

Quantum kinetic equation for thermal
transport of bosons
Or
Seeing the stars

Leon Balents
KITP

Dynamical response and transport in quantum magnets, KITP, 8/28/23

Collaborators



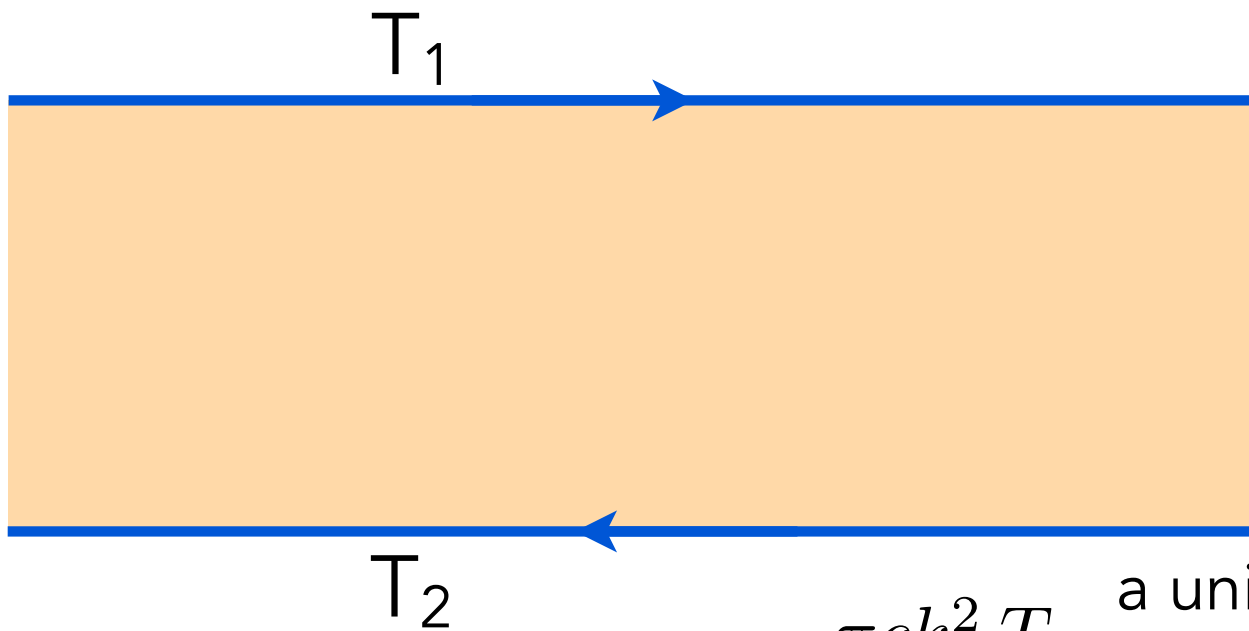
Lucile Savary
ENS Lyon



Léo Mangeolle
ENS Lyon

Thermal Hall effect

- Motivation: a probe of exotic phases.



$$I_x = \kappa_H \Delta T_y$$

Kitaev

$$\kappa_H = \frac{\pi c k_B^2 T}{6\hbar}$$

a universal prediction for chiral
"Ising anyon" phase: *agnostic to
microscopic spin interactions*

Thermal transport

Today

- 09:00AM - Leon Balents (KITP) - *On transport and dynamical response in quantum magnets*
- 09:45AM - Hidenori Takagi (MPI-FKF) - *Thermal transport in quantum magnets*

10:30AM MORNING BREAK

10:30AM - 11:00AM: MORNING BREAK

Gurley Courtyard

11:00AM

Fred Kavli Auditorium (Main)

- 11:00AM - Satoru Nakatsuji (U. Tokyo) - *Anomalous transport and its electrical manipulation in chiral Antiferromagnetic*
- 11:45AM - Léo Mangeolle (ENS Lyon) - *Phonon Thermal Hall Conductivity from Scattering with Collective Fluctuations*

Fred Kavli Auditorium (Main)

- 04:00PM - Elena Hassinger (MPI-CPFS) - *Large magnetic heat transport and plateaux phases in spin-chain compound YbAlO₃*

