picture

Wave packet

Linear response

Summary

Classical picture and Drude model



$$\dot{\mathbf{r}} = \frac{\mathbf{p}}{m}, \quad \dot{\mathbf{p}} = -e\mathbf{E} - \frac{\mathbf{p}}{\tau}$$

- Electric force and friction force
- The two forces encounter an stable value of $\mathbf{p}$:

$$\mathbf{p} = -e\tau\mathbf{E}$$

- The net current

$$\mathbf{J} = -en\dot{\mathbf{r}} = e\mathbf{E} \leftarrow \text{Ohm's law}$$

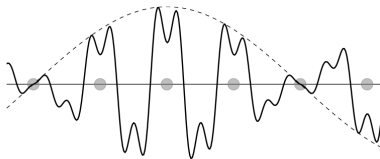
Classical picture and Drude model

Fermi surface, Energy structure, Carrier type, Quantum interference, Localization

- Cannot explain the particle/hole transport
- Cannot recognize metal/semiconductor/insulator
- Quantum interference/localization miss
- Fail in nonlinear transport/high frequency effect

Bloch theorem

Plane wave $\rightarrow$ Bloch wave



$$\psi(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} u_{\mathbf{k}}(\mathbf{r}), \quad u_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r} + \mathbf{R})$$

- Similar with plane wave
- The Amplitude of the plane wave is modulated by periodic potential
- $\mathbf{k}$ is a good quantum number

Why we need to define a wave packet?

The wavefunction of a wave packet:

$$\begin{aligned} |\Psi\rangle &= \int d^3\mathbf{k} a(\mathbf{k}, t) |\psi_{\mathbf{k}}(\mathbf{r}, t)\rangle \\ &= \int d^3\mathbf{k} a(\mathbf{k}, t) e^{i\mathbf{k}\cdot\mathbf{r}} |u_{\mathbf{k}}(\mathbf{r}, t)\rangle \end{aligned}$$

- Linear superposition of Bloch wave near a certain $\mathbf{k}_c \leftarrow$ **Localized in momentum space**

$$\mathbf{k}_c = \langle \Psi | \hat{\mathbf{k}} | \Psi \rangle$$

- What about in real space?

$$\mathbf{r}_c = \langle \Psi | \hat{\mathbf{r}} | \Psi \rangle$$

Outline

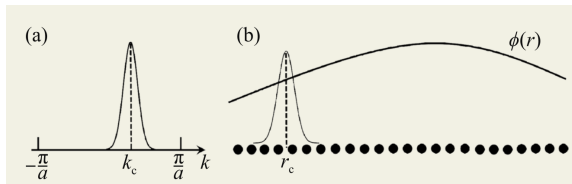
Classical picture

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Summary

Wave packet



- The spread of the wave packet is smaller than length scale of the external field

$$\hbar \dot{\mathbf{k}} = -e\mathbf{E} - e\dot{\mathbf{r}} \times \mathbf{B}$$

$$\dot{\mathbf{r}} = \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial \mathbf{k}}$$

Wave packet

Hamiltonian

$$H[\hat{\mathbf{x}}, \hat{\mathbf{p}}, \beta_1(\hat{\mathbf{x}}, t), \dots, \beta_r(\hat{\mathbf{x}}, t)]$$

- $\{\beta_i(\mathbf{x}, t)\}$ are modulation functions characterizing the perturbation

Linearize the perturbation about the wav packet center

$$H \approx H_c + \sum_i (\hat{\mathbf{x}} - \mathbf{x}_c) \cdot \text{grad}_{\mathbf{x}_c} \beta_i(\mathbf{x}_c, t)$$

Energy spectrum

$$H_c(\mathbf{x}_c, t) |\psi_{\mathbf{q}}(\mathbf{x}_c, t)\rangle = \varepsilon_c(\mathbf{x}_c, \mathbf{q}, t) |\psi_{\mathbf{q}}(\mathbf{x}_c, t)\rangle$$

Wave packet

$$|\Psi\rangle = \int d^3\mathbf{q} a(\mathbf{q}, t) |\psi_{\mathbf{q}}(\mathbf{x}_c, t)\rangle$$

