XIV. More on Transport Properties

A. Looking at $\sigma = \frac{ne^2\tau}{m}$ again

Drude

- didn't know QM
- m = bare electron mass
- τ = collision time

  thought that electrons would scatter off the regular array of ions

Quantum Theory + periodic $V(\vec{r})$ ⇒ Band theory

- $\mathcal{E}_n(\vec{k}) = \mathcal{E}_n(-\vec{k})$; $\vec{v}_n(\vec{k}) = -\vec{v}_n(-\vec{k})$
- Completely filled bands do NOT contribute to electrical conduction ($\because \vec{J} = 0$ always for filled bands) even in the presence of $\vec{\mathcal{E}}$.
- $\sigma = \frac{ne^2\tau}{m^*}$ in cases where m^* can represent band effects
- τ: due to deviations from perfect periodicity

- With band theory ⇒ idea of Fermi surface (FS)
- $$\frac{d(\hbar\vec{k})}{dt} = \vec{F}_{ext} = -e\vec{\mathcal{E}} - \underbrace{\frac{(\hbar\vec{k})}{\tau}}_{\text{damping term due to scatterings}}$$

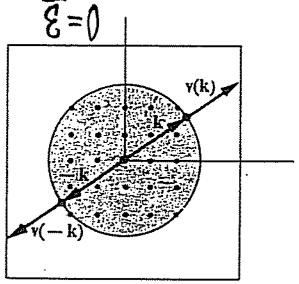
$-e\vec{\mathcal{E}}$ tends to continuously shift FS in k-space

damping term tends to counteract the shift

⇒ Net effect is a steady state corresponding to a shifted FS with every state shifted by

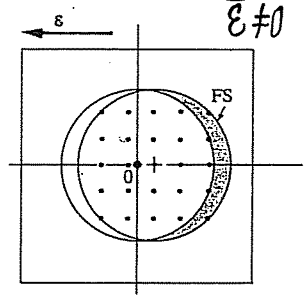
$$\delta k_x = -\frac{e\mathcal{E}}{\hbar}\tau \qquad (\vec{\mathcal{E}} = \mathcal{E}\hat{x})$$

$\vec{\mathcal{E}} = 0$



Cancellation of $\vec{v}_n(\vec{k})$ of occupied states ⇒ $\vec{J}_e = 0$

$\vec{\mathcal{E}} \neq 0$



Some occupied states are not compensated ⇒ $\vec{J}_e \neq 0$

[same physics for more complicated Fermi surfaces]

- Un-compensated states are those states near the Fermi surface at $\vec{\mathcal{E}}=0$ $\Rightarrow$ expect σ to be very sensitive to $\underbrace{g(E_F)}_{\text{DOS at } E_F}$ (Note: $\delta k_x \ll k_F$)

- <u>Write σ in terms of $g(E_F)$</u>

$J_x =$ contributions due to uncompensated electrons

$$= (-e)\underbrace{\overline{v_{F,x}}}_{\text{some averaged value of } x\text{-component of Fermi velocity}} \cdot (\text{concentration of uncompensated electrons})$$

$$= (-e)\overline{v_{F,x}} \cdot g(E_F)\underbrace{\delta\mathcal{E}}_{\text{range of energy near } E_F \text{ affected}} \quad (\text{note}^{+})$$

band

$$= (-e)\overline{v_{F,x}}\, g(E_F)\underbrace{\left(\frac{\partial \mathcal{E}}{\partial k_x}\right)_{E_F}}_{\hbar v_{F,x}}\underbrace{\delta k_x}_{\hookrightarrow -\frac{e\mathcal{E}}{\hbar}\tau}$$

$\vec{\mathcal{E}}$-field

$$= \underbrace{e^2\, \overline{v_{F,x}^2}\, \tau_F\, g(E_F)}_{\sigma}\, \mathcal{E}$$

σ (indicates that it is <u>a Fermi surface effect</u>)

τ may depend on energy of states

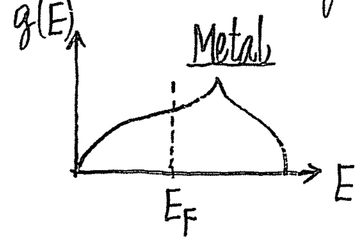
$^{+}$ $g(E_F)$ is the DOS per unit volume, since we need to get the concentration of uncompensated electrons. Thus, it differs from our previous DOS by $1/V$.

