# Semiclassical Electron Transport

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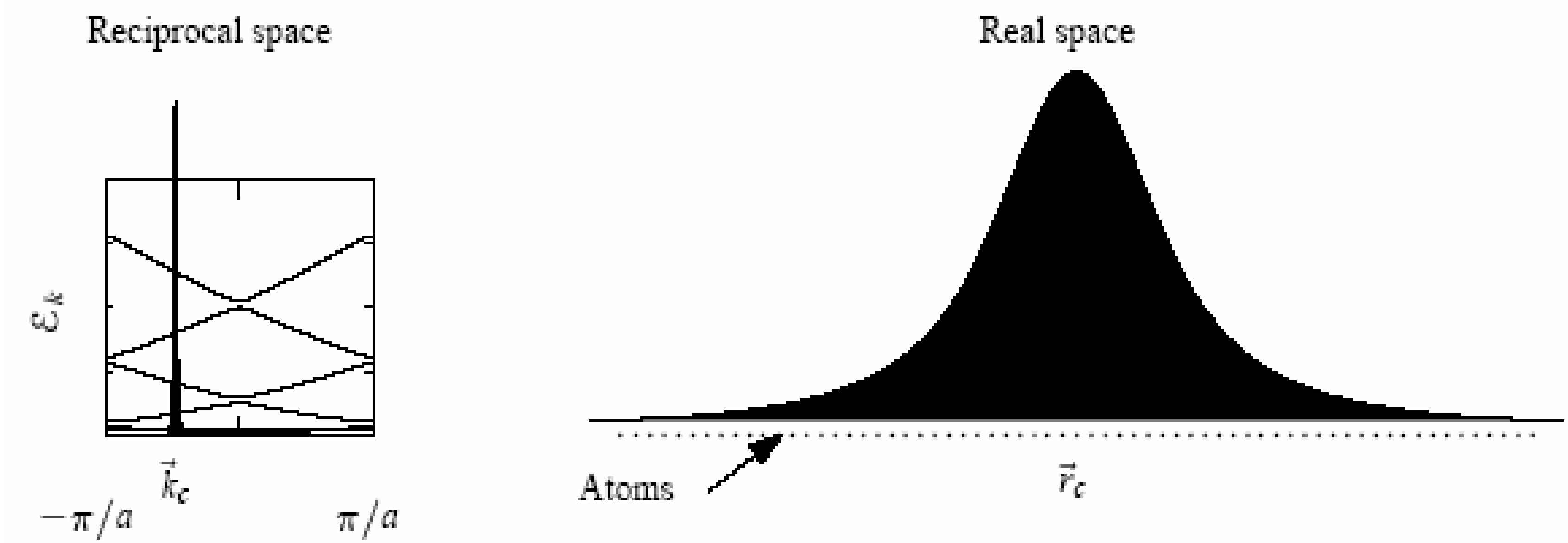
**PHYS 624: Introduction to Solid State Physics**
**http://www.physics.udel.edu/~bnikolic/teaching/phys624/phys624.html**

# Quasiparticle Propagation: Bloch Wavepackets

- Wavepackets represent quasiparticle localized in space:




- In the weak external field we can neglect the transitions between different bands → fix the zone index n=const.

$$\Psi(\vec{r}) = \sum_{\vec{k}} C_{\vec{k}}(t)\Phi_{\vec{k}}(\vec{r})$$

# Semiclassical Dynamics of Bloch Wavepackets

- Wavepacket in external field described by potential $W_{ext}(\vec{r})$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r}) + W_{ext}(\vec{r})\right]\Psi(\vec{r}) = i\hbar\frac{\partial\Psi}{\partial t} \Leftrightarrow \sum_{\vec{k}} C_{\vec{k}}(t)\left[\varepsilon(\vec{k}) + W_{ext}(\vec{r})\right]\Phi_{\vec{k}}(\vec{r}) = i\hbar\frac{\partial\Psi}{\partial t}$$

- Introduce new operator $\varepsilon(-i\nabla)$

- Band energy is periodic function in the reciprocal space $\varepsilon(\vec{k}) = \sum_{\vec{R}} \varepsilon_{\vec{R}} e^{i\vec{R}\vec{k}}$

$$\varepsilon(-i\nabla)\Phi_{\vec{k}}(\vec{r}) = \sum_{\vec{R}} \varepsilon_{\vec{R}} e^{\vec{R}\nabla}\Phi_{\vec{k}}(\vec{r}) = \sum_{\vec{R}} \varepsilon_{\vec{R}} \Phi_{k}(\vec{r}+\vec{R}) = \sum_{\vec{R}} e^{i\vec{k}\vec{R}} \varepsilon_{\vec{R}} \Phi_{\vec{k}}(\vec{r}) = \varepsilon(\vec{k})\Phi_{\vec{k}}(\vec{r})$$