Sundaram et al, PRB 59, 14915 (1999)

$$|\Psi\rangle = \int d^3\mathbf{q} a(\mathbf{q}, t) |\psi_{\mathbf{q}}(\mathbf{x}_c, t)\rangle = \int d^3\mathbf{q} a(\mathbf{q}, t) e^{i\mathbf{q}\cdot\hat{\mathbf{x}}} |u(\mathbf{x}_c, q, t)\rangle$$

$$\begin{cases} \mathbf{q}_c = \int d^3\mathbf{q} \mathbf{q} |a(\mathbf{q}, t)|^2 \\ \mathbf{x}_c = \langle \Psi | \hat{\mathbf{x}} | \Psi \rangle \end{cases}$$

- $\langle \Psi_{\mathbf{q}'} | \Psi_{\mathbf{q}} \rangle = \delta(\mathbf{q}' - \mathbf{q})$
- $|a(\mathbf{q}, t)|^2$ is narrow compared to the size of the Brillouin zone

Center of the wave packet

$$\begin{aligned} \mathbf{x}_c &= \langle \Psi | \hat{\mathbf{x}} | \Psi \rangle = \int d\mathbf{q} d\mathbf{q}' a^*(\mathbf{q}, t) a(\mathbf{q}', t) \langle u_{\mathbf{q}} | e^{-i\mathbf{q} \cdot \mathbf{x}} \mathbf{x} e^{i\mathbf{q}' \cdot \mathbf{x}} | u_{\mathbf{q}'} \rangle \\ &= \int d\mathbf{q} d\mathbf{q}' a^*(\mathbf{q}, t) a(\mathbf{q}', t) \langle u_{\mathbf{q}} | \left(i \partial_{\mathbf{q}} e^{-i\mathbf{q} \cdot \mathbf{x}} \right) e^{i\mathbf{q}' \cdot \mathbf{x}} | u_{\mathbf{q}'} \rangle \\ &= \int d\mathbf{q} d\mathbf{q}' \left[(-i \partial_{\mathbf{q}} a^*(\mathbf{q}, t)) a(\mathbf{q}', t) \langle u_{\mathbf{q}} | u_{\mathbf{q}'} \rangle e^{i(\mathbf{q}' - \mathbf{q}) \cdot \mathbf{x}} \right. \\ &\quad \left. - i a^*(\mathbf{q}, t) a(\mathbf{q}', t) \langle \partial_{\mathbf{q}} u_{\mathbf{q}} | u_{\mathbf{q}'} \rangle e^{i(\mathbf{q}' - \mathbf{q}) \cdot \mathbf{x}} \right] \\ &= \int d\mathbf{q} \left[\frac{\partial \gamma(\mathbf{q}, t)}{\partial \mathbf{q}} \delta(\mathbf{q} - \mathbf{q}_c) + \langle u_{\mathbf{q}} | i \partial_{\mathbf{q}} u_{\mathbf{q}} \rangle \delta(\mathbf{q} - \mathbf{q}_c) \right] \\ &= \frac{\partial \gamma_c}{\partial \mathbf{q}_c} + \langle u | i \partial_{\mathbf{q}_c} u \rangle \end{aligned}$$

Assume $a(\mathbf{q}, t) = |a(\mathbf{q}, t)| e^{-i\gamma(\mathbf{q}, t)}$

$$L = \langle \Psi | i \frac{\partial}{\partial t} - \hat{H} | \Psi \rangle$$

- Lagrangian should be a function of $\mathbf{x}_c$ and $\mathbf{q}_c$, their derivatives, and the time

