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International **C**enter for **Q**uantum **M**aterials

Magnetizations, Thermal Hall Effects and Phonon Hall Effect

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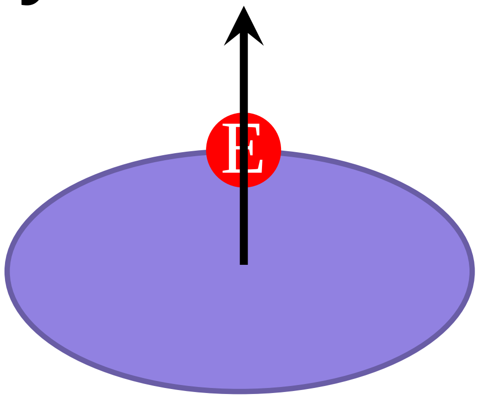
ICQM, Peking University



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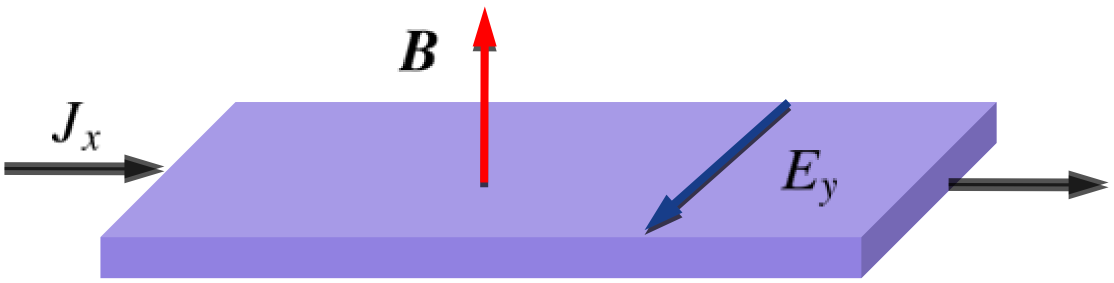
Tao Qin, Qian Niu and Juren Shi, *Energy magnetization and thermal Hall effect* Phys. Rev. Lett. **107**, 236601(2011)
Tao Qin and Junren Shi, *Berry curvature and phonon Hall effect*, arXiv: 1111. 1322 (2011)

Collaborators

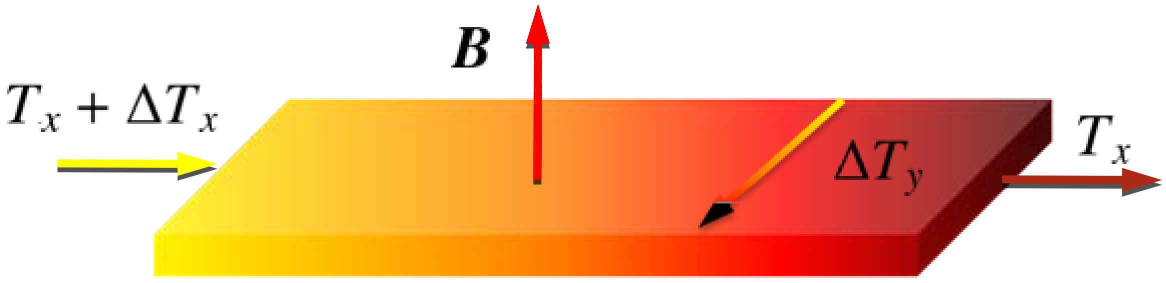
Tao Qin

Qian Niu

Thermal Hall effect



Charge Hall effect



Thermal Hall effect

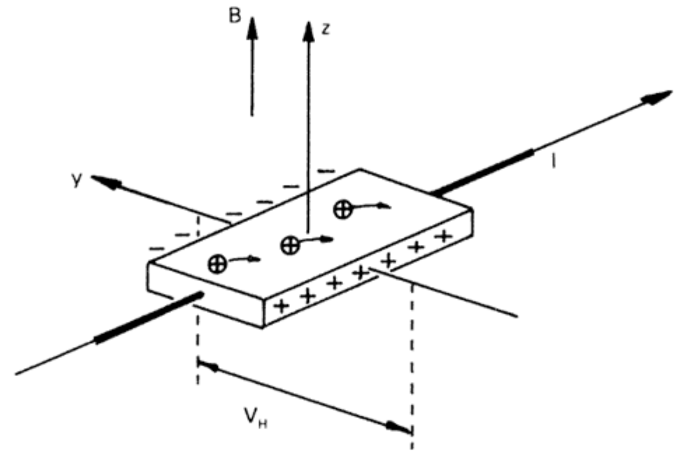
Why Thermal Transport?

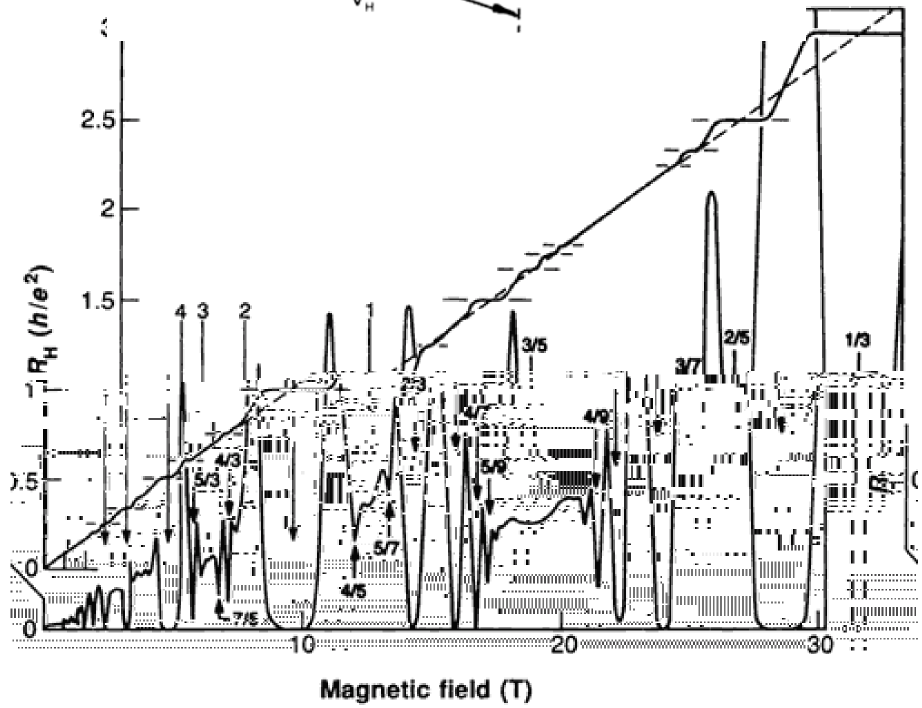
	Charge Transport	Thermal Transport
Carriers	Electrons, Ions	Electrons, Phonons, Magnetic Systems
Statistical Forces	Density Gradient	Temperature Gradient
Individual Forces	Electromagnetic Fields	Gravitational Force
Degree of Freedoms Probed	Charge	Essentially All

Thermal transport -- the more effective ways for probing condensed matter systems!

Why Hall Effect?