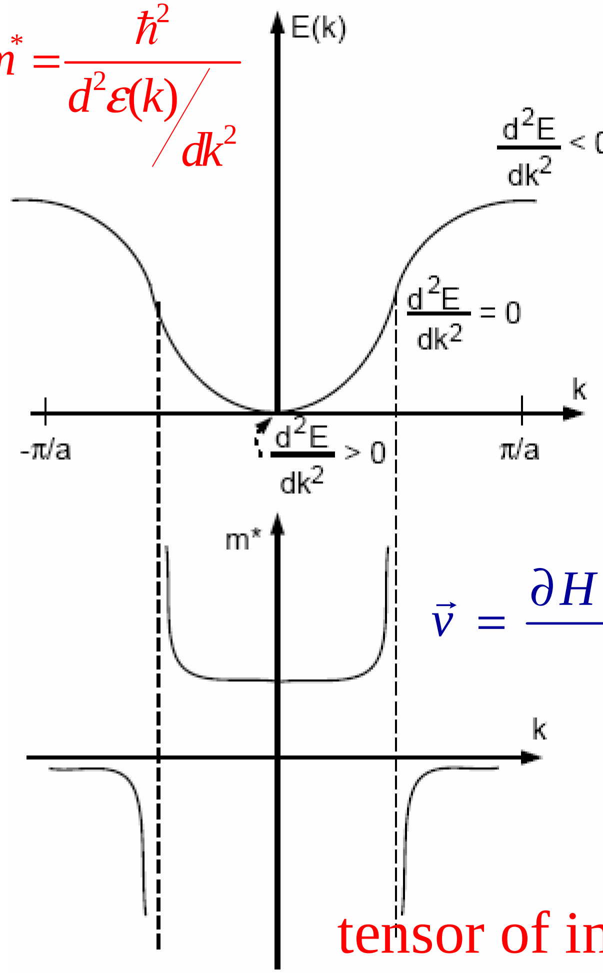
$$\sum_{\vec{k}} C_{\vec{k}}(t)\left[\varepsilon(-i\nabla) + W_{ext}(\vec{r})\right]\Phi_{\vec{k}}(\vec{r}) = i\hbar\frac{\partial\Psi}{\partial t} \Leftrightarrow \left[\varepsilon(-i\nabla) + W_{ext}(\vec{r})\right]\Psi(\vec{r}) = i\hbar\frac{\partial\Psi(\vec{r})}{\partial t}$$

- Electron in a crystal represented as wavepacket of Bloch states propagates as a "free" quasiparticle with charge $-e$, energy $\varepsilon(\vec{k})$, and Hamiltonian $\varepsilon(-i\nabla)$:

$$\left[\hat{\vec{P}}, \varepsilon(-i\nabla)\right] = 0$$

# Hamiltonian, Velocity, and Effective Mass of Bloch Electron

$$m^* = \frac{\hbar^2}{d^2\varepsilon(k)/dk^2}$$




- Ehrenfest theorem: Schrödinger evolution of the center of wavepacket can be obtained from the trajectory of the corresponding classical particle:

correspondence principle: $-i\nabla \rightarrow \frac{p}{\hbar}$

$$H(\vec{r}, \vec{p}) = E\left(\frac{\vec{p}}{\hbar}\right) + W_{ext}(\vec{r})$$

$$\vec{v} = \frac{\partial H(\vec{r}, \vec{p})}{\partial \vec{p}} = \frac{1}{\hbar}\frac{\partial \varepsilon(\vec{k})}{\partial \vec{k}} \qquad \vec{a} = \frac{d}{dt}\left(\frac{1}{\hbar}\frac{\partial \varepsilon(\vec{k})}{\partial \vec{k}}\right) = \left(\frac{1}{\hbar^2}\frac{\partial^2 \varepsilon(\vec{k})}{\partial \vec{k}\partial \vec{k}}\right)\frac{\partial \hbar \vec{k}}{\partial t}$$

$$\frac{\partial \hbar \vec{k}}{\partial t} = -\frac{\partial H}{\partial \vec{r}} = -\nabla W_{ext}(\vec{r})$$

tensor of inverse effective mass: $\left(\frac{1}{m}\right)_{\alpha\beta} = \left(\frac{1}{\hbar^2}\frac{\partial^2 \varepsilon(\vec{k})}{\partial k_\alpha \partial k_\beta}\right)$

# Limitations of Semiclassical Dynamics

- The spatial scale of all external potentials must be much larger than interatomic spacing, making it possible to construct wave packets spanning many unit cells, but seeing the external potential as very slowly varying

- The magnitude of the electric field cannot be too large, or else they induce Zenner tunneling between bands (electrons are quite effective in screening external fields so this strengths are hard to achieve in metals):

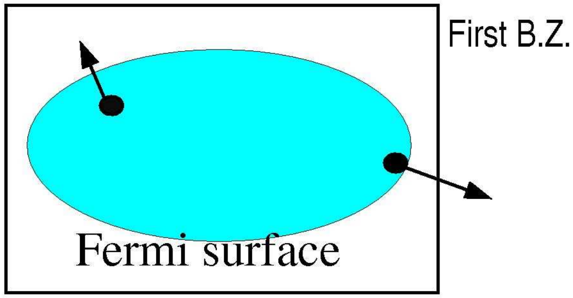
$$\frac{eE}{k_F} \ll \varepsilon_{gap}\sqrt{\frac{\varepsilon_{gap}}{\varepsilon_F}}$$

- The magnitude of magnetic fields cannot be too large: $\frac{\hbar eB}{m} \ll \varepsilon_{gap}\sqrt{\frac{\varepsilon_{gap}}{\varepsilon_F}}$

- The fields must be slowly varying to avoid excitations $\hbar\omega = \varepsilon_{gap}$ across the gap.

