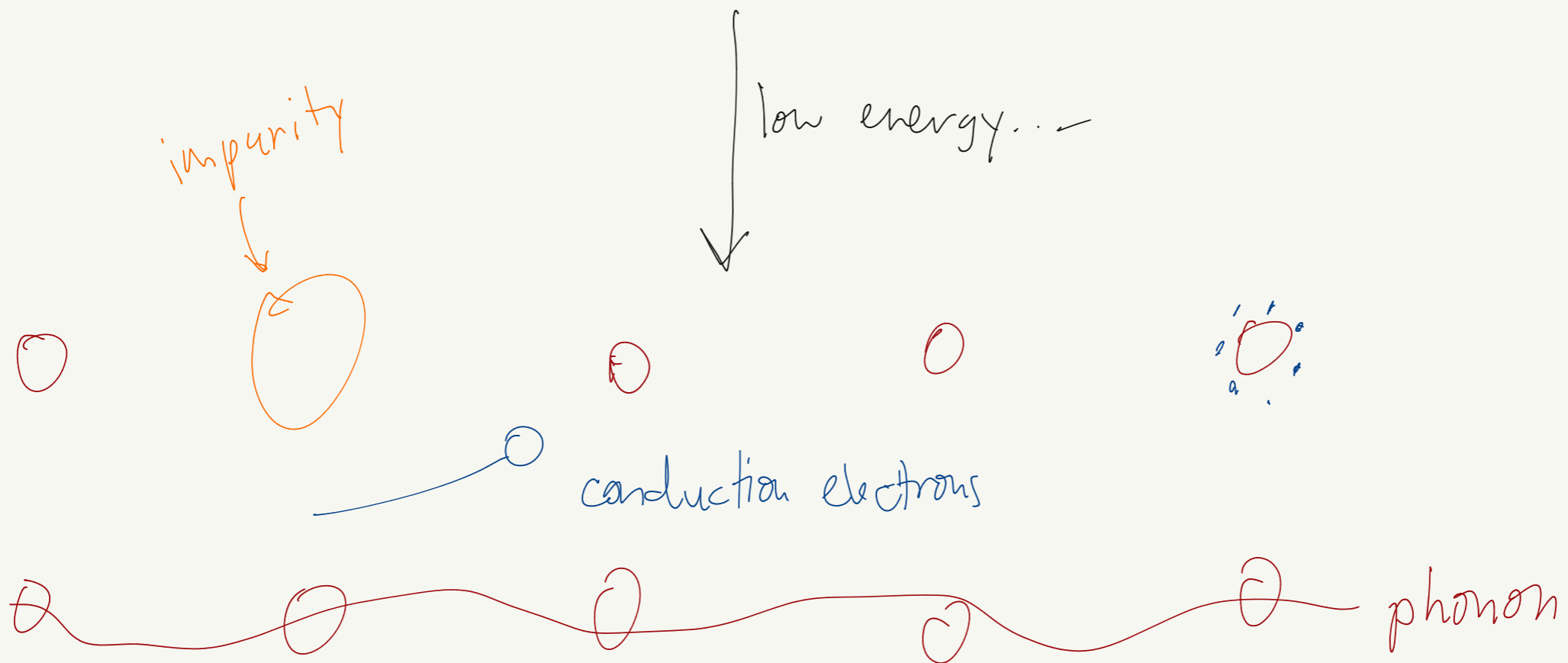


1. Drude model

1.1) Overview of metal physics

This course is about transport in metals. So let's begin by summarizing what we should know about metals coming into this course. Firstly, the microscopic Hamiltonian (unlike particle physics) isn't useful...

$$H = \sum_{a=1}^{N_{ion}} \frac{\vec{p}_a^2}{2M} + \sum_{i=1}^{N_{el}} \frac{\vec{p}_i^2}{2m} + \sum_{a < b} \frac{(Ze)^2}{|\vec{r}_a - \vec{r}_b|} + \sum_{a,i} \frac{-Ze^2}{|\vec{r}_a - \vec{r}_i|} + \sum_{i < j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|}$$



effective theory:

$$H \approx \sum_{q\alpha} \omega_{q\alpha} a_{q\alpha}^\dagger a_{q\alpha} + \sum_{ka} \epsilon_{ka} c_{ka}^\dagger c_{ka}$$

