Kinetic equation approach to the thermal Hall effect of bosons

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Collaborators







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Ye, Savary, Balents arxiv:2103.04223
Mangeolle, Balents, Savary PRB 106, 245139, PRX 12, 041031 (2022)
Mangeolle, Savary, Balents upcoming

Thermal (Hall) conductivity





Hall conductivity:

$$\frac{1}{2}\left(\begin{array}{c} \\ \end{array}\right) = \boldsymbol{\kappa}_{\mathrm{H}}$$

Hall resistivity:

$$\rho = \kappa^{-1}$$

$$\rho_{\rm H}^{\mu\nu} \approx -\frac{\kappa_{\rm H}^{\mu\nu}}{\kappa_{\rm L}^2}$$

if $\kappa_{\rm H} \ll \kappa_{\rm L}$

Thermal Hall conductivity



$$\mathbf{j} = -\boldsymbol{\kappa} \cdot \nabla T$$

$$\mathbf{j} \qquad \mathbf{\kappa} = \boldsymbol{\kappa}(T, \mathbf{B}, \cdots)$$
total energy
current

Motivation:

- Increasingly many experimental measurements, puzzling results, sample dependence
- Some theory but not very much

This work:

- Look for general theory, not fine-tuned
- Mostly study clean systems

H. Katsura, N. Nagaosa, P.A. Lee, 2010 R. Matsumoto, S. Murakami, 2011 R. Matsumoto, R. Shindou, S. Murakami, 2014 T. Qin, J. Zhou, J. Shi, 2012

- 1. We do not really want to do disorder
- 2. Need fine-tuning to break symmetries etc.



- Carriers: phonons, magnons, spinons, ??
- Origin: intrinsic (Berry), scattering (interactions, impurities)
- Theory: methods, transport v/s bulk current/energy magnetization
- Experimental issues

Kinetic equation approach for fermions

PHYSICAL REVIEW B

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ARTICLES

Wave-packet dynamics in slowly perturbed crystals: Gradient corrections and Berry-phase effects

Ganesh Sundaram and Qian Niu Department of Physics, University of Texas at Austin, Austin, Texas 78712-1081 (Received 8 June 1998)

We present a unified theory for wave-packet dynamics of electrons in crystals subject to perturbations varying slowly in space and time. We derive the wave-packet energy up to the first-order gradient correction and obtain all kinds of Berry phase terms for the semiclassical dynamics and the quantization rule. For electromagnetic perturbations, we recover the orbital magnetization energy and the anomalous velocity purely within a single-band picture without invoking interband couplings. For deformations in crystals, besides a deformation potential, we obtain a Berry-phase term in the Lagrangian due to lattice tracking, which gives rise to new terms in the expressions for the wave-packet velocity and the semiclassical force. For multiple-valued displacement fields surrounding dislocations, this term manifests as a Berry phase, which we show to be proportional to the Burgers vector around each dislocation. [S0163-1829(99)07023-X]

PHYSICAL REVIEW B 88, 045308 (2013)

Effective quantum theories for Bloch dynamics in inhomogeneous systems with nontrivial band structure

Christian Wickles^{*} and Wolfgang Belzig[†] Universität Konstanz, Fachbereich Physik, 78457 Konstanz, Germany (Received 26 September 2012; revised manuscript received 5 June 2013; published 11 July 2013)

Starting from a general *N*-band Hamiltonian with weak spatial and temporal variations, we derive a lowenergy effective theory for transport within one or several overlapping bands. To this end, we use the Wigner representation that allows us to systematically construct the unitary transformation that brings the Hamiltonian into band-diagonal form. We address the issue of gauge invariance and discuss the necessity of using kinetic variables in order to obtain a low-energy effective description that is consistent with the original theory. Essentially, our analysis is a semiclassical one and quantum corrections appear as Berry curvatures in addition to quantities that are related to the appearance of persistent currents. We develop a transport framework, which is manifestly gauge invariant, and it is based on a quantum Boltzmann formulation along with suitable definitions of current density operators such that Liouville's theorem is satisfied. Finally, we incorporate the effects of an external electromagnetic field into our theory.

