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International Centre for Theoretical Physics

United Nations
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2035-18

Conference on Superconductor-Insulator Transitions

18 - 23 May 2009

Fluctuations of the superconducting order parameter as an origin of the Nernst effect

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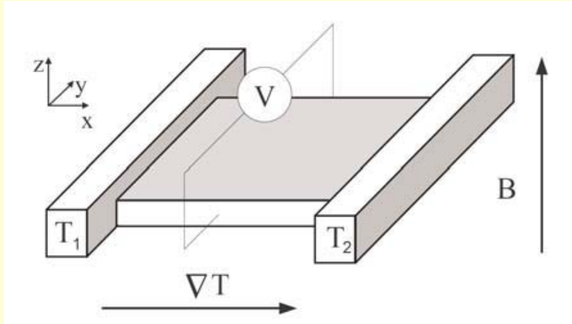


Quantum kinetic approach to the calculation of the Nernst effect

Karen Michaeli and Alexander M. Finkel'stein

Why Not to Use the Kubo Formula?

Luttinger approach – J. M. Luttinger 1964.

Electric conductivity:

- The density matrix at $t = -\infty$ is $\rho_0 = e^{-\beta H_0}$.
- Adiabatically switching on a scalar potential $H = H_0 + e\int e^{-st}\varphi(r)n(r)dr$
- Deriving the Kubo formula for the linear response to the field using the E.O.M for the density matrix and the continuity equation for the density:

$$i\frac{d\rho(t)}{dt} = [H, \rho(t)] \qquad e\dot{n} + \nabla j = 0$$

$$\longrightarrow \quad \langle j_e(r)\rangle = -\langle e^{-\beta H_0} j_e j_e\rangle \nabla\varphi$$

Kubo Formula

Luttinger approach – J. M. Luttinger 1964.

Electric conductivity:

- In the limit s << q (s- the frequency of the electric field), the electro-chemical potential remains constant :

$$\zeta_0 = \mu(r) + e\varphi(r)$$

- The system is at equilibrium:

$$\langle j(r) \rangle = -\sigma \nabla \varphi - eD \nabla n = 0$$

$$\Rightarrow \quad D = -\frac{\sigma \nabla \varphi}{e \nabla n} = \sigma \frac{\nabla \mu}{e^2 \nabla n}$$

Einstein relation

Thermal Conductivity - Kubo Formula

Luttinger approach – J. M. Luttinger 1964.

Thermal conductivity:

- Introducing a mechanical force field that is coupled to the Hamiltonian density:

$$H = \int h_0(r)dr + \int e^{-st}\gamma(r)h_0(r)dr$$

- Deriving the Kubo formula for the linear response to the field:

  The E.O.M for the density matrix:

$$i\frac{d\rho(t)}{dt} = [H, \rho(t)] \qquad \dot{h} + \nabla j_h = 0$$

$$\longrightarrow \qquad \langle j_h \rangle = \langle e^{-\beta H_0} j_h j_h \rangle \nabla\gamma$$

Luttinger connected between the response to the gravitational field and the temperature gradient.

Thermal Conductivity - Kubo Formula

Luttinger approach – J. M. Luttinger 1964.

Thermal conductivity:

- In the limit s << q (s- the frequency of the gravitational field) the system is at equilibrium:

$$j_h^i(\mathbf{r}) = \kappa_{ij} T \nabla_j \left(\frac{1}{T}\right) + \tilde{\kappa}_{ij}\left(-\nabla_j \gamma\right)$$

- - Kubo formula for the energy density yields: $\langle h(-\mathbf{q})\rangle = -\langle h(-\mathbf{q})h(\mathbf{q})\rangle_0 \gamma(\mathbf{q})$

  - Thermodynamic calculation of correlation function: $\lim_{\mathbf{q}\to 0}\langle h(-\mathbf{q})h(\mathbf{q})\rangle_0 = -V\frac{\partial U}{\partial \beta}$

  - and the temperature:

$$\left(\frac{1}{T}\right)_{\mathbf{q}} = \left(\frac{\partial \beta}{\partial h}\right)_N \langle h(\mathbf{q})\rangle$$

Altogether

$$\left(\frac{1}{T}\right)_{\mathbf{q}} = \frac{V}{T}\gamma(\mathbf{q}) \longrightarrow \kappa_{ij} = \tilde{\kappa}_{ij}$$

Thermal Conductivity - Kubo Formula

Luttinger approach – J. M. Luttinger 1964.