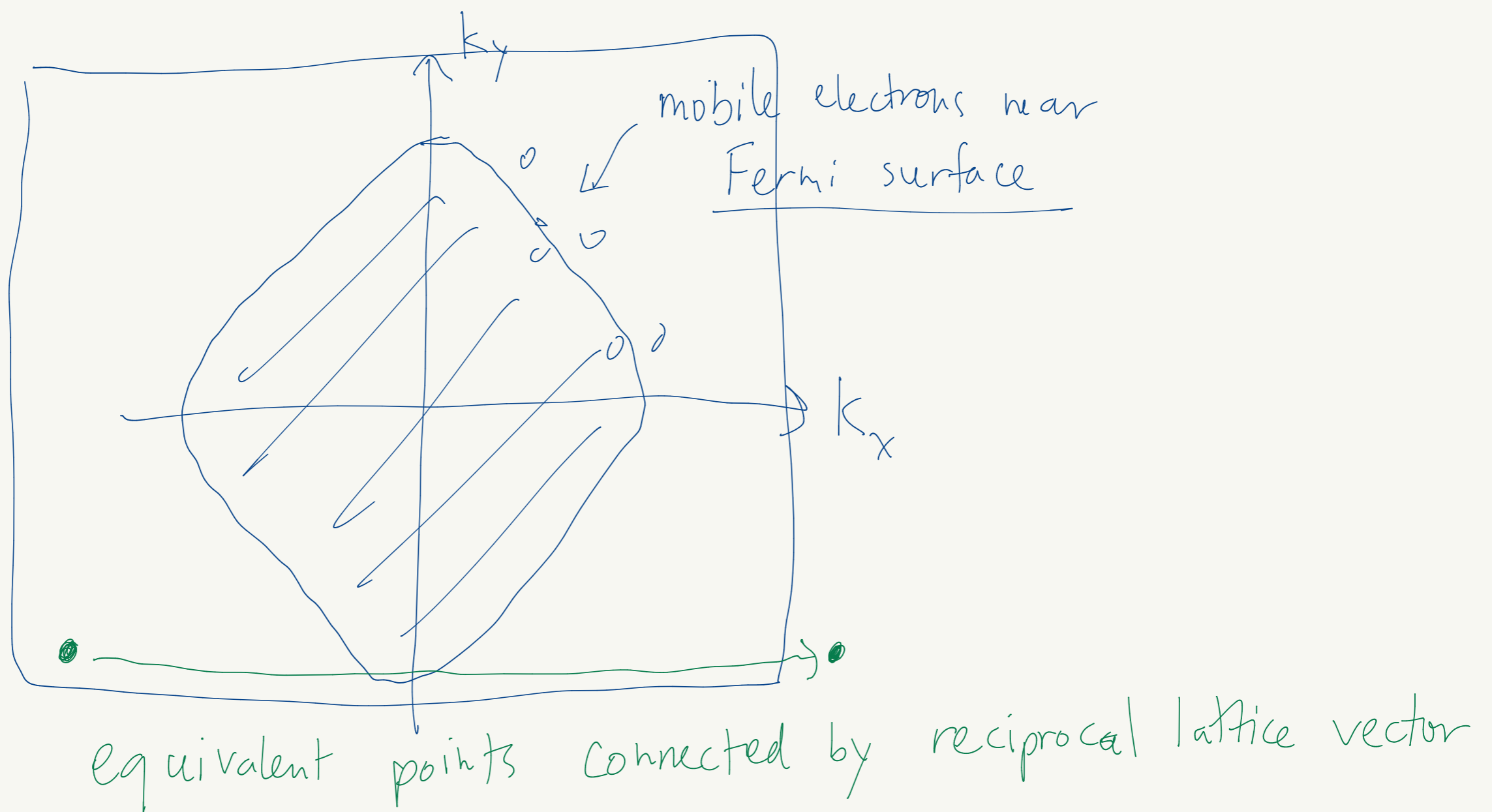
phonons, branch α electron/hole, band a

thermodynamics usually ignores interactions

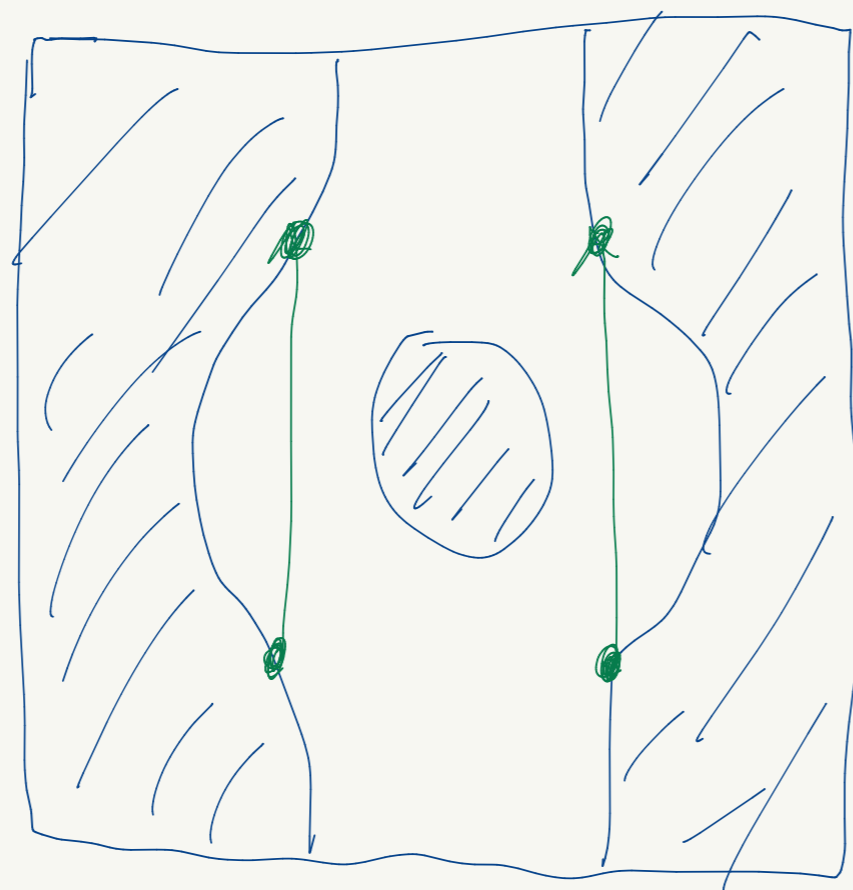
$$+ \sum \lambda_{ph} a^\dagger a a + \sum U c^\dagger c^\dagger c c + \dots$$

transport sensitive to interactions, impurities, etc...