Quantum Hall Effect

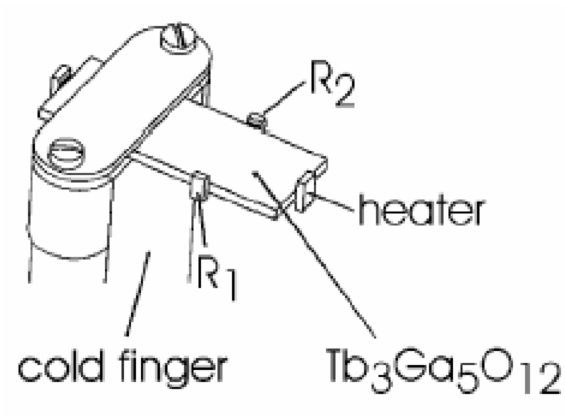


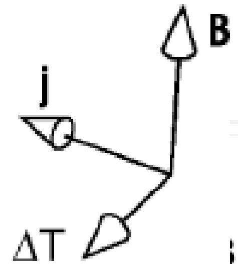


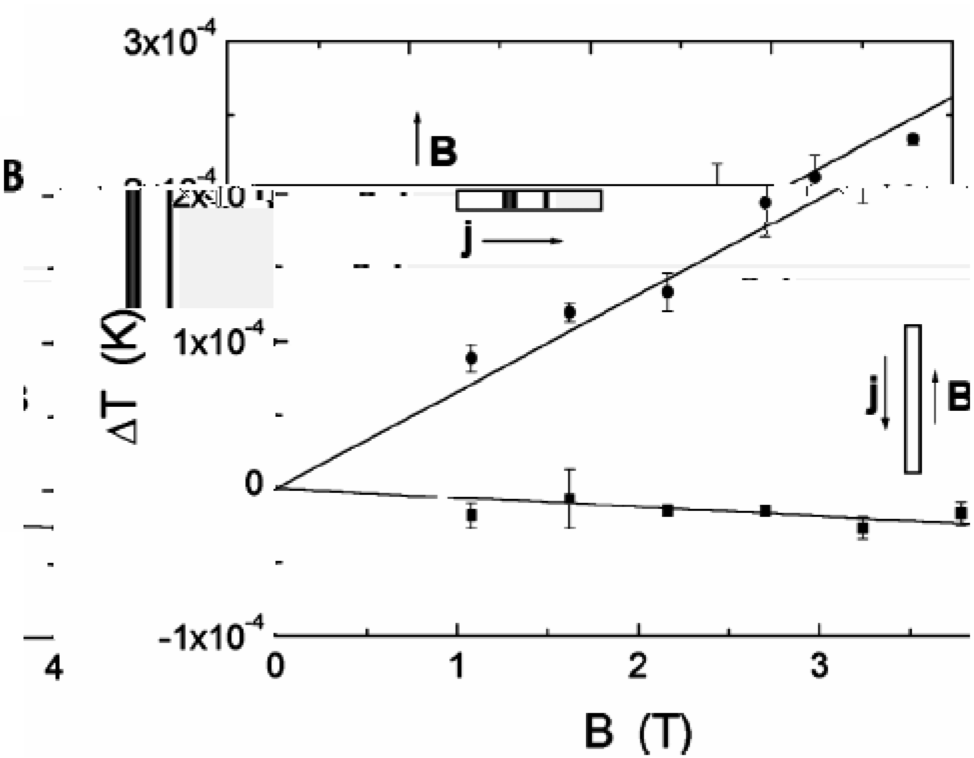
- Klitzing, 1985
- Laughlin, Stormer, Tsui, 1998

- Hall effect for the heat flow?
- Quantum Hall effect for the heat flow?

Phonon Hall effect





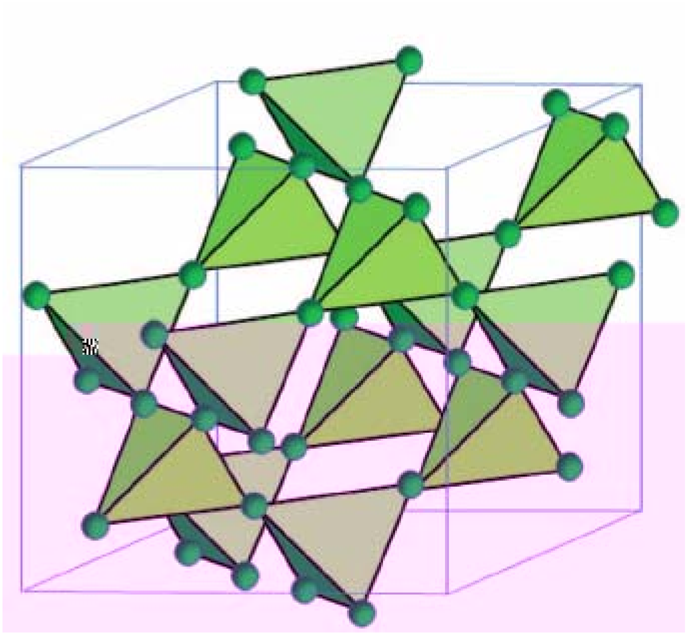


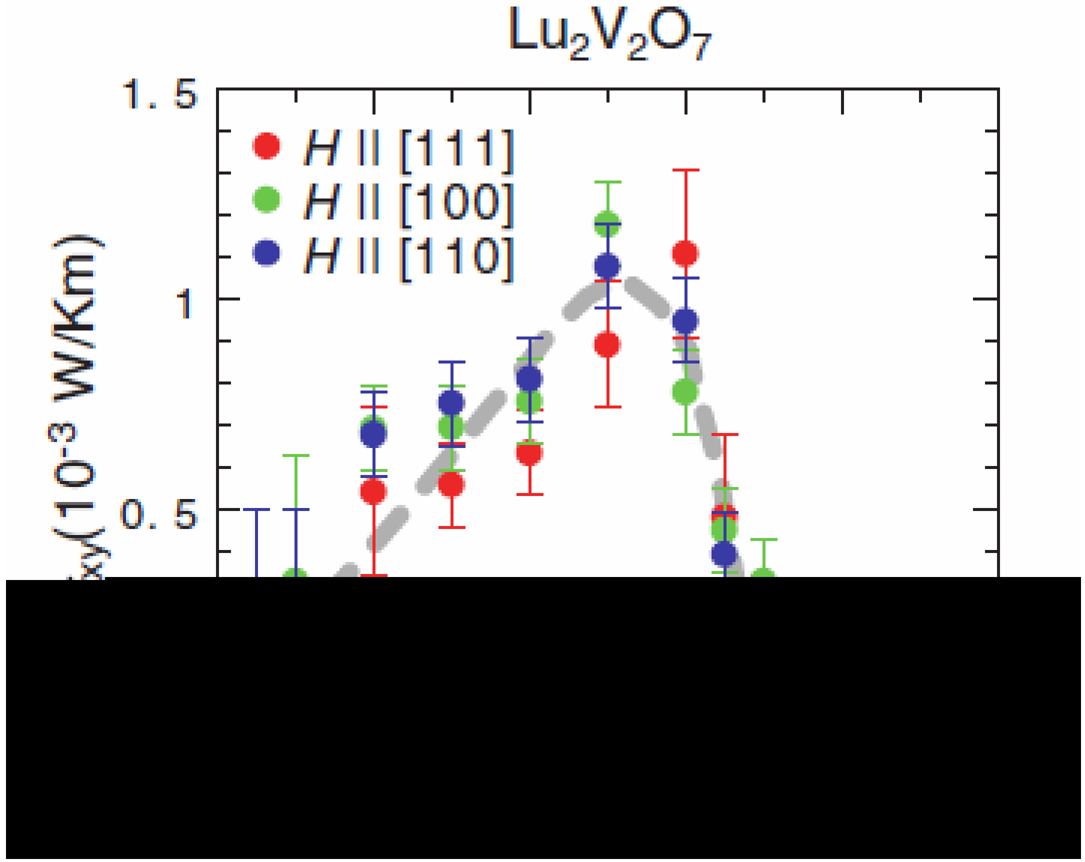
$T = 5.45\text{K}$

$Tb_3Ga_5O_{12}$ Paramagnetic insulator

C. Strohm *et al.*, Phys. Rev. Lett. **95**, 155901(2006).
A.V. Inyushkin *et al.*, JETP Lett. **86**, 379 (2007).

Magnon Hall effect





[redacted]