Thermal conductivity:

- Luttinger's expression for the current operator:

$$j_h^{\upsilon} = \frac{1}{2}\sum_i \left(h_i j_i^{\upsilon}(\mathbf{r}) + j_i^{\upsilon}(\mathbf{r}) h_i\right) - \frac{1}{8m}\sum_{i,i'}\left[\left(p_i^{\upsilon} + p_{i'}^{\upsilon}\right)\left(r_i^{\sigma} - r_{i'}^{\sigma}\right)\frac{\partial u(\mathbf{r}_i, \mathbf{r}_{i'})}{\partial r_i^{\sigma}}\delta(\mathbf{r} - \mathbf{r}_i) + \delta(\mathbf{r} - \mathbf{r}_i)\left(r_i^{\sigma} - r_{i'}^{\sigma}\right)\frac{\partial u(\mathbf{r}_i, \mathbf{r}_{i'})}{\partial r_i^{\sigma}}\left(p_i^{\upsilon} + p_{i'}^{\upsilon}\right)\right]$$

where

$$j_i^{\nu} = \frac{1}{2m}\left(p_i^{\nu}\delta(\mathbf{r} - \mathbf{r}_i) + \delta(\mathbf{r} - \mathbf{r}_i) p_i^{\nu}\right)$$

$$h_i = \frac{p_i^2}{2m} + V_{imp}^i + \frac{1}{2}\sum_{i' \neq i} u(\mathbf{r}_i, \mathbf{r}_{i'})$$

How exactly to use such a vertex?

Thermal Conductivity - Vertex Term

The common expression used in the Kubo formula:

$$j_h^{\upsilon}\left(\mathbf{q},\omega\right)=\frac{2\varepsilon_m+\omega_m}{2e}\,j_e^{\upsilon}\left(\mathbf{k}+\mathbf{q},\omega+\varepsilon\right)$$

i. Where are the corrections due to the interaction?

ii. Should one extract the external frequency from the vertex term?

iii. How to get the Wiedemann-Franz law in the Fermi liquid theory?

Wiedemann-Franz Law in the Fermi Liquid Theory

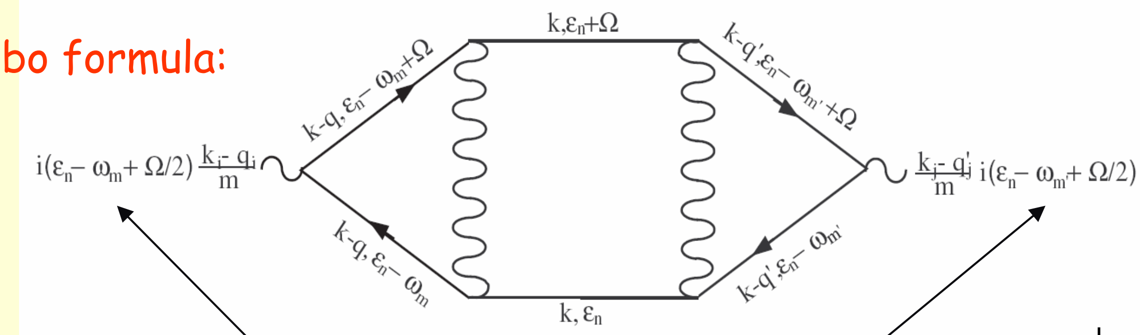
Langer 1962

In the Fermi liquid theory the thermal conductivity is of the form:

$$\kappa = \frac{1}{d}\int \frac{d\mathbf{k}d\varepsilon}{(2\pi)^{d+1}} \frac{\partial \tanh\left(\varepsilon/2T\right)}{\partial \varepsilon} \varepsilon v_i(\mathbf{k},\varepsilon) G_R(\mathbf{k},\varepsilon) \varepsilon v_i(\mathbf{k},\varepsilon) G_A(\mathbf{k},\varepsilon)$$

$$v_i(\mathbf{k},\varepsilon) = \left(\frac{k_i}{m} + \frac{\partial \hat{\Sigma}_{eq}(\mathbf{k},\varepsilon)}{\partial k_i} \right)$$

Using the Kubo formula:



The bosonic frequency in the vertex leads to the violation of the Wiedemann-Franz law.

Nernst Effect - Magnetization

There has been a long discussion about the contribution of magnetization to the thermoelectric transport currents.

For example:
Obraztsov Sov. Phys. Solid State 1965
Smrcka and Streda J. Phys. C 1977
Cooper, Halperin and Ruzin PRB 1997

The heat current that describes the change in the entropy.

In the presence of magnetic field the thermodynamic expression for the heat contains the magnetization term:

$$dQ = TdS = dE - \mu dN + MdB.$$

The Kubo formula is not enough, the contribution from the magnetization must be added.

Quantum Kinetic Approach

The derivation of the transport coefficients using the quantum kinetic approach consists of two stages:

a. Derive the quantum kinetic equation for the Green functions which depend on the external perturbation.

b. Find the expressions for the relevant currents.

$$\begin{pmatrix} j_e \\ j_h \end{pmatrix} = \begin{pmatrix} \sigma & \alpha \\ \tilde{\alpha} & \kappa \end{pmatrix} \begin{pmatrix} E \\ -\nabla T \end{pmatrix}$$

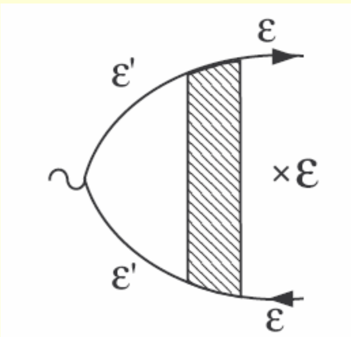
Derivations of the transport coefficients using the kinetic equation already exist, for example:

J.-W. Wu, and G. D. Mahan, 1984.
G. Strinati, C. Castellani, C. DiCastro, and G. Kotliar, 1991.
D. V. Livanov, M. Y. Reizer, and A. V. Sergeev, 1991.
R. Raimondi, G. Savona, P. Schwab, and T. Luck, 2004.
G. Catelani, and I. L. Aleiner, 2005.

