Quantum kinetics, non-linear response, and band geometry

Leon Balents, KITP

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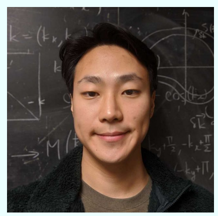

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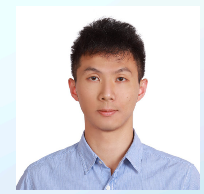

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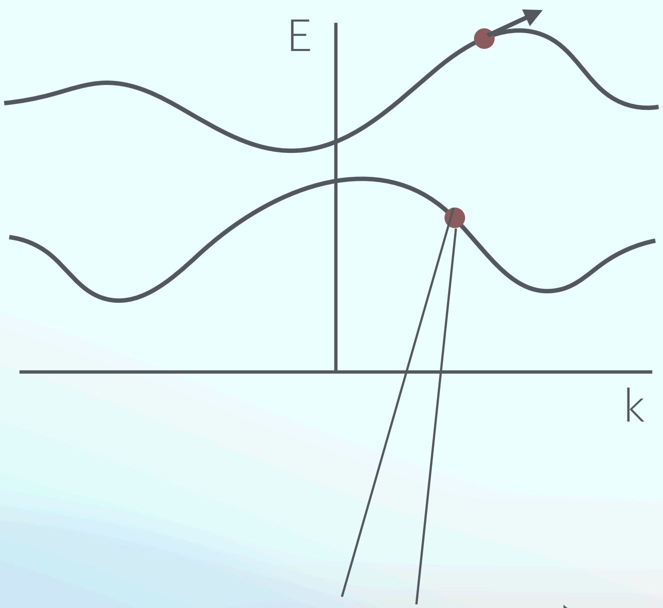
Outline

- Linear and non-linear response as a probe of band geometry and topology
- Semiclassical description: why I like it and you should too
- How to *correctly* use semiclassics beyond leading order

Bands



$|\psi_{nk}\rangle$ → Geometry

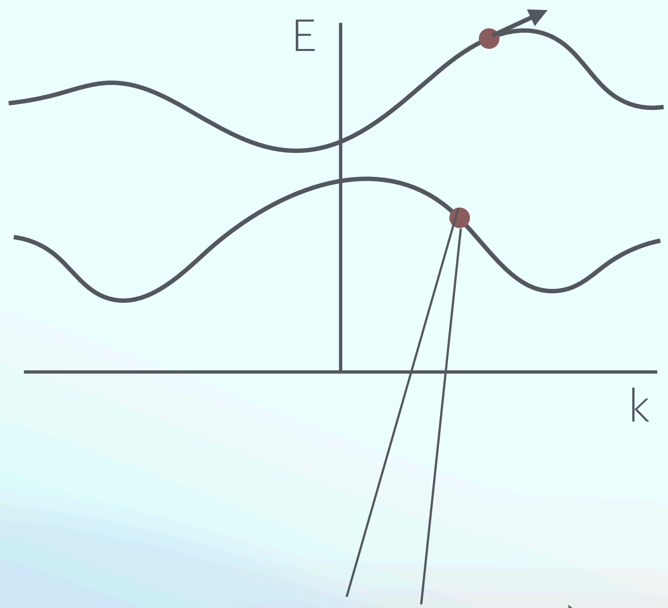
$\epsilon_n(k)$ → $\mathbf{v}_n(k)$

Energetics

$\Omega_{n,\alpha\beta}(k)$ Berry curvature

$g_{n,\alpha\beta}(k)$ Quantum metric

Bands



$|\psi_{nk}\rangle$ → Geometry

$\epsilon_n(k)$ → $\mathbf{v}_n(k)$ $\sigma_{xx} \sim \langle v_n^x v_n^x \rangle$

Energetics

$\Omega_{n,\alpha\beta}(k)$ Berry curvature $\sigma_{xy} \sim \langle \Omega \rangle$

$g_{n,\alpha\beta}(k)$ Quantum metric

Souza, Wilkens, Martin 2000
Various suggestions

Role in interacting systems?

