Application of kinetic theory in condensed matter physics

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Outline

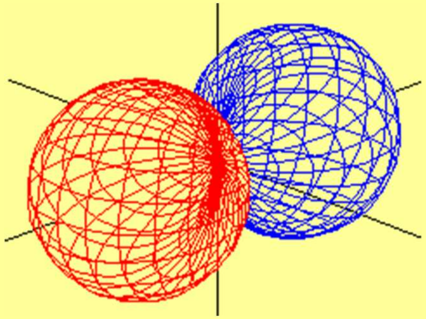
1. Magnetic quadrupole moment and magnetoelectric effect
   - Reference
     Shitade, Watanabe, and Yanase, Phys. Rev. B **98**, 020407(R) (2018).
   - Goal
     to introduce new terms (which may not be related to high energy physics)
2. Thermal Hall effect and gravity
   - References
     Shitade, Prog. Theor. Exp. Phys. **2014**, 123I01 (2014).
     Shitade, J. Phys. Soc. Jpn. **86**, 054601 (2017).
   - Goal
     to motivate high energy physicists to formulate a kinetic theory in curved spacetime

Multipole moments in classical electromagnetism

- Electric (E-)multipole moments: distribution of charge density

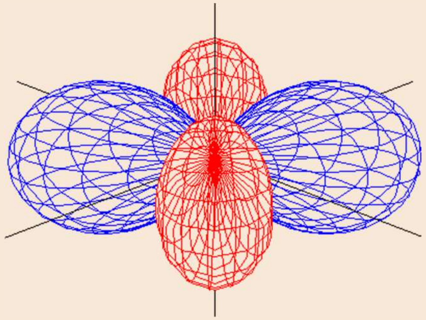
$$\rho(x) = -\partial_i[P^i - \partial_j(Q^{ij} - \cdots)]$$

E-dipole



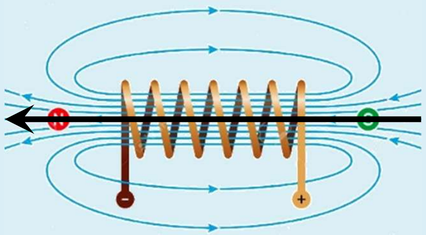
$$\boldsymbol{P} = \int \mathrm{d}V\, \boldsymbol{x}\rho(x)$$

E-quadrupole



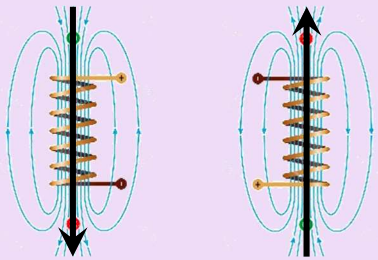
$$Q^{ij} = \frac{1}{2}\int \mathrm{d}V\, x^i x^j \rho(x)$$

M-dipole



$$\boldsymbol{M} = \frac{1}{2}\int \mathrm{d}V\, \boldsymbol{x} \times \boldsymbol{J}(x)$$

M-quadrupole



$$M^k{}_a = \frac{1}{3}\int \mathrm{d}V\, x^k [\boldsymbol{x} \times \boldsymbol{J}(x)]_a$$

- Magnetic (M-)multipole moments: distribution of current density

$$J^i(x) = \partial_t\left[P^i - \partial_j\left(Q^{ij} - \cdots\right)\right] + \epsilon^{ija}\partial_j\left[M_a - \partial_k\left(M^k{}_a - \cdots\right)\right]$$

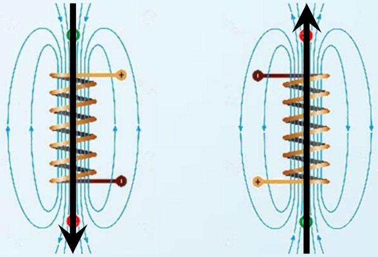
Multipole moments in crystals

- In crystals, $\boldsymbol{x}$ is ill-defined, all the multipole moments are ill-defined.
- We need to seek for alternative definitions.
- E-dipole
  - Charge current in an adiabatic deformation of the Hamiltonian; $J^i = \partial_t P^i$
    King-Smith and Vanderbilt, Phys. Rev. B **47**, 1651 (1993).
  - Expressed by the Berry connection A_n^i.
- M-dipole
  - Energy variation w.r.t. a magnetic field; $d\Omega = -SdT - Nd\mu - M_a dB^a$
    Shi *et al.*, Phys. Rev. Lett. **99**, 197202 (2007).
  - Expressed by the Berry curvature Ω_{an} and magnetic moment m_{an}.
    * magnetic moment=spin tensor
- How about M-quadrupole? Is it interesting?

