Hall conductivity as topological invariant in phase space

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Ariel University, Isreal

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Outlook

Publications

This talk is a report of work in progress, being based on:

C.X. Zhang, M.A. Zubkov,
Hall conductivity as the topological invariant in phase space in the presence of interactions and non-uniform magnetic field,
arXiv:1908.04138 [cond-mat.mes-hall]

I.V.Fialkovsky, M.A.Zubkov,
Elastic deformations and Wigner-Weyl formalism in graphene,
arXiv:1905.11097 [cond-mat.mes-hall]

C.X.Zhang, M.A.Zubkov,
Influence of interactions on the anomalous quantum Hall effect,
arXiv:1902.06545 [cond-mat.mes-hall]

M.A.Zubkov, Xi Wu
Topological invariant in terms of the Green functions for the Quantum Hall Effect in the presence of varying magnetic field,
arXiv:1901.06661 [cond-mat.mes-hall]

M.Suleymanov, M.A.Zubkov,
Wigner - Weyl formalism and the propagator of Wilson fermions in the presence of varying external electromagnetic field,
Nucl. Phys. B 938 (2019), 171-199. arXiv:1811.08233 [hep-lat]

TKNN, 1982

First realization of the topological nature of Hall conductivity is usually attributed to Thouless et al. Phys. Rev. Lett. 49 (1982) 405

Quantized Hall Conductance in a Two-Dimensional Periodic Potential

D. J. Thouless, M. Kohmoto,[a] M. P. Nightingale, and M. den Nijs
Department of Physics, University of Washington, Seattle, Washington 98195
(Received 30 April 1982)

The Hall conductance of a two-dimensional electron gas has been studied in a uniform magnetic field and a periodic substrate potential U. The Kubo formula is written in a form that makes apparent the quantization when the Fermi energy lies in a gap. Explicit expressions have been obtained for the Hall conductance for both large and small $U/\hbar\omega_c$.

PACS numbers: 72.15.Gd, 72.20.Mg, 73.90.+b

Because of the relation between the velocity operator and the derivatives of $\hat{H}$, the Kubo formula can be written as

$$\sigma_H = \frac{ie^2}{A_0\hbar} \sum_{\epsilon_\alpha < E_F} \sum_{\epsilon_\beta > E_F} \frac{(\partial \hat{H}/\partial k_1)_{\alpha\beta}(\partial \hat{H}/\partial k_2)_{\beta\alpha} - (\partial \hat{H}/\partial k_2)_{\alpha\beta}(\partial \hat{H}/\partial k_1)_{\beta\alpha}}{(\epsilon_\alpha - \epsilon_\beta)^2}, \qquad (4)$$

where A_0 is the area of the system and $\epsilon_\alpha, \epsilon_\beta$ are eigenvalues of the Hamiltonian. This can be related to the partial derivatives of the wave functions u, and gives

$$\sigma_H = \frac{ie^2}{2\pi h} \sum \int d^2k \int d^2r \left(\frac{\partial u^*}{\partial k_1}\frac{\partial u}{\partial k_2} - \frac{\partial u^*}{\partial k_2}\frac{\partial u}{\partial k_1} \right)$$
$$= \frac{ie^2}{4\pi h} \sum \oint dk_j \int d^2r \left(u^* \frac{\partial u}{\partial k_j} - \frac{\partial u^*}{\partial k_j} u \right), \qquad (5)$$

only change by an r-independent phase factor θ when k_1 is changed by $2\pi/aq$ or k_2 by $2\pi/b$. The integrand reduces to $\partial\theta/\partial k_j$. The integral is $2i$ times the change in phase around the unit cell and must be an integer multiple of $4\pi i$.

The problem of evaluating this quantum number remains. We have considered the potential

Its relation to (topological) invariants was first recognized a year later in J. E. Avron, R. Seiler, and B. Simon, Phys. Rev. Lett. 51 (1983) 51.

Many a paper followed.

TKNN and mathematics

TKNN can also be written as integral of the Berry curvature $\boldsymbol{A}$ over magnetic Brillouin zone

$$\sigma_{xy} = \frac{e^2}{h}\frac{1}{2\pi \mathrm{i}}\int d^2k[\boldsymbol{\nabla}\times\boldsymbol{A}(k_1,k_2)]_3 \tag{1}$$

$$\boldsymbol{A}(k_1,k_2) = \langle u(k)|\boldsymbol{\nabla}|u(k)\rangle$$

Now it can be recognized as the first Chern class of a $U(1)$ principal fiber bundle on a torus.