Linear response

A host of "conventional" (but still complex) transport coefficients

$$\mathbf{j} = \mathbf{L}^{11}\mathcal{E} + \mathbf{L}^{12}(-\nabla T),$$
$$\mathbf{j}^q = \mathbf{L}^{21}\mathcal{E} + \mathbf{L}^{22}(-\nabla T),$$

Ashcroft+Mermin

And some originating from Berry curvature

Anomalous Hall effect

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

Karplus+Luttinger, 1954!

Gyromagnetic effect

$$\alpha_{ij}^{\mathrm{GME}} = \frac{i\omega\tau e}{1 - i\omega\tau} \sum_n \int [d\boldsymbol{k}](\partial f/\partial \varepsilon_{\boldsymbol{k}n}) v_{\boldsymbol{k}n,i} m_{\boldsymbol{k}n,j}$$

Ma+Pesin 2015; Song *et al* 2016

Chiral anomaly…

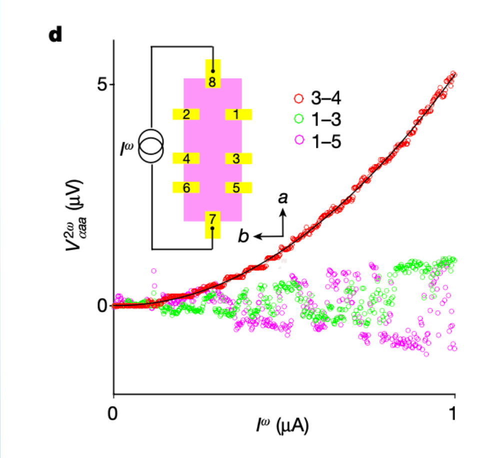
Non-linear response

Non-linear Hall effect

$$j_a^0 = \chi_{\text{abc}} \mathcal{E}_b \mathcal{E}_c^*, \; j_a^{2\omega} = \chi_{\text{abc}} \mathcal{E}_b \mathcal{E}_c,$$

$$\chi_{\text{abc}} = -\varepsilon_{adc} \frac{e^3 \tau}{2(1 + i\omega\tau)} \int_k f_0 (\partial_b \Omega_d)$$

Sodemann+Fu, 2015



Q. Ma *et al*, 2019 (WTe2)

Non-linear response

Quantum metric effects

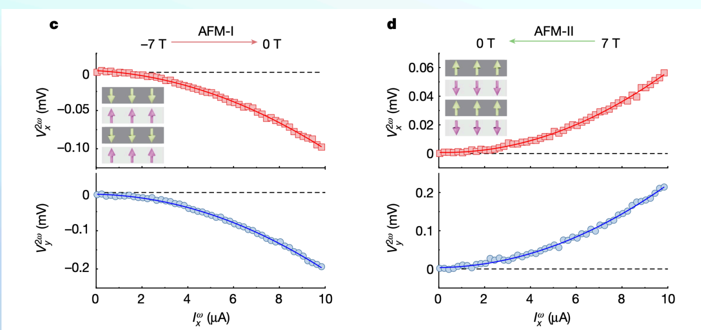
$$\sigma^{\mathrm{BCPD}}_{a;bc} = \frac{e^3}{\hbar} \sum_{m,p,\boldsymbol{k}} \int [d\boldsymbol{k}] f_m \left[\partial_a \tilde{\mathcal{G}}^{bc}_{mp} + \partial_b \tilde{\mathcal{G}}^{ac}_{mp} + \partial_c \tilde{\mathcal{G}}^{ab}_{mp}\right].$$

"Band-resolved quantum metric dipole"

