## Thermoelectric Anomaly in A 2D Electron System with SOI ?



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## Outline

- How does a thermoelectric anomaly appear?
- Is it possible to have one in a semiconductor?
- Is a 2D system with Rashba-Dresselhaus SOI adequate for this purpose?
- Charge and Spin Thermoelectrics
- Results
- Conclusions

## The Seebeck Effect Phenomelogy



 $\mathcal{E} = S \nabla T$ 

#### Semiclassical Picture of Thermoelectric Transport



The cancellation of the states above and below the Fermi energy is exact at T = OK and of the order of  $\binom{k_B T}{\epsilon_F}^2$  at finite temperature

## SMALL!

#### How Can Be S Increased?

Single electron states: momentum  $\vec{k}$ , energy  $\varepsilon(\vec{k})$ , velocity  $\vec{v}(\vec{k})$  and occupation number  $f(\vec{k})$ 



 $\Delta f(\vec{k})$  has to be a strongly varying, asymmetric function of the energy in the neighborhood of the Fermi surface

## What is needed for a thermoelectric anomaly?

#### A. Inelastic scattering

$$\frac{dP(\mathbf{k}', \mathbf{k})}{dt} = -W(\mathbf{k}', \mathbf{k})f(\mathbf{k})[1 - f(\mathbf{k}')] + W(\mathbf{k}, \mathbf{k}')f(\mathbf{k}')[1 - f(\mathbf{k})]$$
In equilibrium:  $W(\mathbf{k}', \mathbf{k})exp\left(\frac{\varepsilon_{k'}}{k_{B}T}\right) = W(\mathbf{k}, \mathbf{k}')exp\left(\frac{\varepsilon_{k}}{k_{B}T}\right)$ 

$$f(\mathbf{k}) = f^{0}(\mathbf{k}) + \Delta f(\mathbf{k})$$

$$\frac{dP(\mathbf{k}', \mathbf{k})}{dt} = W(\mathbf{k}', \mathbf{k})\{\Delta f(\mathbf{k})[1 - f^{0}(\mathbf{k}') + e^{\beta\Delta\varepsilon}f^{0}(\mathbf{k}')] - \Delta f(\mathbf{k}')[f^{0}(\mathbf{k}') + e^{\beta\Delta\varepsilon}(1 - f^{0}(\mathbf{k}'))]$$

$$= W(\mathbf{k}', \mathbf{k}) \left\{ \Delta f(\mathbf{k}) e^{\beta \Delta \varepsilon} \left| \frac{e^{\beta(\varepsilon - \varepsilon_F)} + 1}{e^{\beta(\varepsilon - \varepsilon_F) + \beta \Delta \varepsilon} + 1} - \Delta f(\mathbf{k}') \frac{e^{\beta(\varepsilon - \varepsilon_F) + \beta \Delta \varepsilon} + 1}{e^{\beta(\varepsilon - \varepsilon_F)} + 1} \right] \right\}$$
Summation over k cancels this effect  $\Leftarrow$  
$$= \begin{cases} e^{-\beta \Delta \varepsilon}, \varepsilon > \varepsilon_F \\ 1, & \varepsilon < \varepsilon_F \end{cases}$$

The inelastic scattering has to have unidirectional character.

Spin scattering on magnetic impurities has a one dimensional character as it depends on the relative alignment of the electron and impurity spins

**B.** Population Imbalance



#### Spin Polarized System with Population Imbalance (no magnetic fields allowed)

Classic literature: Spin Density Waves-Itinerant Antiferromagnetism

Contemporary case study: 2D electron system with linear Rashba-Dresselhaus SOI coupling, in the  $\alpha = \beta$  regime

#### 2D Electron System with Rashba-Dresselhaus SOI



## The Spin Instability

In the rotated reference frame, the eigenstates of the single-particle Hamiltonian are



 $S_Q$  and  $S_Q^{\dagger}$  have only zero matrix elements between Slater determinants constructed out of states  $\psi_{k+2Q,\uparrow}$  and  $\psi_{k,\downarrow}$ , since this is a paramagnetic configuration The instability condition leads to a magnetic phase if it is supported by the Coulomb interaction, realizing long-range ordering Non-zero matrix elements are obtained only if the single particle states in the Slater determinant are linear combinations of  $\psi_{k+2Q,\uparrow}$  and  $\psi_{k,\downarrow}$ . Such a superposition will generate a total energy higher than the paramagnetic state