$Lu_2V_2O_7$ Insulating collinear ferromagnet

Y. Onose, *et al.*, Science **329**, 297 (2010).

Kubo Formula

Thermal Hall Coefficient: $\kappa_{xy} = \frac{J_{Qx}}{\partial_y T}$

Standard tool for evaluating transport coefficients:

$$\kappa_{xy} = \frac{1}{T}\int_0^\infty \mathrm{d}t e^{-st}\beta \left\langle \hat{J}_{Qy}(0); \hat{J}_{Qx}(t) \right\rangle$$

$$\left\langle \hat{a};\hat{b} \right\rangle = \frac{1}{\beta}\int_0^\beta \mathrm{d}\lambda \mathrm{Tr}\left\{ \hat{\rho}_0 \exp(\lambda \hat{H}) \hat{a} \exp(-\lambda \hat{H}) \hat{b} \right\}$$

Mahan, *Many Particle Physics*

Kubo, Toda and Hashitsume, *Statistical Physics II*

Kubo formula applicable?

Direct application of Kubo formula in THE often leads to unphysical results:

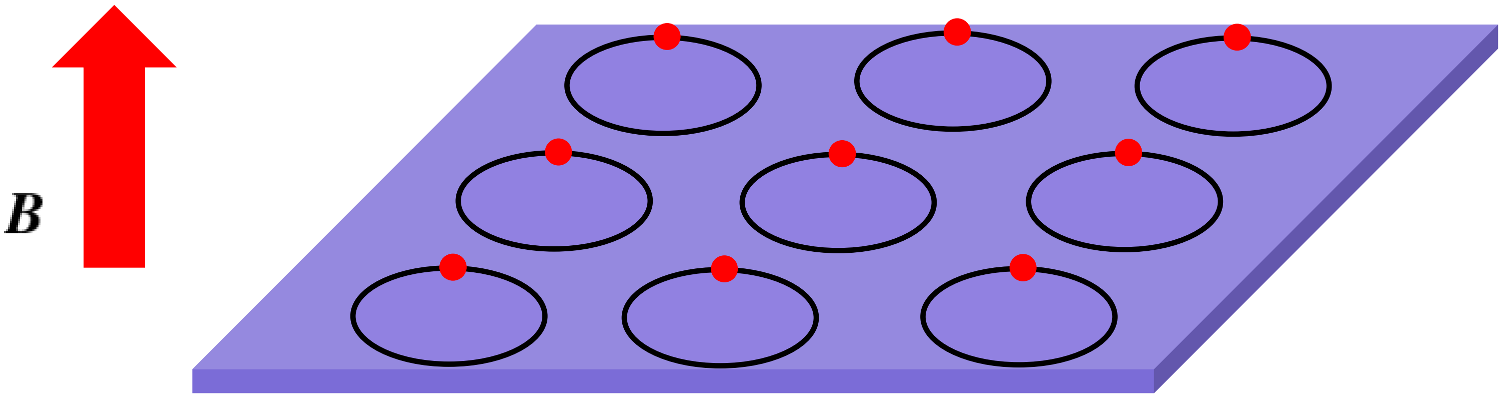
$$\kappa_{xy}^{\text{Kubo}} \propto \frac{1}{T_0}$$

Electron: $$\kappa_{xy}^{\text{Kubo}} = \frac{1}{2T_0\hbar V}\sum_{n\boldsymbol{k}} \text{Im}\left\langle \frac{\partial u_{n\boldsymbol{k}}}{\partial k_x}\right| \left(\hat{\mathcal{H}}_{\boldsymbol{k}} + \epsilon_{n\boldsymbol{k}} - 2\mu_0\right)^2 \left|\frac{\partial u_{n\boldsymbol{k}}}{\partial k_y}\right\rangle f_{n\boldsymbol{k}}$$

Phonon: $$\kappa_{xy}^{\text{Kubo}} = -\frac{\hbar}{2VT_0}\sum_{\boldsymbol{k},i=1}^{3r} \text{Im}\left[\frac{\partial \bar{\Psi}_{\boldsymbol{k}i}}{\partial \boldsymbol{k}} \times \tilde{H}_{\boldsymbol{k}} \frac{\partial \Psi_{\boldsymbol{k}i}}{\partial \boldsymbol{k}}\right]_z \omega_{\boldsymbol{k}i}(2n_{\boldsymbol{k}i}+1)$$

L. Zhang *et al.*, Phys. Rev. Lett. **105**, 225901(2010)
Katsura, Nagaosa& P. A. Lee, Phys. Rev. Lett. **104**, 066403 (2010)

Circular current component



Electric current: Electromagnetic magnetization

Energy current: Energy Magnetization

$$\frac{\partial \hat{h}(\boldsymbol{r})}{\partial t} + \nabla \cdot \hat{\boldsymbol{J}}_E(\boldsymbol{r}) = 0$$

In equilibrium:

$$\nabla \cdot \boldsymbol{J}_E^{\mathrm{eq}}(\boldsymbol{r}) = 0 \quad \Longrightarrow \quad \boldsymbol{J}_E^{\mathrm{eq}}(\boldsymbol{r}) = \boldsymbol{\nabla} \times \boldsymbol{M}_E$$

Transport current

$$\frac{\partial \hat{h}(\boldsymbol{r})}{\partial t} + \nabla \cdot \hat{\boldsymbol{J}}_E(\boldsymbol{r}) = 0$$

- Current is defined only up to a curl:

$$\boldsymbol{J}_E \quad \text{and} \quad \boldsymbol{J}_E - \boldsymbol{\nabla} \times \boldsymbol{M}_E$$

What are we measuring in transport experiments?

- The curl uncertainty does not affect the total current measured
- We can define a transport current that vanishes when equilibrium:

$$\boldsymbol{J}_E^{\mathrm{tr}} = \boldsymbol{J}_E - \boldsymbol{\nabla} \times \boldsymbol{M}_E$$

Einstein Relations

$$\mu_e = \frac{eD}{k_B T}$$

Transport current vanishes in the equilibrium state $\longrightarrow$ Einstein relations

Electron current $J_x = \mu_e n E - D\frac{dn}{dx}$

Equilibrium state $J_x = 0$

Equilibrium distribution $n(x) = N(T)\exp\left\{-\frac{\epsilon - e\phi(x) - \mu}{k_B T}\right\}$

Gravitation Field and Thermal Transport

- Introducing gravitation field:

$$\hat{H} = \int d\boldsymbol{r}\hat{h}(\boldsymbol{r}) \quad \Longrightarrow \quad \hat{H}^{\psi} = \int d\boldsymbol{r}\left[1+\psi(\boldsymbol{r})\right]\hat{h}(\boldsymbol{r})$$

- Equilibrium state:

$$\rho_{\mathrm{eq}} = \frac{1}{Z}e^{-\int d\boldsymbol{r}\beta[1+\psi(\boldsymbol{r})]\hat{h}(\boldsymbol{r})} = \frac{1}{Z}e^{\int d\boldsymbol{r}\frac{\hat{h}(\boldsymbol{r})}{k_B T(\boldsymbol{r})}} \Longrightarrow \beta = \frac{1}{k_B T\left(1+\psi(\boldsymbol{r})\right)}$$

$$\beta = \text{ Constant,} \qquad \boldsymbol{\nabla}\psi + \frac{\boldsymbol{\nabla}T}{T} = 0$$