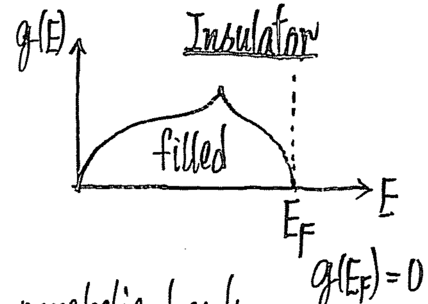
If FS is spherical, $\overline{v_{F,x}^2} = \overline{v_{F,y}^2} = \overline{v_{F,z}^2} = \frac{1}{3}v_F^2$.

Then $$\boxed{\sigma = \frac{1}{3}e^2 v_F^2 \tau_F\, g(E_F)} \qquad (*)$$

contain band effects

(i) This result brings out <u>the importance of $g(E_F)$</u> in determining σ.





(ii) For spherical FS and thus parabolic bands, recall:

$$E_F = \frac{\hbar^2}{2m^*}k_F^2 = \frac{\hbar^2}{2m^*}(3\pi^2 n)^{2/3} = \frac{1}{2}m^* v_F^2$$

$$g(E_F) = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\sqrt{E_F}$$

Using $(*)$, $$\sigma = \frac{ne^2\tau}{m^*}$$

(iii) $(*)$ can be generalized to cases with more complicated FS shapes.

B. $\rho(T)$ of a metal

- $\sigma = \frac{ne^2\tau}{m^*}$; $\rho = \frac{m^*}{ne^2}\left(\frac{1}{\tau}\right)$
- $\frac{1}{\tau}$ can, in principle, be calculated using QM (Fermi Golden rule) for a given mechanism
- Phenomenologically,

$$\frac{1}{\tau} = \sum_{\text{mechanisms}} \frac{1}{\tau_i} \quad \text{(resistances in series)}$$

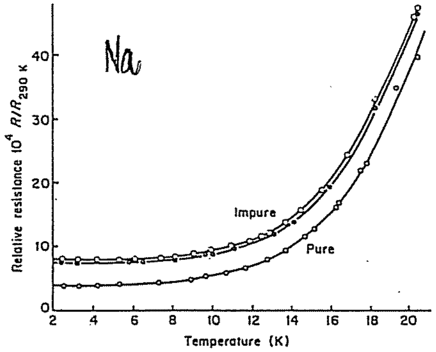
$$\boxed{\text{Mattheisen's rule}} \quad = \underbrace{\frac{1}{\tau_{phonon}}}_{\text{(el-phonon)}} + \underbrace{\frac{1}{\tau_{impurity}}}_{\text{(el-imp)}} + \underbrace{\frac{1}{\tau_{boundary}}}_{\text{(el-boundary)}} + \cdots$$

- Some mechanisms show strong temperature dependence e.g. phonons
- some don't have temperature dependence, e.g. impurities

$$\therefore \rho = \frac{m^*}{ne^2}\left(\frac{1}{\tau}\right) = \underbrace{\rho_0}_{\substack{\text{residual resistivity}\\ (T\to 0 \text{ value})}} + \underbrace{\rho_I(T)}_{\text{ideal resistivity}}$$

$\frac{1}{\tau_{impurity}} \sim$ No temperature dependence ; $\frac{1}{\tau_{phonon}} \sim N_{phonon}$ (has T-dependence)

$\rho(T)$ of a metal:



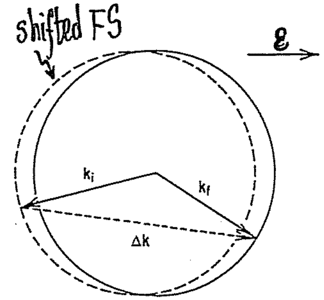
Similar T-dependence for samples of different degrees of impurities

$\Rightarrow$ el-impurity and el-phonon mechanisms act independently

(Mattheisen's rule)

Key Point:

Effective processes that lead to electrical resistivity



Electric-current carrying state with typical relaxation processes

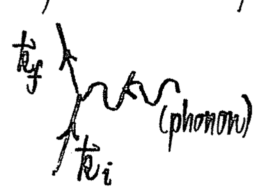
- effective in leading to large change in momentum (e.g. from one side of Fermi surface to another)