## Possible Ground States of a Fermi Liquid

#### Ferromagnetic

Parallel spin alignment decreases the potential energy because of the exchange interaction, but increases the kinetic energy on account of Pauli principle; higher energy than that of the paramagnetic state

# $\uparrow\downarrow$

#### Paramagnetic

Minimizes kinetic energy, but increases the potential energy because it reduces the exchange interaction



#### Spin Density Wave

Balances the kinetic energy with the potential energy by removing the parallel/anti-parallel spin alignment; lowers the energy of the paramagnetic state

A. W. Overhauser, Phys. Rev. Lett., **4**, 462 (1960); A. W. Overhauser, Phys. Rev., **128**, 1437 (1962).

## Giant Spiral Spin Density Waves vs. Itinerant AF

Uniform Fermi liquid

2D + SOI

#### The single particle Hamiltonian:

$$H_1 = -\frac{\hbar^2 \nabla^2}{2m} \qquad \qquad H_1 = -\frac{\hbar^2 (\nabla_x - iQ\sigma_z)^2}{2m}$$

#### The single particle energies

$$\varepsilon_{\uparrow}(k) = \varepsilon_{\downarrow}(k) = \frac{\hbar^2 k^2}{2m}$$
  $\varepsilon_{\sigma}(k) = \frac{\hbar^2 (k_x - Q\sigma)^2}{2m}$ 

A configuration with a single point of degeneracy <u>has to be created</u> by displacing the single particle states of one spin orientation in k space	A configuration with a single point of degeneracy is <u>naturally created</u> by SOI coupling

## New Quasiparticles

#### Uniform Fermi liquid

#### 2D + SOI

$$\psi_{k,-}(r) = \cos \theta_k \, e^{ik \cdot r} |\uparrow\rangle + \sin \theta_k e^{i(k+2Q) \cdot r}$$
  
$$\psi_{k,+}(r) = -\sin \theta_k \, e^{ik \cdot r} |\uparrow\rangle + \cos \theta_k e^{i(k+2Q) \cdot r}$$

$$\psi_{k,-}(r) = \cos \theta_k \, e^{ik \cdot r} |\uparrow\rangle + \sin \theta_k e^{ik \cdot r} |\downarrow\rangle$$
  
$$\psi_{k,+}(r) = -\sin \theta_k \, e^{ik \cdot r} |\uparrow\rangle + \cos \theta_k e^{ik \cdot r} |\downarrow\rangle$$



#### Uniform Fermi liquid

$$\psi(k) = \cos\theta_k e^{ikr} |\uparrow\rangle + \sin\theta_k e^{i(k+2Q)r} |\downarrow\rangle$$

Real space polarization effects are produced by the superposition of the two plain waves of different phases

$$\psi(k) = \cos\theta_k e^{ikr} |\uparrow\rangle + \sin\theta_k e^{ikr} |\downarrow\rangle$$

No real space polarization effects are created because the two plain waves have the same phase

#### The polarization

$$P = \vec{\iota} \sum_{k} \langle \psi_{k} | \sigma_{x} | \psi_{k} \rangle + \vec{j} \sum_{k} \langle \psi_{k} | \sigma_{y} | \psi_{k} \rangle + \vec{k} \sum_{k} \langle \psi_{k} | \sigma_{z} | \psi_{k} \rangle$$

$$P = \sum_{k} \sin 2\theta_{k} (\vec{i} \cos 2Qr + \vec{j} \sin 2Qr) \qquad P = \vec{i} \sum_{k} \sin 2\theta_{k}$$
$$P_{z} = \sum_{k} \cos 2\theta_{k} = 0 \qquad P_{z} = \sum_{k} \cos 2\theta_{k} = 0$$

## Antiferromagnetic Alignment



Koralek et al, Nature 458, 610 (2009)

Fractional Polarization is aligned parallel with the direction of the displacement vector of the single particle states

#### Is the long-range antiferromagnetic alignment real?

Only if supported by the Coulomb interaction

$$v_{k\sigma;k'\sigma'}(q) = \int dr_1 \int dr_2 \psi_{k,\sigma}^{\dagger}(\mathbf{r}_1) \psi_{k'+q,\sigma'}^{\dagger}(\mathbf{r}_2) \frac{e^2}{|\mathbf{r_1} - \mathbf{r_2}|} \psi_{k',\sigma'}(\mathbf{r_2}) \psi_{k+q,\sigma}(\mathbf{r_1})$$

#### The Fundamental Paradigm Of The IAF Formation

The no kinetic energy cost pairing at the point of degeneracy  $|k, \uparrow\rangle \Leftrightarrow |k, \downarrow\rangle$  favors the formation of a new type of quasiparticle whose spin is not constant