Our Scheme Differs in Few Aspects

The kinetic equations and the currents are derived from the action.

For the Coulomb interaction all the continuity currents share a common simple structure:



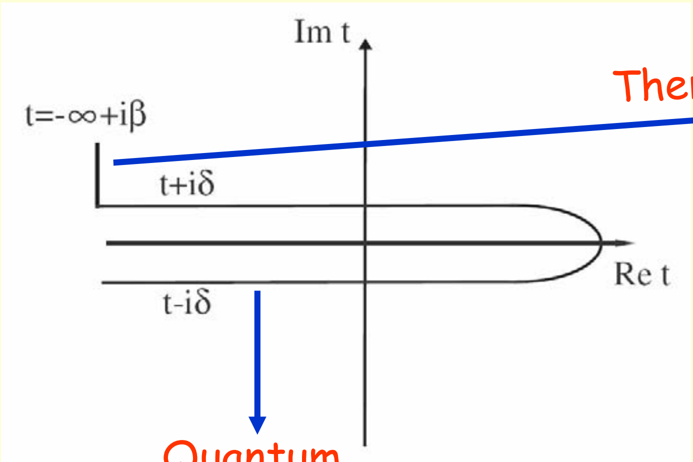
$$\mathbf{j}_e^{con} = -i\int \frac{d\varepsilon}{2\pi}\chi_{e,h}(\varepsilon)\left[\hat{\mathbf{v}}(\varepsilon)\hat{G}(\varepsilon)\right]^{<}$$

$$\chi_e(\varepsilon) = -e \quad , \quad \chi_h(\varepsilon) = \varepsilon$$

The renormalized velocity

Quantum Kinetic Approach

The Keldysh Green function: $\hat{G}(r,t;r't') = \begin{pmatrix} G_T & G^< \\ G^> & G_{\tilde{T}} \end{pmatrix} \Leftrightarrow \begin{pmatrix} G^R & G^K \\ & G^A \end{pmatrix}$



Thermal weight

$$\hat{\rho} = \exp\left\{-i\int d\mathbf{r} \int_{-\infty+i\beta(\mathbf{r})}^{-\infty+i\delta} dt\left[h(\mathbf{r}) - \mu n(\mathbf{r})\right]\right\}$$

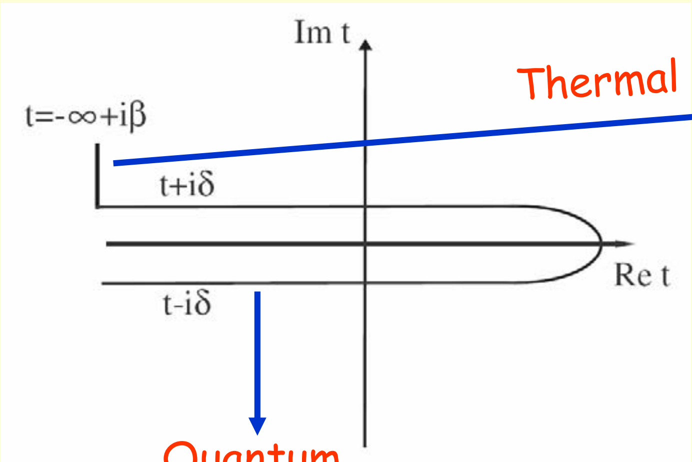
Quantum kinetic equation

Time evolution without any external perturbation.

We have to find highly non-trivial initial state before we even start to study its time evolution

Quantum Kinetic Approach

The Keldysh Green function: $\hat{G}(r,t;r't') = \begin{pmatrix} G_T & G^{<} \\ G^{>} & G_{\tilde{T}} \end{pmatrix} \Leftrightarrow \begin{pmatrix} G^R & G^K \\ & G^A \end{pmatrix}$



Thermal weight

$$\hat{\rho} = \exp\left\{ -i \int d\mathbf{r} \int_{-\infty+i\beta(\mathbf{r})}^{-\infty+i\delta} dt' \gamma(\mathbf{r}) \left[h(\mathbf{r}) - \mu n(\mathbf{r}) \right] \right\}$$

Quantum kinetic equation

We find the response to switching-off the gravitational field.

We introduce the field γ(r) in such a way that the system is initially in fully equilibrium state due to the balancing between the temperature gradient and gravitation field.