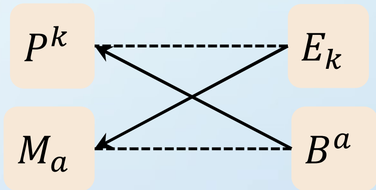
M-quadrupole and ME effect

- M-quadrupole

$$M^k{}_a = \frac{1}{3}\int \mathrm{d}V\, x^k [\boldsymbol{x} \times \boldsymbol{J}(x)]_a$$



- ME effect
  - E-dipole is induced by a M-field; $P^k = \alpha^k{}_a B^a$
  - M-dipole is induced by an E-field; $M_a = \alpha^k{}_a E_k$



- $M^k{}_a$ and $\alpha^k{}_a$ have the same symmetry requirement.
  - Both the inversion and time-reversal symmetries must be broken.
  - Group theory
- More strongly, M-quadrupole has been believed to be a microscopic origin of the ME effect.

Local thermodynamics

1. Local equilibrium

$$d\Omega = -SdT - Nd\mu - \left(M_a - \partial_k M^k{}_a\right)dB^a$$

2. Thermodynamic definitions

$$N = -\frac{\partial\Omega}{\partial\mu}, M^k{}_a = -\frac{\partial\Omega}{\partial(\partial_k B^a)}$$

3. Maxwell relation

$qN = -\partial_k P^k$ for insulators at $T = 0$

$$q\frac{\partial^2\Omega}{\partial\mu\partial(\partial_k B^a)} = -q\frac{\partial M^k{}_a}{\partial\mu} = -q\frac{\partial N}{\partial(\partial_k B^a)} = \frac{\partial\left(\partial_k P^k\right)}{\partial(\partial_k B^a)} = \alpha^k{}_a$$

- General relation between $M^k{}_a$ and $\alpha^k{}_a$
- Stronger than the group-theoretical argument

4. $\partial_k B^a$ can be implemented in a gauge-invariant kinetic theory.

$$A \star B = AB + \left(\frac{i\hbar}{2}\right)\left(\partial_{X^\lambda}A\partial_{p_\lambda}B - \partial_{p_\lambda}A\partial_{X^\lambda}B\right) + \cdots + \frac{1}{3}\left(\frac{i\hbar}{2}\right)^2 q\partial_{X^\lambda}F_{\mu\nu}\left(\partial_{p_\mu}A\partial_{p_\lambda}\partial_{p_\nu}B - \partial_{p_\lambda}\partial_{p_\mu}A\partial_{p_\nu}B\right) + \cdots$$

Comparison to M-dipole

- M-quadrupole

$$M^k{}_a = \frac{q}{\hbar}\sum_n \int \frac{d^d p}{(2\pi\hbar)^d}\left[m^k{}_{an} f(\epsilon_n) + A^k{}_{an}(-\beta^{-1})\ln\left(1 + e^{-\beta(\epsilon_n-\mu)}\right)\right]$$

- M-dipole

$$M_a = \frac{q}{\hbar}\sum_n \int \frac{d^d p}{(2\pi\hbar)^d}\left[m_{an} f(\epsilon_n) + \Omega_{an}(-\beta^{-1})\ln\left(1 + e^{-\beta(\epsilon_n-\mu)}\right)\right]$$

- Semiclassical interpretation

1. 1st term: energy variation

$$\tilde{\epsilon}_n = \epsilon_n - q m_{an} B^a/\hbar - q m^k{}_{an} q \partial_k B^a/\hbar$$

2. 2nd term: volume element correction

$$\tilde{g}_n = 1 - q\Omega_{an} B^a/\hbar - q A^k{}_{an} \partial_k B^a/\hbar$$

Xiao *et al*., Phys. Rev. Lett. **95**, 137204 (2005); Gao *et al*., Phys. Rev. Lett. **112**, 166601 (2014).

Summary of Part 1

- Some of the multipole moments can be defined in crystals by using thermodynamic definitions.
- We find a relation between M-quadrupole and ME coefficient.
  - Based only on local thermodynamics and classical electromagnetism
  - Beyond the group-theoretical argument
- To high-energy physicists
  - Gauge-invariant kinetic theory is useful for derivation of multipole moments in crystal.
  - Be careful if you consider nonuniform EM fields.