In this ground state 
$$\langle c_{k\uparrow}^{\dagger} c_{k\downarrow} \rangle_{0} \neq 0$$

#### Canonical transformation:

$$c_{k\uparrow} = \cos \theta_k a_k + \sin \theta_k b_k$$
$$c_{k\downarrow} = -\sin \theta_k a_k + \cos \theta_k b_k$$



 $\theta_k$  becomes the variational parameter of the problem

#### The Many-Body Hamiltonian

$$H_{0} = \sum_{k} \varepsilon_{k,\uparrow} c_{k,\uparrow}^{\dagger} c_{k,\downarrow} + \varepsilon_{k,\downarrow} c_{k,\downarrow}^{\dagger} c_{k,\downarrow}$$
$$H_{int} = \frac{1}{2} \sum_{k,k',q} \sum_{\sigma,\sigma'} v(q) c_{k,\sigma}^{\dagger} c_{k'+q,\sigma'}^{\dagger} c_{k',\sigma'} c_{k+q,\sigma}$$

Ground state energy is calculated within the Hartree-Fock approximation

$$\left\langle c_{k,\sigma}^{\dagger} c_{k'+q,\sigma'}^{\dagger} c_{k',\sigma'} c_{k+q,\sigma} \right\rangle_{0} = \left\langle c_{k,\sigma}^{\dagger} c_{k+q,\sigma} \right\rangle_{0} \left\langle c_{k'+q,\sigma'}^{\dagger} c_{k',\sigma'} \right\rangle_{0} - \left\langle c_{k,\sigma}^{\dagger} c_{k',\sigma'} \right\rangle_{0} \left\langle c_{k'+q,\sigma'}^{\dagger} c_{k+q,\sigma} \right\rangle_{0}$$

$$\text{Direct interaction} \qquad \text{Exchange}$$

$$\left\langle c_{k\uparrow}^{\dagger} c_{k\uparrow} \right\rangle_{0} \neq 0 \qquad \text{Regular exchange}$$

$$\left\langle c_{k\uparrow}^{\dagger} c_{k\downarrow} \right\rangle_{0} \neq 0 \qquad \text{Itinerant antiferromagnetic exchange}$$

Itinerant antiferromagnetic exchange

$$\langle H \rangle_{HF} = \sum_{k} \varepsilon_{k,\uparrow} (\cos^2 \theta_k f_{1k} + \sin^2 \theta_k f_{2k}) + \sum_{k} \varepsilon_{k,\downarrow} (\sin^2 \theta_k f_{1k} + \cos^2 \theta_k f_{2k})$$

$$- \frac{1}{2} \sum_{k,k'} v(k - k') (\cos^2 \theta_k f_{1k} + \sin^2 \theta_k f_{2k}) (\cos^2 \theta_{k'} f_{1k'} + \sin^2 \theta_{k'} f_{2k'})$$

$$- \frac{1}{2} \sum_{k,k'} v(k - k') (\sin^2 \theta_k f_{1k} + \cos^2 \theta_k f_{2k}) (\sin^2 \theta_{k'} f_{1k'} + \cos^2 \theta_{k'} f_{2k'})$$

$$-\frac{1}{4}\sum_{k,k'}v(k-k')sin2\theta_ksin2\theta_{k'}(f_{1k}-f_{2k})(f_{1k'}-f_{2k'})$$

The IA potential created by the exchange interaction between electrons whose spins are not parallel

#### Finite Temperature Treatment

The Grand Canonical Function

$$\Omega(T, V, \mu) = \langle H_{HF} \rangle - \mu \sum_{k,i} f_{k,i} - k_B T \sum_{k,i} [f_{k,i} ln f_{k,i} + (1 - f_{k,i}) ln (1 - f_{k,i})]$$
$$N = \sum_{k,\sigma} c^{\dagger}_{k\sigma} c_{k\sigma}$$

$$\left\langle a_k^{\dagger} a_k \right\rangle_0 = f_{1k}$$
$$\left\langle b_k^{\dagger} b_k \right\rangle_0 = f_{2k}$$