$$L = L(\mathbf{x}_c, \dot{\mathbf{x}}_c, \mathbf{q}_c, \dot{\mathbf{q}}_c, t)$$

$$\begin{aligned}
 \left\langle \Psi \left| i \frac{\partial}{\partial t} \Psi \right. \right\rangle &= \frac{\partial \gamma_c}{\partial t} + \left\langle u \left| i \frac{\partial u}{\partial t} \right. \right\rangle + \dot{\mathbf{x}}_c \cdot \left\langle u \left| i \frac{\partial u}{\partial \mathbf{x}_c} \right. \right\rangle \\
 &= \frac{d\gamma_c}{dt} - \dot{\mathbf{q}}_c \cdot \frac{\partial \gamma_c}{\partial \mathbf{q}_c} + \dot{\mathbf{x}}_c \cdot \left\langle u \left| i \frac{\partial u}{\partial \mathbf{x}_c} \right. \right\rangle + \left\langle u \left| i \frac{\partial u}{\partial t} \right. \right\rangle \\
 &= \frac{d\gamma_c}{dt} - \dot{\mathbf{q}}_c \cdot \left(\mathbf{x}_c - \left\langle u \left| i \frac{\partial u}{\partial \mathbf{q}_c} \right. \right\rangle \right) + \dot{\mathbf{x}}_c \cdot \left\langle u \left| i \frac{\partial u}{\partial \mathbf{x}_c} \right. \right\rangle + \left\langle u \left| i \frac{\partial u}{\partial t} \right. \right\rangle \\
 &\rightarrow -\dot{\mathbf{q}}_c \cdot \mathbf{x}_c + \dot{\mathbf{q}}_c \cdot \left\langle u \left| i \frac{\partial u}{\partial \mathbf{q}_c} \right. \right\rangle + \dot{\mathbf{x}}_c \cdot \left\langle u \left| i \frac{\partial u}{\partial \mathbf{x}_c} \right. \right\rangle + \left\langle u \left| i \frac{\partial u}{\partial t} \right. \right\rangle
 \end{aligned}$$

$$L = -\varepsilon + \mathbf{q}_c \cdot \dot{\mathbf{x}}_c + \dot{\mathbf{q}}_c \cdot \left\langle u \left| i \frac{\partial u}{\partial \mathbf{q}_c} \right\rangle + \dot{\mathbf{x}}_c \cdot \left\langle u \left| i \frac{\partial u}{\partial \mathbf{x}_c} \right\rangle + \left\langle u \left| i \frac{\partial u}{\partial t} \right\rangle\right.$$

Euler-Lagrange equation

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{\mathbf{x}}} - \frac{\partial L}{\partial \mathbf{x}} = 0, \quad \frac{d}{dt} \frac{\partial L}{\partial \dot{\mathbf{q}}} - \frac{\partial L}{\partial \mathbf{q}} = 0$$

Lagrangian

$$L = -\varepsilon + \mathbf{q} \cdot \dot{\mathbf{x}} + \dot{\mathbf{q}} \cdot \left\langle u \left| i \frac{\partial u}{\partial \mathbf{q}} \right\rangle + \dot{\mathbf{x}} \cdot \left\langle u \left| i \frac{\partial u}{\partial \mathbf{x}} \right\rangle + \left\langle u \left| i \frac{\partial u}{\partial t} \right\rangle\right.$$

Euler-Lagrange equation

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{\mathbf{x}}} - \frac{\partial L}{\partial \mathbf{x}} = 0, \quad \frac{d}{dt} \frac{\partial L}{\partial \dot{\mathbf{q}}} - \frac{\partial L}{\partial \mathbf{q}} = 0$$

Euler-Lagrange equation

$$\frac{\partial L}{\partial \dot{x}_a} = q_a + \langle u | i \partial_{x_a} u \rangle$$

$$\begin{aligned} \frac{\partial L}{\partial x_a} = & - \frac{\partial \varepsilon}{\partial x_a} + \dot{q}_b (\langle \partial_{x_a} u | i \partial_{q_b} u \rangle + \langle u | i \partial_{x_a} \partial_{q_b} u \rangle) \\ & + \dot{x}_b (\langle \partial_{x_a} u | i \partial_{x_b} u \rangle + \langle u | i \partial_{x_a} \partial_{x_b} u \rangle) + \langle \partial_{x_a} u | i \partial_t u \rangle + \langle u | i \partial_{x_a} \partial_t u \rangle \end{aligned}$$