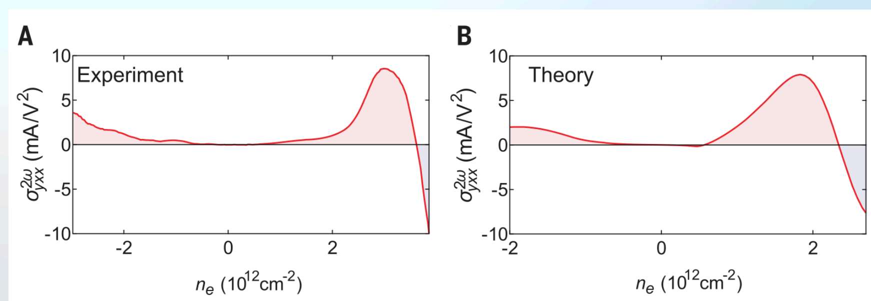
K. Das *et al*,2023

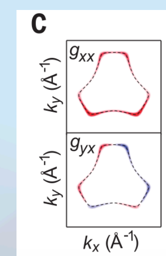
D. Kaplan *et al*, 2024

$MnBi_2Te_4$



N. Wang *et al*, 2023





A. Gao *et al*, 2023

Response to field gradient

$$j^{\mu}_{\text{geom.}}(\mathbf{r}) = -\frac{Q^2}{2\hbar}\int \frac{d^D\mathbf{K}}{(2\pi)^D}\, f_0(\mathbf{K})E^{(0)}_{\nu\lambda}\frac{\partial g^{\nu\lambda}(\mathbf{K})}{\partial K_\mu},$$

Quantum metric dipole

M. Lapa + T. Hughes, 2019

$E_{\mu\nu} = \partial E_\mu / \partial x_\nu$

Theoretical approaches

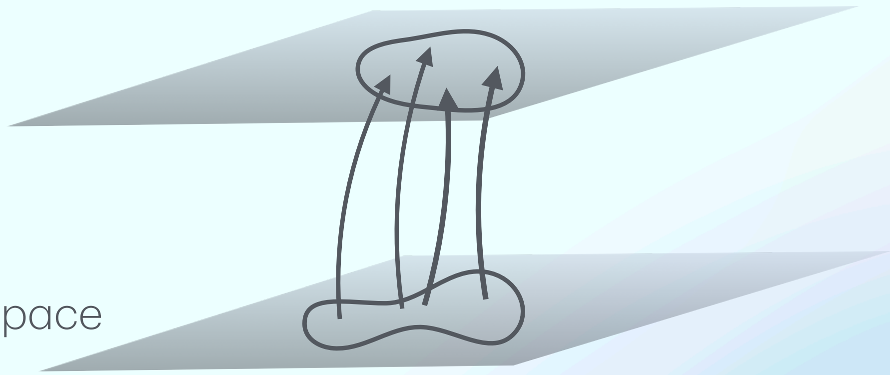
- Quantum response theory (~Kubo)
  - Usually regarded as most rigorous method
  - Formal. Simple results often obtained by very technical route.
  - Does not show dis-equilibrium
- Semi-classics
  - Intuitive
  - Directly reveals deviations from equilibrium
  - Approximate?

Semiclassics

- Boltzmann equation

$$\partial_t f_n + \frac{dx_\mu}{dt}\frac{\partial f_n}{\partial x_\mu} + \frac{dk_\mu}{dt}\frac{\partial f_n}{\partial k_\mu} = \mathcal{C}[f]$$

Incompressible flow of states in phase space



- One particle equations of motion

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{v}_n = \boldsymbol{\nabla}_{\boldsymbol{k}}\tilde{\epsilon}_{n\boldsymbol{k}} - \frac{d\boldsymbol{k}}{dt} \times \boldsymbol{\Omega}_{n\boldsymbol{k}},$$
$$\frac{d\boldsymbol{k}}{dt} = \boldsymbol{F}_n = -e\boldsymbol{E} - e\frac{d\boldsymbol{x}}{dt} \times \boldsymbol{B}.$$

Q. Niu ++

The power of semiclassics

- Anomalous Hall effect

$$\boldsymbol{j}_{ah} = \int_k f_n e \boldsymbol{v}_{ah} = -e \int_k f_n \frac{d\boldsymbol{k}}{dt} \times \boldsymbol{\Omega}_n = e^2 \boldsymbol{E} \times \int_k f_n \boldsymbol{\Omega}_n$$

Immediately gives AHE

- Thermal conductivity

$$f_n = n_F(\epsilon; T(x)) + g_n$$

$$g_n = \tau n_F' \boldsymbol{v}_n \cdot \frac{(\epsilon - \mu)\boldsymbol{\nabla} T}{T^2}$$

n.b. essential to include T(x).

$$j^q_\mu = \int_k (\epsilon_n - \mu) v^\mu_n g_n = -\frac{\partial_\nu T}{T^2} \tau \int_k n_F' (\epsilon - \mu)^2 v^\mu_n v^\nu_n$$

