Thermal Hall effect of magnons

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Related papers:
Outline

1. Spin Hamiltonian
   • Exchange and DM interactions
   • Microscopic origins

2. Elementary excitations

3. Hall effect and thermal Hall effect

4. Main results

5. Summary
Coupling between magnetic moments

- Classical v.s. Quantum
  - Dipole-dipole interaction
  \[ U_{\text{dip}}(r) \propto -\frac{\mu_1 \cdot \mu_2}{r^3} + 3\frac{(\mu_1 \cdot \hat{r})(\mu_2 \cdot \hat{r})}{r^3} \]
  Usually, too small (< 1K) to explain transition temperatures…
  - Exchange interaction
    \[ H_{\text{int}} = J S_i \cdot S_j \quad (S_i: \text{spin at site } i) \]
    Direct exchange: \( J < 0 \rightarrow \text{ferromagnetic (FM)} \)
    Super-exchange: \( J > 0 \rightarrow \text{antiferromagnetic (AFM)} \)

- Anisotropies
  Spin-orbit int. breaks SU(2) symmetry.
  \[ H_{\text{int}} = J_x S_i^x S_j^x + J_y S_i^y S_j^y + J_z S_i^z S_j^z + D_{ij} \cdot (S_i \times S_j) + \cdots \]
  Dzyaloshinskii-Moriya (DM) int.: \( D \)
  NOTE) Inversion breaking is necessary.
  \[ \vec{S}_i \rightarrow \vec{D} \rightarrow \vec{S}_j \]
  Spin tend to be orthogonal
(Crude) derivation

- 2-site Hubbard model
  - Hamiltonian
    \[ H = -t \sum_{\sigma=\uparrow,\downarrow} (c_{1,\sigma}^\dagger c_{2,\sigma} + c_{2,\sigma}^\dagger c_{1,\sigma}) + U \sum_{i=1,2} n_{i,\uparrow} n_{i,\downarrow} \]
  - 2nd order perturbation at half-filling, \( U \gg t \)

\[ H_{\text{eff}} = \frac{4t^2}{U} \left( S_1 \cdot S_2 - \frac{1}{4} \right) \quad S_i^\alpha = \frac{1}{2} \sigma_i^\alpha \]

Origin of exchange int. = electron correlation!
Can explain AFM int. What about FM int.?
(Multi-orbital nature, Kanamori-Goodenough, …)
Origin of DM interaction (1)

- **Spin-dependent hopping**

  \[ H_{\text{hop}} = -t \sum_{\sigma=\uparrow,\downarrow} (c^\dagger_{1,\sigma} c_{2,\sigma} + \text{h.c.}) \]

  \[ \xrightarrow{\text{Due to spin-orbit}} -\sum_{\sigma,\tau} (c^\dagger_{1,\sigma} T_{\sigma,\tau} c_{2,\tau} + \text{h.c.}) \]

  - Hopping matrix

  \[ T = t_0 \exp(i\theta \mathbf{d} \cdot \mathbf{\sigma}/2) \]

  \[ \theta=0 \text{ reduces to the spin-independent case} \]

- **Unitary transformation**

  One can \``absorb\'' the spin-dependent hopping!

  \[ c_i = \begin{pmatrix} c_{i,\uparrow} \\ c_{i,\downarrow} \end{pmatrix} \quad (i = 1, 2) \]

  \[ \xrightarrow{\text{}} f_1 = c_1, \quad f_2 = \exp(i\theta \mathbf{d} \cdot \mathbf{\sigma}/2) c_2 \]

  New fermions satisfy the same anti-commutation relations.

  Number ops. remain unchanged.

  \[ n_i = \sum_{\sigma} c^\dagger_{i,\sigma} c_{i,\sigma} = c^\dagger_i c_i = f^\dagger_i f_i \]

  - Hamiltonian in terms of \( f \)

  \[ H = H_{\text{hop}} + H_U = -t (f^\dagger_1 f_2 + \text{h.c.}) + U \sum_{i=1,2} n_i (n_i - 1) \]
Origin of DM interaction (2)

**Effective Hamiltonian**

\[ H_{\text{eff}} = \frac{4(t_0)^2}{U} \vec{S}_1 \cdot \vec{S}_2 \quad \cdots (1) \]

\[ \vec{S}_i = f_i^\dagger \frac{\vec{\sigma}}{2} f_i \quad (S_i = c_i^\dagger \frac{\vec{\sigma}}{2} c_i) \]

- How does it look like in original spins?

\[ \vec{S}_1 = \vec{S}_1, \quad \vec{S}_2 = c_2^\dagger e^{-i\theta d \cdot \vec{\sigma}/2} \frac{\vec{\sigma}}{2} e^{i\theta d \cdot \vec{\sigma}/2} c_2 \]

\[ = \vec{S}_2 \cos \theta - (d \times \vec{S}_2) \sin \theta + d (d \cdot \vec{S}_2) (1 - \cos \theta) \]

Ex.) Prove the relation.