The Temperature Gradient Dependent Propagators

$$\hat{G}\left(\nabla T;\mathbf{R}=\frac{\mathbf{r}+\mathbf{r}'}{2},\mathbf{r}-\mathbf{r}';\varepsilon\right)$$

$$\frac{\mathbf{R}\cdot\nabla T}{T}\varepsilon\frac{\partial\hat{G}_0\left(\mathbf{R},\mathbf{r}-\mathbf{r}';\varepsilon\right)}{\partial\varepsilon}$$

Local equilibrium part

$$\hat{G}_{\nabla T}\left(\varepsilon\right)=\hat{g}_{eq}\left(\varepsilon\right)\hat{\Sigma}_{\nabla \mathrm{T}}\left(\varepsilon\right)\hat{g}_{eq}\left(\varepsilon\right)$$
$$-i\frac{\nabla \mathrm{T}}{2T}\varepsilon\left[\frac{\partial\hat{g}_{eq}\left(\varepsilon\right)}{\partial\varepsilon}\hat{\mathbf{v}}\left(\varepsilon\right)\hat{g}_{eq}\left(\varepsilon\right)-\hat{g}_{eq}\left(\varepsilon\right)\hat{\mathbf{v}}\left(\varepsilon\right)\frac{\partial\hat{g}_{eq}\left(\varepsilon\right)}{\partial\varepsilon}\right]$$

The propagator of the fluctuations depends on the temperature gradient only through the polarization operator:

$$\hat{L}\left(\nabla T\right)=-L_0\Pi\left(\nabla T\right)L_0$$

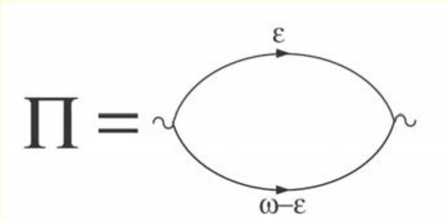
Nernst Effect- Quantum Kinetic Equation

The electric current as a response to a temperature gradient :

$$\mathbf{j}_e = \mathbf{j}_e^{con} + \mathbf{j}_e^{mag}$$

$$\mathbf{j}_e^{con} = ie\int\frac{d\varepsilon}{2\pi}\left[\hat{\mathbf{v}}(\varepsilon)\hat{G}(\varepsilon)\right]^{<} + 2ie\int\frac{d\omega}{2\pi}\left[\hat{\mathbf{v}}_\Delta(\omega)\hat{L}(\omega)\right]^{<} \qquad \mathbf{j}_e^{mag} = \nabla\times\mathbf{M}G^{<}(\nabla T)$$

v_Δ is the notation used for $\hat{\mathbf{v}}_\Delta = \dfrac{\partial\hat{\Pi}(\mathbf{q},\omega)}{\partial\mathbf{q}}$



The contribution from the magnetization current arises due to the local equilibrium Green function.

The Nernst Coefficient

$$\begin{pmatrix} j \\ j_h \end{pmatrix} = \begin{pmatrix} \sigma & \alpha \\ \tilde{\alpha} & \kappa \end{pmatrix} \begin{pmatrix} E \\ -\nabla T \end{pmatrix}$$

$$e_N = \frac{E_y}{-\nabla_x T} = \frac{\alpha_{xy}\sigma_{xx} - \alpha_{xx}\sigma_{xy}}{\sigma_{xy}^2 + \sigma_{xx}^2}$$

$$e_N \approx \frac{\alpha_{xy}}{\sigma_{xx}}$$

α_{xx} is negligible in comparison to α_{xy}

The Peltier coefficient is related to the flow of entropy

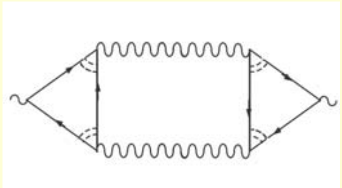
$\equiv$

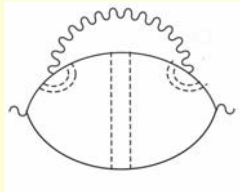
According to the third law of thermodynamics

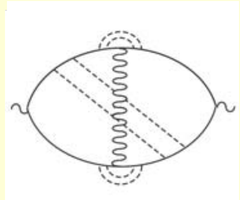
$\alpha \to 0$ when $T \to 0$

The Peltier Coefficient

The contributing diagrams:



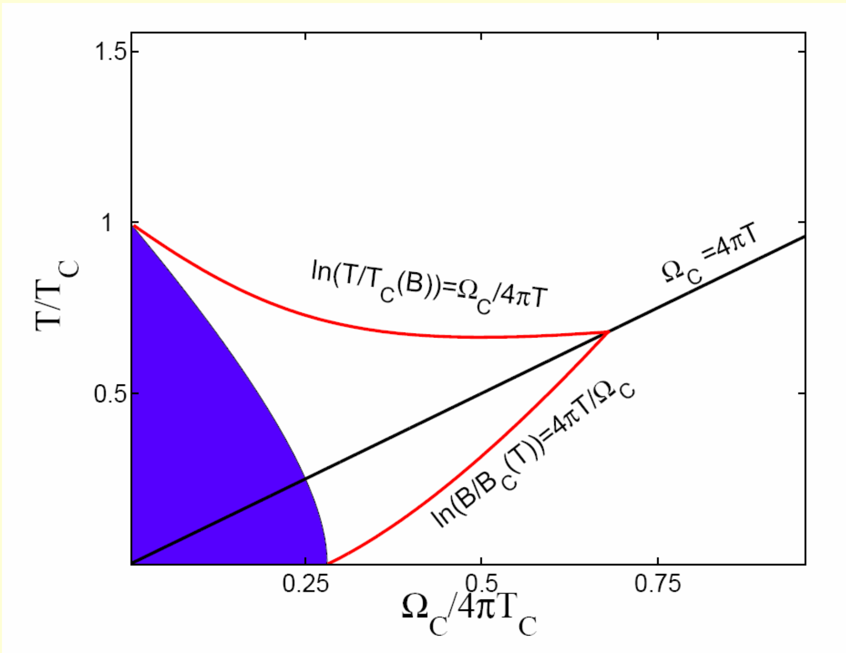




and the magnetization current:

$$\alpha_{xy}^{mag} = -\frac{\partial}{\partial B}\frac{eB}{\pi}\sum_{N=0}^{\infty}\sum_{\omega_m}\ln\left\{-\nu\left[\ln\frac{T}{T_C}-\psi\left(\frac{1}{2}+\frac{|\omega_m|+\Omega_C(N+1/2)}{4\pi T}\right)-\psi\left(\frac{1}{2}\right)\right]\right\}$$

$$\Omega_c = \frac{4eDH}{c}$$



The Origin of the Strong Nernst Signal Created by the Superconducting Fluctuations

- For a Fermi liquid system, the contribution of the quasi-particles to the Nernst signal is negligible: $\propto \omega_c \tau \dfrac{T}{\varepsilon_F}$

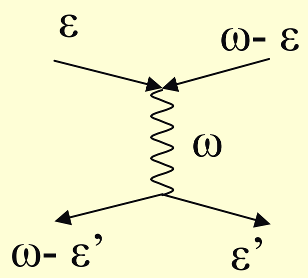
- The neutral modes are not deflected by the Lorentz force.

- The only remaining contribution is form the charged modes.

Transverse current = the difference between two almost equal terms:

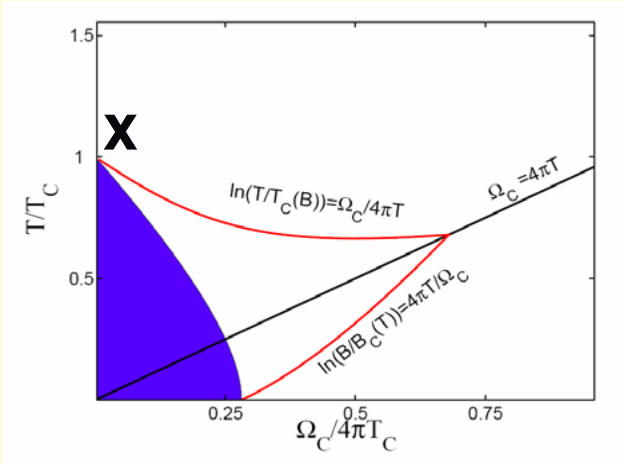
Superconducting fluctuations $\longrightarrow$ odd function of the bosonic frequency.

The fermionic frequency in the vertex transforms into the bosonic frequency through the interaction vertex



The integrand becomes an even function of ω

The Peltier Coefficient



$$\Omega_C << T \qquad \ln\frac{T}{T_C} << 1$$

$$\alpha_{xy} \approx \frac{e\Omega_C}{192\,T\ln\left(T/T_C(B)\right)}$$

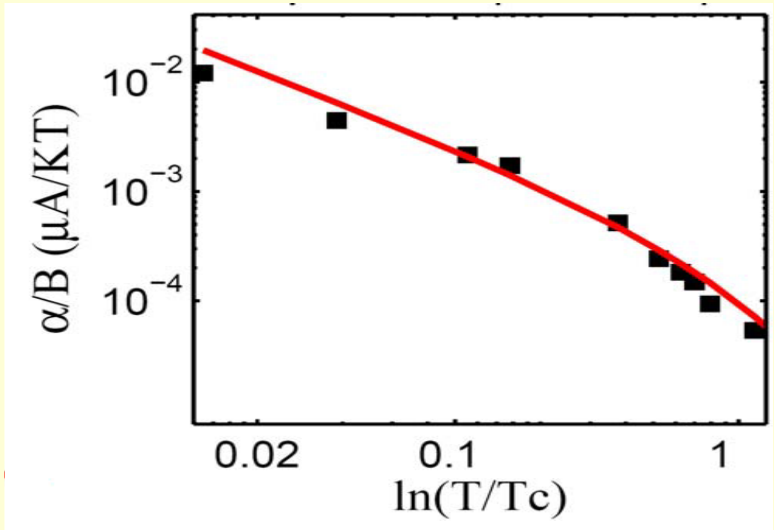
Classical fluctuations – coincide with the phenomenological result of Ussishkin et al, 2002