"Standard" thermal conductivity

The power of semiclassics

- Anomalous Hall effect

$$\boldsymbol{j}_{ah} = \int_k f_n e \boldsymbol{v}_{ah} = -e \int_k f_n \frac{d\boldsymbol{k}}{dt} \times \boldsymbol{\Omega}_n = e^2 \boldsymbol{E} \times \int_k f_n \boldsymbol{\Omega}_n$$

Immediately gives AHE

- Thermal conductivity

These and many other results agree with Kubo exactly. This is because the semiclassical approximation is exact to first order in spatial gradients.

$$f_n = n_F(\epsilon; T(x))$$

$$g_n = \tau n_F' \boldsymbol{v}_n \cdot \frac{(\epsilon - \mu)\boldsymbol{\nabla} T}{T^2}$$

n.b. essential to include T(x).

$$j^q_\mu = \int_k (\epsilon_n - \mu) v^\mu_n g_n = -\frac{\partial_\nu T}{T^2} \tau \int_k n_F' (\epsilon - \mu)^2 v^\mu_n v^\nu_n$$

“Standard” thermal conductivity

Semiclassics

- Boltzmann equation

$$\partial_t f_n + \frac{dx_\mu}{dt}\frac{\partial f_n}{\partial x_\mu} + \frac{dk_\mu}{dt}\frac{\partial f_n}{\partial k_\mu} = \mathcal{C}[f]$$

Incompressible flow of states in phase space

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$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{v}_n = \boldsymbol{\nabla}_{\boldsymbol{k}}\tilde{\epsilon}_{n\boldsymbol{k}} - \frac{d\boldsymbol{k}}{dt}\times\boldsymbol{\Omega}_{n\boldsymbol{k}},$$
$$\frac{d\boldsymbol{k}}{dt} = \boldsymbol{F}_n = -e\boldsymbol{E} - e\frac{d\boldsymbol{x}}{dt}\times\boldsymbol{B}.$$

Q. Niu ++

Just written down! $i\hbar\partial_t\rho = \left[H,\rho\right]$

Wavepacket approximation $i\hbar\partial_t\mathbf{x} = [H,\mathbf{x}]$

Semiclassics

- Boltzmann equation

$$\partial_t f_n + \frac{dx_\mu}{dt}\frac{\partial f_n}{\partial x_\mu} + \frac{dk_\mu}{dt}\frac{\partial f_n}{\partial k_\mu} = \mathcal{C}[f]$$

Incompressible flow of states in phase space

Just written down! $i\hbar\partial_t\rho = [H,\rho]$

Two semiclassical approximations at the same time

- One particle equations of motion

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{v}_n = \boldsymbol{\nabla}_{\boldsymbol{k}}\tilde{\epsilon}_{n\boldsymbol{k}} - \frac{d\boldsymbol{k}}{dt}\times\boldsymbol{\Omega}_{n\boldsymbol{k}},$$
$$\frac{d\boldsymbol{k}}{dt} = \boldsymbol{F}_n = -e\boldsymbol{E} - e\frac{d\boldsymbol{x}}{dt}\times\boldsymbol{B}.$$

Wavepacket approximation $i\hbar\partial_t\mathbf{x} = [H,\mathbf{x}]$

Q. Niu ++

Kinetics

Liouville-von Neumann equation $$i\hbar\partial_t\rho = \left[H, \rho\right]$$

Systematic derivation of Boltzmann-like equations

Intuitively $$f_n(k) \sim \langle n, k \,|\, \rho \,|\, n, k \rangle$$

Two issues:

- Track spatial dependence
- Off-diagonal terms in density matrix (inter-band coherence)

Wigner transformation

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

$$\left\langle X + \frac{x}{2} \middle| \rho \middle| X - \frac{x}{2} \right\rangle$$

Wigner-Weyl quantization

$$C = AB \quad \Longleftrightarrow \quad C(k, X) = A(k, X) \star B(k, X)$$

Operators

Functions on phase space

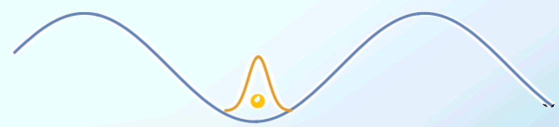
Moyal/star product

$$\star = \exp\left(\frac{i\hbar}{2}\left(\overleftarrow{\nabla}_x \cdot \vec{\nabla}_p - \overleftarrow{\nabla}_p \cdot \vec{\nabla}_x\right)\right) = \exp\left(\frac{i\hbar}{2}\epsilon^{\alpha\beta}\overleftarrow{\partial}_\alpha \vec{\partial}_\beta\right)$$

