Precise Wigner-Weyl calculus for lattice models

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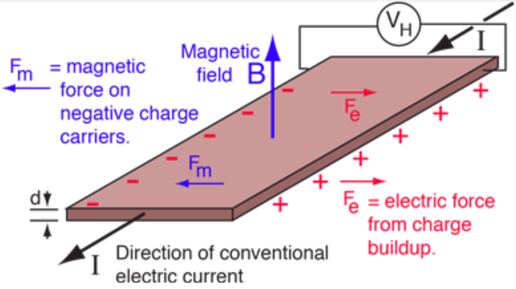
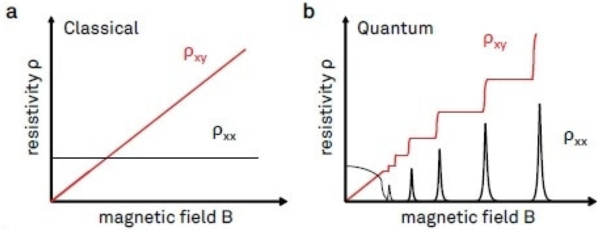
Workshop on Lattice Field Theory and Condensed Matter Physics
e-ICNFP 08/09/2020

Outlook

IF, M. Zubkov, Nucl. Phys. B 938 (2019), 171-199.

Hall system sketch





TKNN and mathematics

TKNN invariant was derived for the Hall conductivity, as an integral of the Berry curvature $\boldsymbol{A}$ over magnetic Brillouin zone

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

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

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

Many other topological invariants discovered later, but all for *homogeneous* systems.

Thouless et al. Phys. Rev. Lett. 49 (1982) 405;
J. E. Avron, R. Seiler, and B. Simon, Phys. Rev. Lett. 51 (1983) 51;
For a review, see, e.g., R. Kaufmann, et al., Rev. Math. Phys., 28(10), 1630003, 2016.

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

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

with some appropriate $\star$ and Tr.

Weyl 1927, Wigner 1932, Groenewold 1946, Moyal 1949

In infinite space, it is given by

$$A_W(x,p) = \int \frac{d^n q}{(2\pi\hbar)^n} e^{\frac{iqx}{\hbar}} \langle p + \tfrac{1}{2}q | \hat{A} | p - \tfrac{1}{2}q \rangle \qquad \star = e^{\frac{i\hbar}{2}(\overleftarrow{\partial}_x \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_x)}$$

Wigner-Weyl field theory

Partition function can be written as

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

The action, in its turn, can written as an operator trace,

$$S[\Psi,\bar{\Psi}] \equiv \int \frac{d\omega d^D \boldsymbol{p}}{2\pi|\mathcal{M}|} \; \bar{\Psi}^T(\omega,\boldsymbol{p}) \, \hat{Q} \, \Psi(\omega,\boldsymbol{p}) = \mathrm{tr}\left(\hat{W}[\Psi,\bar{\Psi}]\hat{Q}\right),$$

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

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

Using the properties Wigner-Weyl formalism,

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

Wigner-Weyl field theory

Now variation of partition function is

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

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

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Finally, the total current is topological invariant

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

Current and conductivity

Thus, we have a Wigner-Weyl expression for the current

$$\bar{J}_k = \mathrm{Tr}(G_W \star \partial_{p_k} Q_W)$$

It is a topological invariant, if we have periodic BC (or decay at infinity in continuous limit).
The averaged conductivity of the systems

$$\bar{\sigma} = \int dx \, \frac{\partial \langle J_k(x) \rangle}{\partial A^{ext}}_{A^{ext}=0} \quad \Rightarrow \quad \bar{\sigma}_H = \frac{\mathcal{N}}{2\pi}$$

where

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

and it is a topological invariant!

Formal definition of Weyl symbol

By Wigner-Weyl formalism we understand $A_W(x,p) \in L^2(\mathcal{M} \times \mathfrak{O})$ (aka Weyl symbol), $\star$-product and trace operation Tr, satisfying the following conditions

1. Star product identity
$$A_W(x,p) \star B_W(x,p) = (\hat{A}\hat{B})_W(x,p)$$
2. First trace identity
$$\mathrm{Tr}\, A_W = \mathrm{tr}\, \hat{A}$$
3. Second trace identity
$$\mathrm{Tr}[A_W(x,p) \star B_W(x,p)] = \mathrm{Tr}[A_W(x,p) B_W(x,p)]$$
4. Weyl symbol of identity operator
$$(\hat{1})_W(x,p) = 1.$$

Examples of would-be Weyl symbols

There were many approaches to build a lattice Wigner-Weyl formalism Buot 1974, Kasperkovitz&Peev 1994, Leonhardt 1995, Ligabó 2012, etc.
To illustrate some problems, let us follow F.Buot 1974 with

$$Q_{\mathcal{B}}(x,p) = \int_{\mathcal{M}} d^D q\, e^{2iqx} Q(p+q, p-q).$$

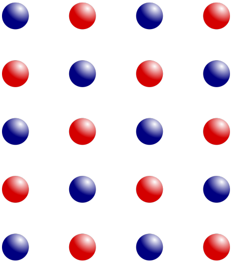
In 1D case (for simplicity) the symbol of a unity operator becomes

$$\begin{aligned}(\hat{1})_{\mathcal{B}} &\equiv \int_{\mathcal{M}} dq\, e^{2ixq} \langle p+q | p-q \rangle = \int_{-\pi/2\ell}^{\pi/2\ell} dq\, e^{2ixq} \delta^{[\pi/\ell]}(2q) \\ &= \frac{1}{2}\int_{-\pi/2\ell}^{\pi/2\ell} dq\, e^{2ixq} \left(\delta(q) + \frac{1}{2}\delta(q-\pi/2\ell) + \frac{1}{2}\delta(q+\pi/2\ell) \right) \\ &= \frac{1}{2}(1+\cos(\pi x/\ell)).\end{aligned}$$

