Electron Dynamics - continued (2)

-- using the semiclassical model

to calculate electrical and thermal conduction in metals

Recall: in the equilibrium case

$$f^0\left(\varepsilon_n(\mathbf{k})\right) = \frac{1}{e^{(\varepsilon-\mu)/k_BT}+1}$$ -- independent of **r**

In the nonequilibrium case

$$f(\mathbf{r},\mathbf{k},t) = \frac{1}{e^{\left(\varepsilon(\mathbf{k})-\mu(\mathbf{r})\right)/k_BT(\mathbf{r})}+1}$$

Nonequilibrium case: H=0, E≠0

$$t - dt \rightarrow t$$

$$\mathbf{r} - v(\mathbf{k})dt$$ -- **r** space

$$\mathbf{k} - (-e)\mathbf{E}\,dt/\hbar$$ -- **k** space

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

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\nabla_r f - \frac{e}{\hbar}E\cdot\nabla_k f = \left(\frac{\partial f}{\partial t}\right)_{scattering}$$

-- Boltzmann Equation

Boltzmann Equation

-- represent the starting point for the treatment of transport problems

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_r f - \frac{e}{\hbar} E \cdot \nabla_k f = \left(\frac{\partial f}{\partial t} \right)_{scattering}$$

Stationary state $\frac{\partial f}{\partial t} = 0$

$$f(\mathbf{k}) \cong f_0(\mathbf{k}) + \frac{e}{\hbar} \boldsymbol{\tau}(k) \mathbf{E} \cdot \nabla_k f_0(\mathbf{k})$$

Small electric field

$$f(\mathbf{k}) \cong f_0\left(\mathbf{k} + \frac{e}{\hbar} \boldsymbol{\tau}(k) \mathbf{E} \right)$$

Calculate: **Thermal Conductivity** in the nonequilibrium condition

Thermodynamics: $TdS = dU - \mu dN$

$$T\,\mathbf{J}^S = \mathbf{J}^\varepsilon - \mu\,\mathbf{J}^N$$

$$\mathbf{J}^\varepsilon = \sum_n \int \varepsilon_n(\mathbf{k})\,\mathbf{v}_n(\mathbf{k}) f_n(\mathbf{k}) \frac{d\mathbf{k}}{4\pi^3}$$

$$\mathbf{J}^N = \sum_n \int \mathbf{v}_n(\mathbf{k}) f_n(\mathbf{k}) \frac{d\mathbf{k}}{4\pi^3}$$

Thermal current:

$$\mathbf{J}^q = T\,\mathbf{J}^S = \mathbf{J}^\varepsilon - \mu\,\mathbf{J}^N = \sum_n \int \left(\varepsilon_n(\mathbf{k}) - \mu\right) \mathbf{v}_n(\mathbf{k}) f_n(\mathbf{k}) \frac{d\,\mathbf{k}}{4\pi^3}$$

From definition: $\mathbf{J}^q = \kappa\left(-\nabla T\right)$

Thermal conductivity:

$$\kappa = \frac{1}{T} \sum_n \int \left(-\frac{\partial f}{\partial \varepsilon}\right) \left(\varepsilon_n(\mathbf{k}) - \mu\right)^2 \mathbf{v}_n(\mathbf{k}) \mathbf{v}_n(\mathbf{k}) \tau\left(\varepsilon(\mathbf{k})\right) \frac{d\,\mathbf{k}}{4\pi^3}$$

-- it is also a tensor

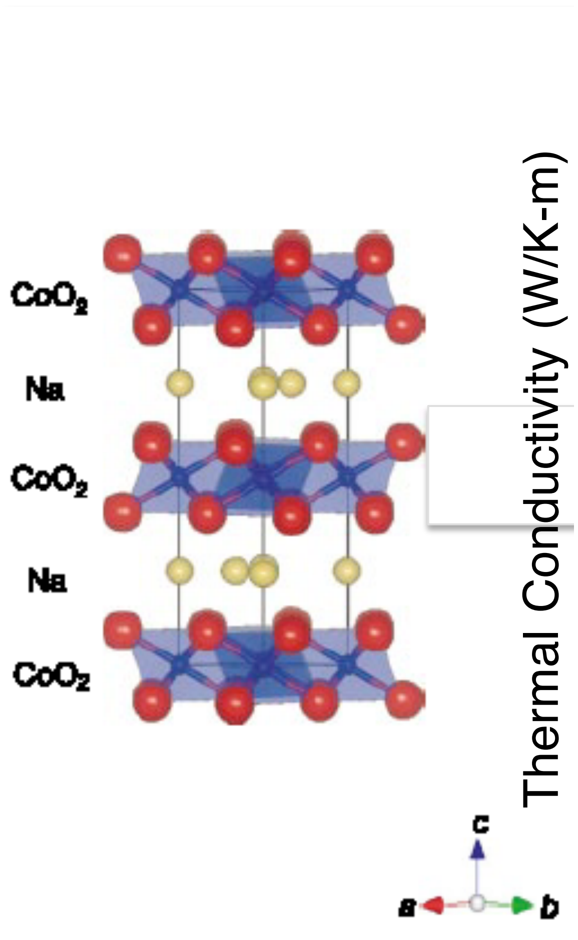
$$\kappa = \frac{1}{T}\sum_n \int \left(-\frac{\partial f}{\partial \varepsilon}\right)\left(\varepsilon_n(\mathbf{k}) - \mu\right)^2 \mathbf{v}_n(\mathbf{k})\mathbf{v}_n(\mathbf{k})\tau\left(\varepsilon(\mathbf{k})\right)\frac{d\mathbf{k}}{4\pi^3}$$