Since a torus does not have a boundary, the application of Stokes theorem would give zero if $\boldsymbol{A}$ were uniquely defined on the entire torus T^2. Non trivial topology makes only integer values possible.

See for instance R. Kaufmann, et al., Rev. Math. Phys., 28(10), 1630003, 2016

Other invariants

The initial discoveries promoted a vast research, and several other physically important invariants were discovered.

Stability of Fermi surface is governed by

$$N_1 = \mathrm{tr} \oint_C \frac{dl}{2\pi \mathrm{i}} G(p_0, p) \partial_l G^{-1}(p_0, p) \qquad (2)$$

C is an arbitrary contour in the 4-momentum space (p_0, p), which encloses the Fermi hypersurface.

G. Volovik, The Universe in a Helium Droplet

Topological stability of Fermi point is protected by
(second Chern class)

$$N_3 = \frac{1}{24\pi^2} \epsilon_{\mu\nu\rho\lambda} \, \mathrm{tr} \int_S dS^\mu G \partial^\nu G^{-1} G \partial^\rho G^{-1} G \partial^\lambda G^{-1} \qquad (3)$$

T. Matsuyama, PTP 77 (1987) 711; G. Volovik
While the latter is applicable for interacting particles, non-homogeneous systems are out of its scope.

Wigner-Weyl formalism

Almost as early as QM itself, a formulation without operators and Hilbert spaces was offered as a correspondence

$$\hat{A} \equiv A(\hat{x}, \hat{p}) \quad \leftrightarrow \quad A_W \equiv A_W(x, p)$$

such that

$$(\hat{A}\hat{B})_W = A_W * B_W, \qquad \mathrm{tr}\,\hat{A} = \mathrm{Tr}\,A_W$$
$$\mathrm{Tr}(A_W * B_W) = \mathrm{Tr}(A_W B_W)$$

with some appropriate $*$ and Tr.

Weyl 1927, Wigner 1932, Groenewold 1946, Moyal 1949

In infinite space, it is given by

$$A_W(x, p) = \frac{1}{(2\pi\hbar)^n} \int d^n q \, e^{\mathrm{i}qx/\hbar} \, \langle p + q/2 | \hat{A} | p - q/2 \rangle$$

Wigner-Weyl formalism

Actually, it can be totally independent formulation of QM, with Schroedinger equation replaced by Moyal equation

$$\frac{\partial \rho}{\partial t} = \frac{H * \rho - \rho * H}{\mathrm{i}\hbar} \equiv \{\!\{H, \rho\}\!\}$$

ρ being the Wigner function, i.e. Weyl symbol of the density matrix. Moyal product is

$$* = e^{\frac{\mathrm{i}\hbar}{2}(\overleftarrow{\partial}_x \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_x)}$$

Rapidly developing area of *deformation quantization* stemmed from this notion, with application to non-commutative geometry among many other fields.

Wigner-Weyl field theory

Partition function of a **lattice** model can be written as

$$Z = \int D\bar{\Psi} D\Psi \; e^{-S[\Psi,\bar{\Psi}]}$$

$$S[\Psi,\bar{\Psi}] = \int_{\mathbb{R}\otimes\mathcal{M}} \frac{d\omega d^D\boldsymbol{p}}{2\pi|\mathcal{M}|} \; \bar{\Psi}^T(\omega,\boldsymbol{p}) \, \hat{Q} \, \Psi(\omega,\boldsymbol{p}),$$

$\mathcal{M}$ is the first Brillouin zone. The action can be written as an operator trace,

$$S[\Psi,\bar{\Psi}] = \mathrm{tr}\left(\hat{W}[\Psi,\bar{\Psi}]\hat{Q}\right)$$

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where $\hat{W}$ (aka. density matrix) is such that

$$\langle p|\hat{W}_{ab}[\Psi,\bar{\Psi}]|q\rangle = \frac{\Psi_b(p)}{\sqrt{2\pi|\mathcal{M}|}} \frac{\bar{\Psi}_a(q)}{\sqrt{2\pi|\mathcal{M}|}}.$$

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$\mathcal{M}$ is the first Brillouin zone. The action can be written as an operator trace,

$$S[\Psi,\bar{\Psi}] = \mathrm{Tr}\left(W_W[\Psi,\bar{\Psi}] * Q_W\right)$$

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Now variation of partition function is

$$\delta Z = -\int D\bar{\Psi} D\Psi\, e^{-S}\, \mathrm{tr}\left(\hat{W}\delta\hat{Q}\right) = -Z\, \mathrm{tr}\left(\langle\hat{W}\rangle\,\delta\hat{Q}\right)$$
$$= \int dpdx\,(G_W(x,p) * \partial_{p_k} Q_W(x,p)\delta A(x))$$
$$= \int dx \delta A(x) \int dp\, G_W(x,p)\partial_{p_k} Q_W(x,p)$$

We used that $\langle\hat{W}\rangle = \hat{G}$ and that introduction of a EM potential A is simply shifting the momenta: $\boldsymbol{p} \to \boldsymbol{p} - \boldsymbol{A}(x)$, i.e. Peierls substitution.