Symplectic form $\quad [q_\alpha, q_\beta] = i\hbar\epsilon^{\alpha\beta}$

Semi-classical expansion

$$\star = \exp\left(\frac{i\hbar}{2}\epsilon^{\alpha\beta}\overleftarrow{\partial}_\alpha \vec{\partial}_\beta\right) = 1 + \frac{i\hbar}{2}\epsilon^{\alpha\beta}\overleftarrow{\partial}_\alpha \vec{\partial}_\beta + \cdots$$



Slow spatial variation

Systematic procedure to carry out gradient expansion while working in both position and momentum.

Star diagonalization

Even with phase space formalism, **H, F**, etc are still matrices

To pass to a semi-classical kinetic equation, we want to eliminate off-diagonal terms.

Diagonalization is compatible with star product

$$\mathsf{H} = U \star \tilde{h} \star U^\dagger \qquad \mathsf{F} = U \star \tilde{f} \star U^\dagger$$

Formal diagonalization carried out order by order in gradient expansion.

Almost the desired diagonal Hamiltonian and distribution

BUT we need to ensure gauge invariance.

Gauge invariance

Quantum mechanics allows an arbitrary phase for each eigenfunction. Within a band this is the usual origin of Berry gauge field.

$$U \to U \star E^{i\theta(x,k)}$$

$$\tilde{f} \to E^{-i\theta} \star \tilde{f} \star E^{i\theta}$$

Transforms non-trivially because of star product

Gauge invariant form

$$f_n = \mathrm{tr}\left[U \star p_n \tilde{f} \star U^\dagger\right]$$

Projector on n^{th} band

Energy density

$$\rho_n^E = \frac{1}{2}\,\mathrm{tr}[U \star p_n(\tilde{h} \star \tilde{f} + \tilde{f} \star \tilde{h}) \star U^\dagger]$$

Gauge invariance

We worked these out to second order in gradients:

$$f_n = \tilde{f}_n + \hbar \varepsilon_{\alpha\beta} \partial_\alpha (\tilde{f}_n A_{n\beta}) + \frac{\hbar^2}{2} \varepsilon_{\alpha\beta} \varepsilon_{\sigma\lambda} \partial^2_{\alpha\sigma} (\tilde{f}_n (\Lambda_\beta \Lambda_\lambda)_{nn})$$

$$h_n \equiv \tilde{h}_n + \hbar \varepsilon_{\alpha\beta} \partial_\alpha \tilde{h}_n \left(A_{n\beta} + \hbar \varepsilon_{\sigma\lambda} A_{n\lambda} \partial_\sigma A_{n\beta} \right) - \hbar^2 \varepsilon_{\alpha\beta} \varepsilon_{\sigma\lambda} \partial^2_{\alpha\sigma} \tilde{h}_n \left(\frac{1}{4} \left\{ \Lambda_\beta, \Lambda_\lambda \right\}_{nn} - A_{n\beta} A_{n\lambda} \right)$$

$$\Lambda_\alpha = -iU^\dagger \star \partial_\alpha U$$

$$A_\alpha = \mathrm{diag}\left(\Lambda_\alpha\right)$$ Berry gauge field

Now simply

$$\mathcal{N} = \int_{x,p} \sum_n f_n$$ f_n is electron density in a band

$$E = \int_{x,p} \sum_n f_n h_n$$ $f_n h_n$ is energy density in a band

Kinetic equation

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

Just continuity equation for density in a band

c.f. simple convection $\mathcal{J}_\alpha = f_n v_\alpha$ $\xrightarrow[\text{Incompressible flow}]{}$ Boltzmann equation