Electron and phonon band structures exist in a Brillouin zone:



It is absolutely crucial for transport that scattering events can take particles and push them all the way around the Brillouin zone in many metals...

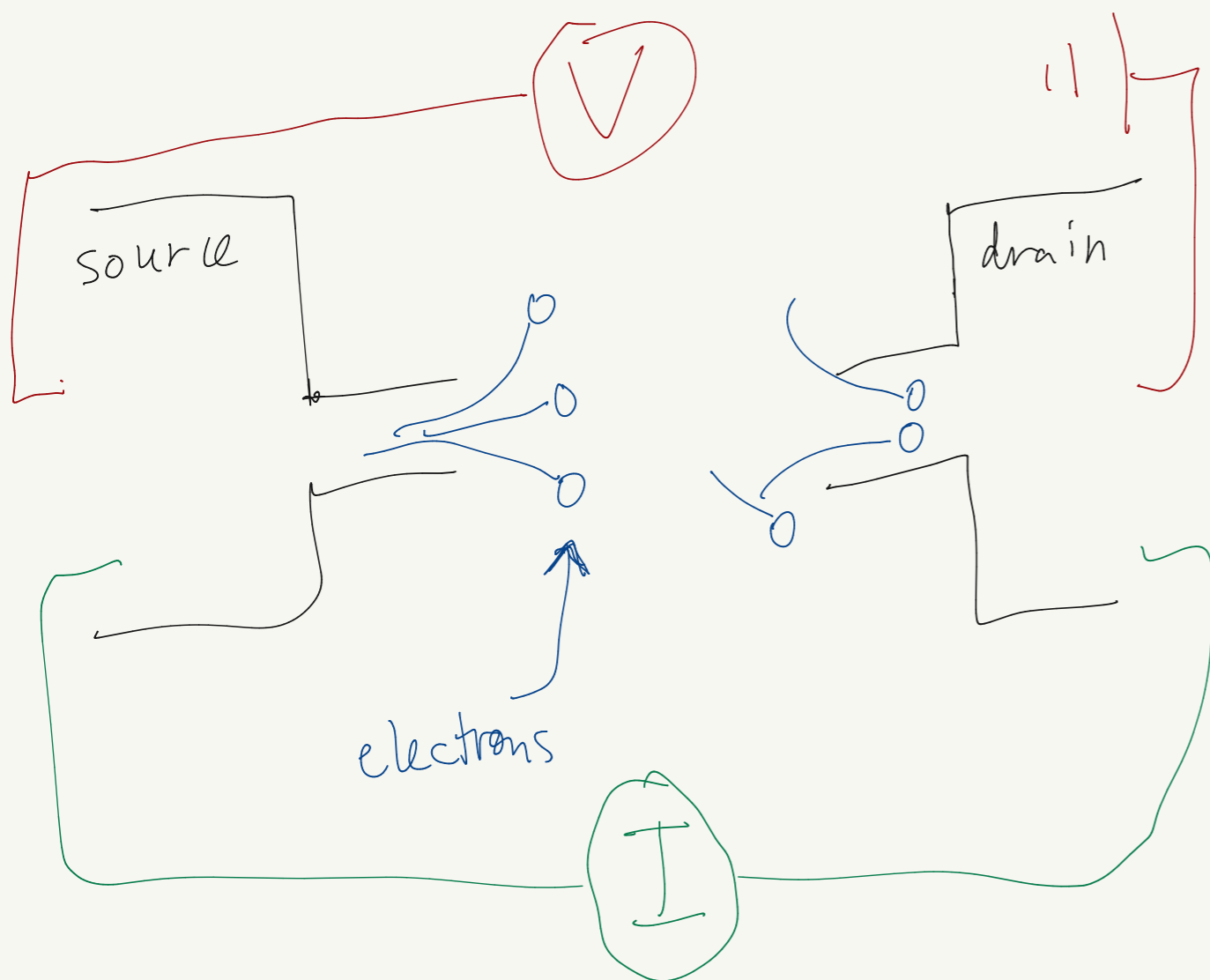


Shape of Fermi surface can be very non-trivial...

New emergent degrees of freedom, can behave very differently. Interplay of fast and slow particles?

Thermo often has a rather universal structure in metals because its sensitive only to existence of electrons, phonons etc ... but transport is sensitive to all the things we like to ignore. Disorder, e-p, e-e, p-p interactions are all controlling factors in the answer. This is why we can have a whole course on Theory of transport but not on metal thermodynamics...

1.2) Introduction to transport



Transport: take things from one place to another. For us, electrons.

This can't come for free

How much energy does it take to transport from one point to another?

beyond linear response!

