Transport in strongly correlated systems

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Lecture 2: Conductivities and their ratios

- Transport coefficients measured experimentally
- Boltzmann transport theory
- Thermopower and Lorenz number
- The Nernst effect

$$J_\alpha = -\mathcal{N}^{11}_{\alpha\beta}\nabla_\beta\bar{\mu} - \mathcal{N}^{12}_{\alpha\beta}\nabla_\beta T$$

$$J^Q_\alpha = -T\mathcal{N}^{21}_{\alpha\beta}\nabla_\beta\bar{\mu} - \frac{\mathcal{N}^{22}_{\alpha\beta}}{T}\nabla_\beta T$$

Charge conductivities: $\nabla T = 0$, apply $\nabla\phi$, measure $\mathbf{J}$

$$\sigma_{\alpha\beta} = \mathcal{N}^{11}_{\alpha\beta}$$

Peltier conductivities: $\nabla T = 0$, apply $\nabla\phi$, measure $\mathbf{J}^Q$

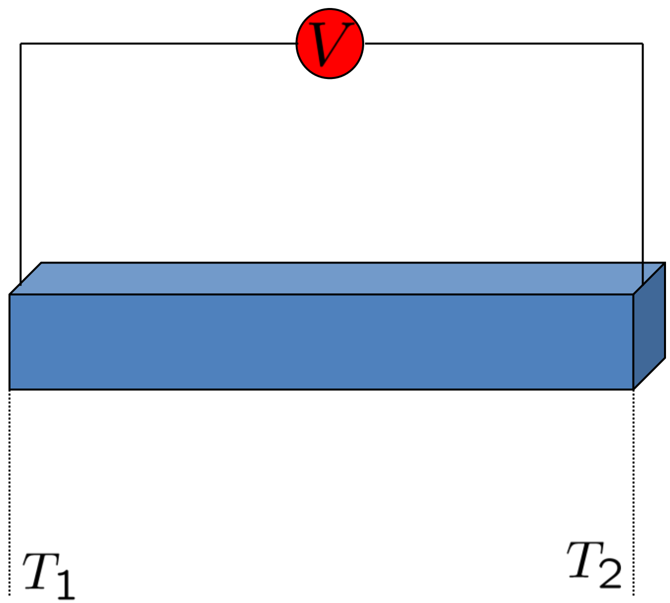
or $\nabla\phi = 0$, apply ∇T, measure $\mathbf{J}$

$$\alpha_{\alpha\beta} = \mathcal{N}^{12}_{\alpha\beta}$$

Heat conductivities: $\nabla\phi = 0$, apply ∇T, measure $\mathbf{J}^Q$

$$Q_{\alpha\beta} = \tfrac{1}{T}\mathcal{N}^{12}_{\alpha\beta}$$

Related quantity thermopower (or Seebeck coefficient) simpler to measure than α_{xx}



Thermopower: $S = \frac{V}{T_2 - T_1}$

S is measured under the condition $\mathbf{J} = 0$, $\nabla_y T = 0$

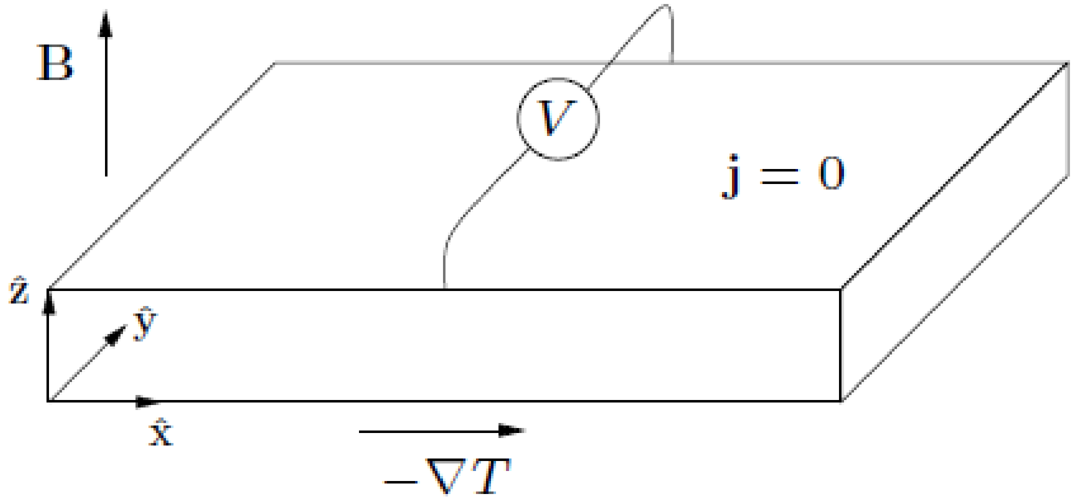
$$S = \left(\mathcal{N}_{xx}^{12}\mathcal{N}_{yy}^{11} + \mathcal{N}_{xy}^{11}\mathcal{N}_{yx}^{12}\right) / \left(\mathcal{N}_{xx}^{11}\mathcal{N}_{yy}^{11} + \mathcal{N}_{xy}^{11}\mathcal{N}_{yx}^{11}\right)$$

$$\mathcal{N}_{xy}^{ab} = 0 \text{ when } \mathbf{B} = 0$$

$$\boxed{S = \frac{\mathcal{N}_{xx}^{12}}{\mathcal{N}_{xx}^{11}} = \frac{\alpha_{xx}}{\sigma_{xx}}}$$

One can also measure V_y when $\nabla_x T \neq 0$ but $\nabla_y T = 0$ and $\mathbf{J} = 0$