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$$\langle J_k(x)\rangle = \int dp\, G_W(x,p)\partial_{p_k} Q_W(x,p)$$

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$$\langle J_k(x)\rangle = \int dp\, G_W(x,p)\partial_{p_k} Q_W(x,p)$$

Finally, the total current is topological invariant

$$\bar{J}_k \equiv \int dx\,\langle J_k(x)\rangle = \mathrm{Tr}(G_W * \partial_{p_k} Q_W)$$

Current and conductivity

Thus, we have a WW expression for the current

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It is a topological invariant, if we have periodic BC (or decay at infinity in continuous limit). However

$$G_W = G_W(A^{ext}) \tag{4}$$

in varying magnetic field or other type of inhomogeneity it is not.

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$$G_W = G_W(A^{ext}) \tag{4}$$

in varying magnetic field or other type of inhomogeneity it is not. Though, we can derive averaged conductivity of the systems as

$$\bar{\sigma} = \int dx \, \frac{\partial \langle J_k(x) \rangle}{\partial A^{ext}}_{A^{ext}=0}$$

and it will be once again <u>a topological invariant</u>.

Conductivity as topological invariant

To obtain the conductivity lets expand the current density in A and its first derivatives.

$$\langle J(x)\rangle \equiv \int dp\, G_W(x,p)\partial_{p_k} Q_W(x,p) \approx j^{(0)} + j_l^{(1)} A^l + j_{lm}^{(2)} F^{lm} + \dots$$

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The Q_W does not depend on the derivatives of A, therefore,

$$Q_W \approx Q_W^{(0)} - \partial_{p_m} Q_W^{(0)} A_m$$

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The Groenewold equation connects G_W and Q_W

$$G_W * Q_W = 1$$

and it can may be solved iteratively

$$G_W \approx G_W^{(0)} + G_W^{(0)} * (\partial_{p_m} Q_W^{(0)} A_m) * G_W^{(0)}.$$

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thus we have

$$Q_W \approx Q_W^{(0)} - \partial_{p_m} Q_W^{(0)} A_m, \qquad G_W \approx G_W^{(0)} + G^{(1)}_{W,m} A_m + G^{(2)}_{W,lm} \partial_l A_m$$

where

$$G^{(1)}_{W,m} = G_W^{(0)} * \partial_{p_m} Q_W^{(0)} * G_W^{(0)}, \qquad G^{(2)}_{W,lm} = \frac{i}{2} G_W^{(0)} * \partial_{p_l} Q_W^{(0)} * G_W^{(0)} * \partial_{p_m} Q_W^{(0)} * G_W^{(0)}$$

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Finally

$$\langle J_k(x)\rangle \approx F_{lm} \frac{i}{2} \int dp \left(G_W^{(0)} * \partial_{p_l} Q_W^{(0)} * G_W^{(0)} * \partial_{p_m} Q_W^{(0)} * G_W^{(0)} \cdot \partial_{p_k} Q_W^{(0)} \right)$$

σ, follow-on

So, we've came to

$$\langle J_k(x)\rangle \approx F_{lm}\frac{\mathrm{i}}{2}\int dp\left(G_W^{(0)}*\partial_{p_l}Q_W^{(0)}*G_W^{(0)}*\partial_{p_m}Q_W^{(0)}*G_W^{(0)}\cdot\partial_{p_k}Q_W^{(0)}\right)$$

then in $2+1$D the average conductivity is given by

$$\bar{\sigma}_H \equiv \int dx\, \sigma_H(x) = \frac{\mathcal{N}}{2\pi}$$

where

$$\mathcal{N} = \frac{\epsilon_{lmk}}{3!4\pi^2}\int d^3p d^3x\ \left(G_W^{(0)}*\partial_{p_l}Q_W^{(0)}*G_W^{(0)}*\partial_{p_m}Q_W^{(0)}*G_W^{(0)}*\partial_{p_k}Q_W^{(0)}\right)$$

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This is a topological invariant, yes!