Experimental data from A. Pourret, et al 2007

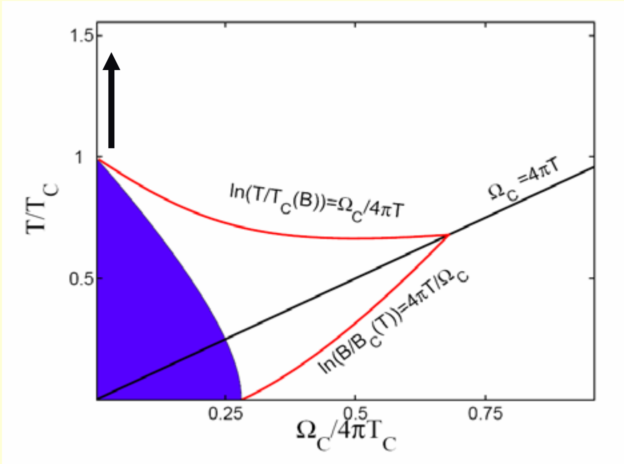
$Nb_{0.15}Si_{0.85}$ film of thickness $35nm$

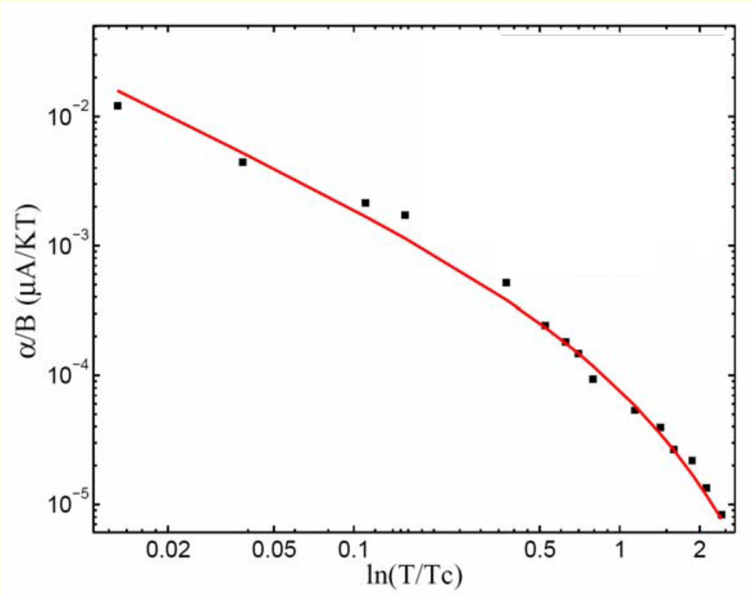
and $T_C = 380mK$

$$D = 0.187\,{cm^2}/{\sec} \qquad T_C^{MF} = 385mK$$



The Peltier Coefficient

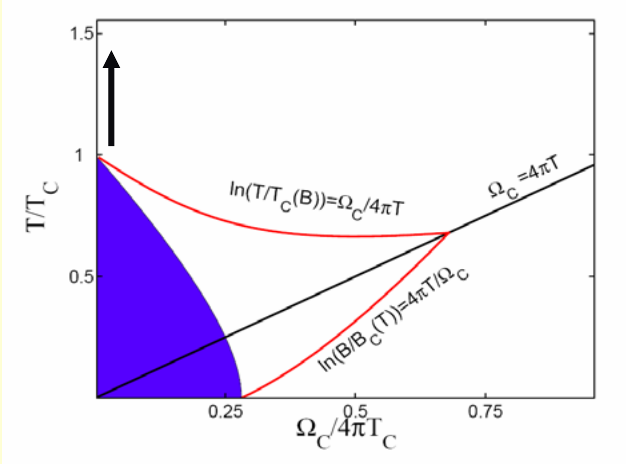


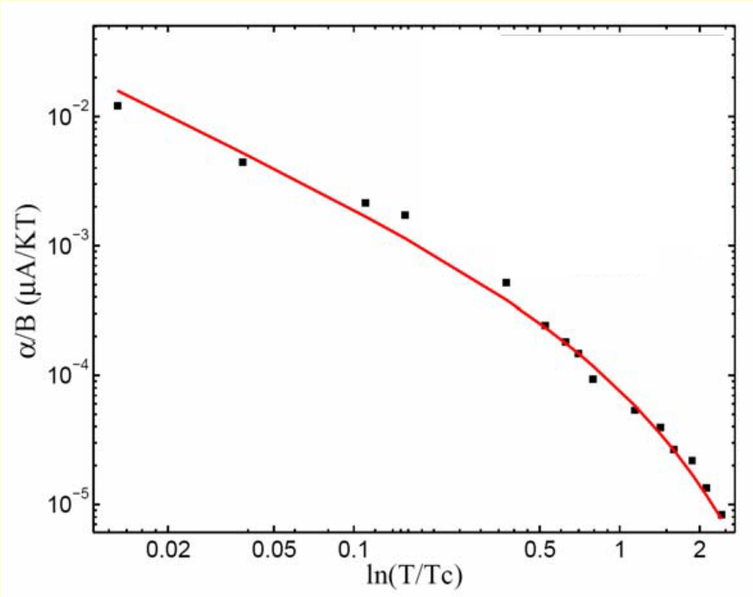


$$\Omega_C << T \qquad \ln\frac{T}{T_C} >> 1$$

$$\alpha_{xy} \approx \frac{e\Omega_C}{24\pi^2 T \ln\left(T / T_C\right)}$$

The Peltier Coefficient





$$\Omega_C << T \qquad \ln\frac{T}{T_C} >> 1$$

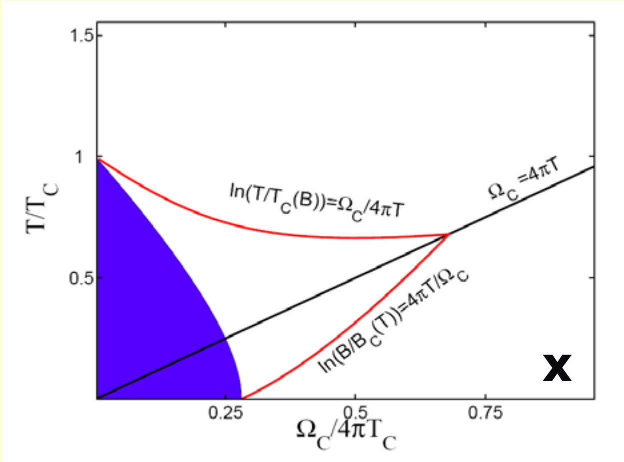
Quantum fluctuations – $T < \omega < 1/\tau$