Here, to second order:

$$\begin{aligned}\mathcal{J}_\alpha =& \varepsilon_{\alpha\beta} \operatorname{tr}\left[f \left(\partial_\beta h + \hbar \left(\varepsilon_{\sigma\lambda} \partial_\sigma h \Omega_{\lambda\beta} - \Omega_{t\beta} \right) \left(1 - \frac{\hbar}{2} \Omega_{\mu\nu} \right) + \frac{\hbar^2}{2} \varepsilon_{\sigma\lambda} \varepsilon_{\mu\nu} \partial^2_{\sigma\mu} h \partial_\beta g_{\nu\lambda} \right) \right] \\ &+ \hbar^2 \varepsilon_{\alpha\beta} \varepsilon_{\sigma\lambda} \partial_\sigma \operatorname{tr}\left[f \left(\frac{1}{2} \varepsilon_{\mu\nu} \partial_\mu h \partial_\nu g_{\beta\lambda} - \frac{1}{2} \partial_t g_{\beta\lambda} + \varepsilon_{\mu\nu} \partial^2_{\mu\beta} h g_{\nu\lambda} \right) \right] - \frac{\hbar^2}{24} \varepsilon_{\alpha\beta} \varepsilon_{\sigma\lambda} \varepsilon_{\mu\nu} \partial^2_{\sigma\mu} \operatorname{tr}\left[f \partial^3_{\beta\lambda\nu} h \right]\end{aligned}$$

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quantum metric $g_{\alpha\beta} = \frac{1}{2}\operatorname{diag}\left(\Lambda_\alpha\Lambda_\beta + \Lambda_\beta\Lambda_\alpha\right) - A_\alpha A_\beta \; = \frac{1}{2}\operatorname{tr}(\partial_\alpha P_n \partial_\beta P_n)$

Kinetic equation

$$\mathcal{J}_\alpha = \varepsilon_{\alpha\beta}\,\mathrm{tr}\left[f\left(\partial_\beta h + \hbar\left(\varepsilon_{\sigma\lambda}\partial_\sigma h\Omega_{\lambda\beta} - \Omega_{t\beta}\right)\left(1 - \frac{\hbar}{2}\Omega_{\mu\nu}\right) + \frac{\hbar^2}{2}\varepsilon_{\sigma\lambda}\varepsilon_{\mu\nu}\partial^2_{\sigma\mu}h\partial_\beta g_{\nu\lambda}\right)\right]$$
$$+ \hbar^2\varepsilon_{\alpha\beta}\varepsilon_{\sigma\lambda}\partial_\sigma\,\mathrm{tr}\left[f\left(\frac{1}{2}\varepsilon_{\mu\nu}\partial_\mu h\partial_\nu g_{\beta\lambda} - \frac{1}{2}\partial_t g_{\beta\lambda} + \varepsilon_{\mu\nu}\partial^2_{\mu\beta}hg_{\nu\lambda}\right)\right] - \frac{\hbar^2}{24}\varepsilon_{\alpha\beta}\varepsilon_{\sigma\lambda}\varepsilon_{\mu\nu}\partial^2_{\sigma\mu}\,\mathrm{tr}\left[f\partial^3_{\beta\lambda\nu}h\right]$$

- General and exact up to second order in semiclassical expansion
- Explicitly contains real space and momentum space, and capable of describing inhomogeneous systems. Magnetic field can be included by modifying $\epsilon_{\alpha\beta}$
- Quantum geometry of bands appears explicitly, takes local band Hamiltonian as input
- Only band-intrinsic quantities appear: but these are bands renormalized by quantum corrections.
- Ready to attack all sorts of problems!

Example: separable problem

$$\mathsf{H}(x,p) = \mathsf{H}_0(p) - eV(x)\mathsf{I}_N$$

Band form   Diagonal potential

Kinetic equation   (relaxation time approx)

$$\partial_t f = -\partial_{x_\alpha} f\Big(v_\alpha + \frac{e}{\hbar}\Omega_{\alpha\beta}\partial_{x_\beta}V + \big[-\frac{e}{2}\partial_{p_\alpha}\mathsf{g}_{\mu\nu} + ev_\mu \mathsf{T}_{\alpha\nu}\big]\partial^2_{x_\mu x_\nu}V + e^2\big[\partial_{p_\mu}\mathsf{T}_{\alpha\nu} - \frac{1}{2}\partial_{p_\alpha}\mathsf{T}_{\mu\nu}\big]\partial_{x_\mu}V\partial_{x_\nu}V\Big)$$
$$- \partial_{p_\alpha} f e \partial_{x_\alpha} V + \frac{\hbar^2}{24}\partial^3_{x_\alpha x_\beta x_\gamma} f \partial^3_{p_\alpha p_\beta p_\gamma}\varepsilon - \tau^{-1}(f - f_{\mathrm{eq}})$$

$$T_{n;\mu\nu} = -\sum_{m\neq n}\frac{\langle\partial_{p_\mu}u_n|u_m\rangle\langle u_m|\partial_{p_\mu}u_n\rangle + (\mu\leftrightarrow\nu)}{\epsilon_n - \epsilon_m}$$