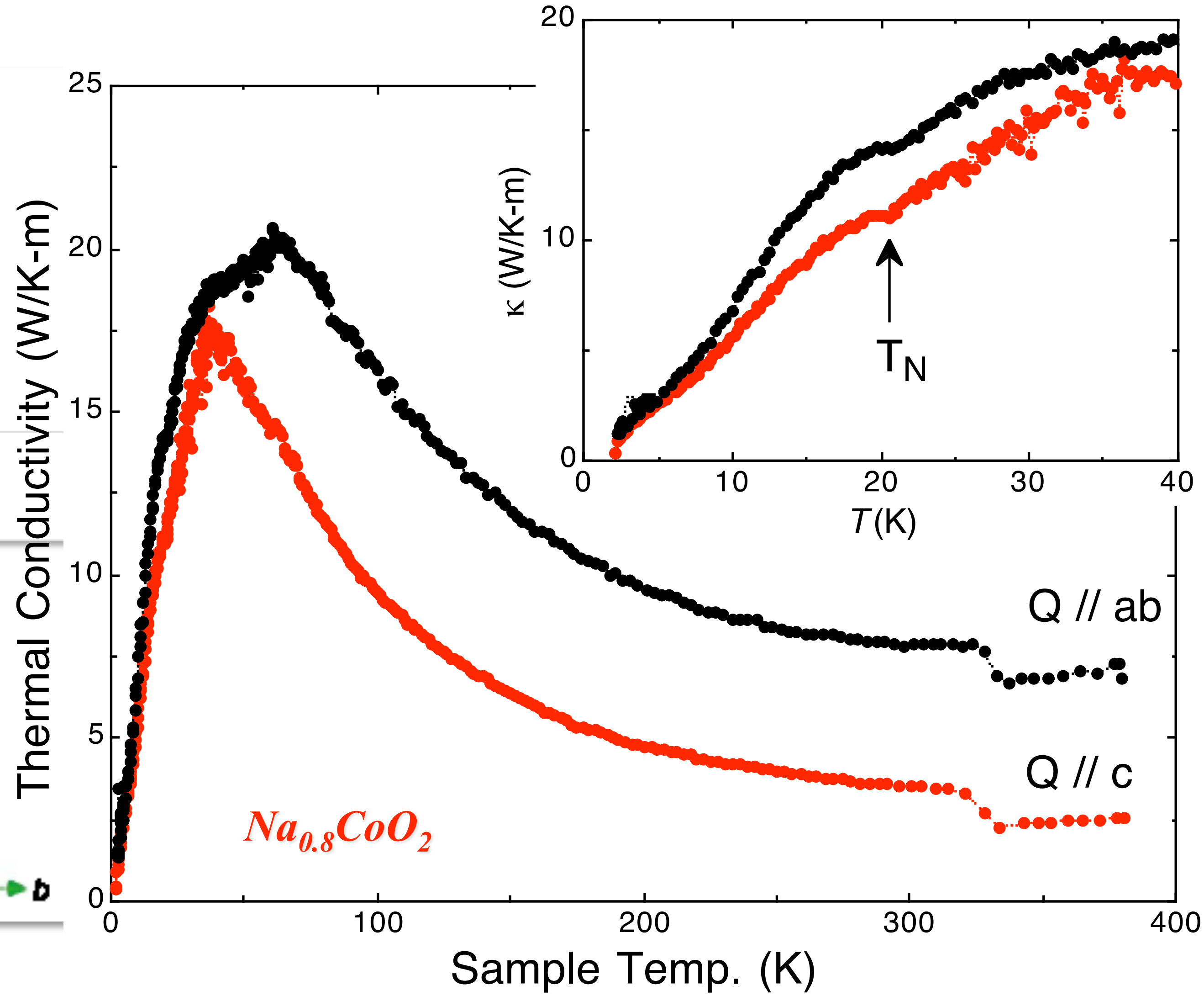
$T \rightarrow 0$ $\varepsilon_F \approx \mu$

$$\kappa \approx \frac{\pi^2 k_B^2 T}{3e^2}\sigma$$

- the thermal conductivity is a tensor - can be different in different direction ⇒ thermal anisotropy
- $\dfrac{\kappa}{\sigma T} \approx \dfrac{\pi^2 k_B^2}{3e^2}$ ⇒ Wiedemann-Franz law holds at $T \rightarrow 0$

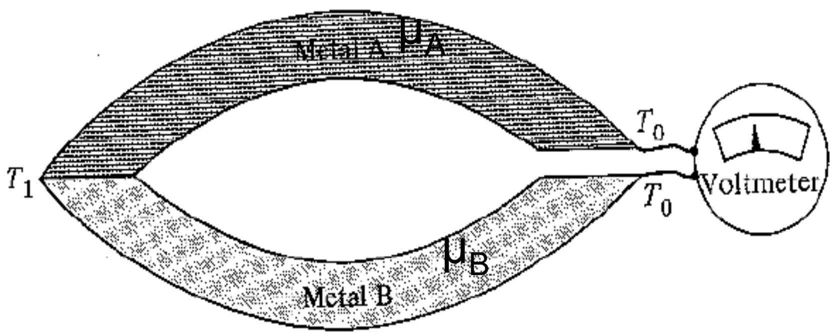
Example: thermal anisotropy





Calculate: **Thermoelectric Power** in the nonequilibrium condition

The chemical potential gradient leads to a diffusion current (field)



$$\mathbf{E}_{diffusion} = \frac{\nabla \mu}{e}$$

Definition: $\mathbf{E}_{diffusion} = Q \nabla T$

$$Q = -\frac{1}{eT} \frac{\sum_n \int \left(-\frac{\partial f}{\partial \varepsilon}\right)\left(\varepsilon_n(\mathbf{k}) - \mu\right) \mathbf{v}_n(\mathbf{k}) \mathbf{v}_n(\mathbf{k}) \tau\left(\varepsilon(\mathbf{k})\right) \frac{d\mathbf{k}}{4\pi^3}}{\sum_n \int \left(-\frac{\partial f}{\partial \varepsilon}\right) \mathbf{v}_n(\mathbf{k}) \mathbf{v}_n(\mathbf{k}) \tau\left(\varepsilon(\mathbf{k})\right) \frac{d\mathbf{k}}{4\pi^3}}$$

$$Q = -\frac{1}{eT}\frac{\sum_n \int \left(-\frac{\partial f}{\partial \varepsilon}\right)\left(\varepsilon_n(\mathbf{k}) - \mu\right)\mathbf{v}_n(\mathbf{k})\mathbf{v}_n(\mathbf{k})\tau\left(\varepsilon(\mathbf{k})\right)\frac{d\mathbf{k}}{4\pi^3}}{\sum_n \int \left(-\frac{\partial f}{\partial \varepsilon}\right)\mathbf{v}_n(\mathbf{k})\mathbf{v}_n(\mathbf{k})\tau\left(\varepsilon(\mathbf{k})\right)\frac{d\mathbf{k}}{4\pi^3}}$$