This is called the Nernst effect



$$\nu = \frac{1}{B}\left(\mathcal{N}^{12}_{xy}\mathcal{N}^{11}_{xx} - \mathcal{N}^{11}_{xy}\mathcal{N}^{12}_{xx}\right) / \left(\mathcal{N}^{11}_{xx}\mathcal{N}^{11}_{yy} + \mathcal{N}^{11}_{xy}\mathcal{N}^{11}_{yx}\right)$$

$$= \frac{1}{B}\left(\alpha_{xy}\sigma_{xx} - \sigma_{xy}\alpha_{xx}\right) / \left(\sigma_{xx}\sigma_{yy} + \sigma_{xy}\sigma_{yx}\right)$$

No Nernst effect for $\mathbf{B} = 0$

If $\sigma_{xy} \ll \sigma_{xx}$

$$\nu = \frac{1}{B}\frac{\alpha_{xy}}{\sigma_{xx}}$$

As we will see later, the Nernst effect is important in superconductors

Generally indicates the presence of mobile vortices

Thermal conductivity

Measure J_x^Q with $\nabla_x T \neq 0$ and $\nabla_y T = 0$ and $\mathbf{J} = 0$

Set $\mathbf{B} = 0$

$$\kappa = \frac{1}{T}\left(\mathcal{N}_{xx}^{22} - T^2 \frac{\mathcal{N}_{xx}^{12}\mathcal{N}_{xx}^{21}}{\mathcal{N}_{xx}^{11}}\right)$$

The heat conductivity $Q_{xx} = \frac{1}{T}\mathcal{N}_{xx}^{22}$

For $\mathbf{B} \neq 0$, $\kappa_{xy} \neq 0$ (Righi-Leduc coefficient)

For a solid state system

$$\boxed{\kappa = \kappa_e + \kappa_{ph}}$$

Before we look at strongly correlated systems

What do these transport coefficients look like for weakly interacting systems?

Such systems can be thought of as consisting of quasiparticles that are scattered in some way

Most efficient way to study transport - Boltzmann transport equation

Scattering parametrized by a momentum dependent scattering rate $\tau(\mathbf{k})$

Semiclassical approach

Distribution function $f(\mathbf{k}, \mathbf{r}, t)$

$$\frac{\partial f}{\partial t} + \mathbf{v}.\nabla_{\mathbf{r}} f + \frac{d\mathbf{k}}{dt}.\nabla_{\mathbf{k}} f = -\left(\frac{\partial f}{\partial t}\right)_{\mathrm{coll}}$$

$$\left(\frac{\partial f}{\partial t}\right)_{\mathrm{coll}} = -\frac{f - f_0}{\tau(\mathbf{k})}$$

f_0 - equilibrium distribution function

Steady state homogeneous situation

$$\frac{d\mathbf{k}}{dt}.\nabla_{\mathbf{k}} f = -\left(\frac{\partial f}{\partial t}\right)_{\mathrm{coll}}$$

$$f = f_0 + \frac{1}{\hbar}\tau(\mathbf{k})\mathbf{F}.\nabla_{\mathbf{k}} f_0$$

$$\frac{d\mathbf{k}}{dt} = \frac{1}{\hbar}\mathbf{F}$$

$$\mathbf{J} = en_0\langle\mathbf{v}\rangle = \frac{e\hbar}{m}\int \frac{d\mathbf{k}}{(2\pi)^d} f(\mathbf{k})\mathbf{k}$$

$$\mathbf{J}^E = n_0\langle\epsilon(\mathbf{k})\mathbf{v}\rangle = \frac{\hbar}{m}\int \frac{d\mathbf{k}}{(2\pi)^d} f(\mathbf{k})\mathbf{k}\epsilon(\mathbf{k})$$

$\mathbf{F} = e\mathbf{E}$ for an applied electric field

$$L^{ab}_{\alpha\beta} = \int d\epsilon \left(-\frac{df_0}{d\epsilon}\right) \Sigma^{ab}_{\alpha\beta}(\epsilon)$$

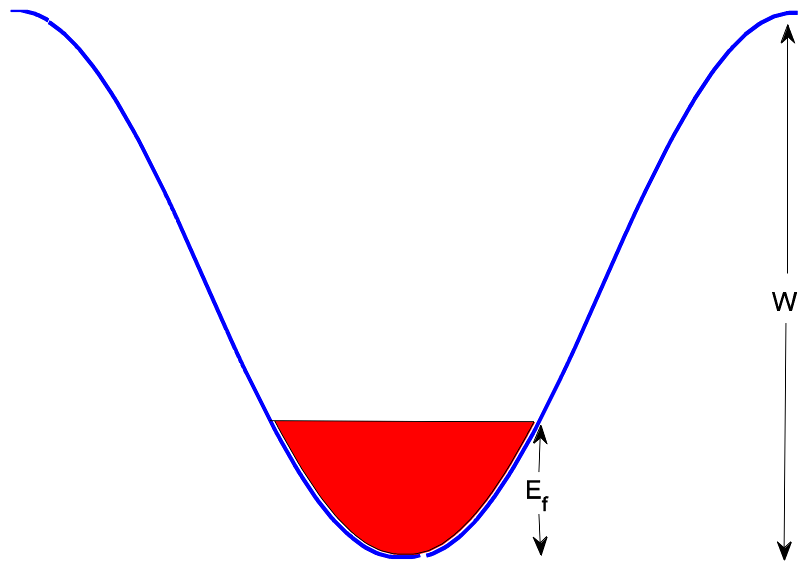
$$\Sigma^{ab}_{\alpha\beta}(\epsilon) = \sum_{\mathbf{k}} \epsilon^{(a+b)} v_\alpha(\mathbf{k}) v_\beta(\mathbf{k}) \tau(\mathbf{k}) \delta[\epsilon - \epsilon(\mathbf{k})]$$

Values of a and b: 0 for charge, 1 for energy

What can we deduce from these relations?