"band-normalized quantum metric"

(*not* a purely geometric quantity)

Solution

Linear conductivity

$$\sigma_{\mu;\alpha}(q,\omega) = -\frac{e^2}{\hbar^2(i\omega+\tau^{-1})}\sum_n\int_k f_n' \mathsf{v}_{n\mu}\mathsf{v}_{n\alpha} + \frac{e^2}{\hbar}\sum_n\int_k f_n\Omega_{\mu\alpha} + \frac{e^2 i q_\gamma}{\hbar^3(i\omega+\tau^{-1})^2}\int_k f_n' \mathsf{v}_{n\mu}\mathsf{v}_{n\alpha}\mathsf{v}_{n\gamma}$$

$$-\frac{e^2 i q_\gamma}{4\hbar}\int_k f_n\left[\underline{\partial_{k_{(\mu}}\mathsf{g}_{n,\gamma\alpha)}} + \mathsf{v}_{n,\{\mu}\mathsf{T}_{n,\gamma\alpha\}}\right] + O(q^2)$$

Lapa+Hughes

Quadratic conductivity

$$\sigma_{\mu;\alpha\beta}(q,\omega;q',\omega') = \frac{e^3}{\hbar^3(i\omega+\tau^{-1})(i\omega'+\tau^{-1})}\sum_n\int_k f_n' \mathsf{v}_\mu\mathsf{v}_\alpha\mathsf{v}_\beta - \frac{e^3}{\hbar^2(i\omega'+\tau^{-1})}\sum_n\underline{\int_k f_n\partial_{k_\alpha}\Omega^{(0)}_{\mu\beta}}$$

Sodemann+Fu

$$+\frac{e^3}{2\hbar}\sum_n\int_k f_n\,\underline{\left(\partial_{k_\mu}\mathsf{T}_{\alpha\beta} - \partial_{k_\alpha}\mathsf{T}_{\mu\beta} - \partial_{k_\beta}\mathsf{T}_{\mu\alpha}\right)} + \mathcal{O}(q).$$

Band-normalized quantum metric dipole

Summary

$$\mathcal{J}_\alpha = \varepsilon_{\alpha\beta}\,\mathrm{tr}\left[f\left(\partial_\beta h + \hbar\left(\varepsilon_{\sigma\lambda}\partial_\sigma h\Omega_{\lambda\beta} - \Omega_{t\beta}\right)\left(1 - \frac{\hbar}{2}\Omega_{\mu\nu}\right) + \frac{\hbar^2}{2}\varepsilon_{\sigma\lambda}\varepsilon_{\mu\nu}\partial^2_{\sigma\mu}h\partial_\beta g_{\nu\lambda}\right)\right]$$
$$+\hbar^2\varepsilon_{\alpha\beta}\varepsilon_{\sigma\lambda}\partial_\sigma\,\mathrm{tr}\left[f\left(\frac{1}{2}\varepsilon_{\mu\nu}\partial_\mu h\partial_\nu g_{\beta\lambda} - \frac{1}{2}\partial_t g_{\beta\lambda} + \varepsilon_{\mu\nu}\partial^2_{\mu\beta}hg_{\nu\lambda}\right)\right] - \frac{\hbar^2}{24}\varepsilon_{\alpha\beta}\varepsilon_{\sigma\lambda}\varepsilon_{\mu\nu}\partial^2_{\sigma\mu}\,\mathrm{tr}\left[f\partial^3_{\beta\lambda\nu}h\right]$$

- We found a procedure to obtain semiclassical electron dynamics organized by spatial gradients
- We found a general result for the phase space current to *second* order in gradients, capable of handling inhomogeneous systems and magnetic fields
- Prior results for linear and non-linear response are recovered, and in some cases corrected
- Still needed: a scattering/interactions theory with the same validity

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