j_e^{con} yield contributions of the order: $$\ln\left(\ln\frac{1}{T\tau}\right) - \ln\left(\ln\frac{T}{T_C}\right)$$

The logarithmically divergent terms are canceled out by the magnetization current.

Trace of the third law of thermodynamics

The Peltier Coefficient – High Magnetic field



$$\Omega_C >> T \qquad \ln\frac{H}{H_{C2}} >> 1$$

j_e^{con} includes contributions proportional to $\frac{\Omega_C}{T}$.

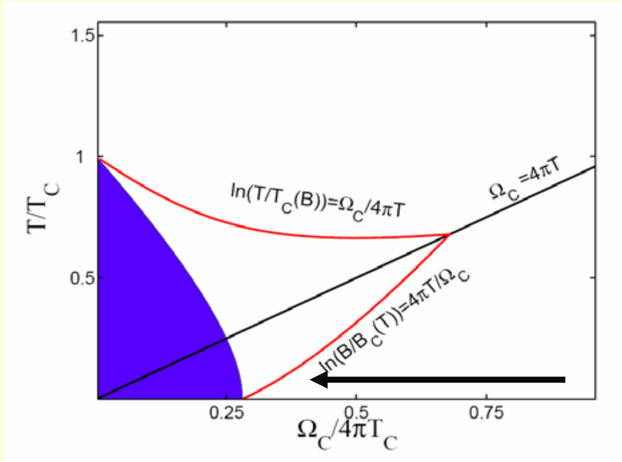
These terms are canceled out by the magnetization current.

$$\alpha_{xy} \approx \frac{2eT}{3\Omega_C \ln\left(H / H_{C2}\right)}$$

The Nernst signal goes to zero at $T \to 0$.

Consistent with the third law of thermodynamics.