At high temperatures†: $T \gg \theta_D$

θ_D: Debye temp. (phonon)

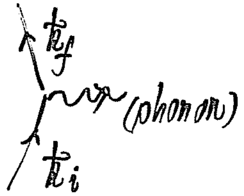
- Electron-phonon interaction plays dominant role

Important el-ph processes:



phonon absorption

$$\hbar\vec{k}_i + \hbar\vec{q} = \hbar\vec{k}_f$$



phonon emission

$$\hbar\vec{k}_i = \hbar\vec{k}_f + \hbar\vec{q}$$

- Maximum energy change of an electron

$\approx$ maximum possible phonon energy

$$\approx \hbar\omega_D = k_B\theta_D$$

k_B: Boltzmann constant; θ_D: Debye temperature

But $k_B\theta_D \ll E_F$ = energy of an electron on Fermi surface

$\Rightarrow$ only electrons close to Fermi surface can be scattered by phonons (we need vacant states with energy $k_B\theta_D$ near E_F) (that's why $g(E_F)$ is important)

† See p. XIII-50

- For $T \gg \theta_D$,

$$\underbrace{q \text{ of phonons} \approx \frac{\pi}{a}}_{\text{sufficient momentum to cause large-momentum transfer collisions that produce electrical resistance}}$$

(modes with $q \sim \frac{\pi}{a}$ can be thermally excited)

- el-ph mechanism is dominant

$\Rightarrow \tau_{ph}$ shortest

$$\rho_I(T) = \frac{m_e}{ne^2\tau_{ph}} = \frac{m_e v_F}{ne^2 l_{ph}}$$

τ_{ph}: relaxation time due to el-ph scattering

l_{ph}: mean free path due to electron-phonon scattering

$$\boxed{\tau_{ph} \sim l_{ph} \sim \frac{1}{\text{Number of phonons present at temp. } T \text{ for scattering}}}$$

Recall: $U_{\text{phonon}}(T \gg \theta_D) \sim T$ so that $C \sim 3Nk_B$ at high T

$\Rightarrow$ Number of phonons $\sim T$

$\therefore \frac{1}{\tau_{ph}} \sim T$ (high T)

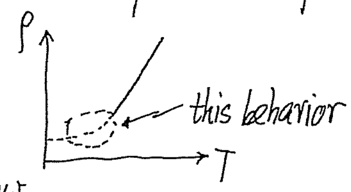
$$\boxed{\therefore \rho_I(T) \propto T \quad (T \gg \theta_D) \quad \text{due to el-ph scattering}}$$

At low temperatures ($T \ll \theta_D$)

ρ shows a more complicated temperature dependence

Often $\rho \sim T^n$ with $n \sim 5$

(but not all metals show this behavior)



Roughly, there are two key factors.

$$\underbrace{\frac{1}{\tau_{el\text{-}ph}}}_{\text{effective for causing resistance}} \sim \underbrace{(\#\,\text{phonons})}_{①} \cdot \underbrace{(\text{effectiveness of phonon to lead to resistance})}_{②}$$

① Recall for $T \ll \theta_D$, $U_{ph}(T) \sim T^4 \sim T^3 \cdot T$ and $C_{ph} \sim T^3$

$\#\,\text{phonons} \sim T^3$

② But for $T \ll \theta_D$, phonons have small wave vectors q → in general, not effective to change the direction of k of electrons

Only $\left(\frac{T}{\theta_D}\right)^2$ of scatterings are effective

$\therefore \frac{1}{\tau_{el\text{-}ph}} \sim T^5 \Rightarrow \rho_I \sim T^5$ at low temperature

Residual Resistivity ρ_0

At very low temperatures: thermal energy can't excite many phonons and phonons q very short

