Elastic deformations and Wigner-Weyl formalism in graphene

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Outlook

1. Conclusions
2. Wigner-Weyl formalism
3. Wigner-Weyl field theory
   - Generalities
   - Current and Conductivity
   - Kubo formula
4. Non-uniform Tight-Binding models
   - Elastic deformations
   - IQH with varying B and elastic deformations
5. Conclusions, once again

Conclusions from a previous talk

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

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

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

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Thus, we need to obtain Weyl symbol of Dirac operator and of its inverse

$$Q_W(\boldsymbol{x}, \boldsymbol{p}), \qquad G_W(\boldsymbol{x}, \boldsymbol{p})$$

$$\boldsymbol{Q} \equiv \boldsymbol{G}^{-1} = \mathrm{i}\omega - \boldsymbol{H}.$$

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,

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

with pseudo-differential operator

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

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Approximately for lattices

$$A_W(\boldsymbol{x}, \boldsymbol{p}) = \frac{1}{|\mathcal{M}|} \int_{\mathcal{M}} d\boldsymbol{q}\, e^{\mathrm{i}\boldsymbol{q}\boldsymbol{x}/\hbar} \langle \boldsymbol{p} + \boldsymbol{q}/2 | \hat{A} | \boldsymbol{p} - \boldsymbol{q}/2 \rangle$$

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Wigner-Weyl field theory

From the previous talks we've learned that partition function is

$$Z = \int D\bar{\Psi} D\Psi \; e^{-\mathrm{Tr}\left(W_W[\Psi,\bar{\Psi}] Q_W\right)}$$

The Weyl symbols in the above are of the **Dirac operator** and **density matrix**

$$Q = \mathrm{i}\omega - H, \qquad \hat{W} = |\Psi\rangle\langle\Psi|$$

The variation of partition function is then

$$\begin{aligned}\delta Z &= -Z\,\mathrm{tr}(\langle\hat{W}\rangle\,\delta\hat{Q}) \\ &= \int dx\delta A(x)\int dp\, G_W(x,p)\partial_{p_k}Q_W(x,p) = \int dx\delta A(x)\langle J_k(x)\rangle\end{aligned}$$

We used that $\langle\hat{W}\rangle = \hat{G}$ and employed Peierls substitution for EM potential A, $\boldsymbol{p}\to\boldsymbol{p}-\boldsymbol{A}(x)$: $\delta Q = -\partial_{p_k}Q\delta A_k$.

The current density thus

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

It is not an invariant, but the total current is

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

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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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We have (using Groenewold equation $G_W * Q_W = 1$)

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

where

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

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where

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

Finally

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

σ, follow-on

So, we've came to

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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

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

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This is a topological invariant, yes!

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

Kubo formula is immediately reconstructed, $\mathcal{H}$, with $\mathcal{H}\,|n\rangle = \mathcal{E}_n\,|n\rangle$

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

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

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

One needed to use that

$$[\partial_{p_j}+\partial_{q_j}]\,\langle \boldsymbol{p}|\mathcal{H}|\boldsymbol{q}\rangle = \mathrm{i}\,\langle \boldsymbol{p}|\mathcal{H}\hat{\boldsymbol{x}}_j - \hat{\boldsymbol{x}}_j\mathcal{H}|\boldsymbol{q}\rangle = \mathrm{i}\,\langle \boldsymbol{p}|[\mathcal{H},\hat{\boldsymbol{x}}_j]|\boldsymbol{q}\rangle\,.$$

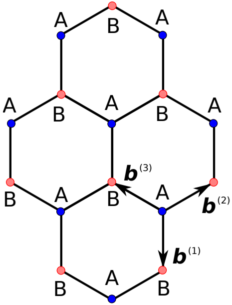
with $\hat{\boldsymbol{x}}$ understood as $i\partial_{\boldsymbol{p}}$ acting on the wave-function in momentum representation

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

Non-uniform Tight-Binding models

The Hamiltonian in external EM field

$$\mathcal{H} = \sum_{\boldsymbol{x},\boldsymbol{y}} \bar{\Psi}(\boldsymbol{y}) f(\boldsymbol{y},\boldsymbol{x}) e^{\mathrm{i}\int_{\boldsymbol{x}}^{\boldsymbol{y}} d\boldsymbol{v} \boldsymbol{A}(\boldsymbol{v})} \Psi(\boldsymbol{x})$$



Nearest neighbour TB with non-uniform varying hopping parameter

$$f(\boldsymbol{y},\boldsymbol{x}) = \sum_{j=1}^{M} \delta(\boldsymbol{y} - (\boldsymbol{x} + \boldsymbol{b}^{(j)})) f^{(j)}(\boldsymbol{y})$$

where $\boldsymbol{b}^{(j)}$ are the vectors connecting each atom to its nearest M neighbors, $j = 1, ..., M$. In Fourier representation we get

$$\mathcal{H} = \frac{1}{|\mathcal{M}|} \sum_{j=1}^{M} \int_{\mathcal{M}} d\boldsymbol{p} d\boldsymbol{q}\, \bar{\Psi}(\boldsymbol{p}) \left[f^{(j)}(\boldsymbol{p} - \boldsymbol{q}) e^{\mathrm{i}\boldsymbol{q}\boldsymbol{b}^{(j)}} \right] \Psi(\boldsymbol{q})$$