Outline

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   - Goal
     to convince high-energy physicists of variety in condensed matter physics
2. Thermal Hall effect and gravity
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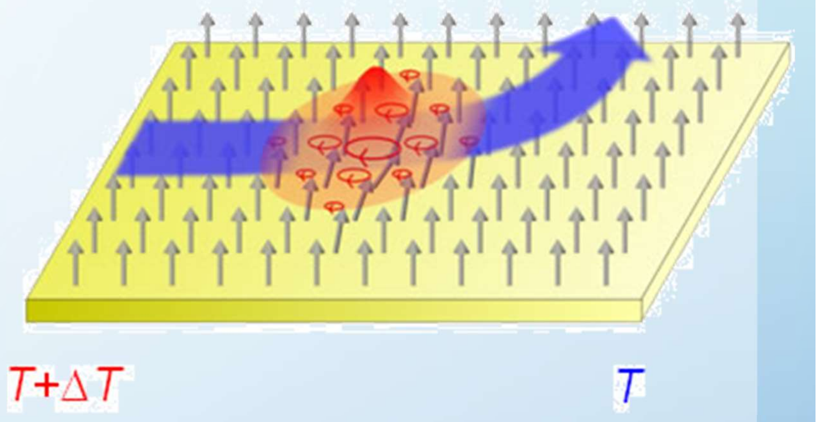
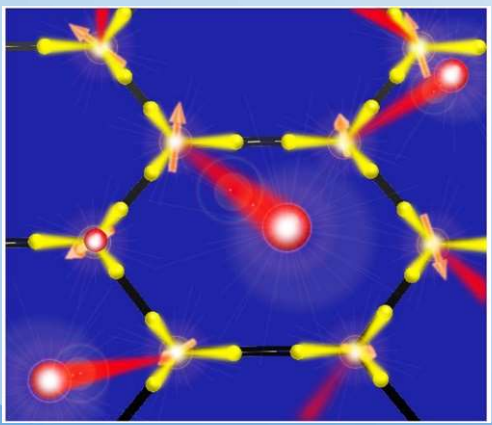
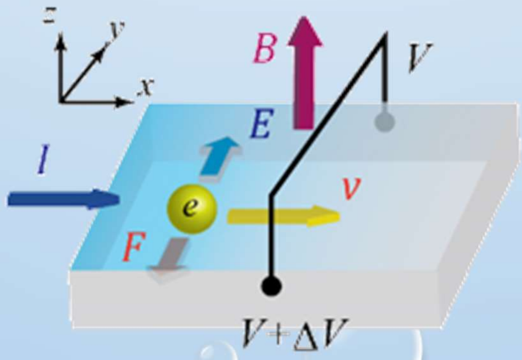
Thermal Hall effect

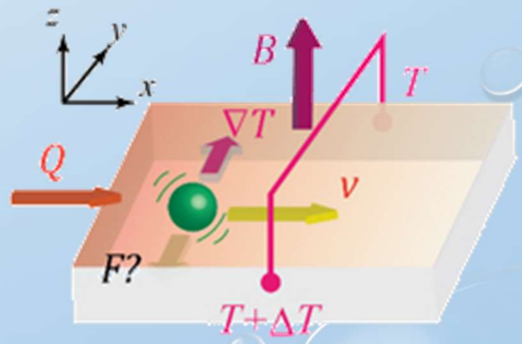
- Heat current flows perpendicular to a temperature gradient.
- Recently investigated in
  - Ferromagnetic metals: anomalous Hall effect
  - Ferromagnets: magnon Hall effect
    Onose *et al.*, Science **329**, 297 (2010).
  - Frustrated kagome antiferromagnets
    Watanabe *et al.*, Proc. Natl. Acad. Sci. **113**, 8653 (2016).
  - Kitaev honeycomb: half-quantized thanks to Majorana fermions
    Kasahara *et al.*, Nature (London) **559**, 227 (2018).



- Most of them are disordered and/or strongly correlated.







Theoretical difficulties (1)

- Assumptions in Kubo formula break down.
  - Existence of a perturbation Hamiltonian,
  - Uniform chemical potential and temperature.
- Gravitational potential Luttinger, Phys. Rev. **135**, A1505 (1964).