Let us make the simplification that τ depnds only on energy

A simple one band system



E_f - Fermi energy

W - Bandwidth $= \#t$

t - hopping

For degenerate electron systems $(T \ll T_F)$

$$\boxed{S = T\frac{\pi^2 k_B^2}{3e^2}\frac{d}{d\epsilon}\log\left[\rho(\epsilon)\langle v^2\rangle_\epsilon \tau(\epsilon)\right]\Big|_{\epsilon=\epsilon_F}} \quad \sim \frac{T}{T_F}$$

Mott formula

Lorenz number $L = \dfrac{\kappa}{T\sigma}$

$$\boxed{L \sim \frac{k_B^2}{e^2}}$$ Wiedemann-Franz law

In many metals at rooms temperature $\kappa_e \gg \kappa_{ph}$
so the WF law holds for total κ as well

For non-degenerate electron systems ($T \ll T_F \ll W$)

$$S \sim \frac{k_B}{e}$$ with a weak (log) dependence on n and T

$$L \sim \frac{k_B^2}{e^2}$$ Semiconductors at room temperature

For very narrow bandwidth systems ($W \ll T$)

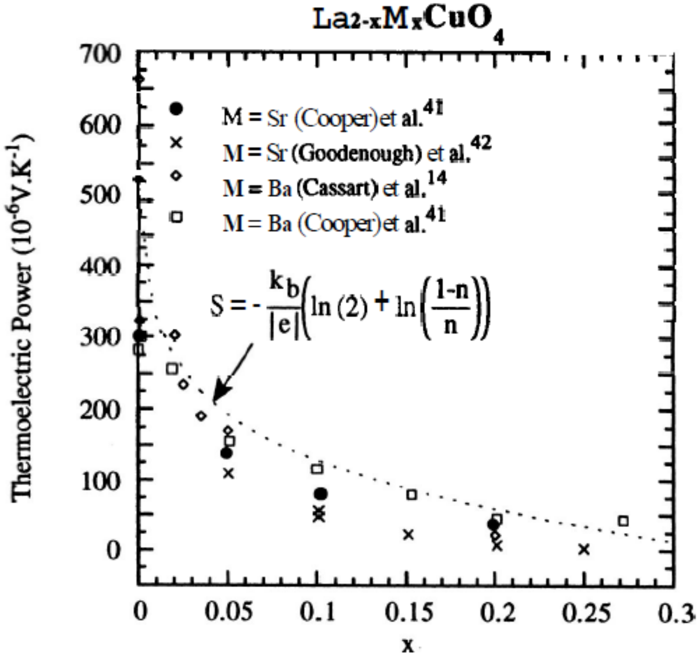
$$S \sim \frac{k_B}{e}$$ log dependence on n, independent of T

Heike's limit

$$L \sim \left(\frac{W}{T}\right)^2$$ Violation of the Wiedemann-Franz law

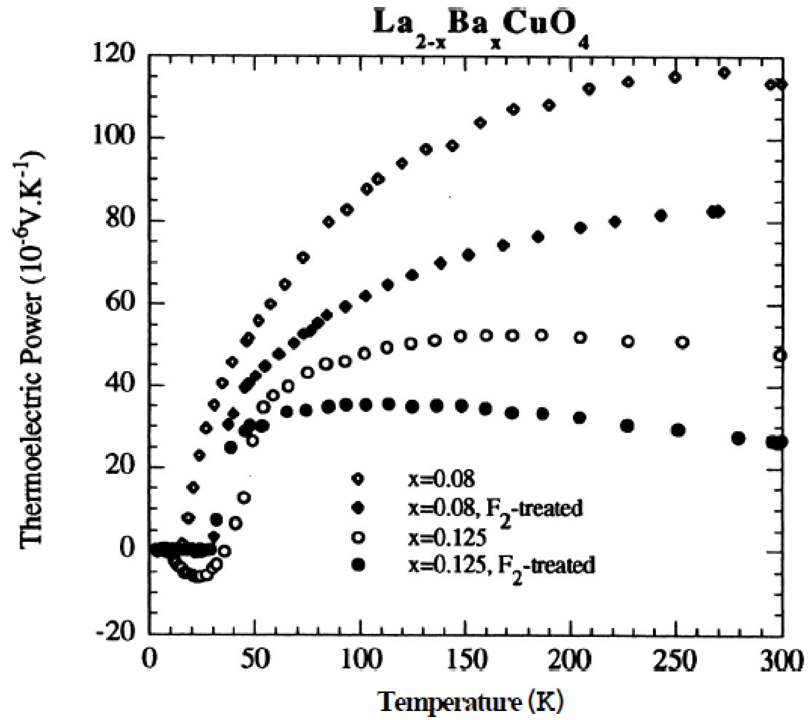
However in both these systems $\kappa_{ph} \gg \kappa_e$