Where is the lattice?

Formally speaking, as soon as you have properly defined Wigner-Weyl transformation, all the above results hold.

By *properly defined* we mean a kind of the following

Weyl-Wigner formalism

Almost as early as QM itself, a formulation without operators and Hilbert spaces was offered as a correspondence

$$\hat{A} \equiv A(\hat{x}, \hat{p}) \quad \leftrightarrow \quad A_W \equiv A_W(x, p)$$

such that

$$(\hat{A}\hat{B})_W = A_W * B_W, \qquad \mathrm{tr}\, \hat{A} = \mathrm{Tr}\, A_W$$
$$\mathrm{Tr}(A_W * B_W) = \mathrm{Tr}(A_W B_W)$$

with some appropriate $*$ and Tr.

Weyl 1927, Wigner 1932, Groenewold 1946, Moyal 1949

In infinite space, it is given by

$$A_W(x, p) = \frac{1}{(2\pi\hbar)^n} \int d^n q \, e^{\mathrm{i}qx/\hbar} \, \langle p + q/2 | \hat{A} | p - q/2 \rangle$$

It is actually not that easy for discrete spaces (lattices).

Where is the lattice?

Formally speaking, as soon as you have properly defined Wigner-Weyl transformation, all the above results hold.

It can be achieved *approximately* by the very same

$$A_W(x,p) = \frac{1}{(2\pi\hbar)^n} \int d^n q \, e^{\mathrm{i}qx/\hbar} \langle p + q/2 | \hat{A} | p - q/2 \rangle$$

It holds for week enough external fields, such that operators remain close to diagonal ones

$$\langle p + q/2 | \hat{A} | p - q/2 \rangle \neq 0 \quad \Leftrightarrow \quad qa \ll 1$$

Development of an exact Wigner-Weyl is in progress.

More details

More details to follow during the Workshop sessions, including

11:30–12:00 Michael Suleymanov
Wigner-Weyl formalism and the propagator of Wilson fermions in the presence of varying external electromagnetic field

12:00–12:30 IVF
Lattice Wigner-Weyl formalism in graphene

Conclusions

Topological invariants in the Wigner-Weyl formalism, applicable to non-uniform systems

Total current

$$\bar{J}_k = \mathrm{Tr}(G_W * \partial_{p_k} G_W^{-1})$$

Average conductivity

$$\bar{\sigma}_H = \frac{\mathcal{N}}{2\pi}$$

$$\mathcal{N} = \frac{\epsilon_{lmk}}{3!4\pi^2} \int d^3p d^3x \, \left(G_W * \partial_{p_l} G_W^{-1} * G_W * \partial_{p_m} G_W^{-1} * G_W * \partial_{p_k} G_W^{-1}\right)$$

Coleman theorem analog: We believe that a proof is ready showing that conductivity σ_H is not renormalized in higher loops.

Possible applications and developments:
- lattice models in non-uniform external EM fields
- under non-uniform strain, etc.

Publications

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Current as topological invariant

If we have time, let us check that

$$\delta \bar{J}_k \equiv -\delta \,\mathrm{Tr}\,[G_W * \partial_{p_k} Q_W] = 0$$

Indeed, if $Q_W \approx Q_W^{(0)} + Q_W^{(1)}$, then $G_W \approx G_W^{(0)} + G_W^{(1)}$, and

$$\delta\left(\mathrm{Tr}\,[G_W * \partial_{p_k} Q_W]\right) = \mathrm{Tr}\left[G_W^{(0)} * \partial_{p_k} Q_W^{(1)} + G_W^{(1)} * \partial_{p_k} Q_W^{(0)}\right]$$

Given that $G_W^{(1)} = -G^{(0)} * Q_W^{(1)} * G^{(0)}$ The latter two terms are

$$\mathrm{Tr}\left[G_W^{(0)} * \partial_{p_k} Q_W^{(1)} - G^{(0)} * Q_W^{(1)} * G^{(0)} * \partial_{p_k} Q_W^{(0)}\right]$$
$$= \mathrm{Tr}\left[G^{(0)} * \partial_{p_k} Q_W^{(0)} * G^{(0)} * Q_W^{(1)} - G^{(0)} * Q_W^{(1)} * G^{(0)} * \partial_{p_k} Q_W^{(0)}\right]$$

we integrated by parts(!) and used that $\partial_{p_l} G_W^{(0)} = -G^{(0)} * \partial_{p_l} Q_W^{(0)} * G^{(0)}$.