Wavepacket approach

Sundaram, Niu 1999

Systematic derivation

Wickles, Belzig 2013

Kinetic equation

- Non-dissipative effects: modifications of intrinsic dynamics of individual quasiparticles, e.g. Berry phase effects, etc.
- Dissipative effects: modifications of scattering of quasiparticles



Boltzmann equation

Typically:

$$rac{\partial f}{\partial t} + rac{\mathbf{p}}{m} \cdot
abla_r f + \mathbf{F} \cdot
abla_p f = \left(rac{\partial f}{\partial t}
ight)_{ ext{coll}}$$

Wikipedia



How chargeless bosons can become chiral

"Topological magnons": sharp consequences for bosons?



Higher energy bosonic bands are only *excited* (e.g. thermally)



- More generally: Berry phase effects
- For phonons: "phonon Hall viscosity"
- Perhaps more relevant: skew scattering





bosons

How chargeless bosons can become chiral



What we do



• Systematic derivation of the kinetic equation

Mangeolle, Savary, Balents upcoming

• Microscopic origin and symmetry constraints for "Hall viscosity" term

Ye, Savary, Balents arxiv:2103.04223

minuscule contribution

$$\left(\frac{d_z \kappa_{xy}^{\Gamma\Gamma'}}{T} \sim \frac{\gamma_{\Gamma\Gamma'} d_z}{\rho v_{\rm ph}} \frac{k_B^2}{\hbar} = \Upsilon \frac{\lambda_{\Gamma} \lambda_{\Gamma'}}{J v_m / d_z} \frac{h}{\rho a_0^2 d_z v_{\rm ph}^2} \frac{k_B^2}{\hbar} \times O(1)\right)$$

 Constraints and systematic effect of phonons (or other bosons) scattering off of magnetic fluctuations (or other, fermions etc)

> Mangeolle, Balents, Savary PRB **106**, 245139, PRX **12**, 041031 (2022)

- Hall and longitudinal have different scaling forms
- Thermal Hall exists out of plane
- Large contribution
- Should look at resistivity
- New "detailed balance"

Kinetic equation

Derivation of a QKE for bosons, including all the Berry curvature effects.

The result is general enough that it can be applied to any bosonic modes directly.

Does not rely on fictitious "gravitational field."

Quantum kinetic equation for bosons

Ingredients:

- Hermitian Bose fields $\Phi_a(m{r})$

 u_i, π_i for phonons m_i, n_i for magnons

• Quadratic Hamiltonian
$$H = \frac{1}{2} \int_{\bm{r},\bm{r}'} \Phi_a(\bm{r}) H_{ab}(\bm{r},\bm{r}') \Phi_b(\bm{r}')$$
 Any hermitian form

• Commutation relations
$$[\Phi_a(\boldsymbol{r}), \Phi_b(\boldsymbol{r}')] = \hbar \Gamma_{ab}(\boldsymbol{r}, \boldsymbol{r}')$$

Build:

• Observables
$$\mathsf{F}_{ab}({m r},{m r}')=rac{1}{2}\left<\{\Phi_a({m r}),\Phi_b({m r}')\}\right>$$

Possible examples

• Example: phonons

$$\mathcal{H}_{\text{elasticity}} = \frac{1}{2\rho(\mathbf{r})} \pi_i(\mathbf{r}) \pi_i(\mathbf{r}) + \frac{c_{ij\mu\nu}(\mathbf{r})}{2} \partial_\mu u_i(\mathbf{r}) \partial_\nu u_j(\mathbf{r})$$

$$\pi_i(\mathbf{r}) = p_i(\mathbf{r}) - \eta_{ij\mu\nu}(\mathbf{r}) \partial_\mu \partial_\nu u_j(\mathbf{r}) \qquad ([\pi_i(\mathbf{r}), \pi_j(\mathbf{r}')] \propto i \eta_{ij\mu\nu})$$