Hint: express \( e^{-i\theta d \cdot \vec{\sigma}/2} \frac{\vec{\sigma}}{2} e^{i\theta d \cdot \vec{\sigma}/2} \) in terms of \( \vec{\sigma} \).

\[(1) = \frac{4t_0^2 \cos \theta}{U} \vec{S}_1 \cdot \vec{S}_2 + \frac{4t_0^2 \sin \theta}{U} d \cdot (\vec{S}_1 \times \vec{S}_2) + \frac{4t_0^2 (1 - \cos \theta)}{U} (d \cdot \vec{S}_1)(d \cdot \vec{S}_2) \]

Heisenberg int. \quad Dzyaloshinskii-Moriya (DM) int. \quad Kaplan-Shekhtman-Aharony-Entin-Wohlman (KSAE) int.

\[ D \propto d \]

**NOTE**) One can eliminate the effect of the DM interaction if there is no loop.
Outline

1. Spin Hamiltonian

2. Elementary excitations
   • What are magnons?
   • From spins to bosons
   • Diagonalization of BdG Hamiltonian

3. Hall effect and thermal Hall effect

4. Main results

5. Summary
What are magnons?

- FM Heisenberg model in a field

\[
H_0 = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j - g \mu_B H \sum_i S_i^z \quad (J > 0)
\]

- Ground state: spins are aligned in the same direction.

\[
E_0 = -N (z J S^2 + g \mu_B H S) \quad z:\text{ coordination number}
\]

- Elementary excitations -- Intuitive picture --

Cf.) non-relativistic Nambu-Goldstone bosons

The picture is classical. But in ferromagnets, ground state and 1-magnon states are *exact* eigenstates of the Hamiltonian.
1-Magnon eigenstates

- "Motion" of flipped spin

\[ -J \vec{S}_i \cdot \vec{S}_j = -\frac{J}{2} (S_i^+ S_j^- + S_i^- S_j^+) + J S_i^z S_j^z \]

Flipped spin hops to the neighboring sites.

\[ -J(\vec{S}_i \cdot \vec{S}_j)|i\rangle = -\frac{J}{2}|j\rangle + \frac{J}{4}|i\rangle \]

- Bloch state

\[ |\psi(\vec{k})\rangle = \frac{1}{\sqrt{N}} \sum_i e^{i\vec{k} \cdot \vec{R}_i} |i\rangle \]

is an exact eigenstate with energy \( E(k) \)

- What about DM int.?

\[ D \text{ vector } // z\text{-axis} \]

\[ -J \vec{S}_i \cdot \vec{S}_j + D[\vec{S}_i \times \vec{S}_j]_z \quad (\tan \phi = D/J) \]

\[ = -\frac{\tilde{J}}{2} (e^{-i\phi} S_i^+ S_j^- + e^{i\phi} S_i^- S_j^+) - JS_i^z S_j^z \]

Magnon picks up a phase factor!

\[ |i\rangle \rightarrow -\frac{\tilde{J}}{2} e^{-i\phi} |j\rangle \]
From spins to bosons

- Holstein-Primakoff transformation
  - Bose operators
    \[ [b_i, b_j^\dagger] = \delta_{ij}, \quad [b_i, b_j] = [b_i^\dagger, b_j^\dagger] = 0 \]
    Number op.: \( n_i = b_i^\dagger b_i \)
  - Spins in terms of \( b \)
    \[ S_j^+ = \sqrt{2S - n_j} b_j, \quad S_j^- = b_j^\dagger \sqrt{2S - n_j}, \quad S_j^z = S - n_j \]
    Obey the commutation relations of spins
    Often neglect nonlinear terms. \( S_j^+ \sim \sqrt{2S} b_j, \quad S_j^- \sim \sqrt{2S} b_j^\dagger \)
    (Good at low temperatures.)
  - Magnetic ground state = vacuum of bosons \( b_j |\text{vac}\rangle = 0 \)