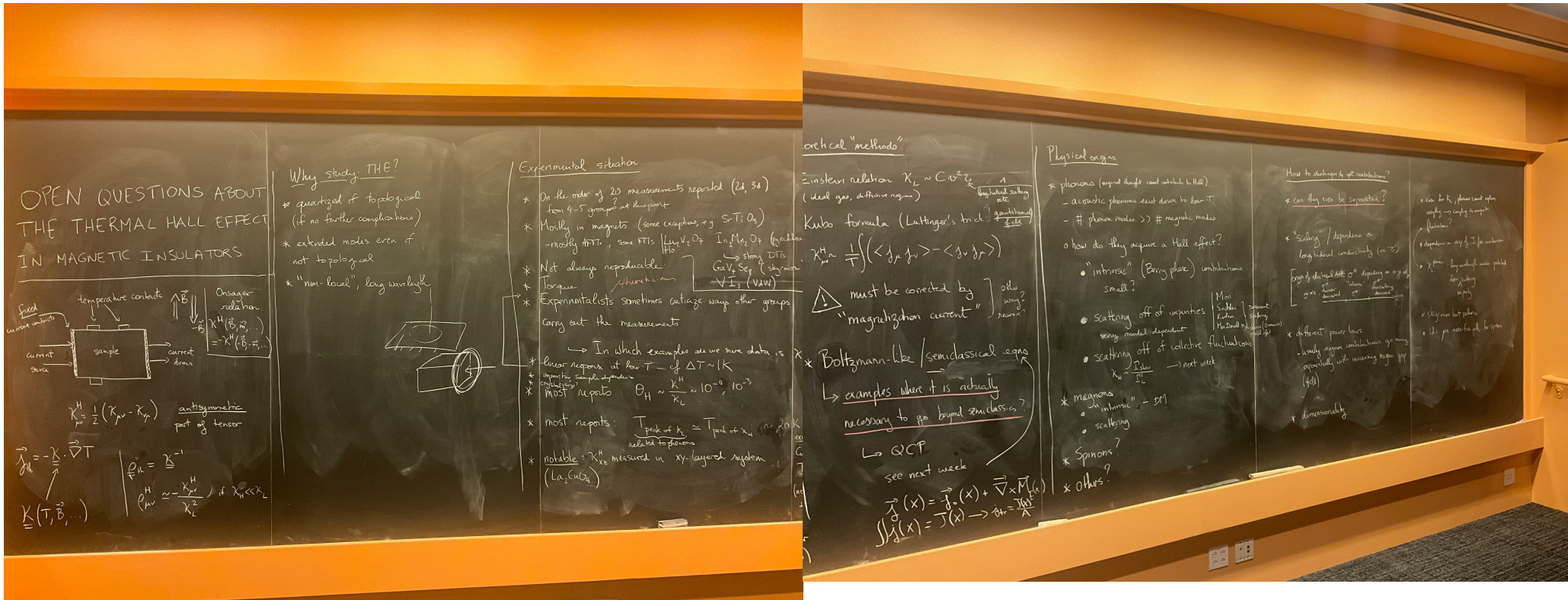
Tuesday

- 02:45PM - Max Hirschberger (RIKEN) - *Detecting spin chirality by the thermal Hall effect*

Wednesday

- 11:45AM - Gábor Halász (Oak Ridge NL) - *Thermal anyon interferometry in phonon-coupled Kitaev spin liquids*

Program discussion



Many issues:

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

Electrical Anomalous Hall effect

Naoto Nagaosa

*Department of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan
and Cross-Correlated Materials Research Group (CMRG), and Correlated Electron
Research Group (CERG), ASI, RIKEN, Wako, 351-0198 Saitama, Japan*

Jairo Sinova

*Department of Physics, Texas A&M University, College Station, Texas 77843-4242, USA
and Institute of Physics ASCR, Cukrovarnická 10, 162 53 Praha 6, Czech Republic*

Shigeki Onoda

Condensed Matter Theory Laboratory, ASI, RIKEN, Wako, 351-0198 Saitama, Japan

A. H. MacDonald

Department of Physics, University of Texas at Austin, Austin, Texas 78712-1081, USA

N. P. Ong

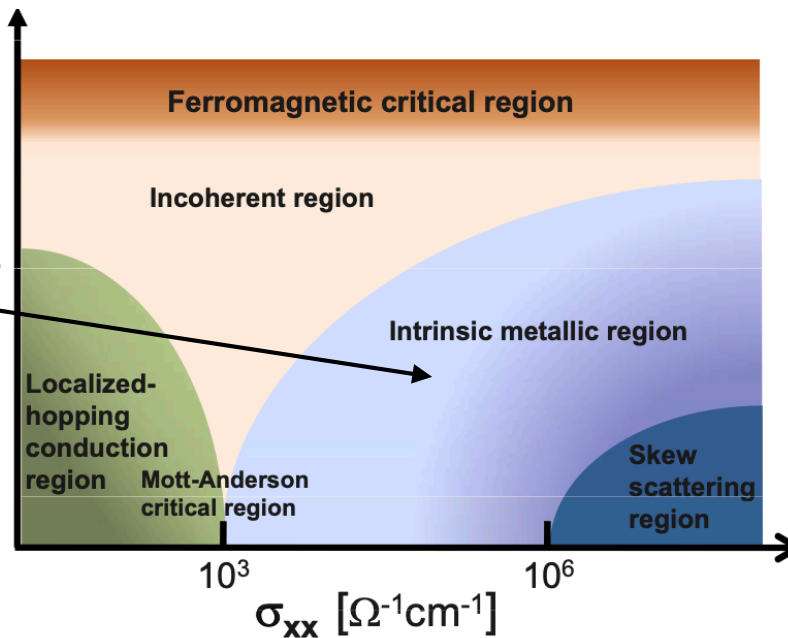
Department of Physics, Princeton University, Princeton, New Jersey 08544, USA