Euler-Lagrange equation

$$\begin{aligned}\frac{d}{dt} \frac{\partial L}{\partial \dot{x}_a} &= \dot{q}_a + \langle \dot{u} | i \partial_{x_a} u \rangle + \langle u | i \partial_{x_a} \dot{u} \rangle \\ &= \dot{q}_a + \dot{q}_b \langle \partial_{q_b} u | i \partial_{x_a} u \rangle + \dot{x}_b \langle \partial_{x_b} u | i \partial_{x_a} u \rangle + \langle \partial_t u | i \partial_{x_a} u \rangle \\ &\quad + \dot{q}_b \langle u | i \partial_{x_a} \partial_{q_b} u \rangle + \dot{x}_b \langle u | i \partial_{x_a} \partial_{x_b} u \rangle + \langle u | i \partial_{x_a} \partial_t u \rangle \\ \frac{\partial L}{\partial x_a} &= - \frac{\partial \varepsilon}{\partial x_a} + \dot{q}_b (\langle \partial_{x_a} u | i \partial_{q_b} u \rangle + \langle u | i \partial_{x_a} \partial_{q_b} u \rangle) \\ &\quad + \dot{x}_b (\langle \partial_{x_a} u | i \partial_{x_b} u \rangle + \langle u | i \partial_{x_a} \partial_{x_b} u \rangle) + \langle \partial_{x_a} u | i \partial_t u \rangle + \langle u | i \partial_{x_a} \partial_t u \rangle\end{aligned}$$

Euler-Lagrange equation

$$\begin{aligned}\frac{d}{dt} \frac{\partial L}{\partial \dot{x}_a} &= \dot{q}_a + \langle \dot{u} | i \partial_{x_a} u \rangle + \langle u | i \partial_{x_a} \dot{u} \rangle \\ &= \dot{q}_a + \dot{q}_b \langle \partial_{q_b} u | i \partial_{x_a} u \rangle + \dot{x}_b \langle \partial_{x_b} u | i \partial_{x_a} u \rangle + \langle \partial_t u | i \partial_{x_a} u \rangle \\ &\quad + \dot{q}_b \langle u | i \partial_{x_a} \partial_{q_b} u \rangle + \dot{x}_b \langle u | i \partial_{x_a} \partial_{x_b} u \rangle + \langle u | i \partial_{x_a} \partial_t u \rangle \\ \frac{\partial L}{\partial x_a} &= - \frac{\partial \varepsilon}{\partial x_a} + \dot{q}_b (\langle \partial_{x_a} u | i \partial_{q_b} u \rangle + \langle u | i \partial_{x_a} \partial_{q_b} u \rangle) \\ &\quad + \dot{x}_b (\langle \partial_{x_a} u | i \partial_{x_b} u \rangle + \langle u | i \partial_{x_a} \partial_{x_b} u \rangle) + \langle \partial_{x_a} u | i \partial_t u \rangle + \langle u | i \partial_{x_a} \partial_t u \rangle\end{aligned}$$

One obtain

$$\begin{aligned}\dot{q}_a &= - \frac{\partial \varepsilon}{\partial x_a} + \dot{q}_b (\langle \partial_{x_a} u | i \partial_{q_b} u \rangle - \langle \partial_{q_b} u | i \partial_{x_a} u \rangle) \\ &\quad + \dot{x}_b (\langle \partial_{x_a} u | i \partial_{x_b} u \rangle - \langle \partial_{x_b} u | i \partial_{x_a} u \rangle) \\ &\quad + \langle \partial_{x_a} u | i \partial_t u \rangle - \langle \partial_t u | i \partial_{x_a} u \rangle\end{aligned}$$