$T \rightarrow 0$ $\quad$ $\varepsilon_F \approx \mu$

$$Q \approx -\frac{\pi^2 k_B^2 T}{3e^2}\frac{\left.\frac{\partial \sigma(\varepsilon)}{\partial \varepsilon}\right|_{\varepsilon=\varepsilon_F}}{\sigma}$$

Semiclassical model: $$Q \approx -\frac{\pi^2 k_B^2 T}{3e^2} \frac{\left.\frac{\partial \sigma(\varepsilon)}{\partial \varepsilon}\right|_{\varepsilon=\varepsilon_F}}{\sigma}$$

Drude model: $$Q \approx -\frac{k_B}{2e}$$ ✘

Sommerfeld model: $$Q \approx -\frac{\pi^2 k_B^2 T}{6e\varepsilon_F}$$

Calculate: **DC Electrical Conductivity** in the nonequilibrium condition

H=0, **E** is static ➔ $f(\mathbf{k}) \cong f_0(\mathbf{k}) + \frac{e}{\hbar}\tau(k)\mathbf{E}\cdot\nabla_k f_0(\mathbf{k})$

$$\mathbf{J} = -e\int \mathbf{v}(\mathbf{k}) f(\mathbf{k}) \frac{d\,\mathbf{k}}{4\pi^3} = \sigma\,\mathbf{E}$$

$$\nabla_k f_0(\mathbf{k}) = \nabla_\varepsilon f_0(\mathbf{k})\hbar\,\mathbf{v}(\mathbf{k})$$

⬇

$$\sigma^n = e^2\int \mathbf{v}_n^2(\mathbf{k})\tau(\varepsilon(\mathbf{k}))\left(-\frac{\partial f}{\partial\varepsilon}\right)\Bigg|_{\varepsilon_n(\mathbf{k})} \frac{d\,\mathbf{k}}{4\pi^3}$$

$$\sigma = \sum \sigma^n$$

$$\sigma = e^2 \int \mathbf{v}^2(\mathbf{k})\tau(\varepsilon(\mathbf{k}))\left(-\frac{\partial f}{\partial \varepsilon}\right)\Bigg|_{\varepsilon(\mathbf{k})} \frac{d\,\mathbf{k}}{4\pi^3}$$

$$\sigma_{xx} = e^2 \int \mathbf{v}_x^2(\mathbf{k})\tau(\varepsilon(\mathbf{k}))\left(-\frac{\partial f}{\partial \varepsilon}\right)\Bigg|_{\varepsilon(\mathbf{k})} \frac{d\,\mathbf{k}}{4\pi^3} \qquad \sigma_{yy} = e^2 \int \mathbf{v}_y^2(\mathbf{k})\tau(\varepsilon(\mathbf{k}))\left(-\frac{\partial f}{\partial \varepsilon}\right)\Bigg|_{\varepsilon(\mathbf{k})} \frac{d\,\mathbf{k}}{4\pi^3}$$

$$\sigma_{zz} = e^2 \int \mathbf{v}_z^2(\mathbf{k})\tau(\varepsilon(\mathbf{k}))\left(-\frac{\partial f}{\partial \varepsilon}\right)\Bigg|_{\varepsilon(\mathbf{k})} \frac{d\,\mathbf{k}}{4\pi^3}$$

$$T \rightarrow 0 \qquad \frac{\partial f}{\partial \varepsilon} \approx -\delta(\varepsilon - \varepsilon_F) \qquad d\,\mathbf{k} = dS_\varepsilon\, dk_\perp = dS_\varepsilon \frac{d\varepsilon}{\hbar\, \mathbf{v}(\mathbf{k})}$$

$$\sigma_{xx} = e^2 \int_{\varepsilon = \varepsilon_F} \frac{\mathbf{v}_x^2(\mathbf{k})}{\mathbf{v}(\mathbf{k})} \tau(\varepsilon(\mathbf{k})) \frac{dS_\varepsilon}{4\pi^3}$$

…

$$\sigma_{xx} = e^2 \int_{\varepsilon=\varepsilon_F} \frac{\mathbf{v}_x^2(\mathbf{k})}{\mathbf{v}(\mathbf{k})} \boldsymbol{\tau}(\varepsilon(\mathbf{k})) \frac{dS_\varepsilon}{4\pi^3}$$

$T \rightarrow 0$ $\quad \frac{\partial f}{\partial \varepsilon} \approx -\delta(\varepsilon - \varepsilon_F)$

Sphere Fermi surface

$$\int_{\varepsilon_F} dS_\varepsilon = 4\pi k_F^2 \qquad v(\varepsilon_F) = \frac{\hbar k_F}{m^*}$$

$$n = \frac{k_F^3}{3\pi^2}$$

$$\sigma = \frac{e^2 \boldsymbol{\tau}(\varepsilon_F)}{m^*} n$$

Drude Model

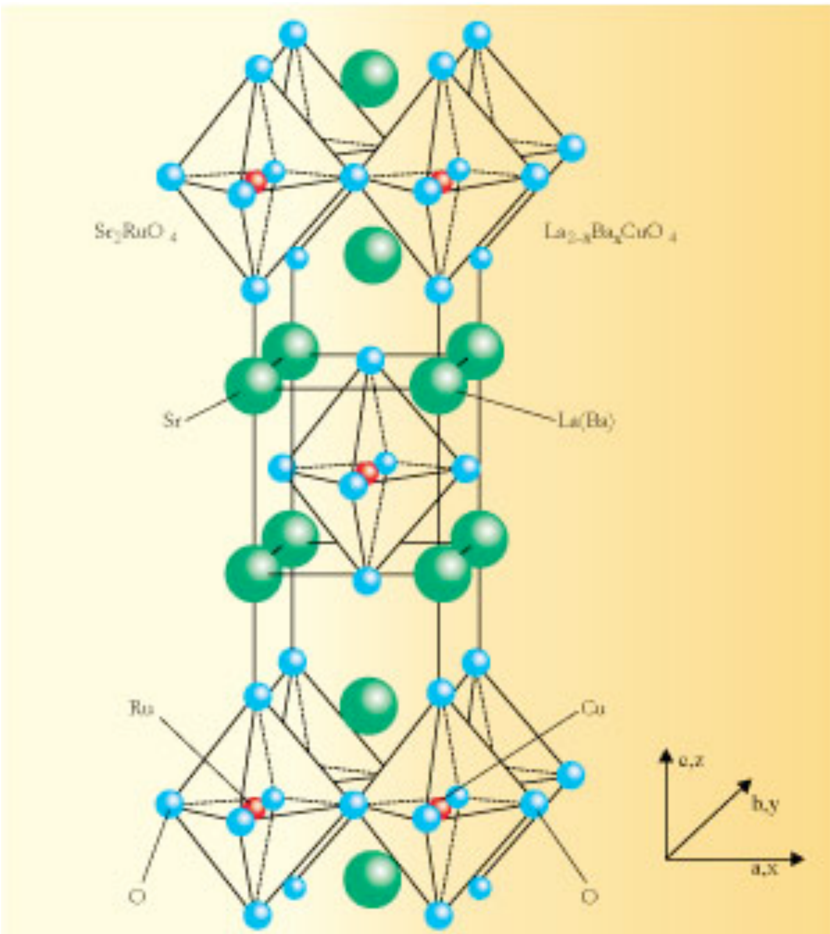
Important Messages:

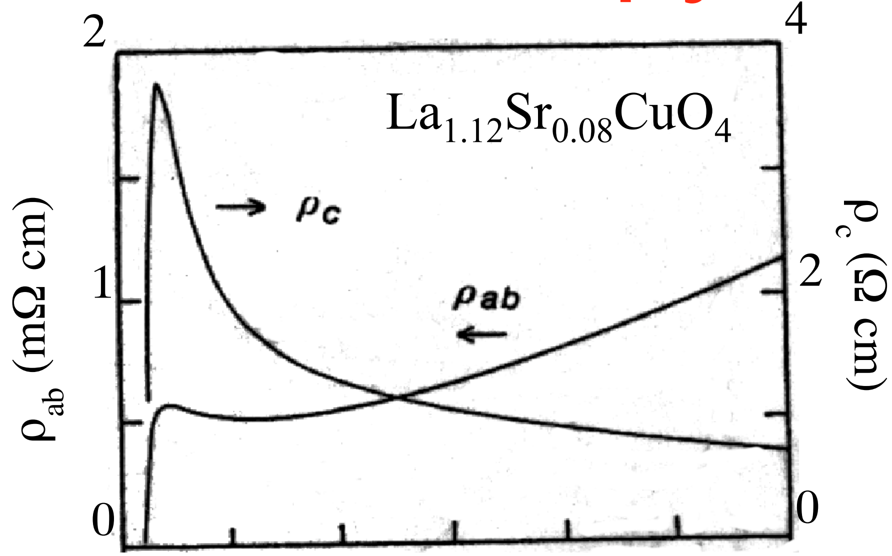
👌 the electrical conductivity is a tensor - can be different in different direction $\Rightarrow$ electric anisotropy

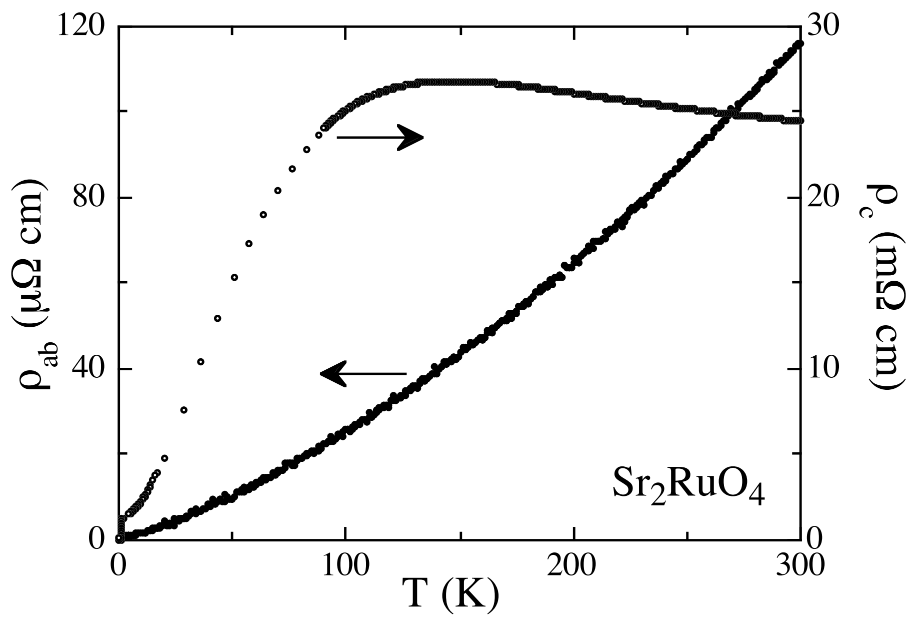
👌 the electrical conductivity depends on $\dfrac{\partial f}{\partial \varepsilon}$
$\Rightarrow$ filled bands give no contribution

👌 when **v** is independent with **k** $\Rightarrow$ free-electron case (Drude form holds)

Example: electrical anisotropy







Temperature Dependence of Electrical Conductivity

$$\sigma = \frac{e^2 \tau(\varepsilon_F)}{m^*} n$$

Recall: $$\frac{1}{\tau_{el-ph}} = 2\pi k^2 \int_{FS} P(\theta)(1-\cos\theta)\sin\theta d\theta$$

$$\langle P(\theta) \rangle \propto \frac{k_B T}{\Theta_D^2}$$ -- scattering transition probability

$$\rho_{e-p} = \frac{AT^5}{M\Theta_D^6} \int_0^{\Theta_D/T} \frac{x^5 dx}{(e^x - 1)(1 - e^{-x})}$$

Bloch-Grüneisen formula

$$x = \frac{\hbar\omega_D}{k_B T}$$

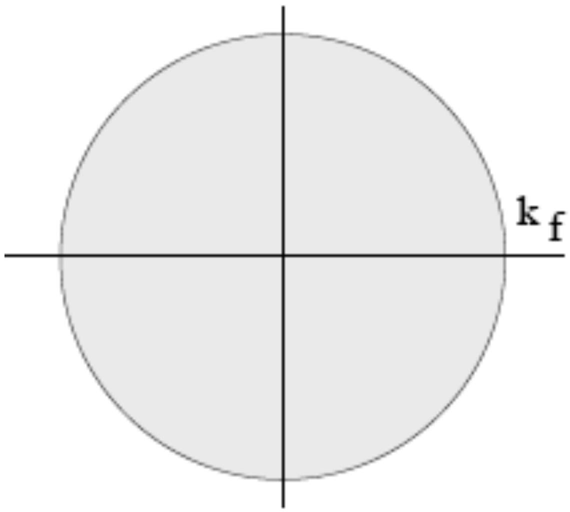
Are there other contributions?