- Einstein relations

$$\left.\begin{array}{c} \boldsymbol{J}_E^{\mathrm{tr}} = \tilde{L}\nabla\psi + L\frac{1}{T}\nabla T \\ \boldsymbol{J}_E^{\mathrm{tr}} \propto \boldsymbol{\nabla}\beta \end{array}\right\} \Longrightarrow \tilde{L} = L, \quad \kappa = \frac{\tilde{L}}{T}$$

J. M. Luttinger, Phys. Rev. **135**, A1505(1964)

Magnetization Correction

$$\boldsymbol{J}_E \to \boldsymbol{J}_E^{\psi} = (1+\psi)^2 \boldsymbol{J}_E$$

$$\boldsymbol{M}_E \to \boldsymbol{M}_E^{\psi} = (1+\psi)^2 \boldsymbol{M}_E$$

$$\times \boldsymbol{M}_E(\mu, T) \to \boldsymbol{\nabla} \times \boldsymbol{M}_E^{\psi} = (1+\psi)^2 \boldsymbol{\nabla} \times \boldsymbol{M}_E + 2\boldsymbol{\nabla}\psi \times \boldsymbol{M}_E$$

Transport current

$$\boldsymbol{J}_E^{\mathrm{tr}} = \boldsymbol{J}_E - \boldsymbol{\nabla} \times \boldsymbol{M}_E$$

$$\Delta \boldsymbol{J}_E^{\mathrm{tr}} = -L\boldsymbol{\nabla}\psi - 2\boldsymbol{\nabla}\psi \times \boldsymbol{M}_E, \qquad \kappa_{xy}^{\mathrm{tr}} = \frac{L}{T} + \frac{2M_E^z}{T}$$

Cooper, Halperin & Ruzin, Phys. Rev. B **55**, 2344 (1997)

Remaining Issues

- How to calculate (energy) magnetization(s) in an open system?

Rigorous derivation for the magnetization correction: Einstein relations maintained?

Tao Qin, Qian Niu and Juren Shi, *Energy magnetization and thermal Hall effect*. Phys. Rev. Lett. **107**, 236601(2011)

Theoretical Difficulty

Orbital magnetization: $\hat{\boldsymbol{M}} = -\frac{e}{2}\boldsymbol{r} \times \hat{\boldsymbol{v}}$

OM is simply the equilibrium expectation value of $\hat{\boldsymbol{M}}$

$$\boldsymbol{M} = \left\langle \Psi_G \middle| \hat{\boldsymbol{M}} \middle| \Psi_G \right\rangle$$

However, for crystalline solid: $\psi_{n\boldsymbol{k}} = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u_{n\boldsymbol{k}}(\boldsymbol{r})$

$\left\langle \psi_{n\boldsymbol{k}} \middle| \hat{\boldsymbol{M}} \middle| \psi_{n\boldsymbol{k}} \right\rangle$ has no deterministic expectation value!

Theory of Orbital Magnetization:

J. Shi, G. Vignale, D. Xiao, Q. Niu, Phys. Rev. Lett. **99**, 197202 (2007).
Thonhauser, Ceresoli, Vanderbilt, Resta, PRL **95,** 137205 (2005).
D. Xiao, J. Shi and Q. Niu, Phys. Rev. Lett. **95**, 137204 (2005).

However, it is only applicable to electrons in crystalline solids

Magnetization Formulas

$$-\frac{\partial \boldsymbol{M}_N}{\partial \mu_0} = \frac{\beta_0}{2\mathrm{i}} \nabla_{\boldsymbol{q}} \times \left\langle \hat{n}_{-\boldsymbol{q}}; \hat{\boldsymbol{J}}_{N,\boldsymbol{q}} \right\rangle_0 \Big|_{\boldsymbol{q}\to 0}$$

$$\boldsymbol{M}_N - T_0 \frac{\partial \boldsymbol{M}_N}{\partial T_0} = \frac{\beta_0}{2\mathrm{i}} \nabla_{\boldsymbol{q}} \times \left\langle \hat{K}_{-\boldsymbol{q}}; \hat{\boldsymbol{J}}_{N,\boldsymbol{q}} \right\rangle_0 \Big|_{\boldsymbol{q}\to 0}$$

$$-\frac{\partial \boldsymbol{M}_Q}{\partial \mu_0} = \frac{\beta_0}{2\mathrm{i}} \nabla_{\boldsymbol{q}} \times \left\langle \hat{n}_{-\boldsymbol{q}}; \hat{\boldsymbol{J}}_{Q,\boldsymbol{q}} \right\rangle_0 \Big|_{\boldsymbol{q}\to 0}$$

$$2\boldsymbol{M}_Q - T_0 \frac{\partial \boldsymbol{M}_Q}{\partial T_0} = \frac{\beta_0}{2\mathrm{i}} \nabla_{\boldsymbol{q}} \times \left\langle \hat{K}_{-\boldsymbol{q}}; \hat{\boldsymbol{J}}_{Q,\boldsymbol{q}} \right\rangle_0 \Big|_{\boldsymbol{q}\to 0}$$

Pre-requisite: In the presence of gravitation field ψ and potential ϕ, the current operators should scale with:

$\hat{\boldsymbol{J}}_Q(\boldsymbol{r}) \equiv \hat{\boldsymbol{J}}_E(\boldsymbol{r}) - \mu_0 \hat{\boldsymbol{J}}_N(\boldsymbol{r})$ $\quad$ $\boldsymbol{M}_Q \equiv \boldsymbol{M}_E - \mu_0 \boldsymbol{M}_N$ $\quad$ $\hat{K}(\boldsymbol{r}) \equiv \hat{h}(\boldsymbol{r}) - \mu_0 \hat{n}(\boldsymbol{r})$

Magnetization Corrections

$$\begin{bmatrix} \boldsymbol{J}_1^{\mathrm{tr}} \\ \boldsymbol{J}_2^{\mathrm{tr}} \end{bmatrix} = \begin{bmatrix} \overleftrightarrow{L}^{(11)} & \overleftrightarrow{L}^{(12)} - \frac{\boldsymbol{M}_N}{\beta_0 V}\times \\ \overleftrightarrow{L}^{(21)} - \frac{\boldsymbol{M}_N}{\beta_0 V}\times & \overleftrightarrow{L}^{(22)} - \frac{2\boldsymbol{M}_Q}{\beta_0 V}\times \end{bmatrix} \begin{bmatrix} \boldsymbol{X}_1 \\ \boldsymbol{X}_2 \end{bmatrix}$$