Ohm's Law:

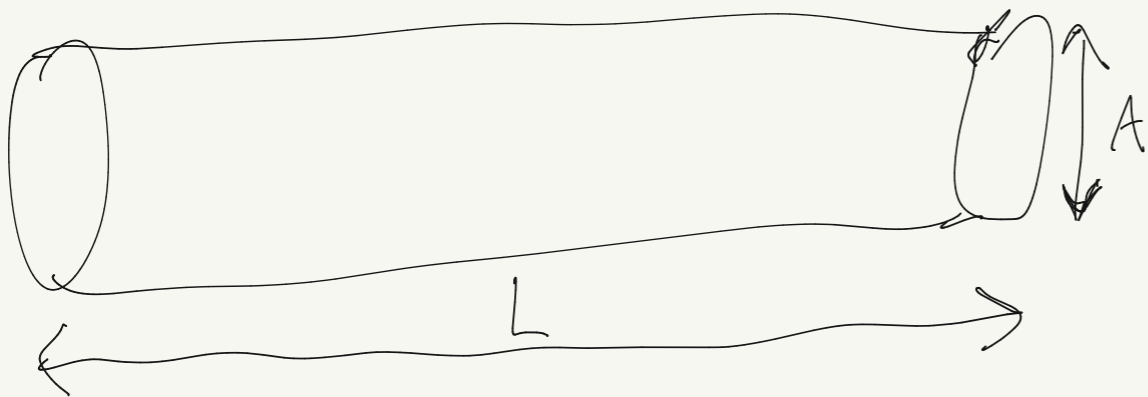
$$V = I \times R$$

↑ user input/output

+ ...
↑ easily measurable quantity

power dissipated:

$$P = I^2 R$$



$$R = \rho \times \frac{L}{A}$$

resistivity ρ ; intrinsic bulk property

$$V = IR$$

$$\frac{V}{L} = \frac{I}{A} \rho$$

$$E = J \rho$$

Lots of experimental data.

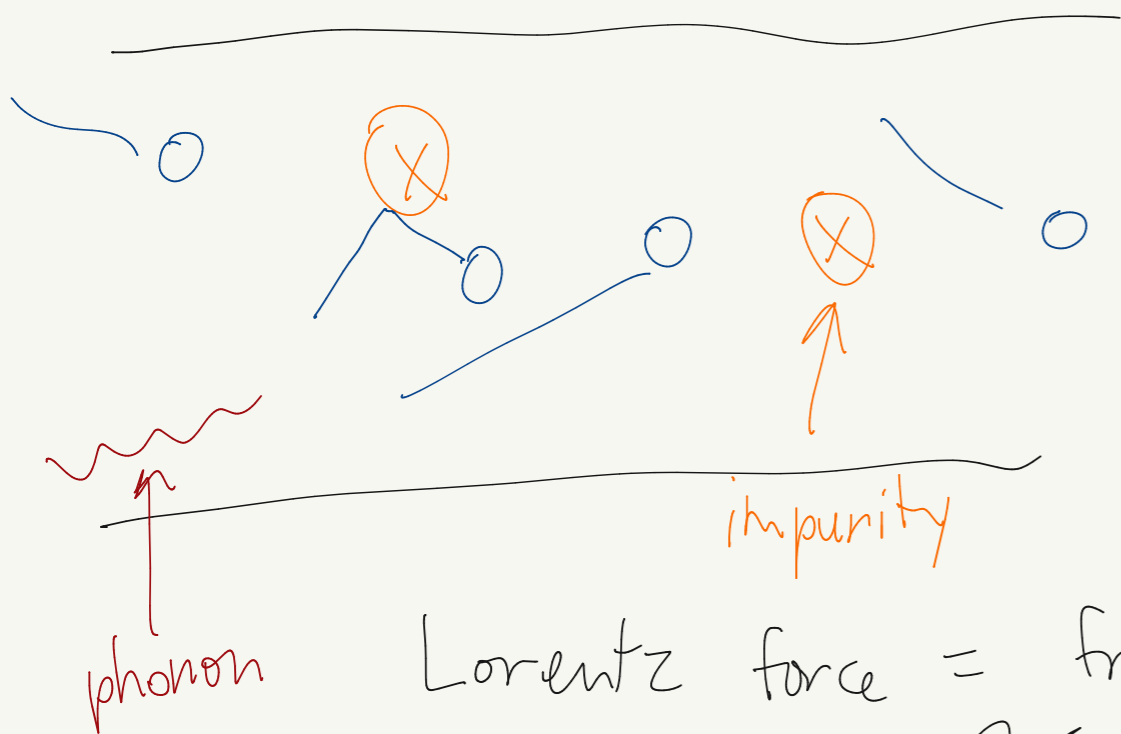
We want to keep track of only the intrinsic material property and learn something about the metal

Transport is the simplest window into dynamics in an experiment.

There are many experimental data sets. But in systems with strong interactions, Theory still hard

1.3) Relaxation time approximation

Begin with simple Drude model of transport in a metal. Think of individual electrons moving around...