Recall:
In the Case of Free Electron Gas

1. Gas potential = $V_{ion} + V_{electron} = 0$

2. Electrons do not collide to each other - many-body excitations are the sum of independent particle excitations.

3. Well-defined Fermi surface.

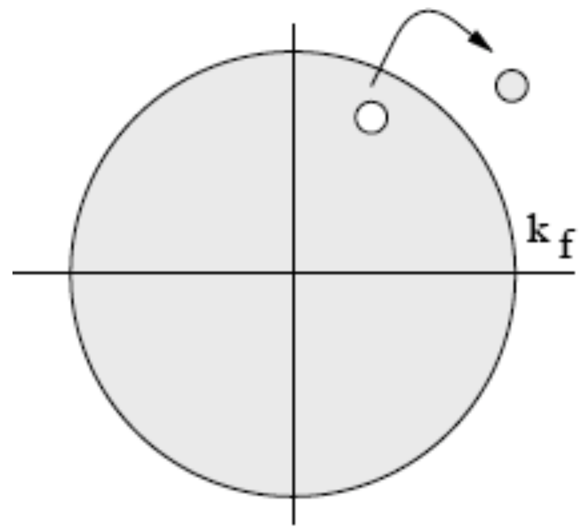


In Reality

$V \neq 0$

$\Rightarrow$ The energies of each one-electron level will be modified;

$\Rightarrow$ Electrons will be scattered in and out of the single electron level.



Electron-Electron Collisions (Interactions)

Electron 1 (momentum p_1, energy ε_1)

Electron 1 (momentum p_2, energy ε_2)

$$p_1 + p_2 = p_1^{'} + p_2^{'}$$

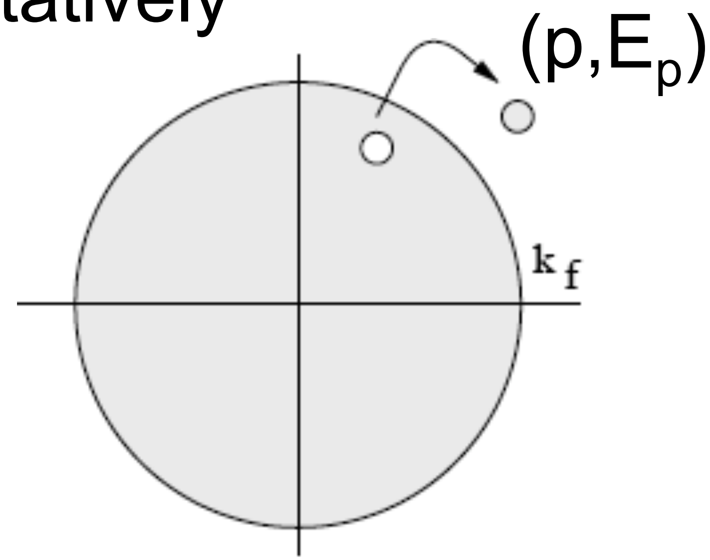
$$\varepsilon_1 + \varepsilon_2 = \varepsilon_1^{'} + \varepsilon_2^{'}$$

Collision rate:

$$\Gamma = \frac{1}{\tau_{e-e}} = \frac{2\pi}{\hbar} \sum_f \left| \langle f | H_{\mathbf{int}} | i \rangle \right|^2 \delta\left(\varepsilon_f - \varepsilon_i\right)$$

In the excited states:

Excitation spectrum remains qualitatively similar as in free Fermi gas but there is a shift in energies:



$$\varepsilon_p - \varepsilon_F = \frac{p^2}{2m} - \varepsilon_F \approx \frac{\hbar k_F}{m^*}\left(k - k_F\right)$$

$$\frac{1}{m^*} = \frac{1}{m} + \frac{1}{2}\int \frac{d\,\mathbf{k}'}{(2\pi)^3}\frac{\mathbf{k}'}{k'}\delta\left(k' - k_F\right)$$

Electrons are called quasi-electrons (or quasi-particles) with effective mass m*

Quasi-particles:

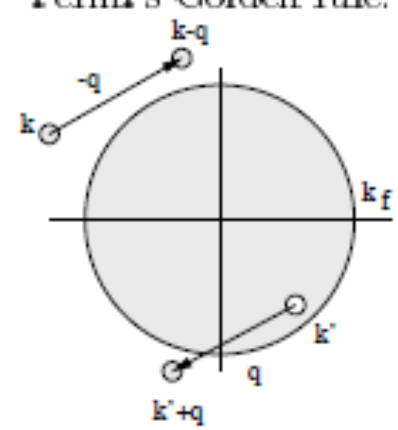
Energy: $$\varepsilon = \varepsilon_k - \varepsilon_F$$

Relaxation time: $$\frac{1}{\tau_{e-e}} = \frac{2\pi}{\hbar} \sum_f \left| \langle f | H_{\mathbf{int}} | i \rangle \right|^2 \delta(\varepsilon_f - \varepsilon_i)$$

$$= \frac{2\pi}{\hbar} \sum_f \left| V_{ij} \right|^2 \delta(\varepsilon_f - \varepsilon_i)$$

$$\frac{1}{\tau} \sim \frac{\pi}{\hbar} \frac{|V|^2}{\varepsilon_F^3} \varepsilon^2 \sim A \frac{1}{\hbar} \frac{(k_B T)^2}{\varepsilon_F}$$

Fermi's Golden rule:



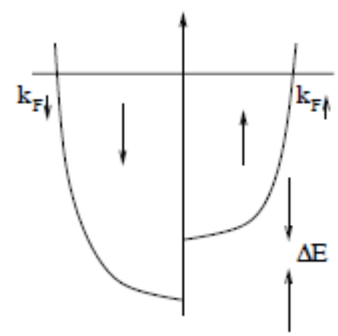
Consequences:

- Density-of-states: $$g(\varepsilon_F) = \frac{m^* \varepsilon_F}{\pi^2 \hbar^2}$$
- Specific heat: $$C_v = \frac{\pi^2}{3} k_B^2 T g(\varepsilon_F) = \gamma T$$