# Currents in Bands: Insulators

- Add Pauli principle to Bloch electron propagation under the influence of an applied electric field




$$\vec{j} = -\frac{e}{8\pi^3\hbar} \int_{First\ BZ} \nabla_{\vec{k}} \varepsilon(\vec{k}) \frac{1}{(2\pi)^3} d^3\vec{k}$$

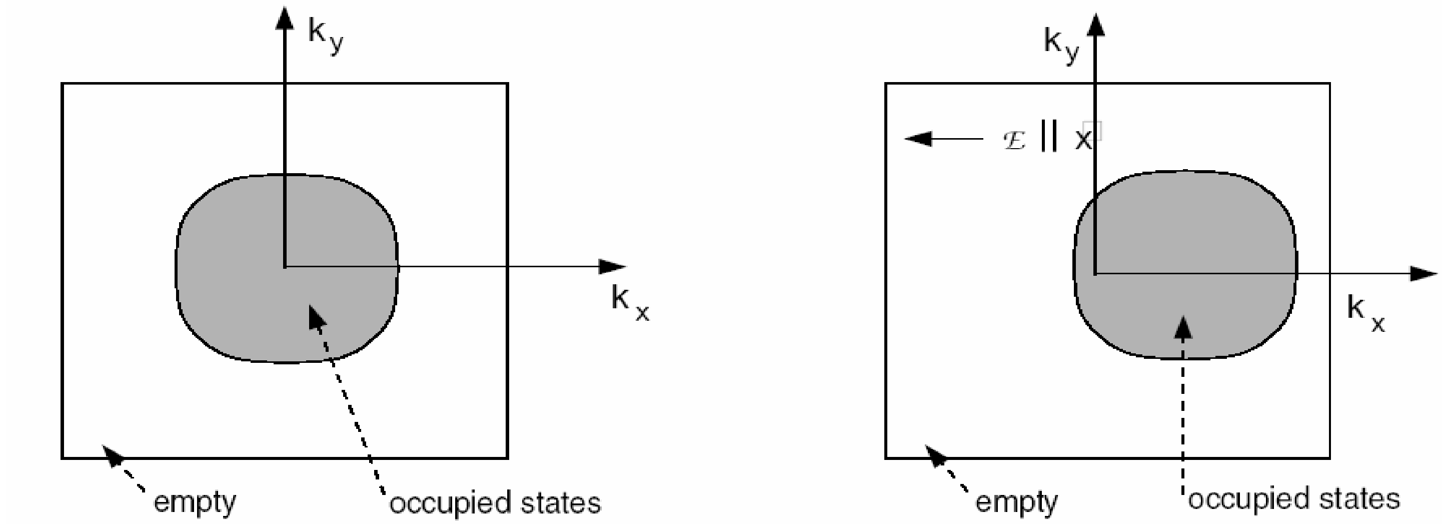
- **Full band of states is insulating!**

$$\text{time reversal invariance:} \varepsilon_{\uparrow}(\vec{k}) = \varepsilon_{\downarrow}(-\vec{k}) \Rightarrow \varepsilon(\vec{k}) = \varepsilon(-\vec{k})$$

$$\vec{v}_{-\vec{k}} = \frac{1}{\hbar} \nabla_{-\vec{k}} \varepsilon(-\vec{k}) = -\nabla_{\vec{k}} \varepsilon(\vec{k}) = -\vec{v}_{\vec{k}} \Rightarrow \vec{j} \equiv 0 \text{ for insulator}$$

# Currents in a Band: Metals

❑Fermi sea of a partially filled band will shift under the influence of an applied electric field → this destroys inversion symmetry of the Fermi sea therefore causing a net current:

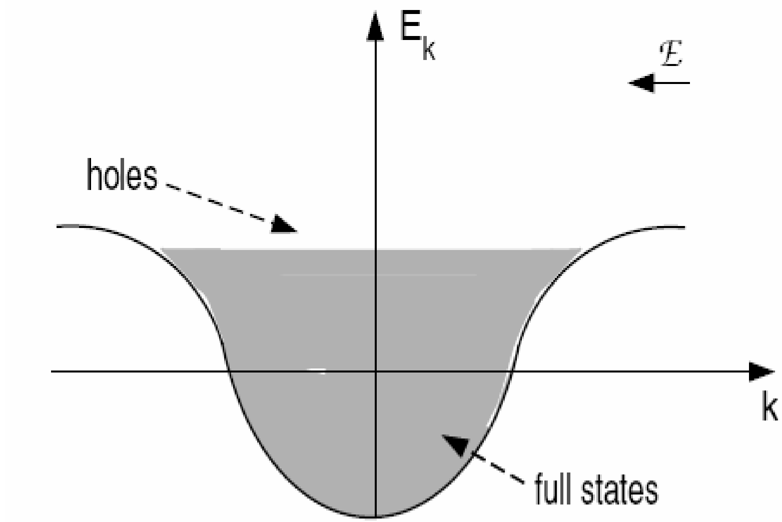


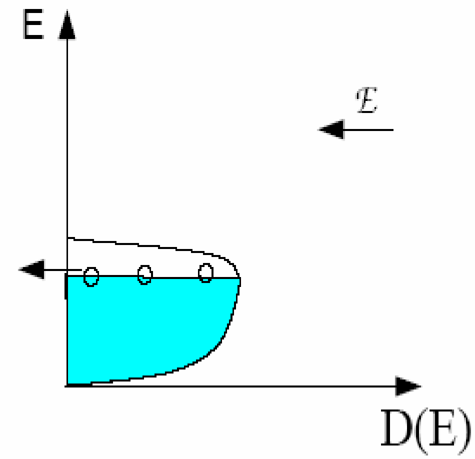

$$\vec{j} = -\frac{e}{8\pi^3\hbar} \int_{Occupied\ \vec{k}} \nabla_{\vec{k}}\varepsilon(\vec{k}) \frac{1}{(2\pi)^3} d^3\vec{k} \qquad \vec{j} = \frac{e}{8\pi^3\hbar} \int_{Empty\ \vec{k}} \nabla_{\vec{k}}\varepsilon(\vec{k}) \frac{1}{(2\pi)^3} d^3\vec{k}$$

$$\vec{j} = -\frac{e}{8\pi^3\hbar} \int_{First\ BZ} \nabla_{\vec{k}}\varepsilon(\vec{k}) \frac{1}{(2\pi)^3} d^3\vec{k} - \frac{-e}{8\pi^3\hbar} \int_{Empty\ \vec{k}} \nabla_{\vec{k}}\varepsilon(\vec{k}) \frac{1}{(2\pi)^3} d^3\vec{k}$$