Assume steady state flow macroscopically

Newton's law gives

Lorentz force = friction

$$-enE = \frac{\rho}{\tau}$$

number density \nearrow ρ ← momentum density
 τ ← momentum relaxation time

If particles all have same mass m :

$$J = -en\langle v \rangle \quad \rho = mn\langle v \rangle$$

But there can be metals where momentum relaxation isn't important for transport ... this is a cartoon for simplest case

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

also often works w/ conductivity

$$\sigma = \frac{1}{\rho}$$

transport time: $\tau_{tr} = \frac{m}{ne^2\rho}$

Useful cartoon but not in general a microscopic time scale of physical significance

material	τ_{tr} (ps)	v_F (m/s)	$l_{tr} = v_F \tau_{tr}$ (nm)
silver (300 K)	~ 0.05	10^6	~ 50
graphene (clean, 100 K)	~ 1	10^6	~ 1000
PdCoO ₂	~ 20	10^6	~ 20000
quantum critical BaFe ₂ (As,P) ₂ (20 K)	~ 0.003 [per band]	10^5	~ 0.3

unit cell: $a \sim 0.1 - 0.3$ nm.

Semiclassical expectation: $\frac{l_{tr}}{a} \gg 1$

- NOT in $\text{BaFe}_2(\text{As,P})_2$!

Mott-Ioffe-Regel bound: a good metal should have

$$\rho \lesssim \frac{m}{ne^2} \frac{v_F}{a} \sim \frac{\hbar}{e^2} a^{d-2}$$

Evidently the MIR bound not always obeyed. Drude argument must go wrong at some point. In the first part of the course we won't be able to calculate anything for such metals, but this is a simple demonstration that this model is insufficient.

Amusingly another problem with this is that near a metal insulator transition (driven by disorder or interactions) the transport time vanishes...but no transport! Drude model is not in general correct.

1.4) Multiple scattering mechanisms

In a real metal there are many scattering mechanisms - phonons, impurities, umklapp with other electrons ... so how should they interact in transport?

$$\sum F = 0 = -en\vec{E} + \vec{F}_{e,e} + \vec{F}_{e,imp} + \vec{F}_{e,ph}$$

\Downarrow

$$-en\vec{E} = P \left(\frac{1}{\tau_{ee}} + \frac{1}{\tau_{e,imp}} + \frac{1}{\tau_{e-ph}} \right)$$

\Downarrow

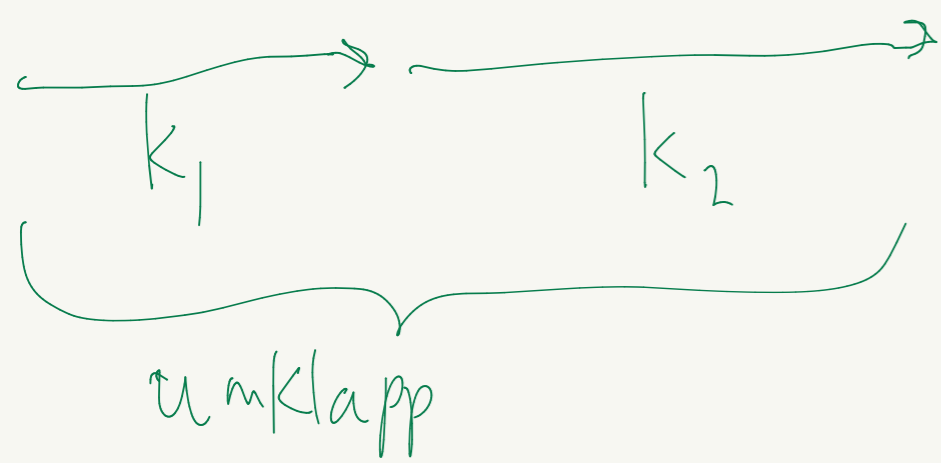
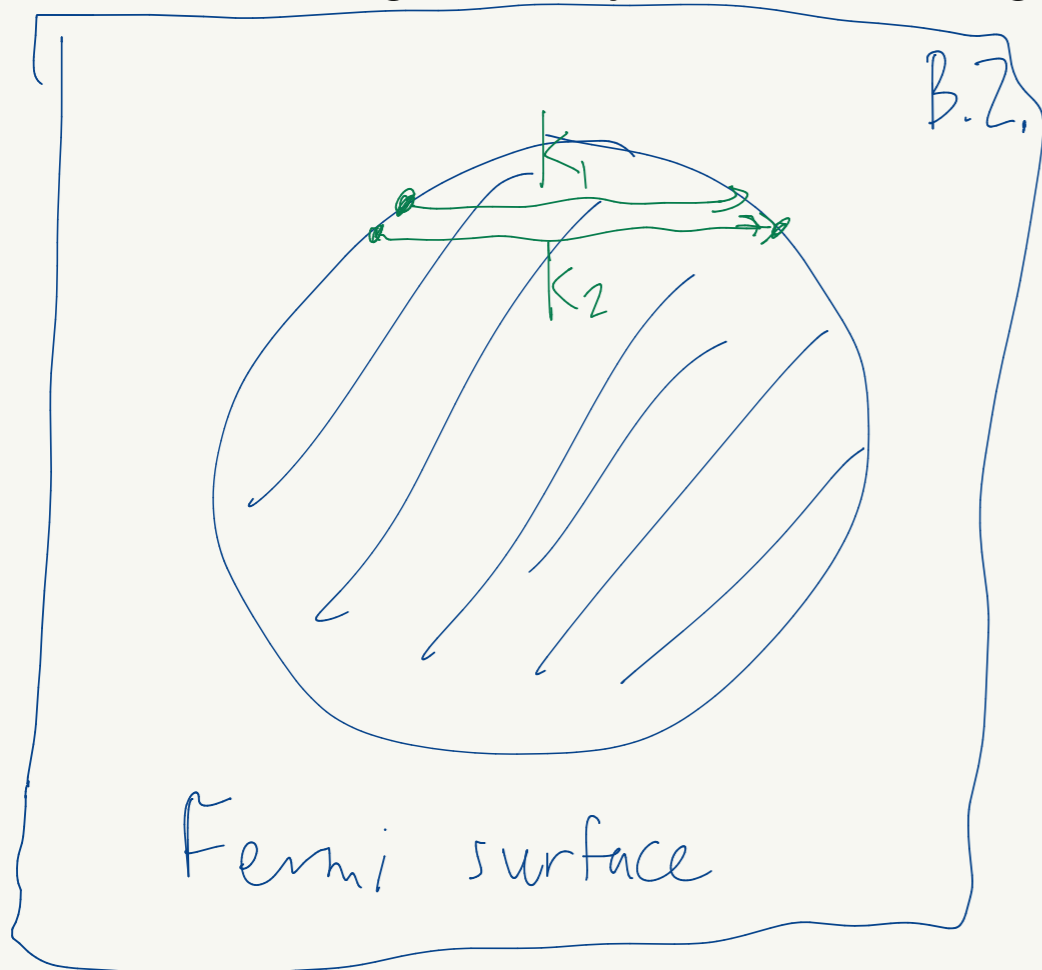
$$\frac{1}{\tau_{eff}} = \sum_{\text{scattering channel } \alpha} \frac{1}{\tau_{\alpha}}$$