("phonon Hall viscosity", e.g. Ye, Savary, Balents 2021)

• Example: magnons

$$\mathcal{H}_{\text{sigma}} = \frac{\rho(\boldsymbol{r})}{2} \partial_{\mu} n^{i} \partial_{\mu} n^{i} + \frac{1}{2\chi(\boldsymbol{r})} m^{i} m^{i} + g_{ij}(\boldsymbol{r}) n^{i} n^{j} + d_{ij}(\boldsymbol{r}) m^{i} n^{j}$$

(e.g. from DM interaction)

m, *n* are Néel and net magnetization *fluctuations*

Note the *inhomogeneous* coefficients

Magnetoelastic coupling

Example:

$$\mathbf{S}_{i} \qquad \mathbf{S}_{j}$$

$$\mathbf{J}(\mathbf{r}_{i} - \mathbf{r}_{j})$$

$$\mathbf{r}_{ij} = \mathbf{r}_{ij}^{0} + \mathbf{u}_{ij}$$

$$\mathbf{r}_{ij} \mathbf{r}_{i}\mathbf{r}_{ij}\mathbf{r}_{j}$$

Phase space formulation

Tools:

• Wigner transform

$$\mathsf{F}(\underline{k},\underline{X}) = \int dx \, e^{ikx} \mathsf{F}(X + \frac{x}{2}, X - \frac{x}{2})$$

transform of relative coordinate

$$[A \otimes B]^W = A(k, x) \star B(k, x)$$

Note: can *exactly* formulate quantum mechanics in this way

 $A \star B = e^{i\frac{\hbar}{2} \left(\nabla_k^A \nabla_x^B - \nabla_x^A \nabla_k^B \right)} AB$

Captures non-commutativity of operators

"Gradient expansion" => semiclassics

Slow variations in real space

Altshuler, Rammer Smith,...

Quantum kinetic equation

$$\partial_t \mathsf{F}(k, X) = -i\left(\mathsf{K} \star \mathsf{F} - \mathsf{F} \star \mathsf{K}^\dagger\right) \qquad \qquad \mathsf{K} = \mathsf{\Gamma} \star \mathsf{H}$$

Not hermitian!

... semiclassical expansion, diagonalization, gauge invariance, tricks ...

$$\begin{aligned} \partial_t \underline{f} + \left(\partial_{\underline{k}_{\mu}} \underline{\omega} + \Omega_{k_{\mu} X_{\nu}} \partial_{\underline{k}_{\nu}} \underline{\omega} + \Omega_{k_{\mu} k_{\nu}} \partial_{\underline{X}_{\nu}} \underline{\omega} \right) \partial_{\underline{X}_{\mu}} \underline{f} \\ + \left(\partial_{\underline{X}_{\mu}} \underline{\omega} + \Omega_{X_{\mu} X_{\nu}} \partial_{\underline{k}_{\nu}} \underline{\omega} + \Omega_{X_{\mu} k_{\nu}} \partial_{\underline{X}_{\nu}} \underline{\omega} \right) \partial_{\underline{k}_{\mu}} \underline{f} = 0 \end{aligned}$$

 $\Omega_{\alpha\beta} = \partial_{\alpha}\mathsf{A}_{\beta} - \partial_{\beta}\mathsf{A}_{\alpha}$

One can recognize all the usual Berry phase effects

Quantum kinetic equation

$$\partial_t \mathsf{F}(k, X) = -i\left(\mathsf{K} \star \mathsf{F} - \mathsf{F} \star \mathsf{K}^{\dagger}\right) \qquad \qquad \mathsf{K} = \mathsf{F} \star \mathsf{F}$$

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 $\Omega_{\alpha\beta} = \partial_{\alpha}\mathsf{A}_{\beta} - \partial_{\beta}\mathsf{A}_{\alpha}$