# Properties of Holes

- A nearly full simple band has states near the Fermi surface that can be thermally or electrically excited of a negative mass → Density of states with holes at the top of the band which have positive charge and positive mass

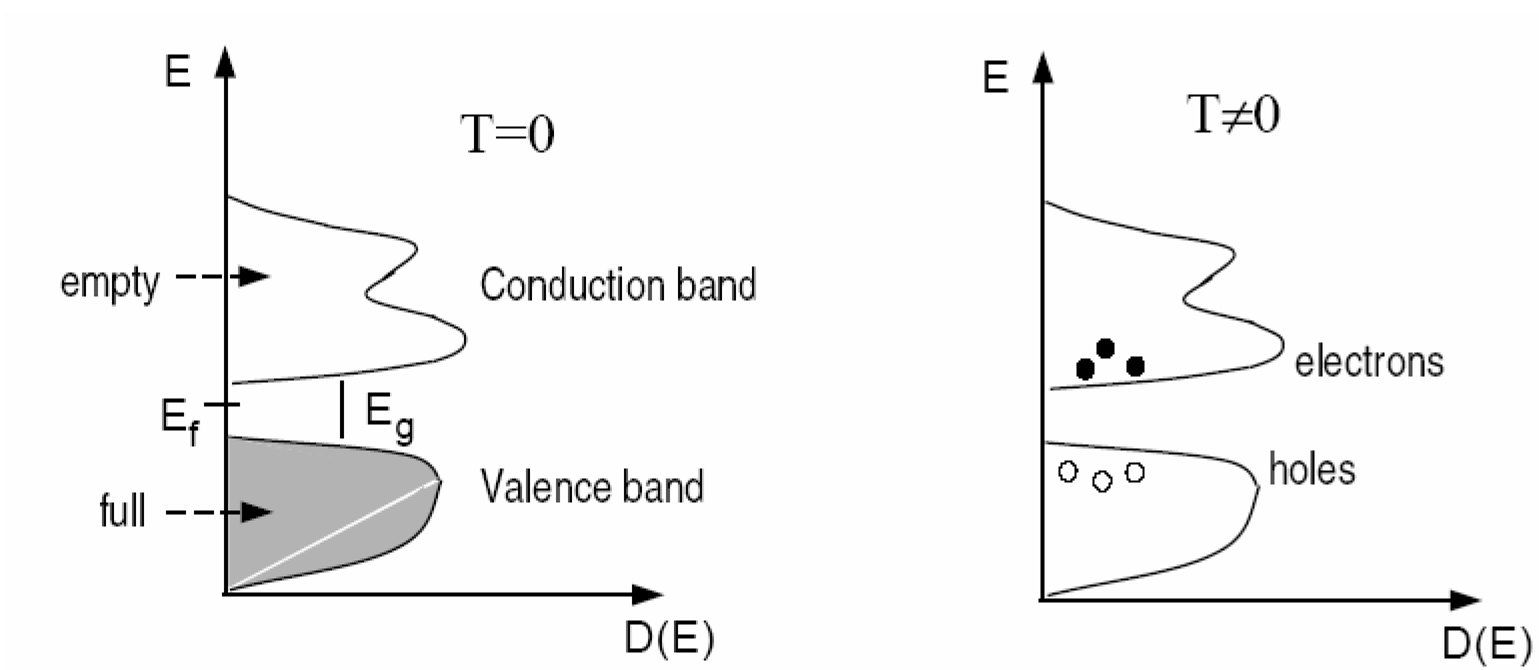



$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2\varepsilon(k)}{dk^2} \Rightarrow m^*_{top} = \hbar^2\left(\left[\frac{d^2\varepsilon(k)}{dk^2}\right]_{k=\pm\pi/a}\right)^{-1} = \frac{\hbar}{2ta^2} < 0$$

$$\varepsilon_{top} = \varepsilon_0 - 2t + ta^2k^2 = \varepsilon_0 - 2t + \frac{\hbar^2k^2}{2m^*} \Rightarrow \dot{v} = \frac{1}{\hbar}\frac{d}{dt}\nabla_k\varepsilon(k) = \frac{eE}{|m^*|}$$