This is known as Matthiessen's rule — scattering rates add to transport independently so the more scattering there is, the higher the resistivity?

Here are a number of important scattering rates to be aware of (we will derive all a little later)

electron-impurity; $\frac{1}{\tau_{e-imp}} \propto d T^0$

Recall that generically, other scattering rates must be momentum relaxing to contribute to transport ...



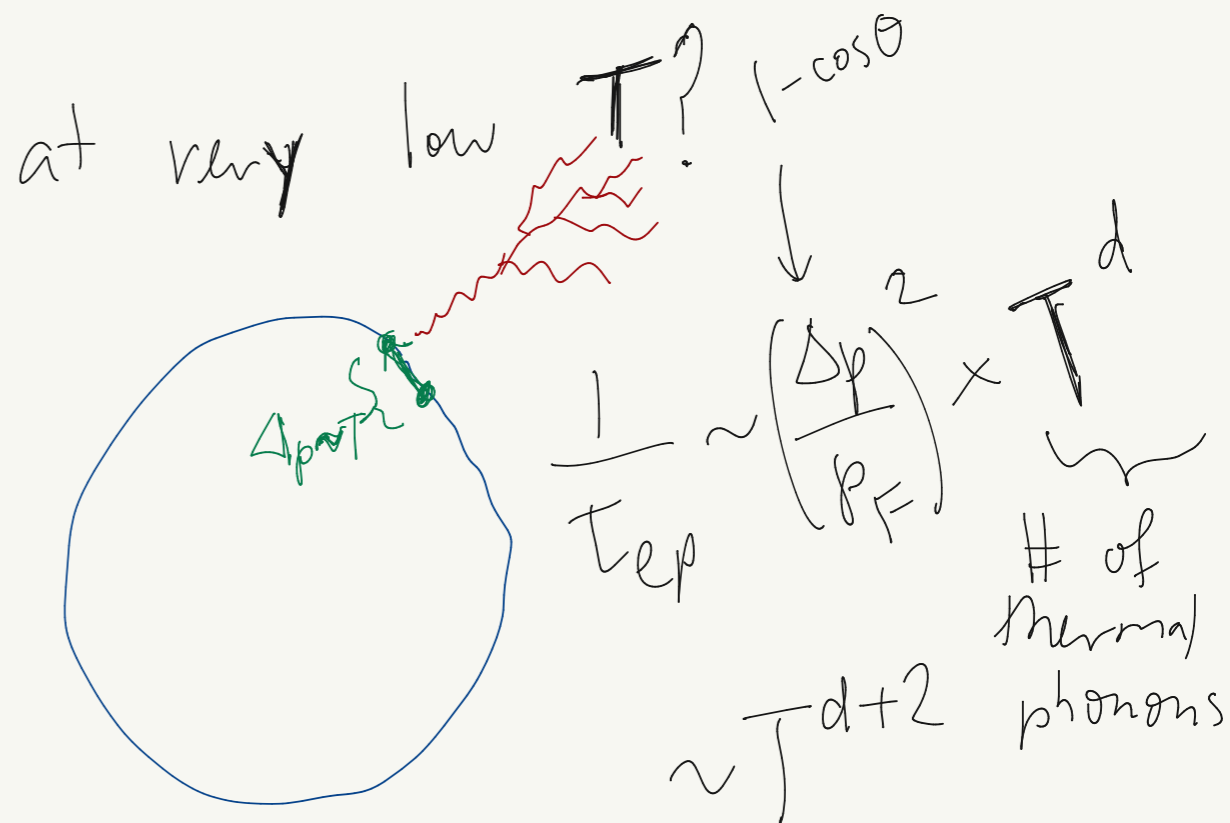
e-e scattering;
(F umklapp...)