Euler-Lagrange equation

$$\begin{aligned}\frac{d}{dt} \frac{\partial L}{\partial \dot{x}_a} &= \dot{q}_a + \langle \dot{u} | i \partial_{x_a} u \rangle + \langle u | i \partial_{x_a} \dot{u} \rangle \\ &= \dot{q}_a + \dot{q}_b \langle \partial_{q_b} u | i \partial_{x_a} u \rangle + \dot{x}_b \langle \partial_{x_b} u | i \partial_{x_a} u \rangle + \langle \partial_t u | i \partial_{x_a} u \rangle \\ &\quad + \dot{q}_b \langle u | i \partial_{x_a} \partial_{q_b} u \rangle + \dot{x}_b \langle u | i \partial_{x_a} \partial_{x_b} u \rangle + \langle u | i \partial_{x_a} \partial_t u \rangle \\ \frac{\partial L}{\partial x_a} &= - \frac{\partial \varepsilon}{\partial x_a} + \dot{q}_b (\langle \partial_{x_a} u | i \partial_{q_b} u \rangle + \langle u | i \partial_{x_a} \partial_{q_b} u \rangle) \\ &\quad + \dot{x}_b (\langle \partial_{x_a} u | i \partial_{x_b} u \rangle + \langle u | i \partial_{x_a} \partial_{x_b} u \rangle) + \langle \partial_{x_a} u | i \partial_t u \rangle + \langle u | i \partial_{x_a} \partial_t u \rangle\end{aligned}$$

One obtain

$$\dot{q}_a = - \frac{\partial \varepsilon}{\partial x_a} + \Omega_{x_a q_b} \dot{q}_b + \Omega_{x_a x_b} \dot{x}_b + \Omega_{x_a t}$$

The tensor is defined as

$$\Omega_{x_a x_b} = i \left(\left\langle \frac{\partial u}{\partial x_a} \middle| \frac{\partial u}{\partial x_b} \right\rangle - \left\langle \frac{\partial u}{\partial x_b} \middle| \frac{\partial u}{\partial x_a} \right\rangle \right)$$

Euler-Lagrange equation

With the same method, one obtain

$$\dot{x}_a = \frac{\partial \varepsilon}{\partial q_a} - (\Omega_{q_a x_b} \dot{x}_b + \Omega_{q_a q_b} \dot{q}_b) + \Omega_{t q_a}$$

Electromagnetic field

- The Hamiltonian is modified by the gauge potential

$$H = H_0[\mathbf{q} + e\mathbf{A}(\mathbf{x}, t)] - e\phi(\mathbf{x}, t)$$

where $\mathbf{k} = \mathbf{q} + e\mathbf{A}(\mathbf{x}_c, t)$ is the gauge invariant crystal momentum.

- The Lagrangian becomes

$$\begin{aligned} L &= -\varepsilon + e\phi(\mathbf{x}_c, t) + \mathbf{q} \cdot \dot{\mathbf{x}} + \dot{\mathbf{k}}_c \cdot \left\langle u \left| i \frac{\partial u}{\partial \mathbf{k}_c} \right. \right\rangle \\ &= -\varepsilon - e\phi(\mathbf{x}_c, t) + \mathbf{k} \cdot \dot{\mathbf{x}} - e\mathbf{A}(\mathbf{x}_c, t) \cdot \dot{\mathbf{x}} + \dot{\mathbf{k}}_c \cdot \left\langle u \left| i \frac{\partial u}{\partial \mathbf{k}_c} \right. \right\rangle \end{aligned}$$

- The equation of motion

$$\begin{aligned} \dot{k}_a &= \frac{\partial \varepsilon}{\partial x_a} + e \left(\frac{\partial \phi}{\partial x_a} + \frac{\partial A_a}{\partial t} \right) - e \dot{x}_b \left(\frac{\partial A_b}{\partial x_a} - \frac{\partial A_a}{\partial x_b} \right) \\ \dot{r}_a &= \frac{\partial \varepsilon}{\partial k_a} + \dot{k}_b (\langle \partial_{k_b} u | i \partial_{k_a} u \rangle - \langle \partial_{k_a} u | i \partial_{k_b} u \rangle) \end{aligned}$$