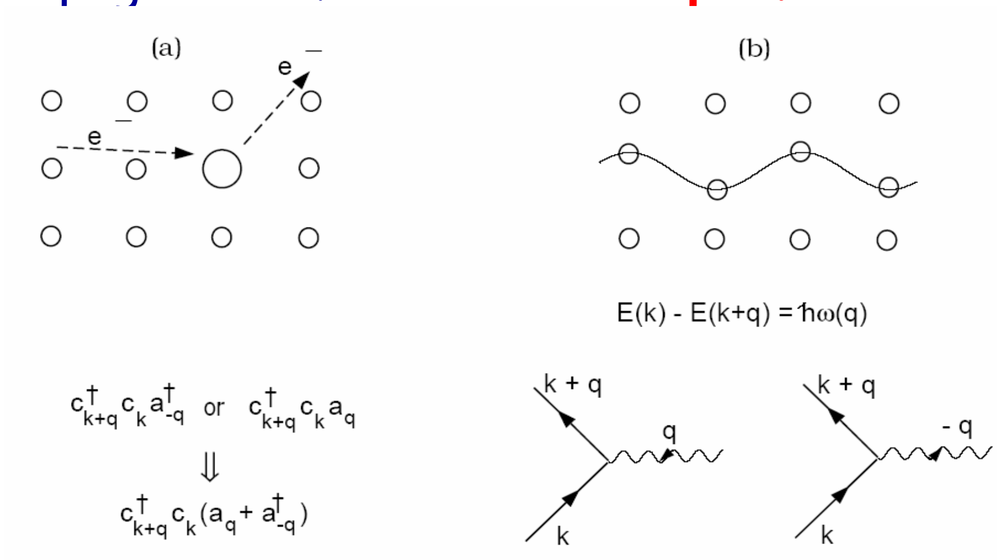
# Currents in Many Bands: Insulators at Finite Temperature

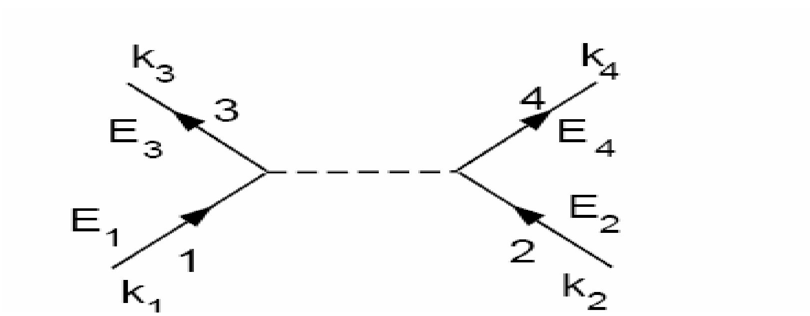



❑An insulator forms when Fermi energy falls within the gap of the density of states → as the temperature is raised, electrons are promoted over the gap $n \sim e^{-E_g/k_B T}$ and both electrons and holes contribute to the conductivity which increases with temperature.

# Sources of Electric Resistivity

- Bloch states are stationary states that describe unperturbed propagation of electrons → **perfect lattice yields no resistivity!**

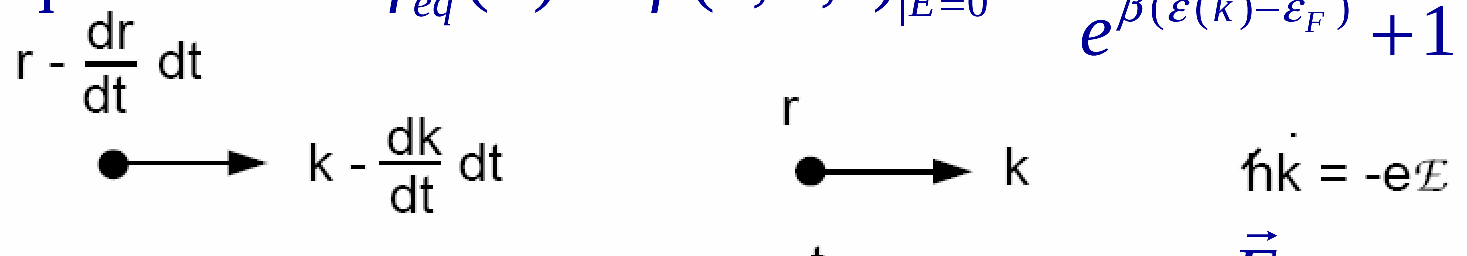


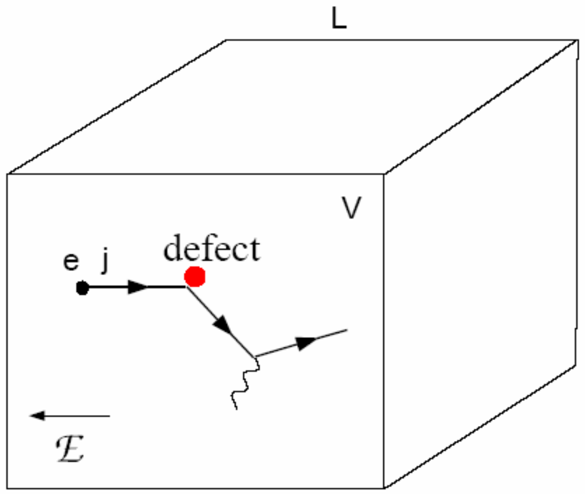

- Resistivity is dominated by the scattering off the deviations from a perfect lattice: defects and lattice vibrations=phonons
- Resistivity arises also due to electron-electron interactions (from simple order of magnitude arguments based on relative strength of the interactions, their contribution should dominate but due to the Pauli principle it does not).