	Current J	Force X
1	Particle current	Electric Field, Density gradient
2	Heat Current	Temperature Gradient, Gravitation Field

$$\boldsymbol{J}_1^{\phi,\psi} = \boldsymbol{J}_N^{\phi,\psi}$$

$$\boldsymbol{J}_2^{\phi,\psi} = \hat{\boldsymbol{J}}_Q^{\phi,\psi} \equiv \boldsymbol{J}_E^{\phi,\psi} - \alpha(\boldsymbol{r})\boldsymbol{J}_N^{\phi,\psi}$$

$$\alpha(\boldsymbol{r}) \equiv [1+\psi(\boldsymbol{r})][\phi(\boldsymbol{r})+\mu(\boldsymbol{r})]$$

$$\beta(\boldsymbol{r}) \equiv 1/k_B[1+\psi(\boldsymbol{r})]T(\boldsymbol{r})$$

$$\boldsymbol{X}_1 = -\beta(\boldsymbol{r})\nabla\alpha(\boldsymbol{r})$$

$$\boldsymbol{X}_2 = \nabla\beta(\boldsymbol{r})$$

Proof--Canonical formulas

- $$\chi_{ij}^{q}(r) = -\mathrm{i}q \times M_{ij}(r) + e^{-\mathrm{i}q\cdot r}\nabla \times \kappa_{ij}^{q}(r)$$

$$\kappa_{11}^{q=0}(r) = \left.\frac{\partial M_N(r)}{\partial \mu_0}\right|_{T_0}, \kappa_{12}^{q=0}(r) = T_0 \left.\frac{\partial M_N(r)}{\partial T_0}\right|_{\mu_0},$$

$$\kappa_{21}^{q=0}(r) = \left.\frac{\partial M_Q(r)}{\partial \mu_0}\right|_{T_0} + M_N(r), \kappa_{22}^{q=0}(r) = T_0 \left.\frac{\partial M_Q(r)}{\partial T_0}\right|_{\mu_0}.$$

- $\nabla_q \times$ both sides of $\chi_{ij}^{q}(r)$, let $q \to 0$ and integrate over r.

Proof—Magnetization corrections

- Density matrix $\hat{\rho} \approx \hat{\rho}_{\text{leq}} + \hat{\rho}_1$

$$\hat{\rho}_{\text{leq}} = \frac{1}{Z} \exp\left[- \int \mathrm{d}\boldsymbol{r} \left(\hat{h}(\boldsymbol{r}) - \mu(\boldsymbol{r}) \hat{n}(\boldsymbol{r}) \right) / \left(k_B T(\boldsymbol{r}) \right) \right]$$

$\hat{\rho}_1$ is determined by $\boxed{ i\hbar \frac{\partial \hat{\rho}}{\partial t} + [\hat{\rho}, \hat{H}_{\phi,\psi}] = 0 }$

- $\boldsymbol{J}_i^{\phi,\psi} = \boldsymbol{J}_i^{\text{leq}} + \boldsymbol{J}_i^{\text{Kubo}}, \ \boldsymbol{J}_i^{\text{leq}} = \mathrm{Tr} \hat{\rho}_{\text{leq}} \hat{\boldsymbol{J}}_i^{\phi,\psi}, \ \boldsymbol{J}_i^{\text{Kubo}} = \mathrm{Tr} \hat{\rho}_1 \hat{\boldsymbol{J}}_i^{\phi,\psi}$

Linear order: $\mu(\boldsymbol{r}) \approx \mu_0 + \delta\mu(\boldsymbol{r})$,

- Local equilibrium current:

$$\boldsymbol{J}_i^{\text{leq}}(\boldsymbol{r}) \approx \boldsymbol{J}_i^{\text{eq}}(\boldsymbol{r}) + \sum_{j=1}^{2} \int \mathrm{d}\boldsymbol{r}' \boxed{\chi_{ij}(\boldsymbol{r}, \boldsymbol{r}')} x_j(\boldsymbol{r}')$$

$$x_1(\boldsymbol{r}) \equiv \delta\mu(\boldsymbol{r}), \quad x_2(\boldsymbol{r}) \equiv -T_0 \delta[1/T(\boldsymbol{r})]$$

Equilibrium current:

$$\boldsymbol{J}_1^{\text{eq}}(\boldsymbol{r}) = [1 + \psi(\boldsymbol{r})] \boldsymbol{\nabla} \times \boldsymbol{M}_N(\boldsymbol{r})$$

$$\boldsymbol{J}_2^{\text{eq}}(\boldsymbol{r}) = [1 + \psi(\boldsymbol{r})]^2 [\boldsymbol{\nabla} \times \boldsymbol{M}_E(\boldsymbol{r}) - \mu(\boldsymbol{r}) \boldsymbol{\nabla} \times \boldsymbol{M}_N(\boldsymbol{r})]$$

Proof—Magnetization corrections

- From $\kappa_{ij}^{q}(\boldsymbol{r}) = -\mathrm{i}\boldsymbol{q}\times\boldsymbol{M}_{ij}(\boldsymbol{r}) + e^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}\nabla\times\kappa_{ij}^{q}(\boldsymbol{r})$, we have:

$$\boldsymbol{J}_1^{\mathrm{leq}}(\boldsymbol{r}) \approx \nabla\times\boldsymbol{M}_N^{\phi,\psi}(\boldsymbol{r}) - \frac{1}{\beta}\boldsymbol{M}_N(\boldsymbol{r})\times\boldsymbol{X}_2$$

$$\boldsymbol{J}_2^{\mathrm{leq}}(\boldsymbol{r}) \approx \nabla\times\boldsymbol{M}_E^{\phi,\psi}(\boldsymbol{r}) - \mu(\boldsymbol{r})\nabla\times\boldsymbol{M}_N^{\phi,\psi}(\boldsymbol{r}) - \frac{1}{\beta}\boldsymbol{M}_N(\boldsymbol{r})\times\boldsymbol{X}_1 - \frac{2}{\beta}\boldsymbol{M}_Q(\boldsymbol{r})\times\boldsymbol{X}_2$$

- Introducing the transport currents:

$$\boldsymbol{J}_{N(E)}^{\phi,\psi,\mathrm{tr}} = \boldsymbol{J}_{N(E)}^{\phi,\psi} - \nabla\times\boldsymbol{M}_{N(E)}^{\phi,\psi}$$

$$\boldsymbol{J}_i^{\phi,\psi,\mathrm{Kubo}} = \boldsymbol{J}_i^{\mathrm{eq}} + \boldsymbol{J}_i^{\mathrm{tr}} \qquad \boldsymbol{J}_i^{\mathrm{Kubo}} \approx \sum_j \overleftrightarrow{L}^{(ij)}\cdot\boldsymbol{X}_j$$

Application to the anomalous Hall system

- The electron energy density:

$$\hat{h}(\boldsymbol{r}) = \left\{\frac{m}{2}[\hat{\boldsymbol{v}}\hat{\varphi}(\boldsymbol{r})]^{\dagger} \cdot [\hat{\boldsymbol{v}}\hat{\varphi}(\boldsymbol{r})] + \hat{\varphi}^{\dagger}(\boldsymbol{r})V(\boldsymbol{r})\hat{\varphi}(\boldsymbol{r})\right\}$$

Energy current operator:

$$\hat{\boldsymbol{J}}_E(\boldsymbol{r}) = \frac{1}{2}\left\{[\hat{\boldsymbol{v}}\hat{\varphi}(\boldsymbol{r})]^{\dagger}\left[\hat{\mathcal{H}}\hat{\varphi}(\boldsymbol{r})\right] + h.c.\right\}$$

$$\hat{\mathcal{H}} = \frac{m}{2}\hat{\boldsymbol{v}}^2 + V(\boldsymbol{r})$$

- Gravitational field $\psi \neq 0,\quad \hat{h}^{\psi}(\boldsymbol{r}) = [1+\psi(\boldsymbol{r})]\,\hat{h}(\boldsymbol{r})$

$$\hat{\boldsymbol{J}}_E^{\psi}(\boldsymbol{r}) = [1+\psi(\boldsymbol{r})]^2\,\hat{\boldsymbol{J}}_E(\boldsymbol{r}) + \boldsymbol{\nabla}(1+\psi(\boldsymbol{r}))^2 \times \hat{\boldsymbol{\Lambda}}(\boldsymbol{r})$$

$$\hat{\boldsymbol{\Lambda}}(\boldsymbol{r}) = \frac{\hbar}{8\mathrm{i}}(\hat{\boldsymbol{v}}\hat{\varphi})^{\dagger} \times (\hat{\boldsymbol{v}}\hat{\varphi})$$