The occupation numbers of the two new quasiparticles

#### The Ground State Configuration



#### Symmetric in k space

$$g_k = \sum_{k'} v(k - k') \sin 2\theta_{k'} (f_{1k'} - f_{2k'})$$

$$\tilde{\varepsilon}_{k,\uparrow} = \varepsilon_{k,\uparrow} - \sum_{k,k'} v(k-k')(\cos^2\theta_k f_{1k} + \sin^2\theta_k f_{2k})$$
$$\tilde{\varepsilon}_{k,\downarrow} = \varepsilon_{k,\downarrow} - \sum_{k,k'} v(k-k')(\sin^2\theta_k f_{1k} + \cos^2\theta_k f_{2k})$$

Single particle energies in HF

## **Quasiparticle Energies**



$$E_{+} - E_{-} = \sqrt{\left(\tilde{\varepsilon}_{k,\uparrow} - \tilde{\varepsilon}_{k,\downarrow}\right)^{2} + g_{k}^{2}}$$

At the point of degeneracy the energy difference is gapped

## The Gap Equation

$$g_k = \sum_{k'} v(k-k') \frac{g_{k'}}{\sqrt{\left(\tilde{\varepsilon}_{k',\uparrow} - \tilde{\varepsilon}_{k',\downarrow}\right)^2 + g_{k'}^2}} \quad (f_{1k'} - f_{2k'})$$

Integral equation that is solved iteratively; major simplifications

- 1. Constant interaction potential:  $\gamma$
- 2. The single particle energies are approximated by the kinetic part only
- 3. Low temperature, such that only the lowest energy eigenstate is occupied

$$g = \frac{\gamma}{(2\pi)^2} \int \frac{g}{\sqrt{\left(\varepsilon_{k,\uparrow} - \varepsilon_{k,\downarrow}\right)^2 + g^2}} dk^2$$

Integration domain is chosen as a rectangle centered at k = 0

$$g = \frac{2\hbar^2 L_x Q}{m^* \mathrm{sinh}\left(\frac{4\hbar^2 Q \pi^2}{m^* \gamma L_y}\right)}$$



#### **Boltzmann Transport Equation**

$$\psi_{k,-}(r) = \cos \theta_k \, e^{ik \cdot r} |\uparrow\rangle + \sin \theta_k e^{ik \cdot r} |\downarrow\rangle$$

Lowest occupied level

$$E_{k,-} = \frac{\varepsilon_{k,\downarrow} + \varepsilon_{k,\uparrow}}{2} - \frac{1}{2}\sqrt{\left(\varepsilon_{k,\uparrow} - \varepsilon_{k,\downarrow}\right)^2 + g_k^2}$$

$$\frac{-e\mathcal{E}\cdot\nabla_k E_k}{\hbar}\frac{df_k^0}{dE_k} = \left(\frac{\partial f_k}{\partial t}\right)_{coll.} = -\frac{f_k - f_k^0}{\tau(k)}$$

$$\left(\frac{\partial f_k}{\partial t}\right)_{coll.} = -\sum_{k'} W(\mathbf{k}', \mathbf{k}) \left\{ \Delta f(\mathbf{k}) \frac{e^{\beta E_{k'}} + e^{\beta \Delta E}}{1 + e^{\beta E_{k'}}} - \Delta f(\mathbf{k}') \frac{1 + e^{\beta \Delta E + \beta E_k}}{1 + e^{\beta E_k}} \right\}$$

#### Charge and Spin Currents

$$j_{c} = -e \sum_{k} \boldsymbol{v}(k) f_{k} = e^{2} \sum_{k} \boldsymbol{v}(k) \tau(k) \boldsymbol{\varepsilon} \cdot \boldsymbol{v}(k) \left(-\frac{df_{k}^{0}}{dE_{k}}\right)$$
$$j_{s}^{x} = \frac{\hbar}{2} \sum_{k} \left\langle \psi_{k} \right| \frac{p}{m} \sigma_{x} \left| \psi_{k} \right\rangle \boldsymbol{v}(k) f_{k} = -e \frac{\hbar}{2} \sum_{k} sin 2\theta_{k} \boldsymbol{v}(k) \tau(k) \boldsymbol{\varepsilon} \cdot \boldsymbol{v}(k) \left(-\frac{df_{k}^{0}}{dE_{k}}\right)$$

$$\sigma_{c} = e^{2} \sum_{k} \tau(k) v(k) v(k) \left( -\frac{df_{k}^{0}}{dE_{k}} \right)$$
$$\sigma_{s} = -e \frac{\hbar}{2} \sum_{k} \tau(k) v(k) v(k) \left( -\frac{df_{k}^{0}}{dE_{k}} \right)$$

The Mott Formula  $S = -\frac{\pi^2 k_B^2 T}{3e\varepsilon_F} \frac{\partial \sigma(E)}{\partial E}|_{\varepsilon_F}$ 