- Sublattice structure
  - AFM int. \( \rightarrow \) Approximate 1-magnon state
  - Spins on the other sublattice:
    \[ S_j^+ = a_j^\dagger \sqrt{2S - n_j}, \quad S_j^- = (S_j^+)^\dagger, \quad S_j^z = -S + n_j \]
    a lowers \( S^z \)

One needs to introduce more species for a more complex order.
Diagonalization of Hamiltonian

Quadratic form of bosons

\[ H_{\text{mag}} = \frac{1}{2} (b^\dagger, b) \begin{pmatrix} h & \Delta \\ \Delta^* & h^T \end{pmatrix} \begin{pmatrix} b \\ b^\dagger \end{pmatrix} \]

\[ h, \Delta: N \times N \text{ matrices} \]
\[ h^\dagger = h, \Delta^T = \Delta \]

• Ferromagnetic case

\[ \Delta = \Delta^* = 0 \]

\[ H_{\text{mag}} = b^\dagger h b + \text{const.} \]

Problem reduces to the diagonalization of \( h \).
Most easily done in \( k \)-space (Fourier tr.).

• AFM (or more general) case

\[ \begin{pmatrix} b \\ b^\dagger \end{pmatrix} = \mathcal{T} \begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} \]

Para-unitary

\[ \mathcal{T} \sigma_3 \mathcal{T}^\dagger = \mathcal{T}^\dagger \sigma_3 \mathcal{T} = \sigma_3 \]

\[ \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]

Transformation leaves the boson commutations unchanged.

\[ \mathcal{T}^\dagger \mathcal{H} \mathcal{T} = \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix} \]

\[ E = \text{diag} (\epsilon_1, \epsilon_2, \ldots, \epsilon_n) \]
\[ \pm \epsilon_k \text{ are e.v. of } \sigma_3 \mathcal{H} \]

Outline

1. Spin Hamiltonian
2. Elementary excitations

3. Hall effect and thermal Hall effect
   • Hall effect and Berry curvature
   • Anomalous and thermal Hall effects
   • General formulation

4. Main results
5. Summary
Hall effect and Berry curvature

Quantum Hall effect (2D el. Gas)

\[ j_x = \sigma_{xx} E_x + \sigma_{xy} E_y \]

\[ \sigma_{xy} = N \frac{e^2}{h} \]

TKNN formula \textit{PRL, 49} (1982)

Integer \( n \) is a topological number!

- Bloch wave function \( \psi_n(k) \)
- Berry connection \( a^{(n)}_\alpha(k) = i \langle \psi_n(k), \frac{\partial}{\partial k_\alpha} \psi_n(k) \rangle \) \( (\alpha = x, y, z) \)
- Berry curvature \( F^{(n)}_{\alpha,\beta}(k) = \partial_\alpha a^{(n)}_\beta(k) - \partial_\beta a^{(n)}_\alpha(k) \)

Chern number

\[ N = - \sum_{n \in \text{occ.}} \int_{\text{BZ}} \frac{d^2k}{(2\pi)^2} F_{xy}(k) \]

Kubo formula relates Chern # and \( \sigma_{xy} \)
Anomalous Hall effect

- QHE without net magnetic field
  - Onsager’s reciprocal relation
    \[ \sigma_{xy}(H) = -\sigma_{xy}(-H) \]  
    Time-reversal symmetry (TRS) must be broken for nonzero \( \sigma_{xy} \)
  - Haldane’s model \((PRL 61, 2015 (1988),\) Nobel prize 2016\)
    Local magnetic field can break TRS!
    n.n. real and n.n.n. complex hopping
    \( \Rightarrow \) Integer QHE without Landau levels

- Spontaneous symmetry breaking
  TRS can be broken by magnetic ordering.
  - Anomalous Hall effect \( \Rightarrow \) Review: Nagaosa et al., \textit{RMP} 82, 1539 (2010).
    \[ \rho_{xy} = R_0 H_z + R_s M_z \]
    \( M_z : \) magnetization
  \textit{Itinerant} electrons in ferromagnets.
  (i) Intrinsic and (ii) extrinsic origins.
  Anomalous velocity by Berry curvature in (i).
  \( \vec{v}_{an} \propto \vec{E} \times \vec{b}_n(\vec{k}) \)
Thermal Hall effect

- **Thermal current**
  \[ J_E = -\kappa \nabla T \]
  \[ J = C_{11}E + C_{12}(-\nabla T) \quad (C_{11} = \sigma) \]
  \[ J_E = C_{21}E + C_{22}(-\nabla T) \]

  Cs are matrix, in general.