- Gauge freedom--curl: $\boldsymbol{\nabla} \times \left((1+\psi(\boldsymbol{r}))^2\,\hat{\boldsymbol{\Lambda}}(\boldsymbol{r})\right)$

New current operator: $\hat{\boldsymbol{J}}_E(\boldsymbol{r}) \to \hat{\boldsymbol{J}}_E(\boldsymbol{r}) - \boldsymbol{\nabla} \times \hat{\boldsymbol{\Lambda}}(\boldsymbol{r})$

Application to the anomalous Hall system

- Kubo formula:

$$\kappa_{xy}^{\mathrm{Kubo}} = \frac{1}{2T_0\hbar V}\sum_{nk}\mathrm{Im}\left\langle\frac{\partial u_{nk}}{\partial k_x}\right|\left(\hat{\mathcal{H}}_{\boldsymbol{k}}+\epsilon_{n\boldsymbol{k}}-2\mu_0\right)^2\left|\frac{\partial u_{nk}}{\partial k_y}\right\rangle f_{n\boldsymbol{k}}$$

- Energy magnetization:

$$\frac{\partial \boldsymbol{M}_Q}{\partial T_0} \quad \beta_0 \quad \boldsymbol{J}_{Q,q} \quad \lim_{q\to 0} \quad \tilde{\boldsymbol{M}}_Q = 2\boldsymbol{M}_Q - T_0\frac{\partial \boldsymbol{M}_Q}{\partial T_0} = \frac{\hat{\ }}{2i}\nabla_q\times\langle \tilde{K}_{q}\rangle$$

$$\tilde{M}_Q = -\frac{1}{\hbar}\sum_{nk}\mathrm{Im}\left[\left\langle\frac{\partial u_{nk}}{\partial k_x}\right|(H_k+\epsilon_{nk}-2\mu_0)^2\left|\frac{\partial u_{nk}}{\partial k_y}\right\rangle\right] f_{nk} \quad M_{Q,z} = \ \cdots$$

$$\sum_{nk}\mathrm{Im}\left[\left\langle\frac{\partial u_{nk}}{\partial k_x}\right|(\epsilon_{nk}-H_k)^2-4(\epsilon_{nk}-\mu_0)(\epsilon_{nk}-H_k)\left|\frac{\partial u_{nk}}{\partial k_y}\right\rangle\right] \quad -\frac{1}{4\hbar}\ \cdots$$

$$\mu_0)\, f' \quad \times(\epsilon_{nk}-\mu_0)\, f_{nk}$$

Application to the anomalous Hall system

$$\kappa_{xy}^{\rm tr} \equiv \kappa_{xy}^{\rm Kubo} + \frac{2M_Q^z}{T_0 V}$$

$$\kappa_{xy}^{\rm tr} = -\frac{1}{e^2 T_0}\int {\rm d}\epsilon (\epsilon - \mu_0)^2 \sigma_{xy}(\epsilon)\frac{df(\epsilon)}{d\epsilon}$$

$$\sigma_{xy}(\epsilon) = -\frac{e^2}{\hbar}\sum_{\epsilon_{nk}\le\epsilon}\Omega_{nk}^z \qquad \Omega_{n\boldsymbol{k}}^z \equiv -2{\rm Im}\left\langle \frac{\partial u_{n\boldsymbol{k}}}{\partial k_x}\middle|\frac{\partial u_{n\boldsymbol{k}}}{\partial k_y}\right\rangle$$

- Wiedemann-Franz law:

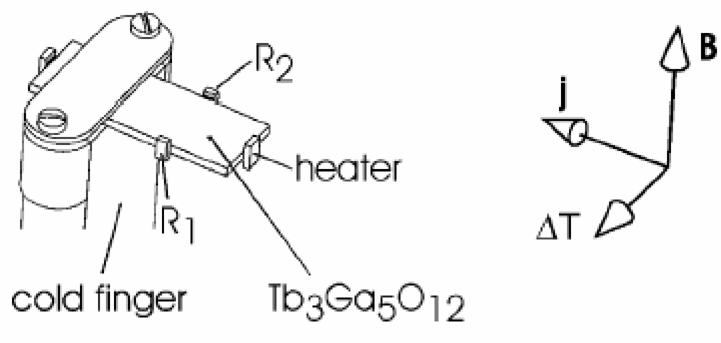
$$\kappa_{xy}^{\rm tr} = \frac{\pi^2}{[illegible]}\left(\frac{k_B}{[illegible]}\right)^2 T [illegible]$$