$\Rightarrow$ el-ph scattering doesn't lead to resistance

Then, impurity scattering and scattering with sample boundary take over

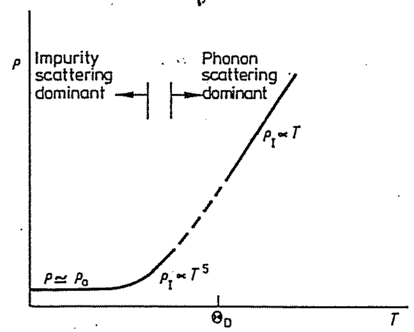
$$\frac{1}{\tau_{el\text{-}ph}} \ll \frac{1}{\tau_{imp}} \text{ or } \frac{1}{\tau_{boundary}}$$

$$\Rightarrow \rho = \frac{m^*}{ne^2\tau_{imp}} = \rho_0$$

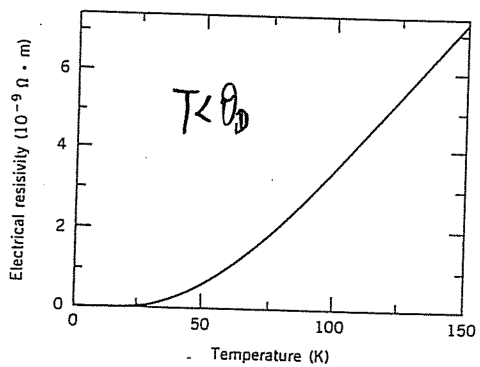
← residual resistivity

[If sample is very clean, then ρ_0 is governed by scatterings off the boundary.]

Schematically:



- Sometimes, for $T < \Theta_D$, the $\sim T^5$ dependence is <u>not</u> clearly seen, since <u>electron-electron scattering</u> gives a $\propto T^2$ dependence that shows up in the same temperature range!



Electrical resistivity of a metal as a function of temperature. For most of the temperature range shown electron-phonon scattering dominates and the resistivity is proportional to T. It does not vanish except perhaps at $T = 0$ K. Low-temperature values are too small to be seen on the graph.

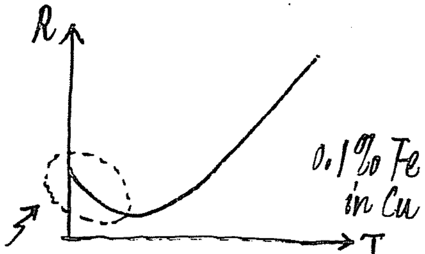
$$\rho = \rho_0 + \underset{\text{el-ph}}{AT^5} + \underset{\text{el-el scattering}}{BT^2}$$

$$\rho(T) = \underset{\text{residual}}{\rho_0} + AT^n + \underbrace{BT^2}_{\text{el-el}} \quad (\text{at low temp. } T \ll \Theta_D)$$

$n \sim 5$ for el-ph scattering

Remarks:

- <u>Kondo effect</u>
  - The observed $\rho(T)$ in some non-magnetic metals with a small amount of <u>magnetic impurity</u> (e.g. Fe impurity in Cu) is very different!



R↓ as T↑ (Kondo effect)

- el-impurity scattering shows special effects with magnetic impurities
- Spin-flip processes $\vec{k}\uparrow \rightarrow \vec{k}'\downarrow$

- <u>Semiconductors</u>
  - conductivity ↑ as T ↑
  - <u>NOT</u> playing with τ, but affecting n (number of carriers (electrons/holes) increases with T)
  - temperature dependence in n_e (and p_v) plays the dominant role, instead of $\tau(T)$.
  - See Ch. XIII.

Refs: Christman Sec. 9.3 - 9.5

C. Electron Contribution to Thermal Conduction

- $K(T)$ of typical metals

(i) Wiedemann-Franz "law"

• Conductors kept at a temperature difference

- electrons coming from a hotter region carry more thermal energy than those from a cooler region → net flow of heat

Recall: There is also a gas of phonons.

Kinetic theory (gas of electrons)

$$\boxed{K_{el} = \frac{1}{3} C_{el}\, v_F\, l_{th}}$$

C_{el}: electronic heat capacity ($\sim T$)

v_F: Fermi velocity

l_{th}: electron mean free path that is relevant to thermal conduction

$$l_{th} = v_F \cdot \tau_{th}^{(el)}$$

$\tau_{th}^{(el)}$: electron relaxation time for processes relevant to thermal conduction

Recall:

$$\sigma = \frac{ne^2\tau}{m}$$

τ: electron relaxation time for processes relevant to electrical conduction.