$$\frac{1}{\tau_{ee}} \sim \underbrace{(\# \text{ of thermal electrons})^2}_{2\text{-body process}}$$

$$\frac{1}{\tau_{ee}} \sim T^2$$



phonons



Implicitly our phonon argument implies rapid phonon umklapp processes since small angle scattering isn't umklapp in general ...

at high T :

$$\frac{1}{\tau_{ep}} \sim (\# \text{ of phonons}) \sim T$$

It isn't always the case that the scattering rates add cleanly. Consider a two band (at the Fermi surface) metal, where we will write down the force balance equation for each band, assuming only impurity scattering (no interband) for simplicity

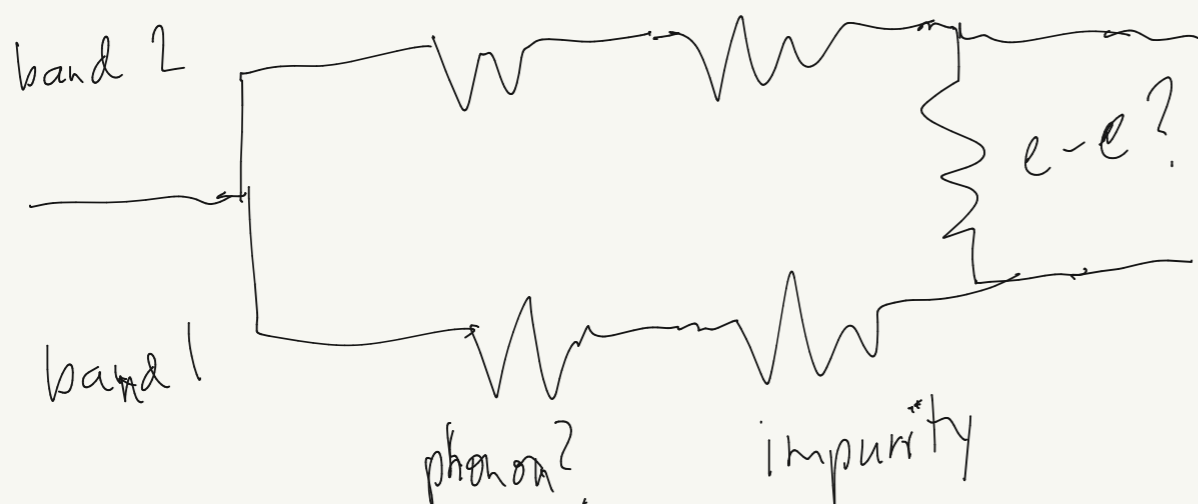
$$-en_1\vec{E} = -\frac{\vec{P}_1}{\tau_1}$$

$$-en_2\vec{E} = -\frac{\vec{P}_2}{\tau_2}$$

$$\vec{J}_{tot} \approx -\frac{e}{m_1}\vec{P}_1 - \frac{e}{m_2}\vec{P}_2 = \left[\frac{n_1 e^2 \tau_1}{m_1} + \frac{n_2 e^2 \tau_2}{m_2} \right] \vec{E}$$

So here the slowest scattering rate controls the conductivity.

Loosely speaking we can imagine a cartoon with a resistor network...



But at least for me it will be easier to instead return to complicated scattering mixtures using the kinetic formalism which we will soon discuss, so I won't say much more on this...

1.5) Thermoelectric conductivity matrix

$$\begin{pmatrix} \vec{J} \\ \vec{Q} \end{pmatrix} = \begin{pmatrix} \sigma & \alpha \\ T\alpha & \bar{\kappa} \end{pmatrix} \begin{pmatrix} E \\ -\nabla T \end{pmatrix}$$

charge current \vec{J}

heat current \vec{Q}

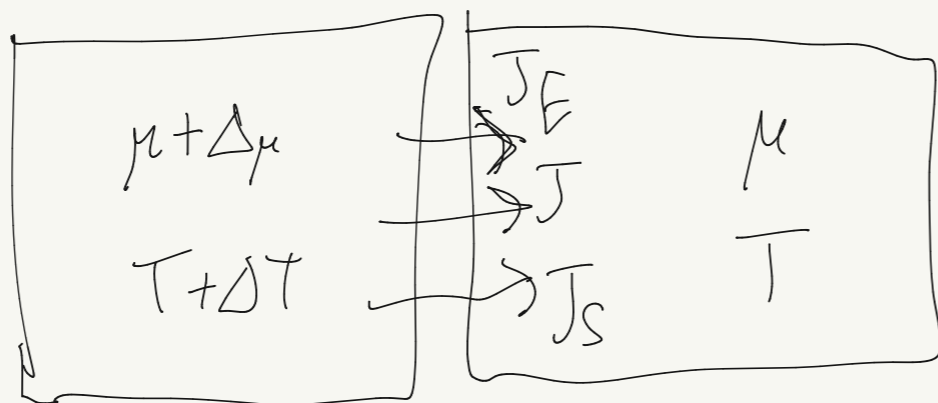
thermal conductivity (theorists')

temperature gradient

Apply small electric fields and temperature gradients and measure charge and heat currents.