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we integrated by parts(!) and used that $\partial_{p_l} G_W^{(0)} = -G^{(0)} * \partial_{p_l} Q_W^{(0)} * G^{(0)}$.
Now simple cycling inside the Trace gives zero.

σ, follow-on

For completeness, lets write it in some other forms

$$\mathcal{N} = \frac{\epsilon_{lmk}}{3!4\pi^2} \int d^3p d^3x \left(G_W^{(0)} * \partial_{p_l} Q_W^{(0)} * G_W^{(0)} * \partial_{p_m} Q_W^{(0)} * G_W^{(0)} * \partial_{p_k} Q_W^{(0)} \right)$$

$$= \frac{\epsilon_{lmk}}{3!4\pi^2} \int d^3p d^3x \left(G_W * \partial_{p_l} G_W^{-1} * G_W * \partial_{p_m} G_W^{-1} * G_W * \partial_{p_k} G_W^{-1} \right)$$

$$= \frac{\epsilon_{lmk}}{3!4\pi^2} \int d^3p d^3x \, \mathrm{tr} \left(G_W * \partial_{p_l} G_W^{-1} * \partial_{p_m} G_W * \partial_{p_k} G_W^{-1} \right)$$

Using Weyl representation in momenta space, we can also rewrite

$$\mathcal{N} = \frac{\epsilon_{abc}}{3!4\pi^2} \int dl \, dk \, dp \, dq$$

$$\mathrm{tr} \left[G(l,k)(\partial_{k_a} + \partial_{p_a}) Q(k,p)(\partial_{p_b} + \partial_{q_b}) G(p,q)(\partial_{q_c} + \partial_{l_c}) Q(q,l) \right]$$

recall $G^{-1} = Q$.

Kubo formula, 2+1D

For 1-particle Hamiltonian, $\mathcal{H}$, with $\mathcal{H}\,|n\rangle = \mathcal{E}_n\,|n\rangle$ the Kubo formula is immediately reconstructed by noting that

$$Q(p^{(1)}, p^{(2)}) \equiv \langle p^{(1)}|\hat{Q}|p^{(2)}\rangle = \left(\delta^{(2)}(\boldsymbol{p}^{(1)} - \boldsymbol{p}^{(2)})\mathrm{i}\omega^{(1)} - \langle \boldsymbol{p}^{(1)}|\mathcal{H}|\boldsymbol{p}^{(2)}\rangle\right)\delta(\omega^{(1)} - \omega^{(2)})$$

where $p = (p_1, p_2, p_3) = (\boldsymbol{p}, \omega)$. At the same time

$$G(p^{(1)}, p^{(2)}) = \sum_n \frac{1}{\mathrm{i}\omega^{(1)} - \mathcal{E}_n}\,\langle \boldsymbol{p}^{(1)}|n\rangle\,\langle n|\boldsymbol{p}^{(2)}\rangle\,\delta(\omega^{(1)} - \omega^{(2)})$$

Thus we will have

$$\mathcal{N} \;=\; -\frac{2\mathrm{i}\,(2\pi)^3}{8\pi^2\,\mathcal{A}}\sum_{n,k}\epsilon_{ij}\,\frac{\theta(-\mathcal{E}_n)\theta(\mathcal{E}_k)}{(\mathcal{E}_k - \mathcal{E}_n)^2}\,\langle n|[\mathcal{H}, \hat{x}_i]|k\rangle\,\langle k|[\mathcal{H}, \hat{x}_j]|n\rangle\,.$$

where one needed to use that

$$[\partial_{p_j^{(4)}} + \partial_{p_j^{(1)}}]\langle \boldsymbol{p}^{(4)}|\mathcal{H}|\boldsymbol{p}^{(1)}\rangle = i\langle \boldsymbol{p}^{(4)}|\mathcal{H}\hat{\boldsymbol{x}}_j - \hat{\boldsymbol{x}}_j\mathcal{H}|\boldsymbol{p}^{(1)}\rangle = i\langle \boldsymbol{p}^{(4)}|[\mathcal{H}, \hat{\boldsymbol{x}}_j]|\boldsymbol{p}^{(1)}\rangle.$$

with $\hat{\boldsymbol{x}}$ understood as $i\partial_{\boldsymbol{p}}$ acting on the wave-function in momentum representation

$$\hat{x}_j\Psi(\boldsymbol{p}) = \langle \boldsymbol{p}|\hat{x}_j|\Psi\rangle = i\partial_{p_j}\langle \boldsymbol{p}|\Psi\rangle = \mathrm{i}\partial_{p_j}\Psi(\boldsymbol{p})$$