[large momentum changes for electrons]

Recall: $C_{el} = \frac{\pi^2}{3} k^2 g(\epsilon_F) T$ (see p. XI-(11)) specific heat (per unit volume)

$$= \frac{\pi^2}{2} n k_B \left(\frac{T}{T_F}\right)$$

$g(\epsilon_F) = \frac{\text{DOS at } \epsilon_F}{\text{Volume}}$

$$K_{el} = \frac{1}{3}\frac{\pi^2}{2} n k_B \left(\frac{T}{T_F}\right) v_F^2 \tau_{th}$$

$$= \frac{\pi^2}{6} n k_B \left(\frac{T}{T_F}\right) \frac{2}{m_e} \epsilon_F \tau_{th}$$

$$\Rightarrow \boxed{K_{el} = \frac{\pi^2 n k_B^2}{3 m_e} \underbrace{\left(T \cdot \tau_{th}\right)}_{\text{controls } K_{el}(T)}}$$

for C_V^{el}

$\sim T \cdot \tau_{th}$

$$\sigma = \frac{ne^2\tau}{m_e}$$

τ: $\tau_{\text{electrical conduction}}$

Lorenz number

$$\frac{K_{el}}{\sigma T} \doteq \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2 \cdot \left(\frac{\tau_{th}}{\tau}\right)$$

condition when the Wiedemann-Franz law is expected to be correct

$$\boxed{\text{if } \tau_{th}^{(el)} = \tau_{\text{electrical conduction}}}$$

$$= \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2$$

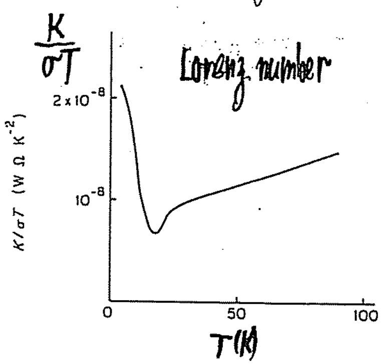
$$= 2.45 \times 10^{-8}\ \mathrm{W\Omega K^{-2}} \quad \text{(a constant)}$$

Wiedemann-Franz law

- Works well for metals at room temperature.

e.g. $2.33 \times 10^{-8}\ \mathrm{W\Omega K^{-2}}$ for Cu at 100°C.

- Deviations from Wiedemann-Franz "law" at certain temperature range indicate that the scattering processes relevant to thermal conduction and electrical conduction (both due to electrons) may be different in that temperature range.



Measured $\frac{K}{\sigma T}$ Vs T for sodium at low temperatures

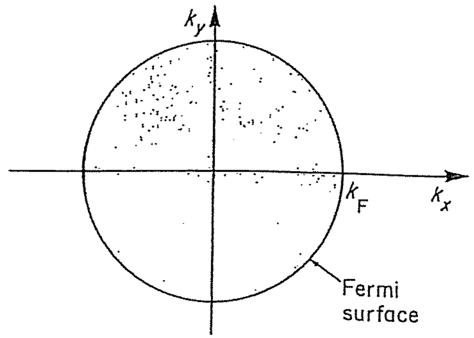
Electrical Conduction

- Phonons with large $\vec{q}$'s that lead to large momentum changes for the electrons → resistance
- Impurities (at low T)

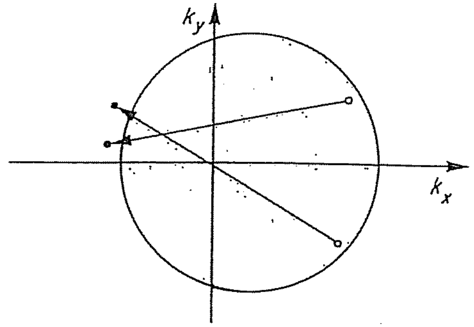
Thermal Conduction

- Even phonons with short $\vec{q}$'s are effective in leading to thermal resistance

Figure taken from Hook and Hall "Solid State Physics"

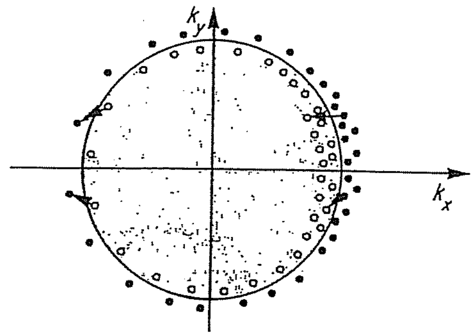


(a) Equilibrium Fermi sphere at $T = 0$.



electrical conduction

(b) Electric-current carrying state with typical relaxation processes



thermal conduction

(c) Heat-current-carrying state in a temperature gradient with small-momentum-change relaxation processes

Schematically showing electrons moving in one direction (positive k_x) are of a higher temperature than those moving in the other (negative k_x) direction.