Electromagnetic field

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- The Lagrangian becomes

$$\begin{aligned} L &= -\varepsilon + e\phi(\mathbf{x}_c, t) + \mathbf{q} \cdot \dot{\mathbf{x}} + \dot{\mathbf{k}}_c \cdot \left\langle u \left| i \frac{\partial u}{\partial \mathbf{k}_c} \right\rangle \right. \\ &= -\varepsilon - e\phi(\mathbf{x}_c, t) + \mathbf{k} \cdot \dot{\mathbf{x}} - e\mathbf{A}(\mathbf{x}_c, t) \cdot \dot{\mathbf{x}} + \dot{\mathbf{k}}_c \cdot \left\langle u \left| i \frac{\partial u}{\partial \mathbf{k}_c} \right\rangle \right. \end{aligned}$$

- The equation of motion

$$\dot{\mathbf{k}} = -e\mathbf{E} - e\dot{\mathbf{x}} \times \mathbf{B}$$

$$\dot{\mathbf{x}} = \frac{\partial \varepsilon}{\partial \mathbf{k}} - \dot{\mathbf{k}} \times \mathbf{\Omega}$$

where $\mathbf{B} = \nabla \times \mathbf{A}$, and $\mathbf{\Omega} = \nabla \times \langle u | i \partial_{\mathbf{k}} u \rangle$

Outline

Classical picture

Wave packet

Linear response

Summary

Boltzmann equation

The distribution function

$$\frac{df}{dt} = \left(\frac{\partial f}{\partial t} \right)_{\text{coll}}$$

- 'coll' is the collision term

Boltzmann equation

The distribution function

$$\frac{\partial f}{\partial t} + \dot{\mathbf{r}} \cdot \frac{\partial f}{\partial \mathbf{r}} + \dot{\mathbf{k}} \cdot \frac{\partial f}{\partial \mathbf{k}} = \left(\frac{\partial f}{\partial t} \right)_{\text{coll}}$$

- 'coll' is the collision term

Boltzmann equation

The distribution function

$$\frac{\partial f}{\partial t} + \dot{\mathbf{r}} \cdot \frac{\partial f}{\partial \mathbf{r}} + \dot{\mathbf{k}} \cdot \frac{\partial f}{\partial \mathbf{k}} = - \frac{f(\mathbf{r}, \mathbf{k}, t) - f_0(\mathbf{r}, \mathbf{k})}{\tau(\mathbf{k})}$$

- Relaxation time approximation
- Non-equilibrium state f decays to f_0

A definite time direction is present

→ The collision term should reverse its sign under time-reversal operation

Boltzmann equation

The distribution function

$$\dot{\mathbf{k}} \cdot \frac{\partial f}{\partial \mathbf{k}} = -\frac{f - f_0}{\tau} \rightarrow f = \sum_{\alpha=0}^{\infty} \left(-\tau \dot{\mathbf{k}} \cdot \nabla_{\mathbf{k}} \right)^{\alpha} f_0$$

Boltzmann equation

The distribution function

$$\dot{\mathbf{k}} \cdot \frac{\partial f}{\partial \mathbf{k}} = -\frac{f - f_0}{\tau} \rightarrow f = \sum_{\alpha=0}^{\infty} (\tau \mathbf{E} \cdot \nabla_{\mathbf{k}})^{\alpha} f_0$$

Linear longitudinal response

Integrate the charge current operator $-e\mathbf{v}$ in k -space:

$$\begin{aligned}j_x &= \frac{1}{(2\pi)^3} \int d\mathbf{k} (-ev_x) \tau \frac{eE_x}{\hbar} \partial_{k_x} f_0 \\&= -\frac{e^2\tau}{\hbar} \frac{1}{(2\pi)^3} \int d\mathbf{k} v_x \frac{\partial f_0}{\partial \varepsilon} \frac{\partial \varepsilon}{\partial k_x} E_x \\&= -\frac{e^2\tau}{(2\pi)^3} \int d\mathbf{k} v_x^2 \frac{\partial f_0}{\partial \varepsilon} E_x\end{aligned}$$

The red part denotes the longitudinal conductivity σ_{xx}

$$j_x = \sigma_{xx} E_x$$

Linear Hall effect

Outline

Classical picture

Wave packet

Linear response

Summary

Summary

- Classical picture of the charge current: Drude model
- Wave packet
- Lagrangian and Euler-Lagrange equation