The Peltier Coefficient –
High Magnetic field



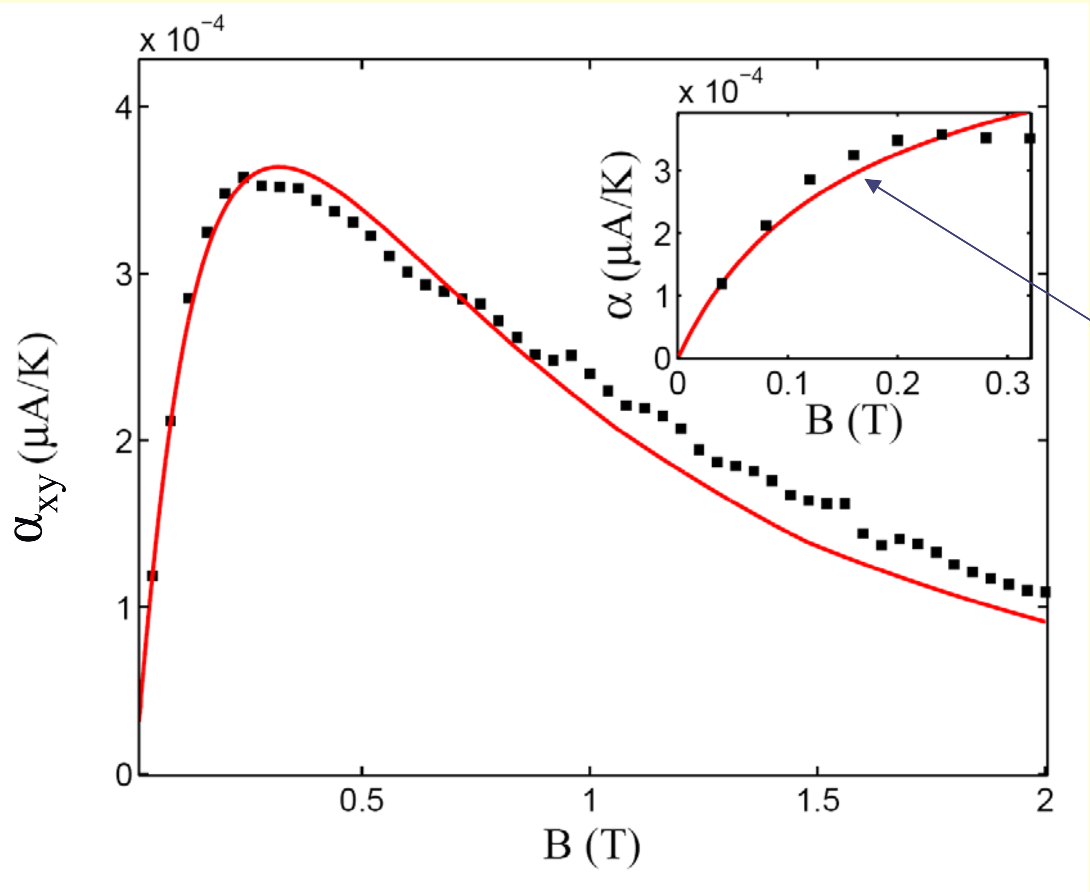
$$\Omega_C >> T \qquad \ln\frac{H}{H_{C2}} << 1$$

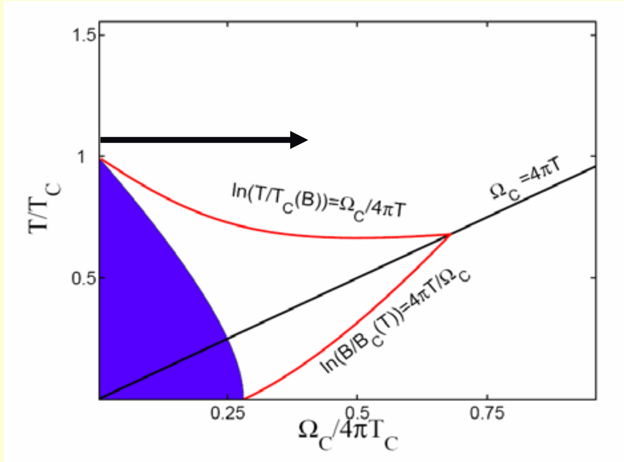
$$\ln\left(\frac{H}{H_{C2}(T)}\right) > \frac{T}{\Omega_C} \qquad \alpha_{xy} \approx -\frac{eT\ln 3}{3\Omega_C \ln^2\left(H/H_{C2}(T)\right)}$$

Since the transverse signal is non-dissipative the sign of the effect is not fixed.

$$\ln\left(\frac{H}{H_{C2}(T)}\right) < \frac{T}{\Omega_C} \qquad \alpha_{xy} \approx -\frac{e\ln 3}{2\pi\ln\left(H/H_{C2}(T)\right)}$$

The Peltier Coefficient as a Function of the Magnetic Field





$$\alpha_{xy} \approx \frac{e\Omega_C}{192\,T\ln\left(T/T_C\left(B\right)\right)}$$

Summary

- In general, the Kubo formula can be used for the calculation of thermal and thermoelectric conductivities. The weak point is in replacing Luttinger's expression for the heat current by the simplified form. The problem with using the full expression for the heat current is that is that it is too complex.

- We have developed an alternative scheme for studying thermal transport using the quantum kinetic equation.

- The novelty of our method is that we were able to derive both the kinetic equation and the currents directly from the action and the corresponding conservation laws.

- All the currents share a uniform and compact structure: $\mathbf{j}_e^{con} = -i\int \frac{d\varepsilon}{2\pi}\chi_{e,h}(\varepsilon)\left[\hat{\mathbf{v}}(\varepsilon)\hat{G}(\varepsilon)\right]^{<}$

- In this method we find $\mathbf{j}_e(\nabla T)$ and $\mathbf{j}_h(\mathbf{E})$ independently from each other. Therefore, we have verified that the two expressions for the currents are connected through the Onsager relation.

Summary

- The contribution from the fluctuations of the superconducting order parameter to the Nernst effect is dominant and can be observed far away from the transition.

- The important role of the magnetization is in canceling the quantum contributions, thus making the Nernst signal compatible with the third law of thermodynamics.

- The third law of thermodynamics (Nernst theorem) imposes a strong constrain on the magnitude of the Nernst signal not only at low temperature ($T \rightarrow 0$), but also at higher temperatures ($T \gg T_C$).

- The Nernst effect provides an excellent opportunity to test the use of the quantum kinetic equation in the description of thermoelectric transport phenomena.

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