  Onsager relation: Absence of \( J \):
  \[ C_{21} = TC_{12} \]
  \[ E = (C_{12}/C_{22})\nabla T \]

  - **Wiedemann-Franz law**
    \[ \frac{\kappa}{\sigma T} = L := \frac{\pi^2 k_B^2}{3 e^2} = 2.45 \times 10^{-8} [\text{W}\Omega/\text{K}^2] \]

  Universal for weakly interacting electrons

- **Righi-Leduc effect**

  Transverse temperature gradient is produced in response to heat current
  \[ \kappa_{xy} = LT \sigma_{xy} \]

  In itinerant electron systems from Wiedemann-Franz

What about Mott insulators? Hall effect without Lorentz force?
\[ \leftarrow \text{Berry curvature plays the role of magnetic field!} \]
General formulation

• TKNN-like formula for bosons
  - Bloch w.f. $\psi_n(k)$, Berry curvature $F_{\alpha\beta}^{(n)}(k)$
  - Earlier work
    - Fujimoto, *PRL* 103, 047203 (2009)

$$\kappa_{xy} \sim \frac{\Delta^2}{4T} \int_{BZ} \frac{d^3k}{(2\pi)^3} \rho_1(k) F_{xy}^{(1)}(k)$$

$\Delta$: energy separation

$$\rho_n(k) = \frac{1}{e^{\beta\omega_n(k)} - 1}$$

Bose distribution

Terms due to the orbital motion of magnon are missing…

• Modified linear-response theory
  - Matsumoto & Murakami, *PRL* 106, 197202; *PRB* 84, 184406 (2011)

$$\kappa_{xy} = -\frac{k_B^2 T}{\hbar} \sum_n \int_{BZ} \frac{d^2k}{(2\pi)^3} c_2(\rho_n(k)) F_{xy}^{(n)}(k)$$

$c_2(\rho) = (1 + \rho) \left( \ln \frac{1 + \rho}{\rho} \right) - (\ln \rho)^2 - 2\text{Li}_2(-\rho)$

Universally applicable to (free) bosonic systems!
Magnons, phonons, triplons, photons (?) … NOTE) No quantization.
Outline

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   • Kagome-lattice FM
   • Pyrochlore FM
   • Comparison of theory and experiment
5. Summary
Magnon Hall effect

Theory
Magnons do not have charge. They do not feel Lorentz force. Nevertheless, they exhibit **thermal Hall effect (THE)!**

Keys:
1. TRS is broken spontaneously in FM
2. DM interaction leads to Berry curvature \( \neq 0 \)

NOTE) Original theory concerned the effect of scalar chirality.

Experiment
Magnon THE was indeed observed in FM insulators!
Role of DM interaction

- **Kagome model**
  \[
  H = \sum_{i,j} \left[ -J S_i \cdot S_j + D_{ij} \cdot (S_i \times S_j) \right]
  \]
  \[
  -\tilde{J} S(e^{i\phi} b_i^\dagger b_j + e^{-i\phi} b_j^\dagger b_i) + \cdots
  \]
  \[
  \tilde{J} = \sqrt{J^2 + D^2}, \quad \tan \phi = D/J
  \]

  Scalar chirality order there \((S_i \cdot (S_j \times S_k)) \leftrightarrow \text{DM.}\)
  Nonzero Berry curvature! \(\kappa_{xy}\) is expected to be nonzero.

- **MOF material Cu(1-3, bdc)**
  FM exchange int. b/w Cu\(^{2+}\) moments

  Nonzero THE response.
  Sign change consistent with theories:
  Mook, Heng & Mertig *PRB* **89**, 134409 (2014),
Pyrochlore ferromagnet Lu$_2$V$_2$O$_7$

Y. Onose et al., Science 329, 297 ('10).

- $V^{4+}$: $(t_{2g})^1$, $S=1/2$
- Trigonal crystal field
  $$|a_{1g}\rangle = \frac{1}{\sqrt{3}}(|xy\rangle + |yz\rangle + |zx\rangle)$$
- Origin of FM: orbital pattern
  Polarized neutron diffraction
  (Ichikawa et al., JPSJ 74 (‘03))

$$T_c=70K$$
Observed thermal Hall conductivity

$\kappa_{xy}$ ≠ 0 at $T < T_C$

$\kappa_{xy}$ ≠ 0 at $H \rightarrow 0^+$  Anomalous? Related to TRS breaking?
Model Hamiltonian