  (γ is called Sommerfeld coefficient or electronic specific heat coefficient)

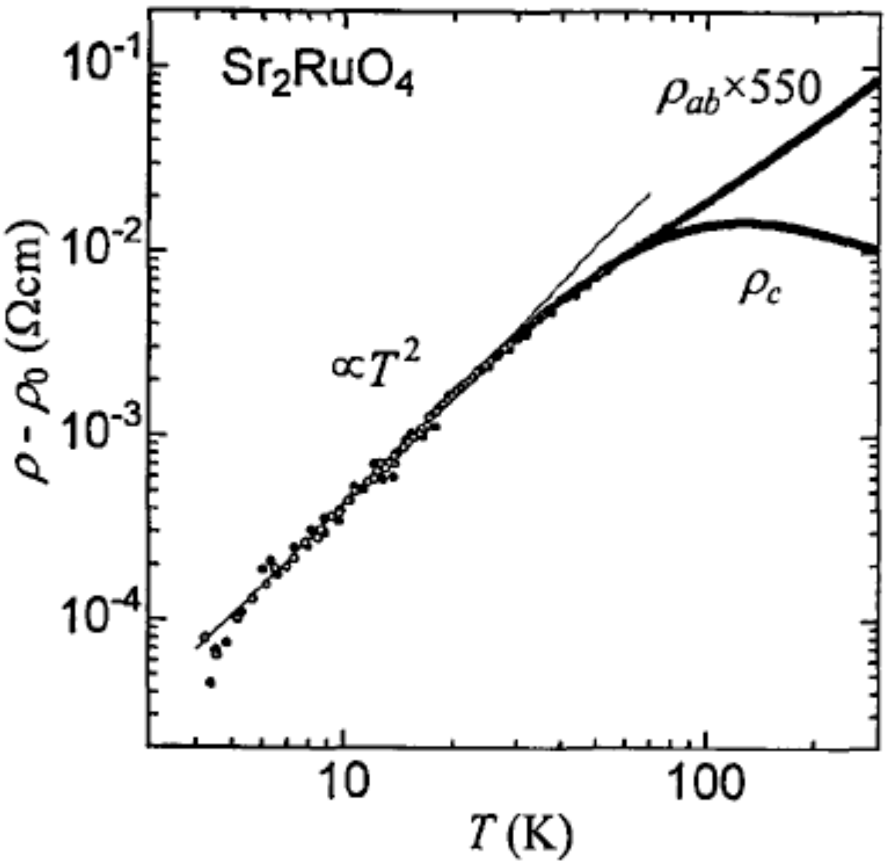
- Pauli spin susceptibility:

$$\chi_{spin} = -\mu_B \sum_k (\delta n_{k\uparrow} - \delta n_{k\downarrow}) = -\frac{\mu_B^2 g(\varepsilon_F)}{1 + F_0^a}$$