(Published 13 May 2010)

Simple, elegant



But a complete description needs
to incorporate all the effects



Two types of effects

Boltzmann 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.

The diagram shows the Boltzmann equation $D_t f = \Gamma[f]$ centered on the page. A blue arrow points down from the text 'Convective derivative. Dynamics.' to the left-hand side of the equation, $D_t f$. A blue arrow points from the left towards the equation. An orange arrow points up from the text 'Collision term' to the right-hand side of the equation, $\Gamma[f]$. An orange arrow points from the left towards the text 'Collision term'.

$$D_t f = \Gamma[f]$$

Collision term

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$$D_t f = \Gamma[f]$$

Collision term

L. Mangeolle, LB, L. Savary, PRX/PRB 2022

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$$D_t f = \Gamma[f]$$



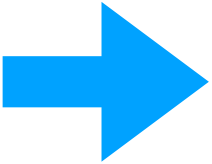
Collision term

Intrinsic Anomalous Hall Effect

- A simple derivation:

- Current
$$\mathbf{j}_e = -e \sum_n \int d^d \mathbf{k} D_n(\mathbf{k}) \mathbf{v}_n(\mathbf{k}) f_n(\mathbf{k})$$

- Velocity
$$\mathbf{v}_n(\mathbf{k}) = \nabla \omega_n(\mathbf{k}) + e\mathbf{E} \times \boldsymbol{\Omega}_n(\mathbf{k})$$


$$\mathbf{j}_e^{ah} = e^2 \sum_n \int \frac{d^d \mathbf{k}}{(2\pi)^d} n_F(\omega_n(\mathbf{k})) \boldsymbol{\Omega}_n(\mathbf{k}) \times \mathbf{E}$$

Karplus+Luttinger, 1954!

Intrinsic thermal Hall effect

- Theory: Magnons

H. Katsura, N. Nagaosa, P.A. Lee, 2010

R. Matsumoto, S. Murakami, 2011

R. Matsumoto, R. Shindou, S. Murakami, 2014

$$\kappa_{xy} = -\frac{k_B^2 T}{\hbar V} \sum_k \sum_{n=1}^N \left\{ c_2[g(\epsilon_{nk})] - \frac{\pi^2}{3} \right\} \Omega_{nk}.$$

s

$$c_2(x) \equiv \int_0^x dt \left(\ln \frac{1+t}{t} \right)^2 = (1+x) \left(\ln \frac{1+x}{x} \right)^2 - (\ln x)^2 - 2\text{Li}_2(-x),$$

- Theory: Phonons

T. Qin, J. Zhou, J. Shi, 2012

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

where

$$\sigma_{xy}(\epsilon) = -\frac{1}{V\hbar} \sum_{\hbar\omega_{ki} \leq \epsilon} \Omega_{ki}^z$$

and

$$Z_{\text{ph}} = \frac{2\pi}{V} \sum_{k;i=1}^{3r} \Omega_{ki}^z.$$

Actually they are identical

Intrinsic THE

- A simple derivation?

PRL **104**, 066403 (2010)

PHYSICAL REVIEW LETTERS

week ending
12 FEBRUARY 2010

Theory of the Thermal Hall Effect in Quantum Magnets

Hosho Katsura,¹ Naoto Nagaosa,^{1,2} and Patrick A. Lee³

PHYSICAL REVIEW B **84**, 184406 (2011)



Rotational motion of magnons and the thermal Hall effect

Ryo Matsumoto and Shuichi Murakami*

Department of Physics, Tokyo Institute of Technology, Tokyo 152-8551, Japan

(Received 10 June 2011; published 7 November 2011)

PHYSICAL REVIEW B **86**, 104305 (2012)

Berry curvature and the phonon Hall effect

Tao Qin,¹ Jianhui Zhou,¹ and Junren Shi²

¹Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

²International Center for Quantum Materials, Peking University, Beijing 100871, China

(Received 6 December 2011; published 13 September 2012)

 actually incorrect

Mistake fixed

Semi-classical model *assuming magnon chemical potential*

Kubo/Luttinger formula

Kubo/Luttinger formula

No kinetic equation formulation

Kinetic equation

What I want to describe is a *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.