# Distribution Function In and Out of Equilibrium

equilibrium: $f_{eq}(k) = f(r,k,t)_{|E=0} = \dfrac{1}{e^{\beta(\varepsilon(k)-\varepsilon_F)}+1}$




no scattering: $f(\vec{r},\vec{k},t) = f\left(\vec{r}-\vec{v}dt, \vec{k}+\dfrac{e\vec{E}}{\hbar}dt, t-dt\right)$




$$f(\vec{r},\vec{k},t) = f\left(\vec{r}-\vec{v}dt, \vec{k}+\frac{e\vec{E}}{\hbar}dt, t-dt\right) + \left(\frac{\partial f}{\partial t}\right)_{scattering} dt$$

$$n(\vec{r}) = -\frac{e}{8\pi^3}\int d\vec{k}\; f(\vec{r},\vec{k},t)$$

$$j(\vec{r}) = -\frac{e}{8\pi^3}\int d\vec{k}\; v(\vec{k})\, f(\vec{r},\vec{k},t)$$

# Boltzmann Equation

$$f(\vec{r},\vec{k},t) = f(\vec{r},\vec{k},t) - \vec{v}\frac{\partial}{\partial \vec{r}} + \frac{eE}{\hbar}\frac{\partial}{\partial \vec{k}} f - \frac{\partial}{\partial t} f + \left(\frac{\partial f}{\partial t}\right)_{scattering}$$

$$\frac{\partial}{\partial t} f + \vec{v}\frac{\partial}{\partial \vec{r}} f + \frac{eE}{\hbar}\frac{\partial}{\partial \vec{k}} f = \left(\frac{\partial f}{\partial t}\right)_{scattering}$$

- If the phonon and defect perturbations are small, time-independent, and described by Hamiltonian $\hat{H}$, then the scattering rate from a Bloch state $\vec{k}$ to $\vec{k}'$ (occupied to unoccupied) is $w_{\vec{k}'\vec{k}} = 2\pi \left|\left\langle \vec{k}' \middle| \hat{H} \middle| \vec{k} \right\rangle\right|^2 / \hbar$

$$\left(\frac{\partial f}{\partial t}\right)_{scattering} = \frac{V}{(2\pi)^3}\int d\vec{k}' \left[(1 - f(\vec{k}))w_{\vec{k}\vec{k}'} f(\vec{k}') - (1 - f(\vec{k}'))w_{\vec{k}'\vec{k}} f(\vec{k})\right]$$

- **The Boltzmann equation is valid under assumptions of semi-classical transport:** Effective mass approximation (which incorporates the quantum effects due to periodicity of the crystal); Born approximation for the collisions, in the limit of small perturbation for the electron-phonon interaction and instantaneous collisions; no memory effects, i.e. no dependence on initial condition terms. The phonons are usually treated as in equilibrium, although the condition of non-equilibrium phonons may be included through an additional equation.

# Relaxation Time Approximation

- Ansatz: The rate at which a system returns to equilibrium is proportional to its deviation from equilibrium (i.e., we make the assumption that scattering merely acts to drive a non-equilibrium system back to equilibrium):

$$\left(\frac{\partial f}{\partial t}\right)_{scattering} = -\frac{f(\vec{k}) - f_{eq}(\vec{k})}{\tau(\vec{k})}$$

- If $E \neq 0, t < 0$ and then at $t \geq 0, E \equiv 0$ the external electric field is switched off, then for a homogeneous system we find:

$$\left(\frac{\partial f}{\partial t}\right) = \left(\frac{\partial f}{\partial t}\right)_{scattering} = -\frac{f - f_{eq}}{\tau} \Rightarrow f - f_{eq} = \left[f(t=0) - f_{eq}\right]e^{-t/\tau}$$

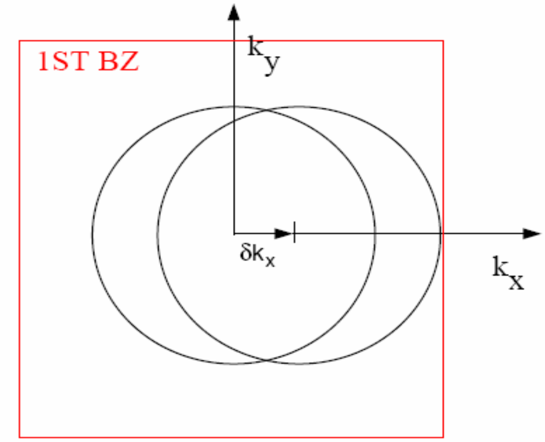
- In the steady state transport regime induced by a time-independent external electric field:

$$\left(\frac{\partial f}{\partial t}\right) = 0, \frac{\partial f}{\partial \vec{r}} = 0 \Rightarrow -\frac{e}{\hbar}\vec{E} \cdot \frac{\partial f}{\partial \vec{k}} = \left(\frac{\partial f}{\partial t}\right)_{scattering} = -\frac{f(\vec{k}) - f(\vec{k})}{\tau(\vec{k})}$$

$$f(\vec{k}) = f_{eq}(\vec{k}) + \frac{e}{\hbar}\tau(\vec{k})\vec{E} \cdot \frac{\partial f(\vec{k})}{\partial \vec{k}}$$

# Linear Semiclassical Response

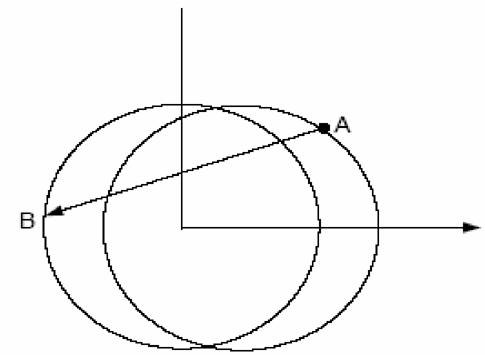
- For small electric field (Ohmic regime), the relaxation time approximation solution can be linearized:




$$f(k) \simeq f_{eq}(k) + \frac{e}{\hbar}\tau(\vec{k})\vec{E} \cdot \frac{\partial}{\partial k} f_{eq}(k)$$

$$\vec{E} = E_x \hat{\mathbf{x}} \Rightarrow f(k) \simeq f_{eq}\left(k + \frac{e}{\hbar}\tau(k)E_x\right)$$