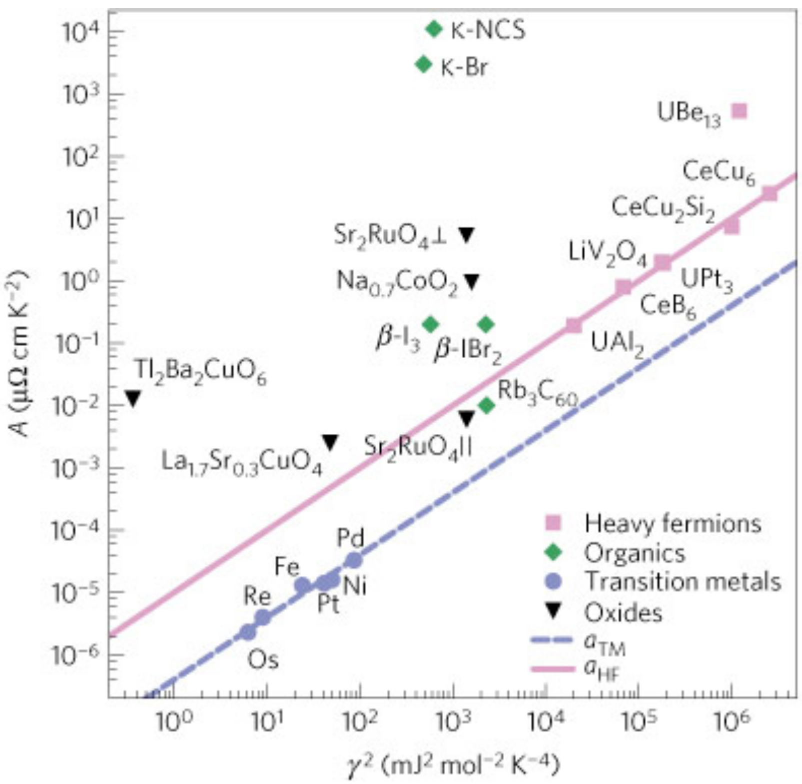


- Electrical Resistivity: $$\rho = \frac{m^*}{ne^2}\frac{1}{\tau} \propto T^2$$

Example: Fermi-liquid Behavior



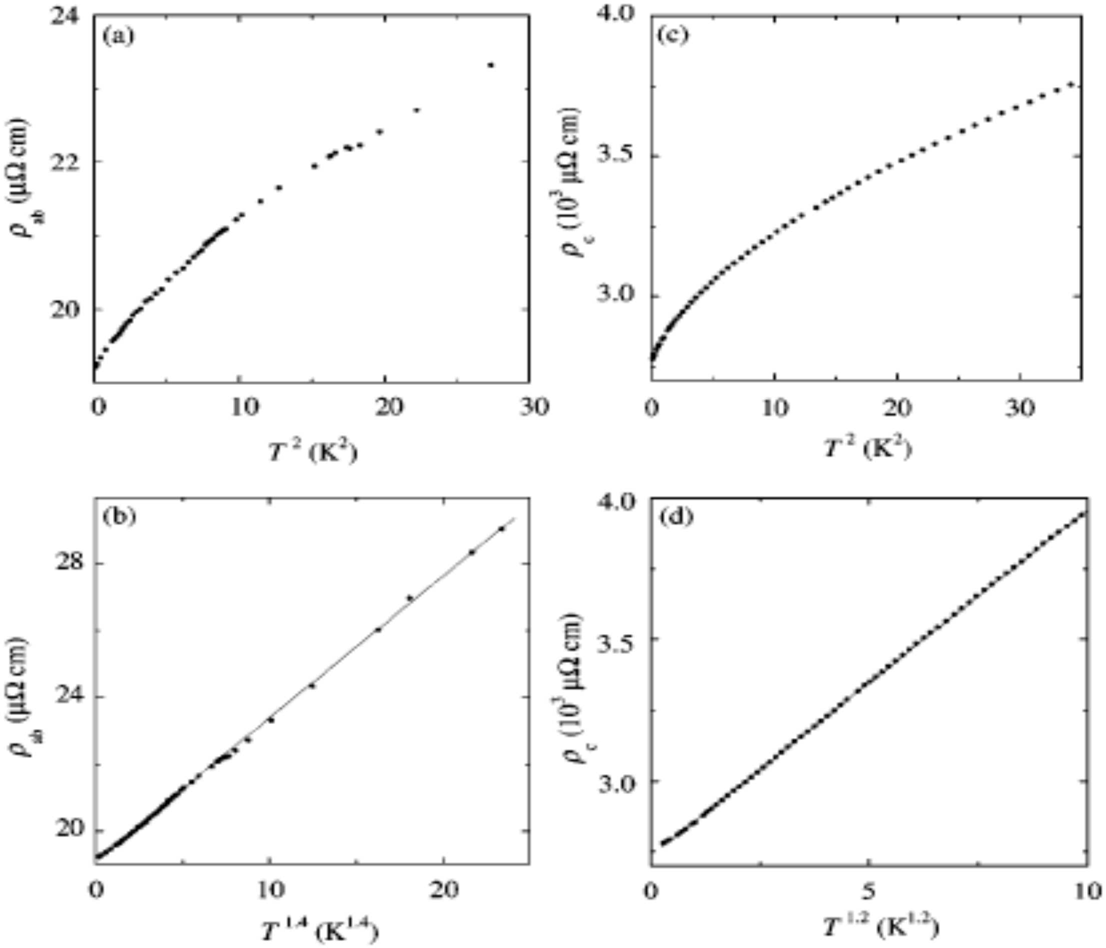
Kadowaki-Woods ratio

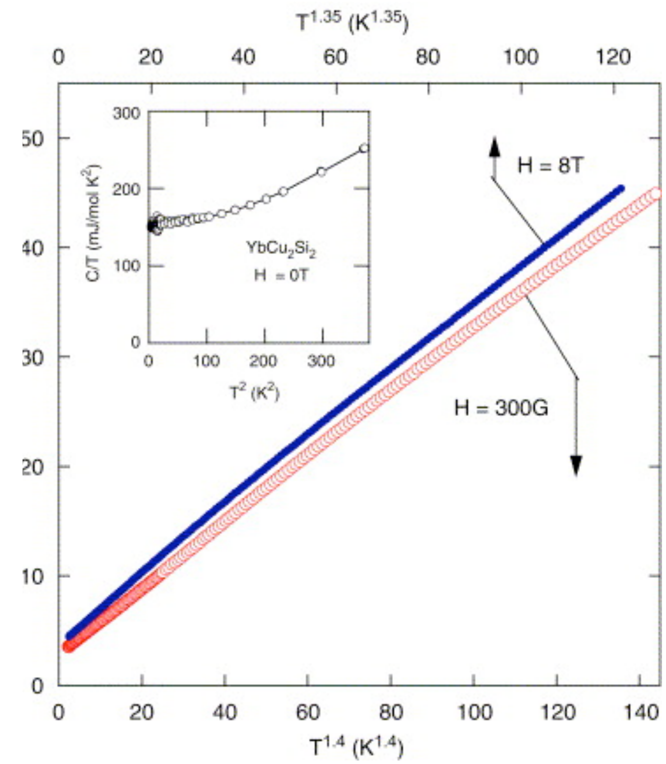


$\frac{A}{\gamma^2} \sim 10^{-5}$ For strong-interacting systems

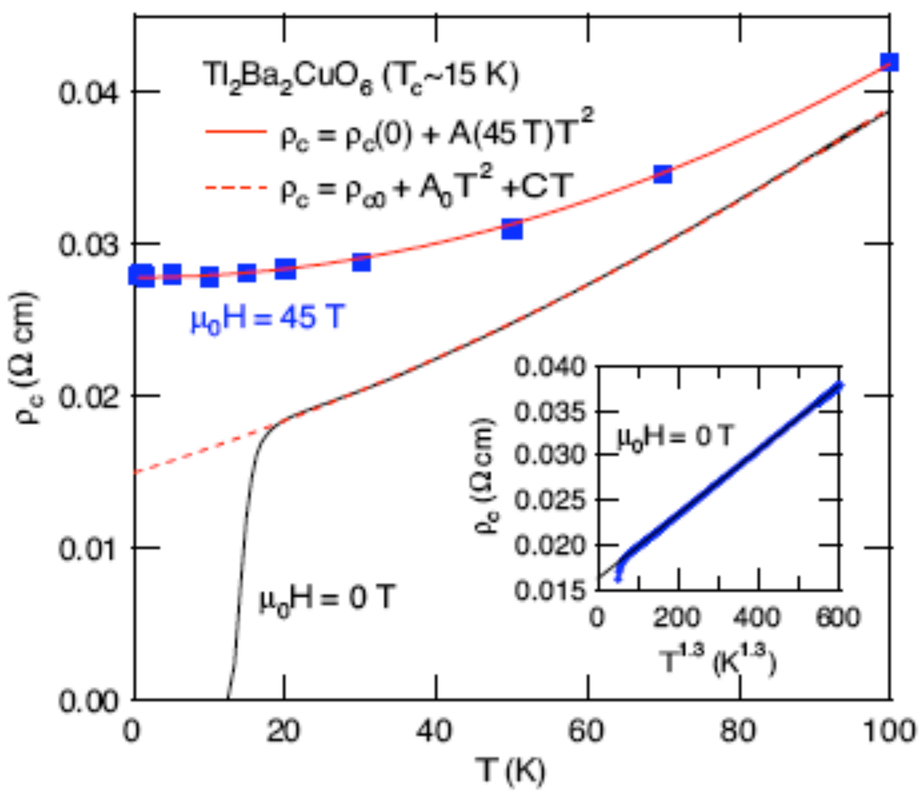
$\frac{A}{\gamma^2} \sim 10^{-6}$ For non-interacting systems