But first I have to tell you a story about my sabbatical

Paris, May 2022









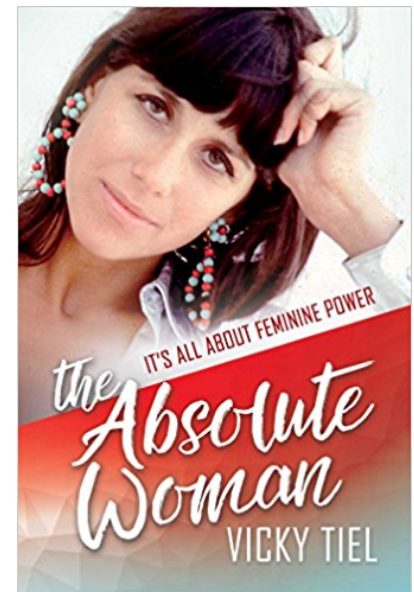
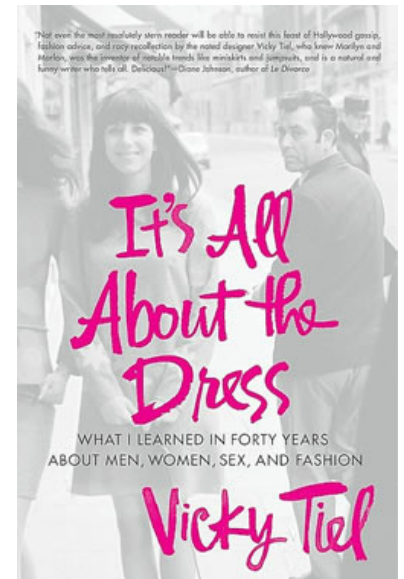
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VICKY TIEL

Vicky Tiel Is An American Born French Couturier Designing Since 1964, When She Went To Paris With Her Partner, Mia Fonnagrives. They Created A Storm With Their Miniskirts, Hot Pants And Jumpsuits. Vicky Did The Costumes For 15 Films And In 1975 She Sold Couture To Henri Bendel's And 45 Leading Shops In 2011 She Joined HSN TV, Wrote Her First Book "Its All About The Dress" And Has Written A Second Book "The Absolute Woman It's All About Feminine Power" Which She Recently Launched On HSN.



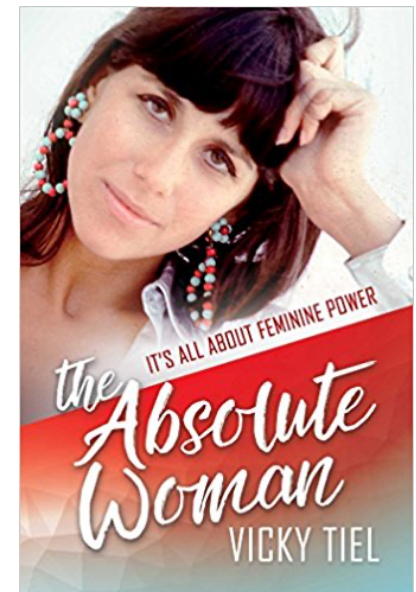
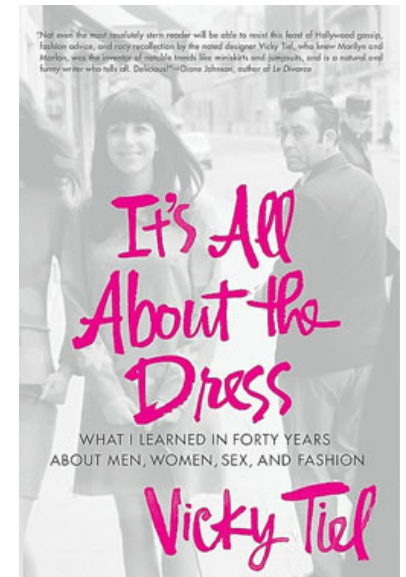
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"Elle est très **star**"