1. Assume local equilibrium

$$\rho = Z^{-1} \exp\left\{ - \int dV\, \beta(x) [H(x) - \mu(x) N(x)] \right\}$$

2. Introduce mechanical potentials
   - $\mu(x) = [1 + \phi_{\mathrm{g}}(x)]^{-1} [\mu_0 - q\phi(x)]$ → scalar potential
   - $\beta(x) = \beta_0 [1 + \phi_{\mathrm{g}}(x)]$ → gravitational potential
   - $H^{\phi,\phi_{\mathrm{g}}}(x) = [1 + \phi_{\mathrm{g}}(x)] H(x) + q\phi(x) N(x)$

$$\rho = Z^{-1} \exp\left\{ - \int dV\, \beta_0 [H^{\phi,\phi_{\mathrm{g}}}(x) - \mu_0 N(x)] \right\}$$

Theoretical difficulties (2)

1. Gravitational potential perturbs observables.
   Smrčka and Středa, J. Phys. C **10**, 2153 (1977).

- $\boldsymbol{J}^{\phi,\phi_{\mathrm{g}}}(x) = [1+\phi_{\mathrm{g}}(x)]\boldsymbol{J}(x)$ * comes from $\sqrt{-g}$
- $\boldsymbol{J}_{\mathrm{Q}}^{\phi,\phi_{\mathrm{g}}}(x) = [1+2\phi_{\mathrm{g}}(x)]\boldsymbol{J}_{\mathrm{Q}}(x) + \phi(x)\boldsymbol{J}(x)$ * depends on the definition

2. These perturbations give additional terms.

- $$\begin{aligned}\mathrm{tr}\left[\rho^{\phi,\phi_{\mathrm{g}}}\boldsymbol{J}^{\phi,\phi_{\mathrm{g}}}(x)\right] &= [1+\phi_{\mathrm{g}}(x)]\mathrm{tr}[\rho\boldsymbol{J}(x)] + \mathrm{tr}[\rho'\boldsymbol{J}(x)] \\ &= \boldsymbol{\nabla}\times\{[1+\phi_{\mathrm{g}}(x)]\boldsymbol{M}(x)\} + \mathrm{tr}[\rho'\boldsymbol{J}(x)] + [-\boldsymbol{\nabla}\phi_{\mathrm{g}}(x)]\times\boldsymbol{M}(x)\end{aligned}$$
- $$\begin{aligned}\mathrm{tr}\left[\rho^{\phi,\phi_{\mathrm{g}}}\boldsymbol{J}_{\mathrm{Q}}^{\phi,\phi_{\mathrm{g}}}(x)\right] &= [1+2\phi_{\mathrm{g}}(x)]\mathrm{tr}[\rho\boldsymbol{J}_{\mathrm{Q}}(x)] + \phi(x)\mathrm{tr}[\rho\boldsymbol{J}(x)] + \mathrm{tr}[\rho'\boldsymbol{J}_{\mathrm{Q}}(x)] \\ &= \boldsymbol{\nabla}\times\{[1+2\phi_{\mathrm{g}}(x)]\boldsymbol{M}_{\mathrm{Q}}(x) + \phi(x)\boldsymbol{M}(x)\} + \mathrm{tr}[\rho'\boldsymbol{J}_{\mathrm{Q}}(x)] \\ &\quad + [-\boldsymbol{\nabla}\phi(x)]\times\boldsymbol{M}(x) + 2[-\boldsymbol{\nabla}\phi_{\mathrm{g}}(x)]\times\boldsymbol{M}_{\mathrm{Q}}(x)\end{aligned}$$
- $\mathrm{tr}[\rho\boldsymbol{J}(x)] \equiv \boldsymbol{\nabla}\times\boldsymbol{M}(x)$ and $\mathrm{tr}[\rho\boldsymbol{J}_{\mathrm{Q}}(x)] \equiv \boldsymbol{\nabla}\times\boldsymbol{M}_{\mathrm{Q}}(x)$.

Multipole corrections

- Kubo formulas (denoted by tilde below) may not be sufficient when we are interested in temperature-gradient-induced phenomena.
  - Nernst effect; $J^i = \alpha^{ij}(-\partial_j T)$

$$T\alpha^{ij} = T\tilde{\alpha}^{ij} + \epsilon^{ijk} M_k$$

  - Thermal Hall effect; $J_{\mathrm{Q}}^i = \kappa^{ij}(-\partial_j T)$

$$T\kappa^{ij} = T\tilde{\kappa}^{ij} + 2\epsilon^{ijk} M_{\mathrm{Q}k}$$

  - Gravito-ME effect; $M_a = \beta^i{}_a(-\partial_i T)$

    Shitade, Daido, and Yanase, Phys. Rev. B **99**, 024404 (2019).

$$T\beta^i{}_a = T\tilde{\beta}^i{}_a + M^i{}_a$$

- In general, the Kubo formulas diverge at $T \to 0$ when their electric counterparts are nonzero.
- We need to define heat M-dipole $M_{\mathrm{Q}k}$.

Gauging translation symmetry

- Let us follow the derivation of M-dipole.