(ii) $K(T)$ of a typical metal.

- at high temperatures ($T \gg \theta_D$) (recall: $K(\text{metal}) > K(\text{insulator})$ ∵ electrons' contribution)

  el-$\underbrace{\text{phonon}}_{\text{large } \vec{q}\text{'s phonons are available}}$ scatterings: dominant process [Wiedemann-Franz law holds]

  el-ph $\rightarrow$ $\tau_{th} \sim \frac{1}{N_{phonon}}^{+} \sim \frac{1}{T} \Rightarrow \tau_{th} \cdot T \sim$ constant (no temp. dependence)

  $$\therefore K_{el} = \frac{\pi^2}{3} \frac{n k_B^2}{m_e} \cdot \text{constant} \sim T^0 \text{ (a constant)}$$

  [Wiedemann-Franz law obeyed]

- at low temperatures ($T \ll \theta_D$) $\quad [\sigma \sim \frac{1}{\rho} \sim \frac{1}{T} \Rightarrow \sigma T \sim \text{const}]$

  typical phonon energy $\sim k_B T$

  thermal conduction: even phonons with short $\vec{q}$'s are effective

  $$\tau_{th} \sim \frac{1}{N_{phonon}}^{+} \sim \frac{1}{T^3} \Rightarrow \tau_{th} \cdot T \sim \frac{1}{T^2}$$

  $$\therefore K_{el} \sim \frac{1}{T^2} \text{ for } T \ll \theta_D$$

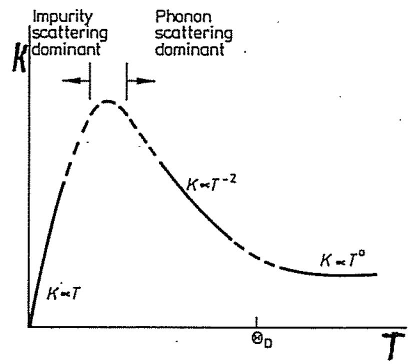
  [deviate from Wiedemann-Franz law]

$^{+}\ \frac{1}{\tau_{el\text{-}ph}} \sim N_{phonon}$ and $N_{phonon} = \sum_{\lambda, \vec{q}} \frac{1}{e^{\hbar\omega(\vec{q})/k_BT} - 1}$. At low temperatures, N_{phonon} can be estimated using the Debye model to be $\sim T^3$.

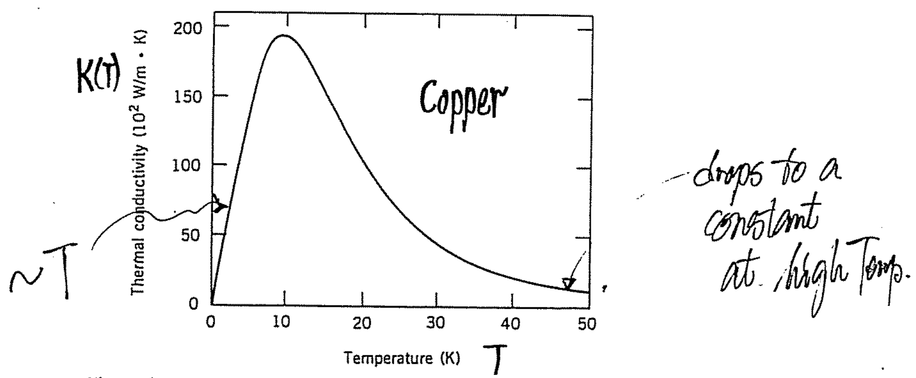
- at very low temperatures
  - electron-impurity scattering becomes dominant

    $\tau_{th} = \tau \sim$ No T-dependence [Wiedemann-Franz law holds]

    $K_{el} \sim T$ (from specific heat)



Schematic temperature dependence of $K(T)$ of a metal



Thermal conductivity of copper as a function of temperature. It approaches a constant at high temperature. Defect scattering dominates at low temperature and the conductivity is proportional to T.

Ref. Christman Sec. 9.4