Turns out that being très star is key to getting the QKE to work properly

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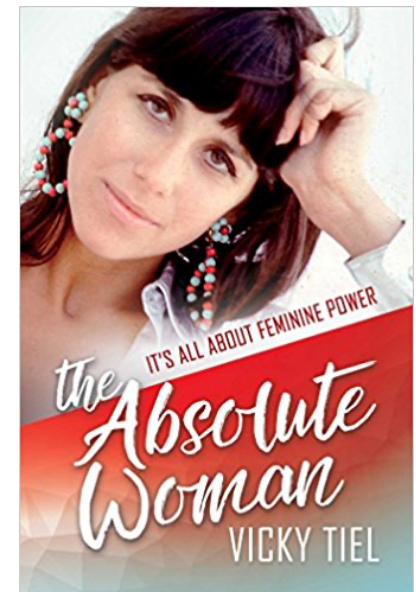
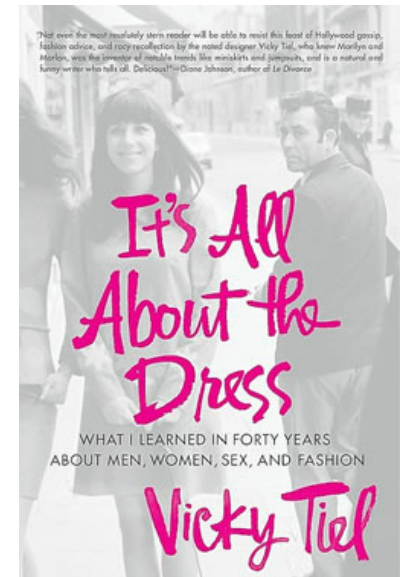


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"Elle est très **star**"



c.f. fermions: Wickles+Belzig, 2013

QKE for bosons

- Basic ingredients

- Hermitian bose fields

$$[\Phi_a(x)]^\dagger = \Phi_a(x)$$

- A quadratic Hamiltonian

$$H = \int_{x_1, x_2} \frac{1}{2} h_{ab}(x_1, x_2) \Phi_a(x_1) \Phi_b(x_2)$$

- Commutation relations

$$[\Phi_a(x), \Phi_b(x')] = \Gamma_{ab}(x, x')$$

- Requirements

- Hermiticity, symmetry

$$h_{ab}(x, x') = h_{ba}(x', x)$$

$$h_{ba}(x', x) = [h_{ab}(x, x')]^*$$

$$\Gamma_{ba}(x', x) = [\Gamma_{ab}(x, x')]^*$$

$$\Gamma_{ab}(x, x') = -\Gamma_{ba}(x', x)$$

QKE for bosons (2)

- Observable

$$F_{ab}(x_1, x_2) = \frac{1}{2} \langle \{ \Phi_a(x_1), \Phi_b(x_2) \} \rangle \quad \text{"Density matrix"}$$

- Matrix notation

$$[A \otimes B]_{ab}(x_1, x_2) = \int_{x'} A_{ac}(x_1, x') B_{cb}(x', x_2)$$

- Equation of motion

$$\partial_t \Phi = -i [\Phi, H] = -i \Gamma \otimes h \otimes \Phi \equiv -i \mathcal{K} \otimes \Phi$$

QKE for bosons (3)

- Density matrix $\partial_t F = -i (K \otimes F - F \otimes K^\dagger)$
- Wigner transform $F(k, X) = \int dx e^{ikx} F(X + \frac{x}{2}, X - \frac{x}{2})$

This is the basis of a semi-classical correspondence.

- We need to Wigner transform the first equation
 - What is the Wigner transform of a convolution?

Moyal/star product

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

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



Joseph Moyal

- Expansion of exponential corresponds to semi-classical expansion
 - Note: it is justified when A/B are slowly-varying in x.
- Other nice properties:

$$(A \star B) \star C = A \star (B \star C) \qquad (A \star B)^\dagger = B^\dagger \star A^\dagger$$

QKE for bosons

- Exact QKE:
$$\partial_t F(k, X) = -i (K \star F - F \star K^\dagger)$$
$$K = \Gamma \star h$$
- What do we do with it??
 - Diagonalize it: remove the matrix structure
 - Carry out semi-classical expansion
 - Then express physical quantities in terms of the distribution

Diagonalization

- Tricky point: K is not hermitian
- BUT can show that it is diagonalizable:

$$S^{-1} \star K \star S = K_d = \text{diag}(\omega_a) \qquad S^\dagger \star h \star S = 1$$

$$S^{-1} \star F \star h \star S = F_d = \text{diag}(f_a)$$



"Stargenvalues"

Diagonalization

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$$S^{-1} \star K \star S = K_d = \text{diag}(\omega_a) \qquad S^\dagger \star h \star S = 1$$

$$S^{-1} \star F \star h \star S = F_d = \text{diag}(f_a)$$

Conceptually, the first two equations are to be solved order by order in \hbar , and then this determines F which is physical, in terms of f_a .