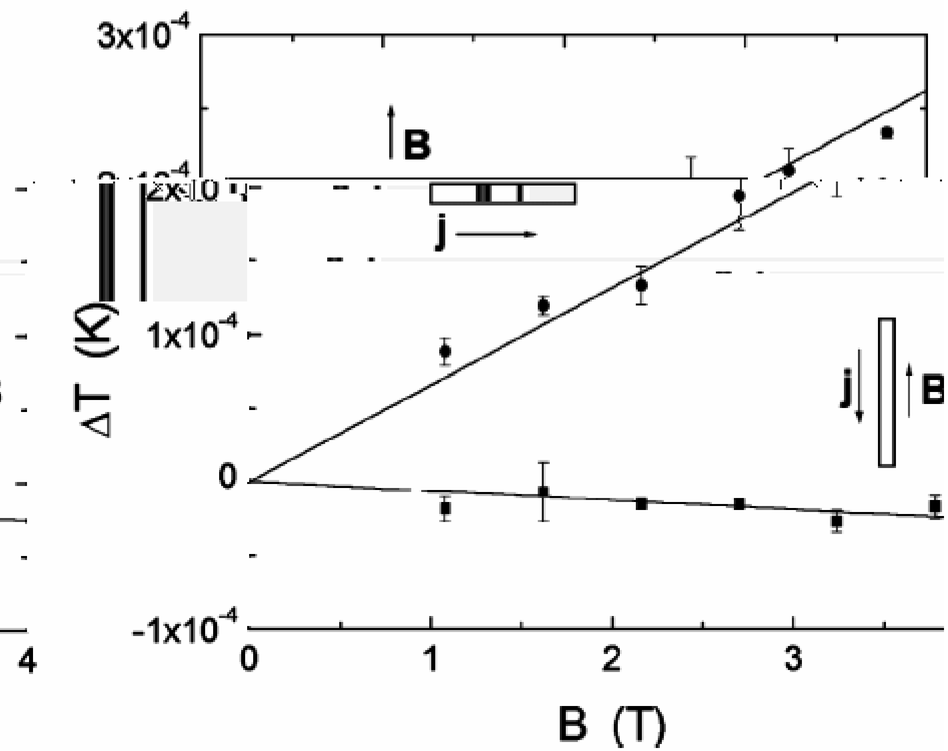
Theory for the phonon Hall effect

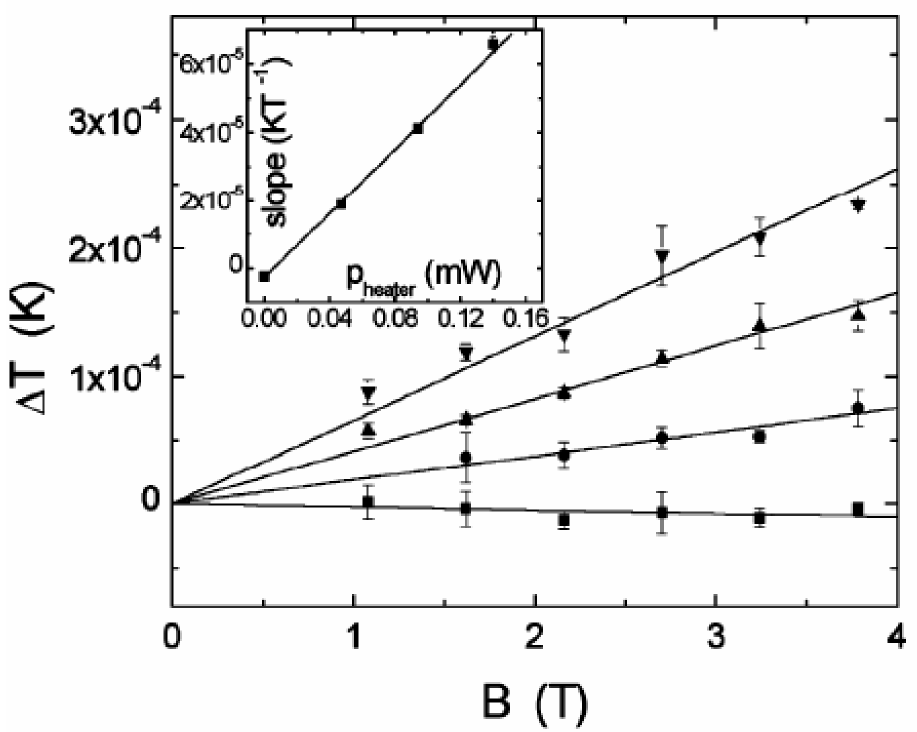
- Experiments on phonon Hall effect
- Issues of existing theories
- **Our theory**
  - General phonon dynamics for magnetic systems
  - Proper evaluation of phonon Hall coefficient
  - Topological phonon system
  - Low temperature behavior

Tao Qin and Junren Shi, *Berry curvature and phonon Hall effect*, arXiv: 1111. 1322v1

Experiments on phonon Hall effect





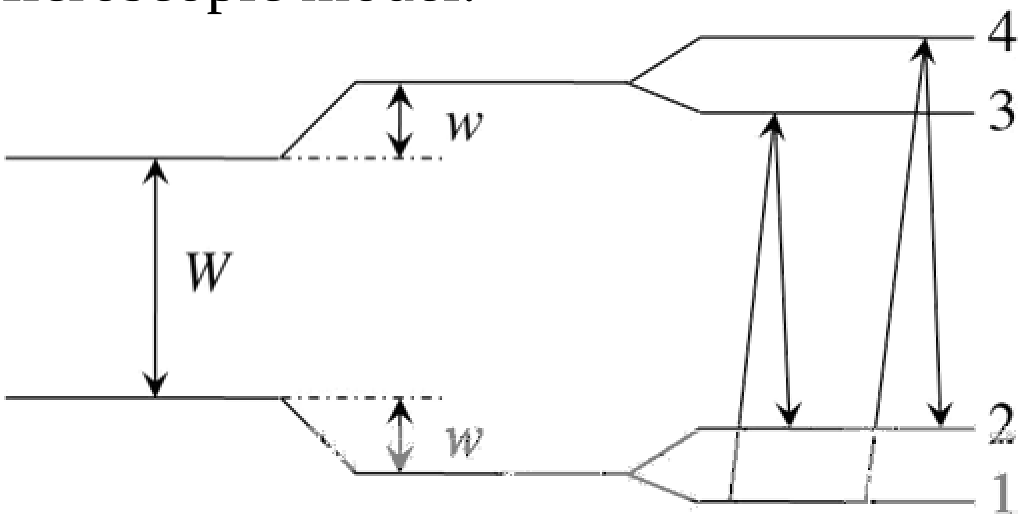


C. Strohm *et al*., Phys. Rev. Lett. **95**, 155901(2006)

A. Inyushkin *et al*., JETP Lett. **86**, 379 (2007)

Existing theories: Spin-lattice Raman interaction

- Microscopic model:



$$H_R = K \sum_m \boldsymbol{M} \cdot \Omega_m$$

$$\Omega_m = \boldsymbol{u}_m \times \boldsymbol{p}_m$$

Kronig, Physica **6**, 33(1939)

L. Sheng *et al.*, Phys. Rev. Lett. **96**, 155901(2006)

Yu. Kagan *et al.*, Phys. Rev. Lett. **100**, 145902 (2008)

L. Zhang, *et al.*, Phys. Rev. Lett. **105**, 225901(2010)

- Kubo formula or its equivalents is employed

Issue #1: inappropriate microscopic model

$$H_R = K \sum_m \boldsymbol{M} \cdot \Omega_m$$

$$\Omega_m = \boldsymbol{u}_m \times \boldsymbol{p}_m$$

Considering a rigid-body motion: $\boldsymbol{u}_m = \boldsymbol{u}$

$$H_R \to K\boldsymbol{M} \cdot (\boldsymbol{u} \times \boldsymbol{P})$$

A magnetic solid will experience a Lorentz force!?

The microscopic model breaks Principle of Relativity!

Issue #2: Kubo formula

$$\kappa_{xy}^{\text{Kubo}} = \frac{1}{Vk_B T^2} \lim_{s\to 0} \lim_{\boldsymbol{q}\to 0} \int_0^\infty \mathrm{d}t e^{-st} \left\langle \hat{J}^y_{E,-\boldsymbol{q}};\ \hat{J}^x_{E,\boldsymbol{q}}(t) \right\rangle$$

However, this formula is not applicable for magnetic systems!

$$\kappa_{xy}^{\text{tr}} \equiv \kappa_{xy}^{\text{Kubo}} + \frac{2M_Q^z}{T_0 V}$$

$$2\boldsymbol{M}_Q - T_0 \frac{\partial \boldsymbol{M}_Q}{\partial T_0} = \frac{\beta_0}{2\mathrm{i}} \boldsymbol{\nabla}_q \times \left\langle \hat{K}_{-\boldsymbol{q}}; \hat{\boldsymbol{J}}_{Q,\boldsymbol{q}} \right\rangle_0 \Big|_{\boldsymbol{q}\to 0}$$

Tao Qin, Qian Niu and Juren Shi, Energy magnetization and thermal Hall effect. Phys. Rev. Lett. **107**, 236601(2011)

Our theory: Phonon Dynamics

- The electron Berry phase ⟹ The effective magnetic field
- The effective Hamiltonian

$$\hat{H} = \sum_{l\kappa} \frac{\left(-\mathrm{i}\hbar\boldsymbol{\nabla}_{l\kappa} - \boldsymbol{A}_{l\kappa}(\{\boldsymbol{R}\})\right)^2}{2M_\kappa} + V_{\mathrm{eff}}(\{\boldsymbol{R}\})$$

$$\boldsymbol{A}_{l\kappa}(\{\boldsymbol{R}\}) \equiv \mathrm{i}\hbar \langle \Phi_0(\{\boldsymbol{R}\}) | \boldsymbol{\nabla}_{l\kappa} \Phi_0(\{\boldsymbol{R}\}) \rangle$$

Mead-Truhlar term: $\boxed{\boldsymbol{A}_{l\kappa}(\{\boldsymbol{R}\}) \cdot \frac{\hbar}{\mathrm{i}} \boldsymbol{\nabla}_{l\kappa}}$

C. A. Mead and D. G. Truhlar, J. Chem. Phys. **70**, 2284 (1979)

Effective magnetic field acting on phonons

The effective magnetic field:

$$G^{\kappa\kappa'}_{\alpha\beta}(\boldsymbol{R}^0_l - \boldsymbol{R}^0_{l'}) = 2\hbar \mathrm{Im} \left\langle \frac{\partial \Phi_0}{\partial u_{\beta,l'\kappa'}} \middle| \frac{\partial \Phi_0}{\partial u_{\alpha,l\kappa}} \right\rangle \bigg|_{u_{l\kappa} \to 0}$$

A constraint naturally emerges from the translational symmetry:

$$\sum_{l\kappa\kappa'} G^{\kappa\kappa'}_{\alpha\beta}(\boldsymbol{R}^0_l) = 0$$

Principle of Relativity recovers.