One can recognize all the usual Berry phase effects

Observables

• Energy density

$$H = \int_{k,X} \mathcal{H}(k,X)$$

$$\mathcal{H}(k, X) = \frac{1}{4} \mathrm{Tr} \, \left(\mathsf{H} \star \mathsf{F} + \mathsf{F} \star \mathsf{H} \right)$$

Use conservation of energy
 => continuity equation in phase space



$$\partial_t \mathcal{H} + \partial_\alpha \mathcal{J}_\alpha = 0$$

$$\mathcal{J}_{\alpha}(k, X) = \frac{1}{2} \epsilon_{\alpha\beta} \operatorname{Re} \operatorname{Tr} \left(\partial_{\beta} \mathsf{K}(\mathsf{F} \star \mathsf{H}) \right)$$

$$\left(\epsilon_{X_{\mu}k_{\nu}} = -\epsilon_{k_{\mu}X_{\nu}} = \delta_{\mu\nu}\right)$$

Phase space current

... semiclassical expansion, diagonalization, gauge invariance, tricks ...

$$\mathcal{J}_{\alpha} = \mathcal{J}_{\alpha}^{(1)} + \mathcal{J}_{\alpha}^{(2)}$$

$$\mathcal{J}_{\alpha}^{(1)} = \frac{1}{2} \epsilon_{\alpha\beta} \left(1 - \frac{1}{2} \epsilon_{\gamma\lambda} \Omega_{\gamma\lambda} \right) \left(\partial_{\beta} \underline{\omega}_{a} + \epsilon_{\sigma\rho} \Omega_{\beta\rho} \partial_{\sigma} \underline{\omega}_{a} \right) \underline{f}_{a}$$

$$\mathcal{J}_{\alpha}^{(2)} = \frac{1}{2} \epsilon_{\alpha\beta} \epsilon_{\gamma\lambda} \partial_{\gamma} \left(\mathfrak{M}_{\lambda\beta} \underline{f}_{a} \right)$$

with $\mathfrak{M}_{\alpha\beta} = rac{1}{2} \left\{ \Lambda_{\beta}, \left[\Lambda_{\alpha}, \mathsf{K}_{d} \right] \right\}^{(\mathrm{d})}$

Real space component of local current

Transport current

$$\mathcal{J}_{X_{\mu}}^{(1)} = \frac{1}{2} \left(1 + \Omega_{k_{\nu}X_{\nu}} \right) \left(\frac{\partial \underline{\omega}_{a}}{\partial k_{\mu}} + \Omega_{k_{\mu}X_{\nu}} \frac{\partial \underline{\omega}_{a}}{\partial k_{\nu}} + \Omega_{k_{\mu}k_{\nu}} \frac{\partial \underline{\omega}_{a}}{\partial X_{\nu}} \right) \underline{f}_{a}$$

Momentum integral gives the transport current

Magnetization current

$$\mathcal{J}_{X_{\mu}}^{(2)} = \frac{1}{2} \left(\frac{\partial}{\partial k_{\nu}} \left(\mathfrak{M}_{X_{\nu}k_{\mu}}^{(a)} \underline{f}_{a} \right) - \frac{\partial}{\partial X_{\nu}} \left(\mathfrak{M}_{k_{\nu}k_{\mu}}^{(a)} \underline{f}_{a} \right) \right)$$

Momentum integral gives **pure magnetization current** Can one measure it?

• Global total current through a surface: $J_{\text{tot}}^Y = \int_{X,Z} \int_{\mathbf{k}} \left(\mathcal{J}_Y^{(1)} + \mathcal{J}_Y^{(2)} \right)$

total derivatives drop

Local currents





Also recover Murakami / Shi's formula



$$\kappa_{xy}^{\rm tr} = \frac{1}{L\partial_y T} \int dy \, J_x^{\rm tr}(y)$$

$$\sigma(\epsilon, Y) = \sum_{n} \int_{\boldsymbol{k}} \Theta(\epsilon - \omega_n(\boldsymbol{k}, Y)) \Omega_n(\boldsymbol{k})$$