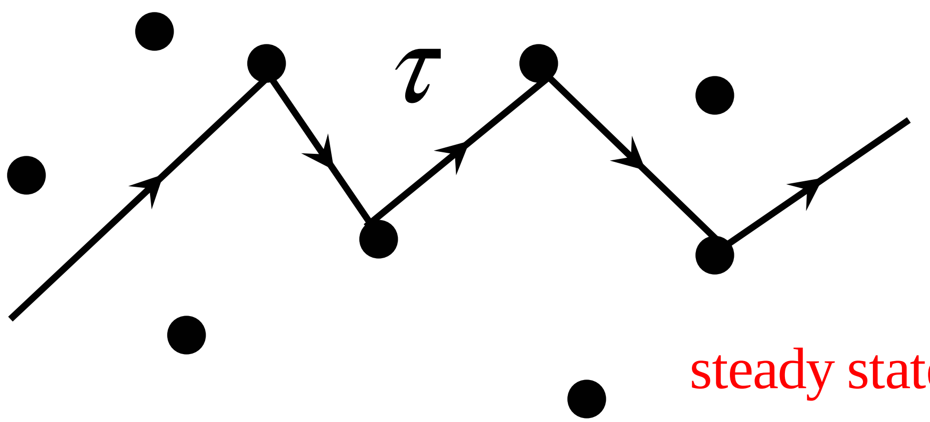
- According to the linear Boltzmann equation, the effect of the electric field $E_x$ is to shift the Fermi surface by $\delta k_x = -e\tau E_x / \hbar$




- Note that elastic scattering cannot restore equilibrium; rather they would cause Fermi surface to expand →inelastic scattering (i.e., from phonons) is needed to explain relaxation.

# Drude Conductivity: Naïve Derivation

- Drude (1900) assumptions: all electrons participate and electron-lattice scattering yields a scattering rate $\tau^{-1}$ which introduces the mean free time (or relaxation time or collision time which electrons travel, on average, between collisions):




$$m\dot{v} + \frac{m}{\tau}(v - v_{therm}) = -eE$$

drift velocity: $v - v_{therm} = v_{Drift}$

friction: $\frac{m}{\tau} v_D$

steady state: $v_D = -\frac{e\tau}{m}E \Rightarrow j = -env_D = \frac{ne^2\tau}{m}E$

Ohmic conductivity: $j = \sigma E \Leftrightarrow \sigma = \frac{ne^2\tau}{m}$

Mobility: $\sigma = \mu ne \Rightarrow \mu = \frac{e\tau}{m}$

# Drude Conductivity: Bloch-Boltzmann Derivation

❑Quantum Mechanics (1927) makes Drude reasoning problematic → not all electrons can participate in the conduction due to the Pauli principle!

$$\vec{j} = -\frac{e}{8\pi^3}\int d\vec{k}\, v(\vec{k})\, f(\vec{k}) \simeq -\frac{e}{8\pi^3}\int d\vec{k}\, v(\vec{k})\left[ f_{eq}(\vec{k}) + \frac{e\tau(\vec{k})}{\hbar} E_x \frac{\partial f_{eq}}{\partial k_x}\right]$$

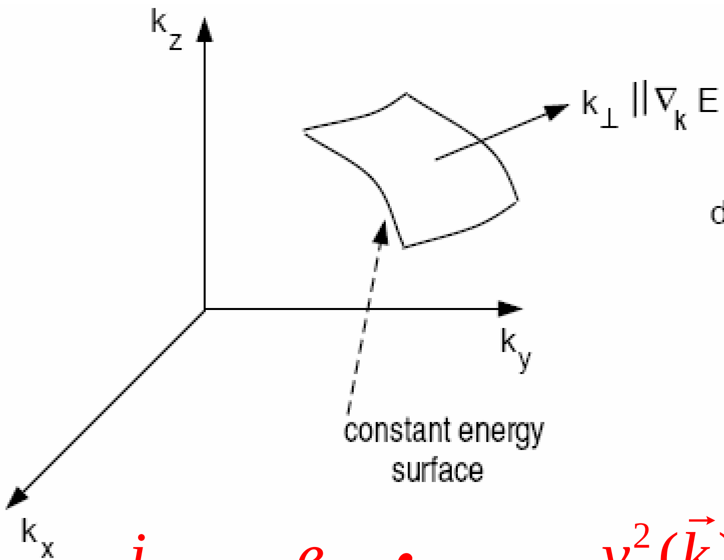
isotropic material: $j_y = j_z = 0$

$$\vec{v}_{-\vec{k}} = -\vec{v}_{\vec{k}} \Rightarrow \int \vec{v}_{\vec{k}}\, f_{eq}(\vec{k}) d\vec{k} = 0$$

$$\frac{\partial f_{eq}(\vec{k})}{\partial k_x} = \frac{\partial f}{\partial E}\frac{\partial E}{\partial k_x} = \frac{\partial f_{eq}}{\partial E}\hbar v_x \simeq -\delta(E - E_F)\hbar v_x$$