Strongly correlated system

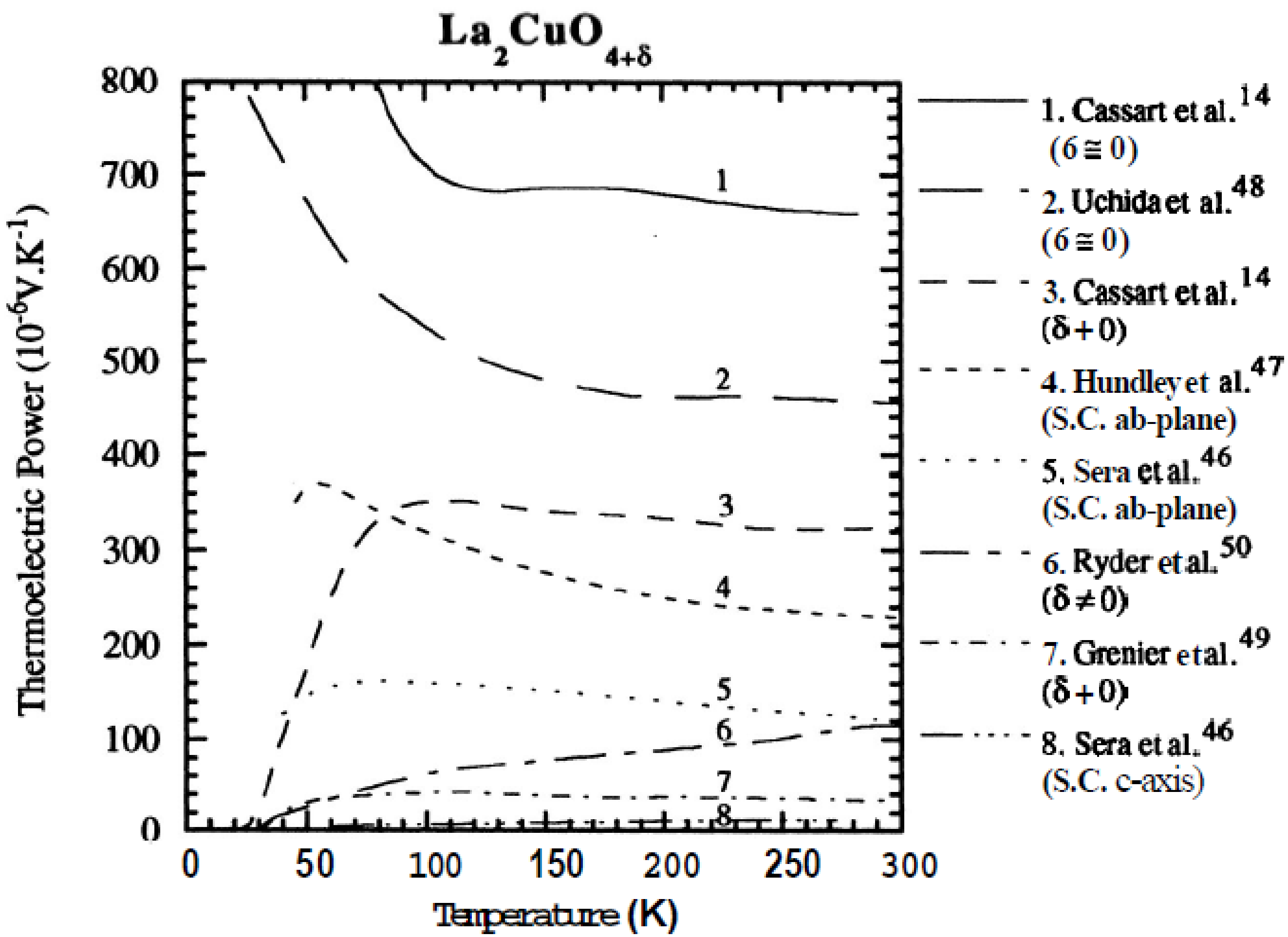


at room temperature

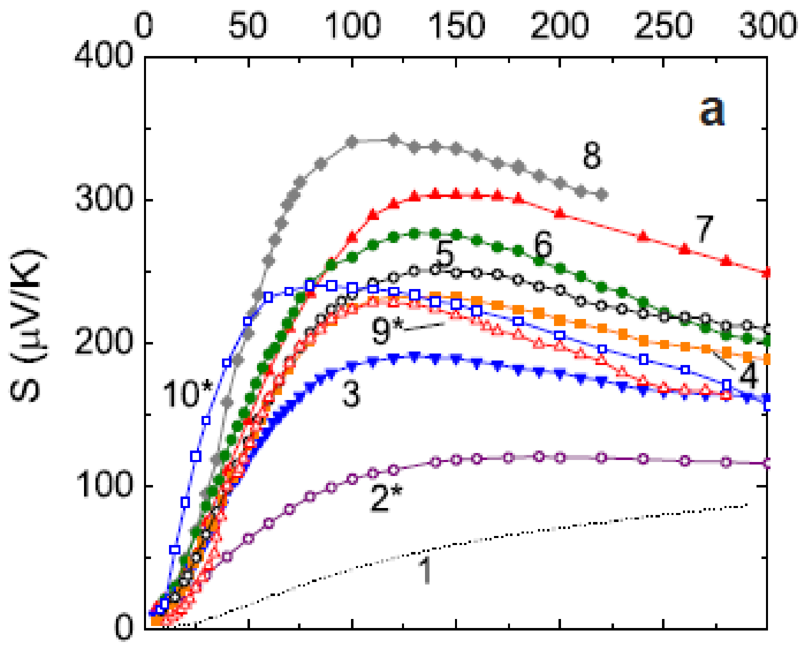
Dotted line (Heikes fit) with strong correlations