#### Impurity Scattering and The Relaxation Time

$$\sum_{i} V\delta(r-R_i) + J\bar{\sigma} \cdot S\delta(r-R_i)$$

 $\bar{\sigma}$  is the the electron spin along the direction of the local polarization

$$\bar{\sigma}_z = \sigma_x \quad \bar{\sigma}_x = -\sigma_z \quad \bar{\sigma}_y = \sigma_y$$

#### Fermi's Golden Rule

$$W(k',k) = \frac{2\pi N_i}{\hbar} \left[ |\langle \psi_{k'}|V|\psi_k\rangle|^2 \delta(E_k - E_{k'}) + \left| \left| \left| \psi_{k'} \right| J \frac{\bar{\sigma}^+ S^-}{2} \left| \psi_k \right| \right|^2 \delta(E_{k'} - E_k + \Delta E) \right]$$
$$+ \left| \left| \left| \psi_{k'} \right| J \frac{\bar{\sigma}^- S^+}{2} \left| \psi_k \right| \right|^2 \delta(E_{k'} - E_k - \Delta E) \right]$$

#### The Transverse Relaxation Rate

$$\left(\frac{\partial f_k}{\partial t}\right)_{coll.} = -\sum_{k'} W(\mathbf{k}', \mathbf{k}) \left\{ \Delta f(\mathbf{k}) \frac{e^{\beta E_{k'}} + e^{\beta \Delta E}}{1 + e^{\beta E_{k'}}} - \Delta f(\mathbf{k}') \frac{1 + e^{\beta \Delta E + \beta E_k}}{1 + e^{\beta E_k}} \right\}$$

$$\begin{split} \Delta f(k) &= -e \frac{1}{\hbar} \nabla_k E_k \cdot \mathcal{E} \left( \frac{df_k^0}{dE_k} \right) \\ &\frac{1}{\hbar} \nabla_k E_k \cdot \mathcal{E} = \begin{cases} \frac{\hbar k}{m} \cdot \mathcal{E}, & \mathcal{E} \perp Q \\ \left( \frac{\hbar k}{m} - \frac{\hbar Q}{m} \cos \theta_k \right), \mathcal{E} \parallel Q \end{split}$$

$$\begin{aligned} \frac{1}{\tau_n} &= \frac{\pi N_i}{\hbar} \left[ (V^2 + \langle S_z^2 \rangle) (N_0 + P_0 \sin 2\theta_k) + 2VJ \langle S_z \rangle (N_0 \sin 2\theta_k + P_0) \right. \\ &\quad + \frac{e^{\beta E_k} + 1}{e^{\beta E_k} + e^{-\beta \Delta E}} \frac{(J^2 \langle S_+^2 \rangle)}{2} (N_0 - P_0) (1 + \sin 2\theta_k) \\ &\quad + \frac{e^{\beta E_k} + 1}{e^{\beta E_k} + e^{-\beta \Delta E}} \frac{(J^2 \langle S_-^2 \rangle)}{2} (N_0 - P_0) (1 + \sin 2\theta_k) \right] \\ N_0 &= \sum_k \delta(E_k - E_F) \qquad \qquad P_0 = \sum_k \sin 2\theta_k \delta(E_k - E_F) \end{aligned}$$

## The Longitudinal Relaxation Time

$$\tau_{p} = \tau_{n} \left[ 1 + \frac{\left(1 - \frac{J^{2}}{V^{2}} \langle S_{z}^{2} \rangle\right) \cos 2\theta_{k}}{\nu_{p}(k)} \times \frac{\tau_{0}^{-1} \sum_{k'} \cos 2\theta_{k'} \nu_{p}(k') \tau_{n}(k') \delta(E_{k'} - E_{F})}{1 - \tau_{0}^{-1} \sum_{k'} \cos^{2}\theta_{k'} \tau_{n}(k') \delta(E_{k'} - E_{F})} \right]$$

$$\tau_0^{-1} = \frac{\pi N_i}{\hbar} V^2$$

#### **Experimental Numbers**

PRB **86**, 081306(R) (2012), Khoda et al.



#### Results



## Conclusions

- 1. In the presence of the Coulomb interaction, the state of an electron system with SOI at  $\alpha = \beta$  is that of a paramagnet or an itenerant antiferromagnet polarized along the direction of Q.
- 2. If the AF state exists, they are highly susceptible to variations in the particle density, screening, etc.
- 3. Thermoelectric measurements in this state should indicate a thermoelectric anomaly