The Groenewold equation (i.e. symbol of $\hat{Q}\hat{G} = \hat{1}$) becomes

$$Q_{\mathcal{B}}(x,p) \star G_{\mathcal{B}}(x,p) = (\hat{1})_{\mathcal{B}} = \begin{cases} 1, & x = 2k\ell \\ 0, & x = (2k+1)\ell \end{cases}.$$

The indication for solution is to separate two lattices



$$\mathfrak{O} = \{\ell k, k \in \mathbb{Z}\} \equiv \mathcal{O} \cup \mathcal{O}',$$

$$\mathcal{O} = \{2\ell k, k \in \mathbb{Z}\}, \quad \mathcal{O}' = \{2\ell(k + \tfrac{1}{2}), k \in \mathbb{Z}\}.$$

To build a lattice Wigner transformation we now enlarge operators acting on $\mathcal{O}$ to act on $\mathfrak{O}$:

$$\langle x|\hat{Q}|y\rangle = \langle x + \ell|\hat{Q}|y + \ell\rangle\,, \quad x, y \in \mathcal{O}.$$

Moreover, we demand that the inter-lattice matrix elements vanish

$$\langle x|\hat{Q}|y\rangle = \langle y|\hat{Q}|x\rangle = 0 \quad \forall x \in \mathcal{O}, y \in \mathcal{O}'$$

Then, the matrix elements in momentum space of such operators become

$$\langle p|\hat{Q}|q\rangle = \frac{1}{2} Q(p,q)(1 + e^{\mathrm{i}(q-p)\ell})$$

Exact Weyl symbol

It leads to the following lattice Weyl symbol of operator $\hat{Q}$ (in D)

$$Q_W(x,p) = \int_{\mathcal{M}} d^D q\, e^{2\mathrm{i}qx} Q(p+q, p-q) \prod_{j=1}^{D} \left(1 + e^{-2\mathrm{i}q\ell^{(j)}}\right).$$

The trace operation has the form

$$\mathrm{Tr}\, Q_W = \frac{1}{2^D|\mathcal{M}|} \int_{\mathcal{M}} d^D p \sum_{x\in\mathcal{O}\cup\mathcal{O}'} \mathrm{tr}\, Q_W(x,p).$$

The $\star$-product is the original Moyal one

$$\star \equiv \star_{x,p} = e^{-\frac{\mathrm{i}}{2}\overleftarrow{\partial}_x\overrightarrow{\partial}_p + \frac{\mathrm{i}}{2}\overrightarrow{\partial}_x\overleftarrow{\partial}_p}.$$

IVF, M. Zubkov 2019

For operators, possessing a series representation of a function of two variables

$$\hat{Q} = \mathcal{Q}(x,p)\big|_{x\to \mathrm{i}\partial_p} = \sum_n (\mathrm{i}\partial_p)^n Q_n(p)$$

its Weyl symbol can be defined as

$$Q_{\mathcal{W}}\,(x,p) = \sum_n x^n q_n(p),$$

with

$$q_n(p) = \sum_{k_i \geq n_i} \prod_i C^{n_i}_{k_i} \left(\frac{\mathrm{i}}{2}\partial_p\right)^{k-n} Q_n(p).$$

Moreover,

$$Q_{\mathcal{W}}\,(x,p) = Q_W\,(x,p)\,, \quad \forall x \in \mathfrak{O}$$

provided that (practically $\langle x|\hat{Q}|y\rangle = \langle x+\ell|\hat{Q}|y+\ell\rangle$)

$$\mathcal{Q}(x+\ell,p) = \mathcal{Q}(x,p), \quad \forall x \in \mathcal{O}.$$

Conclusions

Non-uniform Topological invariants in Wigner-Weyl formalism:

Total current

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

Average conductivity

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

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

Exact and convenient Wigner transformation:

$$Q_W(x,p) = \int_{\mathcal{M}} d^3q \, e^{2\mathrm{i}qx} Q(p+q, p-q) \prod_{j=1}^{3} \left(1 + e^{-2\mathrm{i}q\ell^{(j)}} \right)$$

Possible applications and developments:

- lattice models in non-uniform external EM fields, non-uniform strain, etc.
- non-equilibrium models under the same conditions.

Publications

I.V. Fialkovsky, M.A. Zubkov,
Precise Wigner-Weyl calculus for lattice models,
Nucl. Phys. B 20 114999 (2020), arXiv:1912.02786 [math-ph]

See also

I.V.Fialkovsky, M.A.Zubkov,
Elastic deformations and Wigner-Weyl formalism in graphene,
2. Symmetry 2020, 12(2), 317, arXiv:1905.11097 [cond-mat.mes-hall]

I.V.Fialkovsky, M.Suleymanov, Xi Wu, C. X. Zhang, , M.A.Zubkov,
Hall conductivity as topological invariant in phase space,
Phys. Scr. 95 064003 (2020), arXiv:1910.04730 [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]