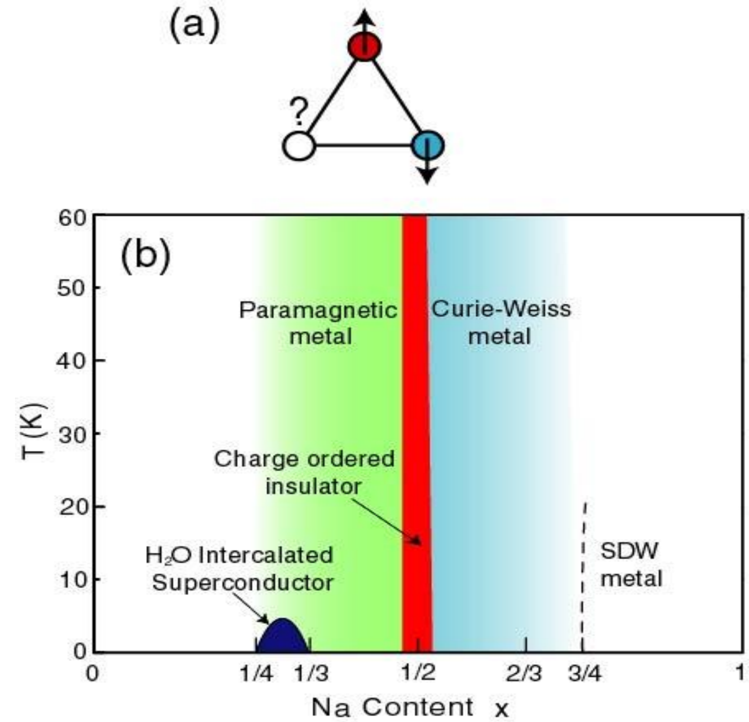
S shows signs of saturation around 200-300 K



La2CuO4+δ
Thermoelectric Power (10-6V.K-1)
800
700
600
500
400
300
200
100
0
0
50
100
150
200
250
300
Temperature (K)
1
2
3
4
5
6
7
8
1. Cassart et al.14
(6 ≅ 0)
2. Uchida et al.48
(6 ≅ 0)
3. Cassart et al.14
(δ + 0)
4. Hundley et al.47
(S.C. ab-plane)
5. Sera et al.46
(S.C. ab-plane)
6. Ryder et al.50
(δ ≠ 0)
7. Grenier et al.49
(δ + 0)
8. Sera et al.46
(S.C. c-axis)



Na_xCoO_2



Electron doped Mott insulator

Metallic but also large S

[M. Lee *et. al.*, *Nature Materials* **5** 237 (2006)]

What is so interesting?

Heikes like saturation even with strong interactions

What sets the energy scale above which the saturation sets in?

Theory with strong correlations

What about the Lorenz number?
In these materials κ_{ph} can dominate κ_e

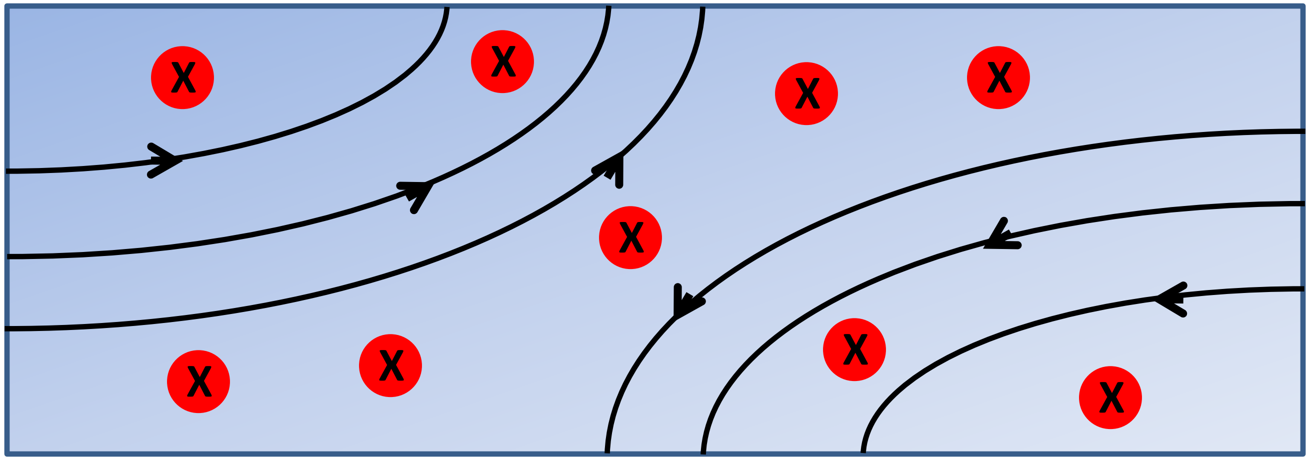
The Nernst effect

$$\nu = \frac{1}{B}\left(\alpha_{xy}\sigma_{xx} - \sigma_{xy}\alpha_{xx}\right) / \left(\sigma_{xx}\sigma_{yy} + \sigma_{xy}\sigma_{yx}\right)$$

In Boltzmann theory with energy independent relaxation time (Drude theory)