- FM Heisenberg + DM
  \[ H = \sum_{\langle i,j \rangle} \left[ -JS_i \cdot S_j + D_{ij} \cdot (S_i \times S_j) \right] - H \cdot \sum_i S_i \]

  - Allowed DM vectors
    Elhajal et al., PRB 71; Kotov et al., PRB 72 (2005).

  - Stability of FM g.s. against DM

- Spin-wave Hamiltonian
  Only \( D \parallel H \) is important.

  \[ H_{\text{eff}} = \sum_{\langle i,j \rangle} \left[ -JS_i \cdot S_j + (D_{ij} \cdot \hat{\zeta})(S_i \times S_j) \right] - H \sum_i S_i^\zeta \]

  \[ -J_{ij} S(e^{-i\phi_{ij}} b_i^\dagger b_j + e^{i\phi_{ij}} b_i b_j^\dagger ) + \ldots \]

  - Hamiltonian in k-space
    \[ H_{\text{mag}}(k) = -2JS \Lambda(k, \{\phi_{ij}\}) + \text{const.} \]
    \[ \Lambda: \text{4x4 matrix. } \rightarrow \text{4 bands} \]

  \[ \omega_1(k) \sim 2JS|k|^2 + H \]
Comparison of theory and experiment

- Formula (at $H=0^+$)

\[ \kappa_{\alpha\beta} = \Phi_{\alpha\beta} \frac{4k_B^2 T}{3\pi^2 \hbar \alpha} \left( \frac{k_B T}{2JS} \right)^{5/2} \int_0^\infty c_2 [(e^t - 1)^{-1}] t^{3/2} \, dt \]

\[ \Phi_{\alpha\beta} = \frac{D}{8\sqrt{2} J} \epsilon_{\alpha\beta\gamma} n_\gamma \quad (\alpha, \beta, \gamma = x, y, z) \]

Berry curvature around $k=0$ can be obtained analytically

- Explains the observed isotropy
- $D/J$ is the only fitting parameter

- Fitting

The fit yields $|D/J| \sim 0.38$

Observed in other pyrochlore FM insulators
- $\text{Ho}_2\text{V}_2\text{O}_7$: $D/J \sim 0.07$
- $\text{In}_2\text{Mn}_2\text{O}_7$: $D/J \sim -0.02$

Reasonable!

Cf.) $D/J \sim 0.19$ in pyrochlore AFM $\text{CdCr}_2\text{O}_4$

What about other lattices

- Provskite-like lattices
  - Absence of THE in La$_2$NiMnO$_6$ and YTiO$_3$
    - Ideal cubic perovskite $\rightarrow$ No DM
    - In reality, it’s distorted $\rightarrow$ nonzero DM

What’s the reason?
Flux pattern $\rightarrow$ staggered
Berry curvature is zero because of pseudo TRS in

- Presence of THE in BiMnO$_3$
  - The origin is unclear…
  May be due to complex orbital order
Summary

Thermal Hall effect in FM insulators

- Mechanism
  Heat current is carried by magnons.
  Driven by Berry curvature due to DM int. $\mathbf{D} \cdot (\mathbf{S}_i \times \mathbf{S}_j)$

- TKNN-like formula
  $$\kappa_{xy} = -\frac{k_B T}{\hbar} \sum_n \int_{\text{BZ}} \frac{d^2 k}{(2\pi)^3} c_2(\rho_n(k)) F_{xy}^{(n)}(k)$$

- Observation in pyrochlore FMs
  Lu$_2$V$_2$O$_7$, Ho$_2$V$_2$O$_7$, In$_2$Mn$_2$O$_7$

Consistency
- Below FM transition
- Isotropy of $\kappa_{xy}$
- Reasonable $D/J$
  Agreement is excellent!

Mysteries
- Nonzero $\kappa_{xy}$ in BiMnO$_3$
- Effect of int. between magnons
Other directions

- Thermal Hall effects of bosonic particles
  - Phonon:

- Topological magnon physics
  - Dirac magnon
  - Weyl magnon
  - Topological magnon insulators