	M-dipole	Heat M-dipole
	$\boldsymbol{M}=\frac{1}{2}\int \mathrm{d}V\,\boldsymbol{x}\times\boldsymbol{J}(x)$	$\boldsymbol{M}_{\mathrm{Q}}=\frac{1}{2}\int \mathrm{d}V\,\boldsymbol{x}\times\boldsymbol{J}_{\mathrm{Q}}(x)$
Definitions	$\boldsymbol{M}=-\partial\Omega/\partial\boldsymbol{B}$	$\boldsymbol{M}_{\mathrm{Q}}/T=-\partial\Omega/\partial\left(T\boldsymbol{B}_{\mathrm{g}}\right)$
"magnetic fields"	$\boldsymbol{B}=\boldsymbol{\nabla}\times\boldsymbol{A}$	$\boldsymbol{B}_{\mathrm{g}}=\boldsymbol{\nabla}\times\boldsymbol{A}_{\mathrm{g}}$
"gauge fields"	U(1) gauge symmetry • $t'=t,\boldsymbol{x}'=\boldsymbol{x}$ • $\psi'(t',\boldsymbol{x}')=e^{iq\epsilon(t,\boldsymbol{x})/\hbar}\psi(t,\boldsymbol{x})$ • $\boldsymbol{A}'=\boldsymbol{A}+\boldsymbol{\nabla}\epsilon,\phi'=\phi-\partial_t\epsilon$	Time translation symmetry • $t'=t-\xi(t,\boldsymbol{x}),\boldsymbol{x}'=\boldsymbol{x}$ • $\psi'(t',\boldsymbol{x}')=\psi(t,\boldsymbol{x})$ • $\boldsymbol{A}_{\mathrm{g}}'=\cdots,\phi_{\mathrm{g}}'=\cdots$
Noether theorem	Charge conservation	Energy (non)conservation

- The above gravitational gauge field $(1+\phi_{\mathrm{g}},-\boldsymbol{A}_{\mathrm{g}})$ is identified as a part of vielbein $e^{\hat{0}}{}_{\mu}$, which induces torsion $T^{\hat{0}}{}_{\mu\nu}$.

Thermal Hall effect as torsional responses

- Thermal Hall conductivity consists of two terms.
  1. Kubo formula: response to a torsional E-field $T_{\hat{0}j0} = \partial_j e_{\hat{0}0} - \partial_0 e_{\hat{0}j}$
  2. Heat M-dipole: response to a torsional M-field $T_{\hat{0}ij} = \partial_i e_{\hat{0}j} - \partial_j e_{\hat{0}i}$
- Try to combine vielbein with Keldysh Green's function
  - Wigner transformation
  - And then Peierls transformation $\pi_a = e_a{}^{\mu}(p_\mu - qA_\mu)$
  - This procedure is known to be incorrect. Green's function does not satisfy the local gauge covariance (even for U(1)).
- Correct kinetic theory in curved spacetime with collision?
  - Anomalous (thermal) Hall effect
    - Disorder as well as the Berry curvature is important.
    - Effects of interactions with phonons and/or magnons are future problems.
  - Nonlinear phenomena w.r.t a temperature gradient and others

Is torsion necessary or not?

- Traditionally, in the semiclassical Boltzmann theory we deal with E-field and temperature gradient in parallel.
  - Analogy based on symmetries and gauge fields is beautiful.
  - Temperature gradient may be described by a spin connection, but it is not a field strength.
- Effective action for the quantized thermal Hall effect
  - Gravitational Chern-Simons term? Stone, Phys. Rev. B 85, 184503 (2012).

$$S = \frac{1}{96\pi} \int d^3x \, e\epsilon^{\mu\nu\lambda} \omega^a{}_{b\mu} D_\nu \omega^b{}_{c\lambda}$$

    - Order counting; $\omega \sim \partial T$
    - Not explain the Wiedemann-Franz law; $T\kappa^{xy} \to (\pi^2 k_B^2/3q^2) T^2 \sigma^{xy}$ as $T \to 0$
  - Torsional Chern-Simons term? Huang *et al.*, arXiv:1911.00174.

$$S = \frac{1}{4\pi l^2} \int d^3x \, e\epsilon^{\mu\nu\lambda} e^a{}_\mu D_\nu e_{a\lambda}$$

Summary of Part 2

- Condensed matter physics meets high energy physics in temperature-gradient-induced phenomena.
  - Multipole corrections may be necessary in some cases.
  - I believe that I did convince you of a relation between Parts 1 and 2.
- Thermal Hall effect
  - Heat analog of M-dipole is necessary.
  - Gauging time translation symmetry introduces vielbein and torsion, which defines heat M-dipole.
- Kinetic theory in curved spacetime
  - How to deal with convolution and derive Moyal product