 $f_n = \omega_n \left(n_{\rm B}(\omega_n) + \frac{1}{2} \right)$

Next: Textures



Skyrmion lattice

Superconducting vortex lattice

Collision integral

Hall and longitudinal have different scaling forms

New "detailed balance"

General formulas can be directly applied to fluctuations of any origin

Thermal Hall exists out of plane Large contribution

Should look at resistivity

Kinetic equation

- Non-dissipative effects: modifications of intrinsic dynamics of individual quasiparticles, e.g. Berry phase effects, etc.
- Dissipative effects: modifications of scattering of quasiparticles

Convective derivative. Dynamics. \downarrow $D_t f = \Gamma[f]$ \uparrow Collision term

Boltzmann equation

Mangeolle, Balents, Savary PRX **12**, 041031 (2022) PRB **106**, 245139 (2022)

Phonons coupled to other degrees of freedom

Boltzmann's equation (simple version):

$$(\partial_t + \boldsymbol{v}_{n,\mathbf{k}} \boldsymbol{\nabla}_r) N_{n,\mathbf{k}} = \mathcal{I}_{n,\mathbf{k}} [\{N_{n',\mathbf{k}'}\}]$$

$$egin{aligned} oldsymbol{v}_{n,\mathbf{k}} &= oldsymbol{
aligned}_{oldsymbol{k}} \, \omega_{n,\mathbf{k}} \, \omega_{n,\mathbf{k}} \, \omega_{n,\mathbf{k}} \, N_{n,\mathbf{k}} \, \mathbf{j}_{\mathrm{E}} &= \sum_{n,\mathbf{k}} oldsymbol{v}_{n,\mathbf{k}} \, \omega_{n,\mathbf{k}} \, N_{n,\mathbf{k}} \, \mathbf{j}_{n,\mathbf{k}} \, \mathbf{j}_{n,\mathbf{k$$

- scattering with collective excitations
- <u>extrinsic</u> phonon Hall conductivity (but no disorder/impurities)

Formulation: $H_{\text{tot}} = H_{\text{ph}} + H_Q + H_{\text{int}}$



Recall: spin-phonon coupling:

General results

 $\kappa_{\rm H}\,$ involves mainly 4-point correlators:

Involves only <u>equilibrium</u> properties of the Q system \longrightarrow 'ready for use' formula

$$\mathsf{Model} \longrightarrow \boxed{Q_{n\mathbf{k}}} \longrightarrow [\langle [Q,Q']\{Q,Q'\}\rangle \longrightarrow [\Sigma] \longrightarrow \kappa_{\mathrm{L}}, \kappa_{\mathrm{H}}$$

Application to an AFM



Skew-scattering-induced extrinsic thermal Hall effect of phonons:

- Hall resistivity displays 'universal' scaling

(cf $\kappa_{
m H} \sim W/D^2$ whereas $\varrho_{
m H} \sim W$)

- 'isotropic' Hall conductivity: κ_{H}^{XY}

$$pprox \kappa_{\mathrm{H}}^{xz}$$

only phonon-magnon scattering (inelastic scattering, no impurities)

Quantitative estimate:

- 'large' Hall angle: $\theta_{\rm H} \simeq \kappa_{\rm L} \varrho_{\rm H} \sim 10^{-3}$

Parameter values: inspired by copper formate tetradeuterate (CFTD)

 $T_0 = 54 \,\mathrm{K}$ $\varrho_0 = 5.9 \,\mathrm{m \cdot K \cdot W^{-1}}$ $\lambda_{\mathrm{soc}} \sim 5\% \,\lambda_{\mathrm{iso}}$ $\mathrm{m}_0^{\perp} \sim 5\% \,J_{\mathrm{iso}}$ Ronnow *et al.*, PRL 87, 037202

Phonons and out-of-plane Hall effect

Cuprates – Grissonnanche *et al.,* Nature 571, 376–380 & Nat. Phys. 16, 1108-1111



Thank you