Phonon dynamics and Berry curvature

- The equations of motion

$$\dot{\tilde{\boldsymbol{u}}}_k = \boldsymbol{P}_k$$

$$\dot{\boldsymbol{P}}_k = -D_k \tilde{\boldsymbol{u}}_k + G_k \boldsymbol{P}_k$$

$$\omega_{ki} \Psi_{ki} = \begin{pmatrix} 0 & \mathrm{i} \\ -\mathrm{i} D_k & \mathrm{i} G_k \end{pmatrix} \Psi_{ki} \equiv \tilde{H}_k \Psi_{ki}$$

6r branches of phonons satisfing:

$$\omega_{ki}^{(-)} = -\omega_{-ki}^{(+)} \qquad \Psi_{ki}^{(-)} = \Psi_{-ki}^{(+)*}$$

$$\bar{\Psi}_{ki} \Psi_{ki} = 1 \qquad \bar{\Psi}_{ki} = \Psi_{ki}^{\dagger} \tilde{D}_k$$

- The phonon Berry connection and Berry curvature

$$\mathcal{A}_{ki} = \mathrm{i} \bar{\Psi}_{ki} \frac{\partial \Psi_{ki}}{\partial \boldsymbol{k}} \qquad \Omega_{ki} = -\mathrm{Im}\left[\frac{\partial \bar{\Psi}_{ki}}{\partial \boldsymbol{k}} \times \frac{\partial \Psi_{ki}}{\partial \boldsymbol{k}}\right]$$

Phonon Hall coefficient

- Kubo formula

$$\kappa_{xy}^{Kubo} = \frac{\hbar}{VT_0}\sum_{k;i=1}^{3r} \omega_{ki}\left(n_{ki}+\frac{1}{2}\right)$$

$$\mathcal{M}_{ki} = \mathrm{Im}\left[\frac{\partial \bar{\psi}_{ki}}{\partial \boldsymbol{k}} \times \tilde{H}_{\boldsymbol{k}} \frac{\partial \psi_{ki}}{\partial \boldsymbol{k}}\right]$$

- Energy magnetization

$$\tilde{M}_E^z = -\frac{\hbar}{2}\sum_{k;i=1}^{3r}\left[\Omega^z_{ki}\omega^3_{ki}n'_{ki} + \mathcal{M}^z_{ki}\left(2\omega_{ki}n_{ki} + \omega^2_{ki}n'_{ki} + 1\right)\right]$$

$$2M_E^z - T\frac{\partial M_E^z}{\partial T} = \tilde{M}_E^z$$

Phonon Hall coefficient

$$\kappa_{xy}^{\mathrm{tr}} \equiv \kappa_{xy}^{\mathrm{Kubo}} + \frac{2M_Q^z}{T_0 V}$$

$$\kappa_{xy}^{\mathrm{tr}} = -\frac{(\pi k_B)^2}{3h} Z_{\mathrm{ph}} T - \frac{1}{T} \int d\epsilon \epsilon^2 \sigma_{xy}(\epsilon) \frac{dn(\epsilon)}{d\epsilon}$$

$$Z_{\mathrm{ph}} = \frac{2\pi}{V} \sum_{\boldsymbol{k};i=1}^{3r} \Omega_{\boldsymbol{k}i}^z, \qquad \sigma_{xy}(\epsilon) = -\frac{1}{V\hbar} \sum_{\hbar\omega_{\boldsymbol{k}i} \le \epsilon} \Omega_{\boldsymbol{k}i}^z$$

Topological Phonon System

$$Z_{\mathrm{ph}} \neq 0$$

$$\kappa_{xy}^{\mathrm{topo.}} = -\frac{(\pi k_B)^2}{3h} Z_{\mathrm{ph}} T$$

$$Z_{\mathrm{ph}} = \begin{cases} \text{Integer}, & 2D \\ \frac{G_z}{2\pi}, & 3D \end{cases}$$

G_z: *z*-component of a reciprocal lattice vector *G*

Halperin, Jpn. J. Appl. Phys. 26S3, 1913 (1987)

Our theory: long wave limit

- Constraint on the effective magnetic field acting on atoms:

$$\sum_{l\kappa\kappa'} G_{\alpha\beta}^{\kappa\kappa'}(\boldsymbol{R}_l^0) = 0$$

- Phonon Hall coefficient

$$\kappa_{xy}^{\mathrm{tr}} \propto T^3$$

Instead of $\kappa_{xy}^{\mathrm{tr}} \propto T$

L. Sheng *et al*., Phys. Rev. Lett. **96**, 155901(2006). J. Wang *et al*., Phys. Rev. B **80**, 012301 (2009)

Summary

$$-\frac{\partial \boldsymbol{M}_N}{\partial \mu_0} = \frac{\beta_0}{2\mathrm{i}} \boldsymbol{\nabla}_{\boldsymbol{q}} \times \left\langle \hat{n}_{-\boldsymbol{q}}; \hat{\boldsymbol{J}}_{N,\boldsymbol{q}} \right\rangle_0 \Big|_{\boldsymbol{q}\to 0}$$

$$\boldsymbol{M}_N - T_0 \frac{\partial \boldsymbol{M}_N}{\partial T_0} = \frac{\beta_0}{2\mathrm{i}} \boldsymbol{\nabla}_{\boldsymbol{q}} \times \left\langle \hat{K}_{-\boldsymbol{q}}; \hat{\boldsymbol{J}}_{N,\boldsymbol{q}} \right\rangle_0 \Big|_{\boldsymbol{q}\to 0}$$

$$-\frac{\partial \boldsymbol{M}_Q}{\partial \mu_0} = \frac{\beta_0}{2\mathrm{i}} \boldsymbol{\nabla}_{\boldsymbol{q}} \times \left\langle \hat{n}_{-\boldsymbol{q}}; \hat{\boldsymbol{J}}_{Q,\boldsymbol{q}} \right\rangle_0 \Big|_{\boldsymbol{q}\to 0}$$

$$2\boldsymbol{M}_Q - T_0 \frac{\partial \boldsymbol{M}_Q}{\partial T_0} = \frac{\beta_0}{2\mathrm{i}} \boldsymbol{\nabla}_{\boldsymbol{q}} \times \left\langle \hat{K}_{-\boldsymbol{q}}; \hat{\boldsymbol{J}}_{Q,\boldsymbol{q}} \right\rangle_0 \Big|_{\boldsymbol{q}\to 0}$$

Summary

- A general phonon dynamics for magnetic systems
- Emergent “magnetic field” for phonon
- Phonon Hall coefficient and phonon Berry curvature
- Topological phonon systems – Quantum Hall Effect of Phonon Systems
- Low temperature behavior of ordinary phonon systems: T^3 instead of T
- Linear T with quantized coefficient may suggest Topological Phonon System

Tao Qin, Qian Niu and Juren Shi, *Energy magnetization and thermal Hall effect* Phys. Rev. Lett. **107**, 236601(2011)

Tao Qin and Junren Shi, *Berry curvature and phonon Hall effect*, arXiv: 1111. 1322