$\boxed{\nu = 0}$ Sondheimer cancellation

For general $\tau(\epsilon)$ ν is non-zero but typically small for metals



$-\nabla T \rightarrow$

Backflow of charged particles needed for $\mathbf{J} = 0$

No voltage if identical motion in both directions

Energy dependent scattering can give non-zero voltage

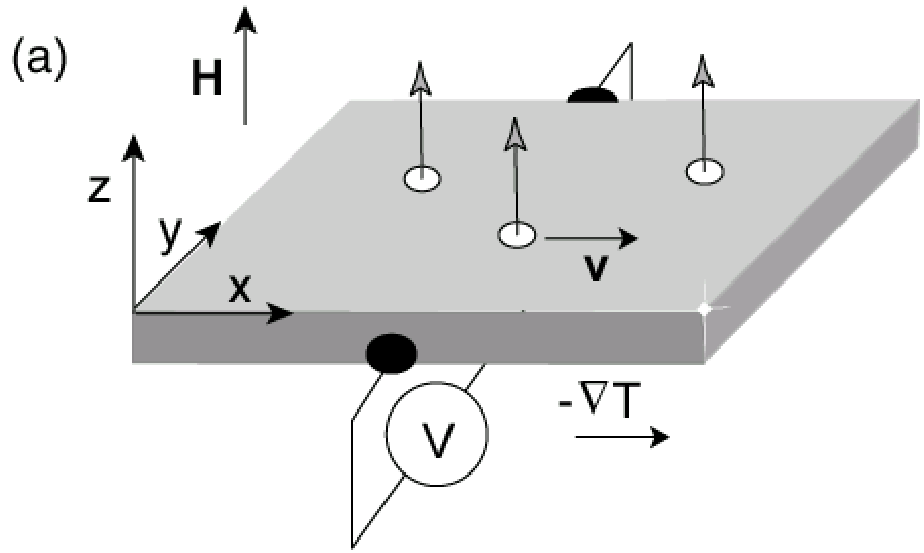
One way to get a large Nernst effect

Excitations transporting heat do not carry charge

(no backflow required for zero charge current)