What exactly is the heat current? Recall the first law of thermodynamics

$$dS = \frac{dE}{T} - \frac{\mu}{T} dQ$$



$$Q = T J_S = J_E - \mu J$$

Why is this heat current special? Because it is what naturally couples to a temperature gradient. Consider an unsourced medium

$$T \partial_t S = \partial_t \epsilon - \mu \partial_t \rho$$

entropy density energy density charge density

[local first law]

conservation laws:

$$\begin{cases} \partial_t \epsilon + \nabla \cdot J_E = 0 \\ \partial_t \rho + \nabla \cdot J = 0 \end{cases}$$

convective derivative

$$= -\nabla \cdot J_E + \mu \nabla \cdot J$$

$$= -\nabla \cdot Q - J \cdot \nabla \mu$$

$$T \frac{ds}{dt} = T(\partial_t S + \nabla \cdot J_S) = -J \cdot \nabla \mu - \frac{Q}{T} \cdot \nabla T$$

local heating

So the generalization of Ohm's law is

$$P = J \cdot E - Q \cdot \frac{\nabla T}{T} = \begin{pmatrix} E \\ -\frac{\nabla T}{T} \end{pmatrix} \underbrace{\begin{pmatrix} \sigma & T\alpha \\ T\alpha & T\bar{\kappa} \end{pmatrix}}_{\text{positive semidefinite}} \begin{pmatrix} E \\ -\frac{\nabla T}{T} \end{pmatrix}$$

Second law of thermodynamics implies that

$$\sigma \geq 0, \quad \bar{\kappa} \geq 0, \quad \bar{\kappa}\sigma \geq T\alpha^2$$

The thermoelectric conductivity matrix must be symmetric if there is time reversal symmetry (Onsager reciprocity)

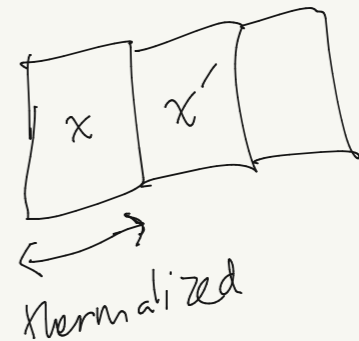
$$J_a = \begin{pmatrix} J \\ Q \end{pmatrix}, \quad E_a = \begin{pmatrix} E \\ -\nabla T/T \end{pmatrix}, \quad \sigma_{ab} = \begin{pmatrix} \sigma & T\alpha \\ T\alpha & T\bar{\kappa} \end{pmatrix}$$

$$= -\nabla \mu_a$$

Now we work in the grand canonical ensemble where pressure is the thermodynamic State Function

$$dP = p d\mu + s dT$$

$$= n_a d\mu_a \quad \leftarrow \text{volume}$$



thermally fluctuating variables

$$\langle n_a^{(x)} \mu_b^{(y)} \rangle = \int d\vec{\mu} \mu_b^{(y)} \frac{\partial P}{\partial \mu_a^{(x)}} e^{-PV/T} = -\frac{T}{V} \int d\vec{\mu} \mu_b \frac{\partial}{\partial \mu_a^{(x)}} e^{-PV/T}$$

$$= \frac{T}{V} \delta_{ab} \delta_{xy}$$

This logic holds if $|x-y| \gg$ thermalization length...

$$\langle n_a(t, x) n_b(t, x') \rangle = \langle n_a(0, x) n_b(t, x') \rangle \quad [\text{time reversal}]$$

$$\partial_t \langle n_a(t) n_b(0) \rangle = -\langle n_b(0) \nabla \cdot J_a(t) \rangle = -\langle n_a(0) \nabla \cdot J_b(t) \rangle$$

$$= -\langle \sigma_{ac} \nabla n_b(0) \cdot \nabla \mu_c(0) \rangle$$

$$= -\langle \sigma_{bc} \nabla n_a(0) \cdot \nabla \mu_c(0) \rangle$$

$$\sigma_{ac} \langle \nabla n_b(0, x) \cdot \nabla \mu_c(0, x') \rangle = \frac{T}{V} \sigma_{ac} (-\nabla^2 \delta(x-x')) \delta_{bc} \sim \sigma_{ab}$$

Hence,

$$\sigma_{ab} = \sigma_{ba}$$

In experiments one often measures the thermoelectric conductivity matrix in a weird way. For example,

$$Q = -\kappa \nabla T \Big|_{J=0} \quad : \quad 0 = \sigma E - \alpha \nabla T$$

$$\kappa = \bar{\kappa} - \frac{T \alpha^2}{\sigma} \quad \kappa \geq 0$$

Seebeck coefficient:

$$S = -\frac{\Delta V}{\Delta T} \Big|_{J=0} = \frac{\alpha}{\sigma}$$

Lastly we have thus far assumed isotropic systems, but it is straightforward to generalize all previous arguments to obtain that in an anisotropic system

$$\begin{pmatrix} J_i \\ Q_i \end{pmatrix} = \begin{pmatrix} \sigma_{ij} & \alpha_{ij} \\ T \alpha_{ji} & \bar{\kappa}_{ij} \end{pmatrix} \begin{pmatrix} E_j \\ -\partial_j T \end{pmatrix}$$

where now σ_{ij} is positive-semidefinite, etc....

$$\kappa_{ij} = \bar{\kappa}_{ij} - T \alpha_{ik} \sigma_{kl}^{-1} \alpha_{lj}$$

$$S_{ij} = \sigma_{ik}^{-1} \alpha_{kl}$$