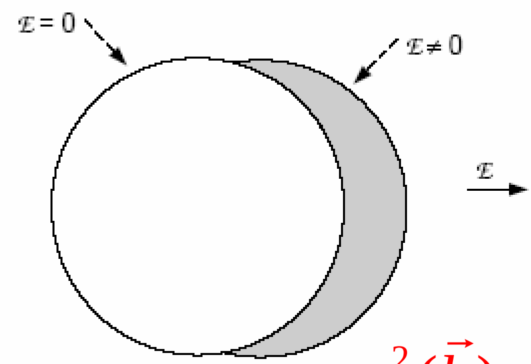
$$j_x \simeq -\frac{e}{8\pi^3} E_x \int d\vec{k}\, v_x^2 \tau(\vec{k}) \frac{\partial f_{eq}}{\partial E} = \sigma E_x$$

# Drude-Boltzmann Conductivity as a Fermi Surface Property




$$d\vec{k} = dS_E dk_\perp = dS_E \frac{dE}{\hbar v(\vec{k})}$$

$$dk_\perp = \frac{dE}{|\nabla_k E|}$$




$$\sigma = \frac{j_x}{E_x} = \frac{e}{8\pi^3\hbar}\int dS_E dE \frac{v_x^2(\vec{k})}{v(\vec{k})}\tau(\vec{k})\delta(E-E_F) = \frac{e}{8\pi^3\hbar}\int_{E=E_F} dS_E \frac{v_x^2(\vec{k})}{v(\vec{k})}\tau(\vec{k})$$

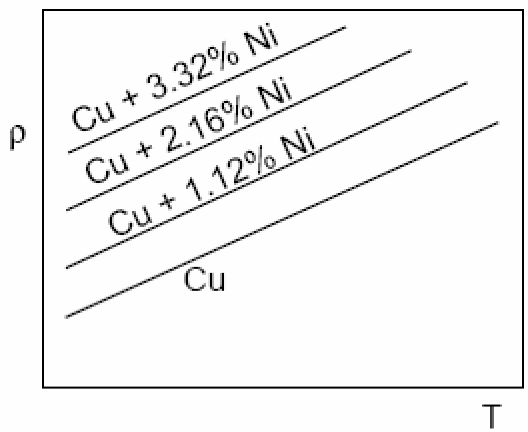
spherical Fermi surface: $\int_{E=E_F} dS_E \frac{v_x^2(\vec{k})}{v(\vec{k})}\tau(\vec{k}) = \frac{4\pi}{3}k_F^3\tau(E_F)v(E_F) = \frac{4\pi}{3}k_F^3\tau(E_F)\frac{\hbar k_F}{m^*}$

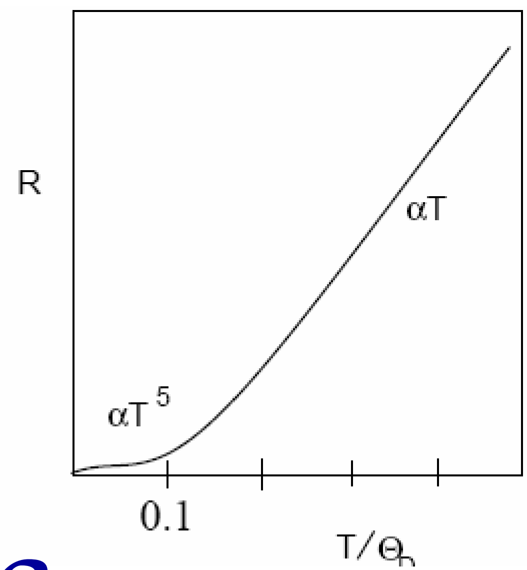
$$\sigma = \frac{e^2}{8\pi^3\hbar}\frac{4\pi}{3}k_F^3\tau(E_F)\frac{\hbar k_F}{m^*} \overset{k_B T \ll E_F}{\underset{k_F^3 = 3\pi^2 n}{=}} \frac{e^2\tau(E_F)}{m^*}n$$

# Temperature Dependence of Drude-Boltzmann Conductivity

❑ Mattheiesen Rule: the phonon and defect scattering mechanism are independent

$$\frac{1}{\tau} = \frac{1}{\tau_{phonon}} + \frac{1}{\tau_{defect}} \Rightarrow \rho = \rho_{phonon} + \rho_{defect}$$




$$T \gg T_{Debye} \Rightarrow \rho = aT + \rho_{defect}$$

# Drift-Diffusion approximation to Boltzmann Equation for Semiconductors

- The drift-diffusion equations are derived introducing the mobility $\mu = e\tau / m^*$ and replacing $\langle v^2 \rangle = k_B T / m^*$ with its average equilibrium value, therefore neglecting thermal effects. The diffusion coefficient $D = \mu k_B T / e$ (Einstein's relation) is also introduced, and the resulting drift-diffusion current is:

$$j_n = e\mu_n n(x) E(x) + eD_n \frac{dn(x)}{dx}$$

$$j_p = e\mu_p p(x) E(x) - eD_p \frac{dp(x)}{dx}$$

$$\text{Continuity:} \begin{cases} \dfrac{\partial n}{\partial t} = \dfrac{1}{e} \nabla j_n + U_n \\ \dfrac{\partial p}{\partial t} = -\dfrac{1}{e} \nabla j_p + U_p \end{cases}$$

$$\text{Poisson: } \nabla^2 V = \frac{q(n - p + N_A^- - N_D^+)}{\varepsilon_0}$$

- The choice of equilibrium (thermal) velocity means that the drift-diffusion equations are only valid for very small perturbations of the equilibrium state (low fields).

- The validity of the drift-diffusion equations is empirically extended by introducing field-dependent mobility $\mu(E)$ and diffusion coefficient $D(E)$, obtained from empirical models or detailed calculations.