They are capable of producing voltages

Vortices in superconductors satisfy these criteria



Vortices induced by magnetic field

Move from hot end to cold end without transporting charge

Induce transverse voltage through phase slips

Very simple minded phenomenological theory

Thermal force $\mathbf{F}_T = -S_\phi \nabla T$

Drag force $\mathbf{F}_D = -\eta \mathbf{v}_\phi$

$$\mathbf{E} = -\mathbf{v}_\phi \times \mathbf{B}$$

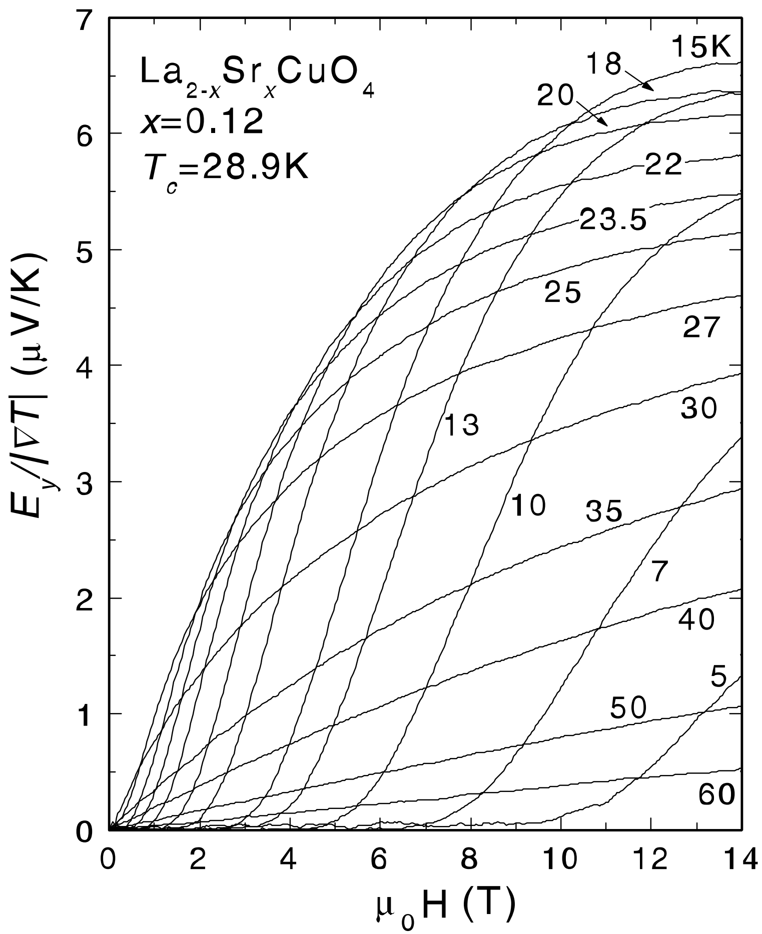
$$\mathbf{F}_D + \mathbf{F}_T = 0$$

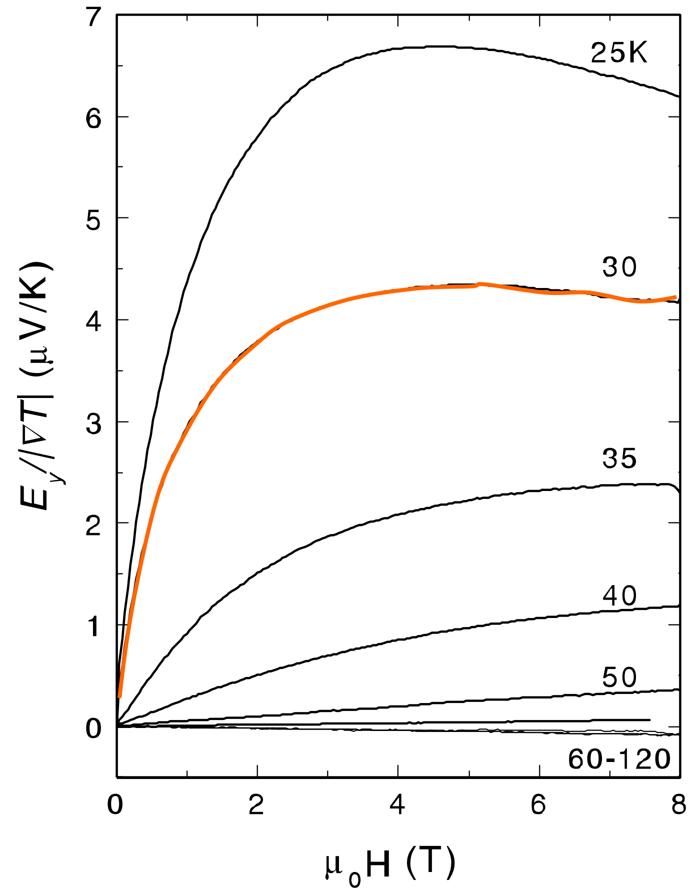
$$\nu = \frac{S_\phi}{\eta}$$

How do we obtain S_ϕ and η from an appropriate model?