Diagonalization

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$$S^{-1} \star K \star S = K_d = \text{diag}(\omega_a) \qquad S^\dagger \star h \star S = 1$$

$$S^{-1} \star F \star h \star S = F_d = \text{diag}(f_a)$$



$$\partial_t f_a = -i(\omega_a \star f_a - f_a \star \omega_a) \approx \nabla_x \omega_a \nabla_k f_a - \nabla_k \omega_a \nabla_x f_a$$

Gauge invariance

- Phase freedom of similarity transformation S

$$S \rightarrow S \star \Lambda$$

$$\Lambda = \text{diag} \left(e^{i\theta_a(k,x)} \right)$$

- This keeps K and F diagonal as matrices
- BUT it does transform $\omega_a(k, x)$ and $f_a(k, x)$ as functions

$$\omega_a \rightarrow \omega_a - \epsilon_{\alpha\beta} \partial_\beta \theta_a \partial_\alpha \omega_a$$

$$f_a \rightarrow f_a - \epsilon_{\alpha\beta} \partial_\beta \theta_a \partial_\alpha f_a$$

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

Berry gauge fields

- Define $M_\alpha = S^{-1} \star \partial_\alpha S$

$$A_\alpha = \text{Im } M_\alpha^{(d)} = \text{diag}(A_{a,\alpha})$$

- To leading semi-classical order,

$$A_\alpha \rightarrow A_\alpha + \partial_\alpha \theta$$

- This allows one to define gauge-invariant quantities

$$\underline{\omega}_a(q_\alpha) = \omega_a(q_\alpha + \epsilon_{\alpha\beta} A_{a,\beta})$$

“Kinetic coordinates” $\underline{q}_\alpha = q_\alpha + \epsilon_{\alpha\beta} A_{a,\beta}$

Final QKE

$$\partial_t f = \epsilon_{\alpha\beta} \partial_{\underline{\alpha}} \omega \partial_{\underline{\beta}} f = \left(\epsilon_{\alpha\beta} \partial_{\underline{\alpha}} \omega + \frac{1}{2} (\epsilon_{\alpha\beta} \epsilon_{\gamma\sigma} + \epsilon_{\gamma\alpha} \epsilon_{\beta\sigma}) \bar{\Omega}_{\alpha\sigma}^{(d)} \partial_{\underline{\gamma}} \omega \right) \partial_{\underline{\beta}} f.$$

Unravelling it...

$$\begin{aligned} \partial_t \underline{f} + \left(\partial_{\underline{k}_\mu} \omega + \bar{\Omega}_{\underline{k}_\mu \underline{X}_\nu}^{(d)} \partial_{\underline{k}_\nu} \omega - \bar{\Omega}_{\underline{k}_\mu \underline{k}_\nu}^{(d)} \partial_{\underline{X}_\nu} \omega \right) \partial_{\underline{X}_\mu} \underline{f} \\ + \left(-\partial_{\underline{X}_\mu} \omega - \bar{\Omega}_{\underline{X}_\mu \underline{X}_\nu}^{(d)} \partial_{\underline{k}_\nu} \omega + \bar{\Omega}_{\underline{X}_\mu \underline{k}_\nu}^{(d)} \partial_{\underline{X}_\nu} \omega \right) \partial_{\underline{k}_\mu} \underline{f} = 0 \end{aligned}$$

One can recognize all the usual Berry phase effects

Current

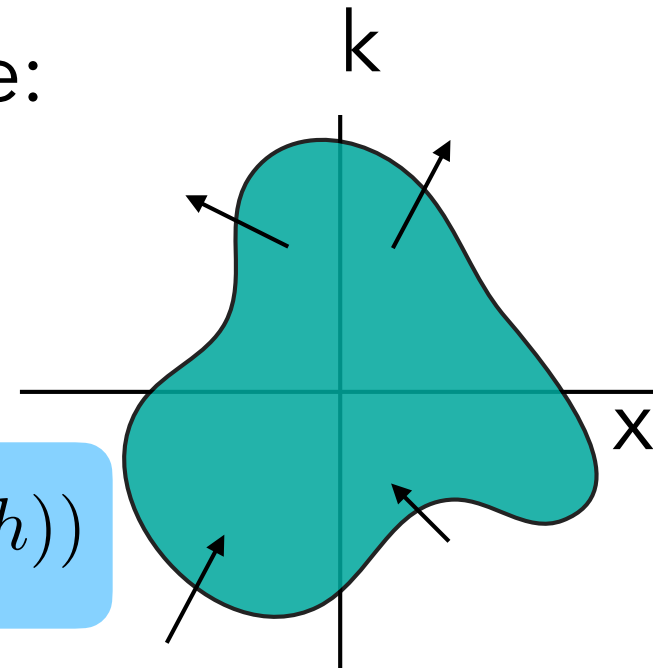
Use conservation of energy

$$H = \int_{k,x} \mathcal{H}(k, x)$$
$$\mathcal{H}(k, x) = \frac{1}{4} \text{Tr} (h \star F + F \star h)$$