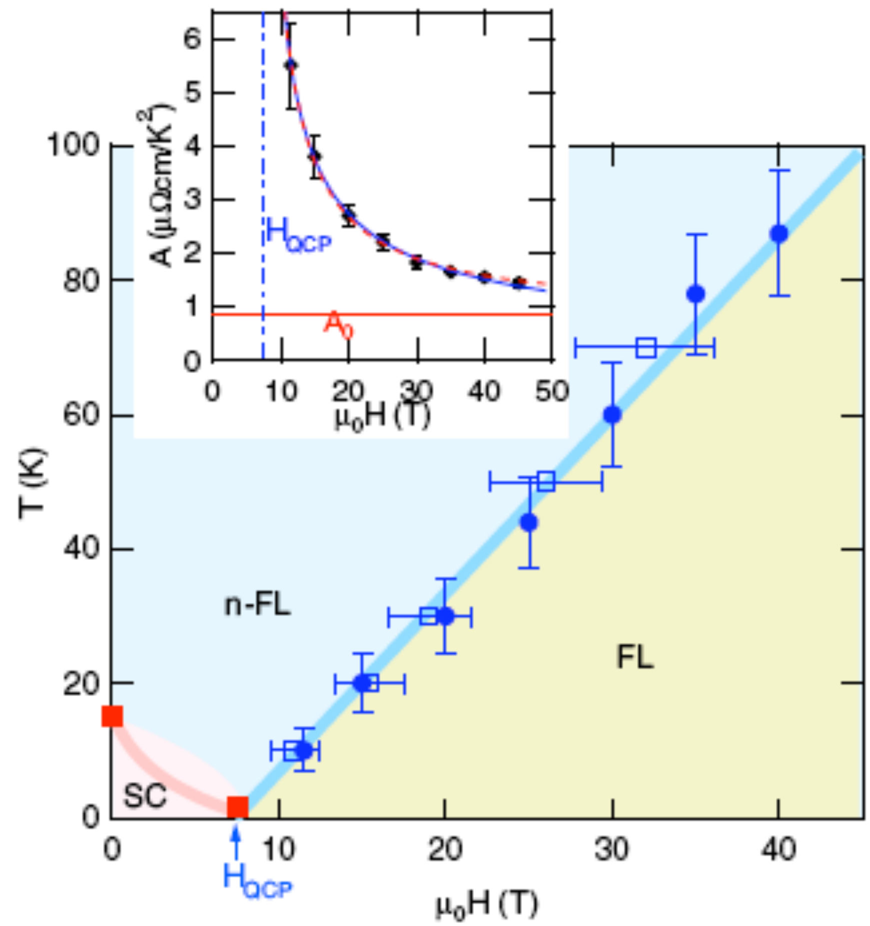
Example:
Non-Fermi-liquid Behavior



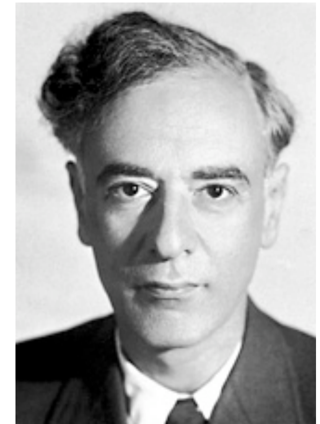


Example: Fermi-Liquid--Non-Fermi-liquid Crossover

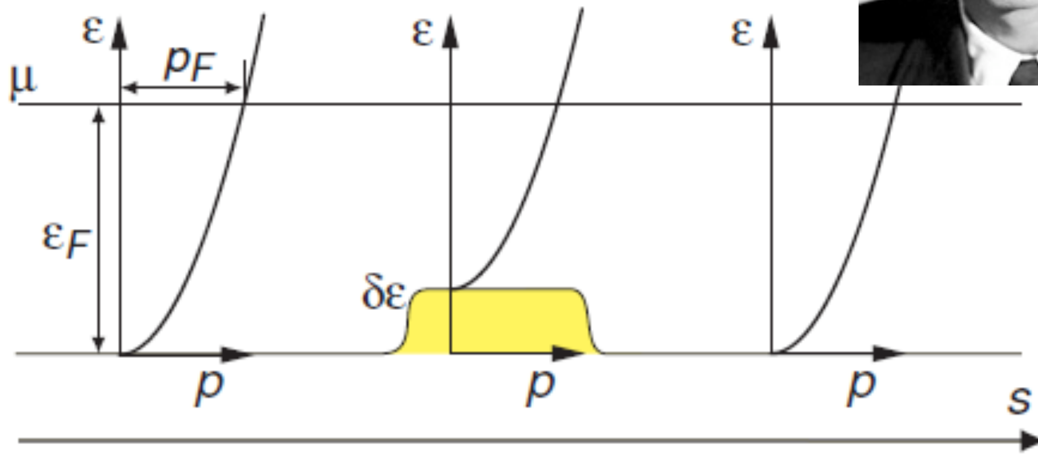




Landau Fermi Liquid Theory:



While the fundamental symmetries remain unbroken, there will be a one-to-one correspondence between new and old states – new states can be labeled by the same quantum numbers.



The basic assumption of the Fermi-liquid theory is that the potential is small compared to the Fermi energy ϵ_F, i.e. $\delta\epsilon \ll \epsilon_F$. This means that a quasiparticle is slightly decelerated when it enters the beam and it is accelerated back when it leaves the crossing region. In the energy point of view (figure above), the quasiparticle flies at constant energy $\epsilon \approx \mu$ and the potential is effectively compensated by depletion of fermions with the same momentum direction in the crossing region. If there were a second quasiparticle beam along the trajectory, there appears to be no interaction between the two stationary beams.

Total Electrical Resistivity in a Metal

$$\rho = \rho_{el-el} + \rho_{el-ph}$$

$$\rho = \begin{cases} AT^2 + BT \sim BT & T >> \Theta_D \\ AT^2 + BT^5 \sim AT^2 & T << \Theta_D \end{cases}$$

Homework (due on 11/4/2010)

1. $Cd_2Re_2O_7$ is a superconductor below 1.5 K. We found that, at 2 K < T < 30 K, the electrical resistivity can be described as $\rho=\rho_0+AT^2$ with A = 0.024 μΩ cm/K^2, and electronic specific heat coefficient γ = 30 mJ/mol-K^2. Discuss the electron-electron Interaction strength in this material.