Nernst effect in high T_c superconductors

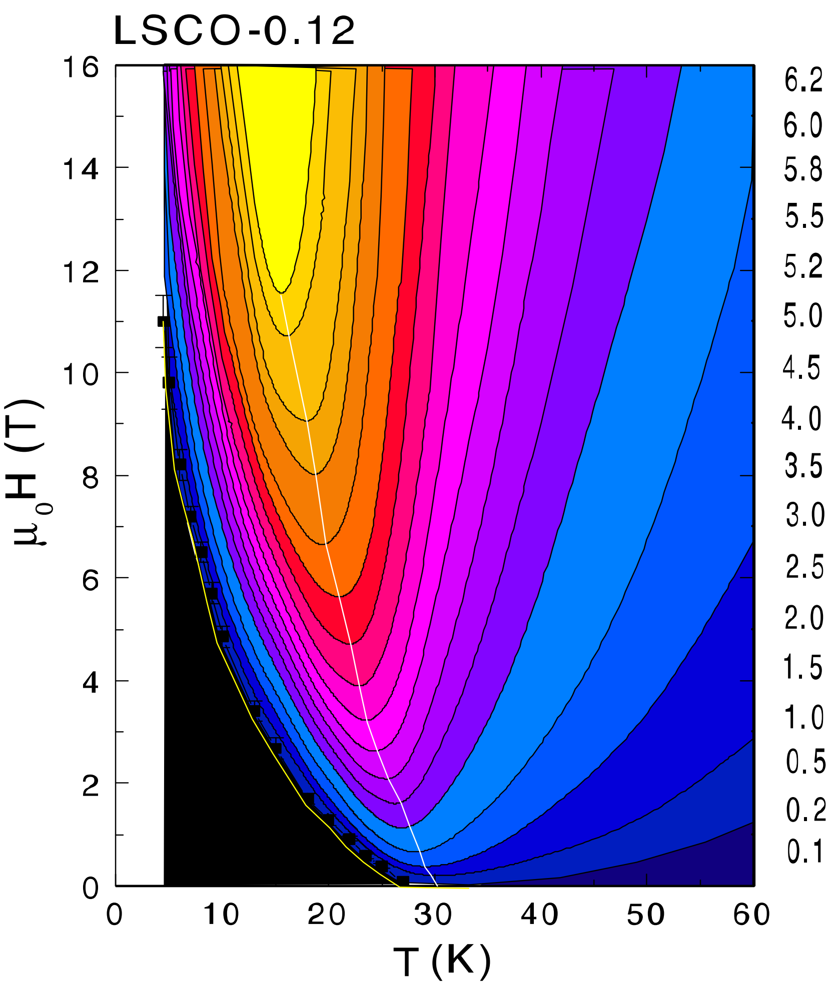
$Bi_2Sr_{2-y}La_yCu_2O_6$

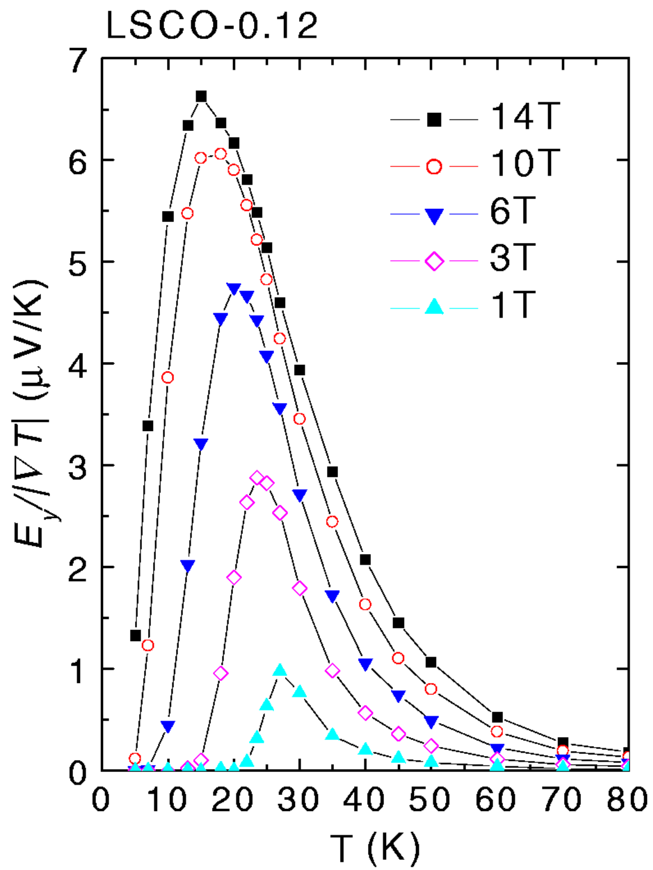




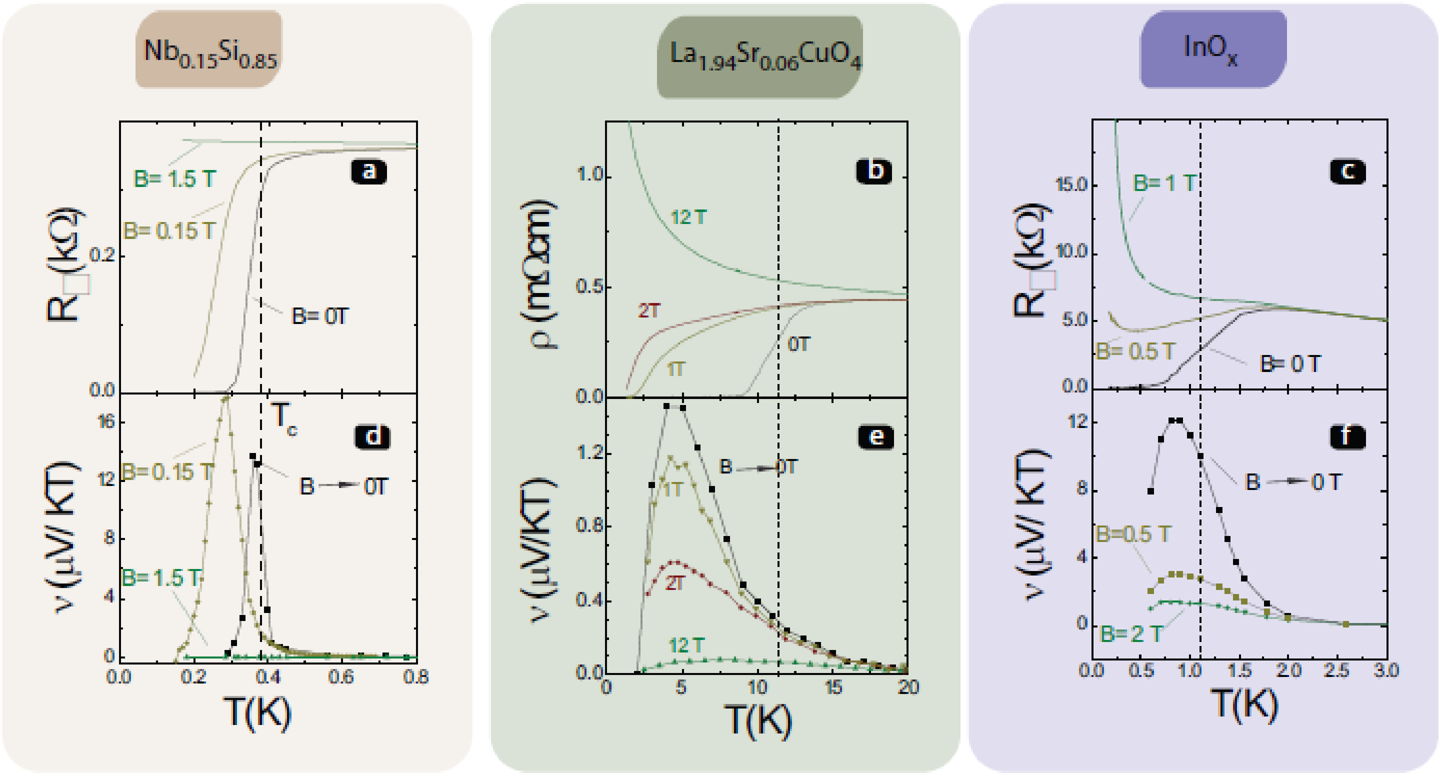
[Z. A. Xu *et. al.*, *Nature* **406** 486 (2000)]

[Y. Wang *et. al.*, *Phys. Rev. B* **64** 224519 (2001)]


LSCO-0.12
μ0H (T)
T (K)
0
2
4
6
8
10
12
14
16
0
10
20
30
40
50
60
6.2
6.0
5.8
5.5
5.2
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.2
0.1


LSCO-0.12
14T
10T
6T
3T
1T
Ey/|∇T| (μV/K)
T (K)
0
1
2
3
4
5
6
7
0
10
20
30
40
50
60
70
80

Disordered thin films



[A. Pourret *et. al.*, *Nature Physics* **2** 683 (2006)]

What is interesting here?

Are we seeing vortices well above T_c?

Do these "vortices" have anything to do with the pseudogap state that forms after superconductivty is lost above T_c?

Can we come up with a theory to explain the B and T dependence?

Is there any universality across different types of systems?

(To be discussed in the last lecture)

References

1. H. B. Callen *Phys. Rev.* **73** 1349 (1948)
2. Y. Wang, L. Li and N. P. Ong, *Phys. Rev. B* **73** 024510 (2006)
3. G. D. Mahan, *Many Particle Physics* (Plenum Publishers)
4. S. R. de Groot and P. Mazur, *Non-equilibrium Thermodynamics* (Dover Publications)
5. J. M. Ziman, *Principles of the theory of solids*

Lecture 3: Transport with strong interactions

- Thermopower, Lorenz number, figure of merit
- Hubbard model in the atomic limit
- Comparison to experimental data
- Single molecules with strong interactions