Continuity equation in phase space:

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

$$j_\alpha(k, x) = \frac{1}{2} \epsilon_{\alpha\beta} \text{Re} \text{Tr} (\partial_\beta K(F \star h))$$



Current (2)

$$j_\alpha(k, x) = \frac{1}{2} \epsilon_{\alpha\beta} \text{Re Tr} (\partial_\beta K(F \star h))$$

- Use $S^{-1} \star K \star S = K_d = \text{diag}(\omega_a)$
 $S^{-1} \star F \star h \star S = F_d = \text{diag}(f_a)$

In reverse

- Lot's of algebra and tricks, to leading order in \hbar

$$j_\alpha = j_\alpha^{(1)} + j_\alpha^{(2)}$$

$$j_\alpha^{(1)} = \frac{1}{2} \epsilon_{\alpha\beta} \left(1 - \frac{1}{2} \epsilon_{\gamma\lambda} \bar{\Omega}_{\gamma\lambda} \right) \left(\partial_\beta \underline{\omega}_a + \epsilon_{\sigma\rho} \bar{\Omega}_{\beta\rho} \partial_\sigma \underline{\omega}_a \right) \underline{f}_a$$

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

Current (3)

- Unravel it

$$j_{x_\mu}^{(1)} = \frac{1}{2} (1 + \bar{\Omega}_{k_\nu x_\nu}) \left(\frac{\partial \omega_a}{\partial k_\mu} + \bar{\Omega}_{k_\mu x_\nu} \frac{\partial \omega_a}{\partial k_\nu} - \bar{\Omega}_{k_\mu k_\nu} \frac{\partial \omega_a}{\partial x_\nu} \right) \underline{f}_a$$

- Momentum integral gives the transport current

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

- Momentum integral gives pure magnetization current

(i.e. until we figure out how to measure it, you can forget this one!)

Summary

Diagonalization

$$S^{-1} \star K \star S = K_d = \text{diag}(\omega_a)$$

$$S^\dagger \star h \star S = 1$$

- Must calculate S and ω_a order by order in \hbar

Kinetic equation

$$\begin{aligned} \partial_t \underline{f} + \left(\partial_{\underline{k}_\mu} \underline{\omega} + \bar{\Omega}_{\underline{k}_\mu \underline{x}_\nu}^{(d)} \partial_{\underline{k}_\nu} \underline{\omega} - \bar{\Omega}_{\underline{k}_\mu \underline{k}_\nu}^{(d)} \partial_{\underline{x}_\nu} \underline{\omega} \right) \partial_{\underline{x}_\mu} \underline{f} \\ + \left(-\partial_{\underline{x}_\mu} \underline{\omega} - \bar{\Omega}_{\underline{x}_\mu \underline{x}_\nu}^{(d)} \partial_{\underline{k}_\nu} \underline{\omega} + \bar{\Omega}_{\underline{x}_\mu \underline{k}_\nu}^{(d)} \partial_{\underline{x}_\nu} \underline{\omega} \right) \partial_{\underline{k}_\mu} \underline{f} = \partial_t \underline{f} |_{\text{coll}} \end{aligned}$$

- Solve for local distribution

Obtain current, other observables

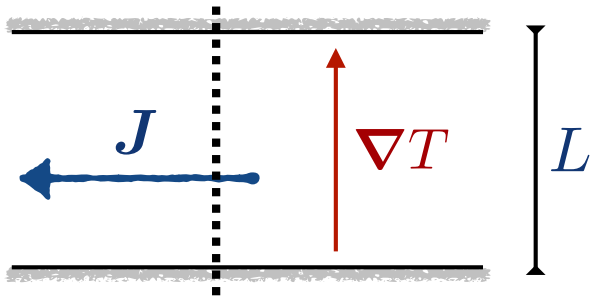
$$j_{x_\mu}^{(\text{tr})} = \frac{1}{2} (1 + \bar{\Omega}_{\underline{k}_\nu \underline{x}_\nu}) \left(\frac{\partial \omega_a}{\partial k_\mu} + \bar{\Omega}_{\underline{k}_\mu \underline{x}_\nu} \frac{\partial \omega_a}{\partial k_\nu} - \bar{\Omega}_{\underline{k}_\mu \underline{k}_\nu} \frac{\partial \omega_a}{\partial x_\nu} \right) \underline{f}_a$$

Applications

- Separate transport current automatically
- Calculate local current *density*
- Calculate local *temperature*
- Formalism ready to combine interactions, scattering and Berry curvature

Check

- Can we recover κ_{xy}^{tr} ?



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

$$j_{x_\mu}^{(\text{tr})} = \frac{1}{2} \left(1 + \bar{\Omega}_{k_\nu x_\nu} \right) \left(\frac{\partial \omega_a}{\partial k_\mu} + \bar{\Omega}_{k_\mu x_\nu} \frac{\partial \omega_a}{\partial k_\nu} - \bar{\Omega}_{k_\mu k_\nu} \frac{\partial \omega_a}{\partial x_\nu} \right) \underline{f}_a$$

$$\kappa_{xy}^{\text{tr}} = -\frac{1}{L\partial_y T} \sum_{n=1}^N \int_{\mathbf{k}} \int dy \bar{\Omega}_n(\mathbf{k}) \frac{\partial \omega_n}{\partial y} f_n(\omega_n; T(y))$$

Check

$$\kappa_{xy}^{\text{tr}} = \frac{1}{L\partial_y T} \sum_{n=1}^N \int_{\mathbf{k}} \int dy \Omega_n(\mathbf{k}) \frac{\partial \omega_n}{\partial y} f_n(\omega_n; T(y))$$

• Define $\sigma(\epsilon, y) = \sum_n \int_{\mathbf{k}} \Theta(\epsilon - \omega_n(\mathbf{k}, y)) \Omega_n(\mathbf{k})$ $f_n = \omega_n (n(\omega_n) + \frac{1}{2})$

$$\kappa_{xy}^{\text{tr}} = \frac{1}{L\partial_y T} \int d\epsilon \int dy \partial_y \sigma(\epsilon, y) \epsilon (n(\epsilon; T(y)) + \frac{1}{2})$$

$$= -\frac{1}{L\partial_y T} \int d\epsilon \int dy \sigma(\epsilon, y) \epsilon \partial_y n(\epsilon; T(y))$$

$$= -\frac{1}{L\partial_y T} \int d\epsilon \int dy \sigma(\epsilon, y) \epsilon \left(-\frac{\epsilon}{T} \partial_y T \right) n'(\epsilon; T(y))$$

$$\xrightarrow{L \rightarrow \infty} \frac{1}{T} \int d\epsilon \sigma(\epsilon) \epsilon^2 n'(\epsilon) \quad \text{Agrees with results for magnons and phonons.}$$



Summary



Diagonalization

$$S^{-1} \star K \star S = K_d = \text{diag}(\omega_a)$$

$$S^\dagger \star h \star S = 1$$

- Must calculate S and ω_a order by order in \hbar



Applications



- Separate transport current automatically
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Kinetic equation

$$\partial_t \underline{f} + \left(\partial_{\underline{k}_\mu} \underline{\omega} + \bar{\Omega}_{\underline{k}_\mu \underline{x}_\nu}^{(d)} \partial_{\underline{k}_\nu} \underline{\omega} - \bar{\Omega}_{\underline{k}_\mu \underline{k}_\nu}^{(d)} \partial_{\underline{x}_\nu} \underline{\omega} \right) \partial_{\underline{x}_\mu} \underline{f} + \left(-\partial_{\underline{x}_\mu} \underline{\omega} - \bar{\Omega}_{\underline{x}_\mu \underline{x}_\nu}^{(d)} \partial_{\underline{k}_\nu} \underline{\omega} + \bar{\Omega}_{\underline{x}_\mu \underline{k}_\nu}^{(d)} \partial_{\underline{x}_\nu} \underline{\omega} \right) \partial_{\underline{k}_\mu} \underline{f} = \partial_t \underline{f} |_{\text{coll}}$$

- Solve for local distribution



Obtain current, other observables

$$j_{x_\mu}^{(\text{tr})} = \frac{1}{2} (1 + \bar{\Omega}_{\underline{k}_\nu \underline{x}_\nu}) \left(\frac{\partial \omega_a}{\partial k_\mu} + \bar{\Omega}_{\underline{k}_\mu \underline{x}_\nu} \frac{\partial \omega_a}{\partial k_\nu} - \bar{\Omega}_{\underline{k}_\mu \underline{k}_\nu} \frac{\partial \omega_a}{\partial x_\nu} \right) \underline{f}_a$$



c.f. Léo's talk