And those with $\mathbb{Z}_2$ symmetry

The lattice consist of two Bravais sub-lattices

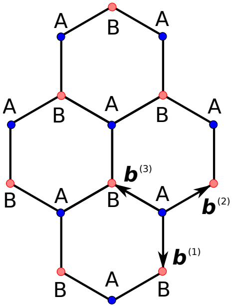
$$\mathcal{O} = \mathcal{O}_1 \cup \mathcal{O}_2, \qquad \mathcal{O}_2 = \mathcal{O}_1 + \boldsymbol{b}^{(1)}$$

then we introduce a vector wave function

$$\Psi \to \left(\Psi_1(\boldsymbol{y}_1),\ \Psi_2(\boldsymbol{y}_2)\right)^{\mathrm{T}}, \qquad \begin{matrix} \boldsymbol{y}_1 \in \mathcal{O}_1 \\ \boldsymbol{y}_2 \in \mathcal{O}_2 \end{matrix}$$

and Dirac Hamiltonian becomes

$$\mathcal{H} = \sum_{\substack{\boldsymbol{x}\in\mathcal{O}_1 \\ \boldsymbol{y}\in\mathcal{O}_2}} \begin{pmatrix} \Psi_1^*(\boldsymbol{x}) \\ \Psi_2^*(\boldsymbol{y}) \end{pmatrix} \boldsymbol{H}(\boldsymbol{x},\boldsymbol{y}) \begin{pmatrix} \Psi_1(\boldsymbol{x}) \\ \Psi_2(\boldsymbol{y}) \end{pmatrix}^{\mathrm{T}}$$



where

$$\boldsymbol{H} = \begin{pmatrix} 0 & H_{12} \\ H_{21} & 0 \end{pmatrix} \qquad \begin{aligned} H_{21}(\boldsymbol{y}_2,\boldsymbol{y}_1) &= -\sum_{j=1}^{M} \delta\left(\boldsymbol{y}_2 - (\boldsymbol{y}_1 + \boldsymbol{b}^{(j)})\right) t^{(j)}\left(\tfrac{\boldsymbol{y}_1+\boldsymbol{y}_2}{2}\right) \\ H_{12}(\boldsymbol{y}_1,\boldsymbol{y}_2) &= H_{21}(\boldsymbol{y}_2,\boldsymbol{y}_1) \end{aligned}$$

Momentum representation

In momentum representation the Hamiltonian becomes

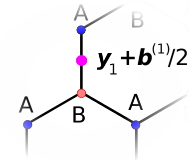
$$\mathcal{H}_{21} = \frac{1}{|\mathcal{M}|}\int_{\mathcal{M}} d\boldsymbol{p}d\boldsymbol{q}\,\bar{\Psi}_2(\boldsymbol{p})H_{21}(\boldsymbol{p},\boldsymbol{q})\Psi_1(\boldsymbol{q})$$

we have

$$H_{12}(\boldsymbol{q},\boldsymbol{p}) = \frac{1}{|\mathcal{M}|}\sum_{j=1}^{M}\sum_{\boldsymbol{y}_1\in\mathcal{O}_1} e^{-\mathrm{i}(\boldsymbol{q}-\boldsymbol{p})\boldsymbol{y}_1+\mathrm{i}\boldsymbol{q}\boldsymbol{b}^{(j)}}\, t^{(j)}\left(\boldsymbol{y}_1+\boldsymbol{b}^{(j)}/2\right)$$

it can be rewritten as

$$H_{21}(\boldsymbol{p},\boldsymbol{q}) = \sum_{j=1}^{M} t^{(j)}(\boldsymbol{p}-\boldsymbol{q})e^{\mathrm{i}(\boldsymbol{p}+\boldsymbol{q})\boldsymbol{b}^{(j)}/2}$$



if we introduce a shifted Fourier transform

$$t^{(j)}(\boldsymbol{p}) = \frac{1}{|\mathcal{M}|}\sum_{\boldsymbol{x}\in\mathcal{O}^{(j)}_{1/2}} t^{(j)}(\boldsymbol{x})e^{-\mathrm{i}\boldsymbol{x}\boldsymbol{p}}$$

we introduced a new set of points: $\mathcal{O}^{(j)}_{1/2} = \{\boldsymbol{y}_1+\boldsymbol{b}^{(j)}/2,\ \boldsymbol{y}_1\in\mathcal{O}_1\}$, i.e. points situated in the middle of the lattice links along the j-th direction.

Weyl symbol of Dirac operator

We use the following definition of the Weyl symbol of an operator $\hat{A}$:

$$(\hat{A})_W(\boldsymbol{x}, \boldsymbol{p}) = \int_{\mathcal{M}} d\boldsymbol{q}\, A(\boldsymbol{p} + \boldsymbol{q}/2, \boldsymbol{p} - \boldsymbol{q}/2) e^{\mathrm{i}\boldsymbol{q}\boldsymbol{x}}.$$

For off-diagonal components of $\boldsymbol{H}$ from above it gives

$$H_{21,W}(\boldsymbol{x}, \boldsymbol{p}) = \int_{\mathcal{M}} d\boldsymbol{q}\, e^{\mathrm{i}\boldsymbol{q}\boldsymbol{x}} \sum_{j=1}^{M} t^{(j)}(\boldsymbol{q})\, e^{\mathrm{i}\boldsymbol{p}\boldsymbol{b}^{(j)}} = \sum_{j=1}^{M} e^{\mathrm{i}\boldsymbol{p}\boldsymbol{b}^{(j)}} \int_{\mathcal{M}} d\boldsymbol{q}\, t^{(j)}(\boldsymbol{q}) e^{\mathrm{i}\boldsymbol{q}\boldsymbol{x}}$$

If the hopping parameters are homogeneous, then

$$H_{21,W}(\boldsymbol{x}, \boldsymbol{p}) = e^{\mathrm{i}\boldsymbol{p}\boldsymbol{b}^{(j)}} t^{(j)}$$

On the other hand, when the hopping parameters vary, we have

$$H_{21,W}(\boldsymbol{x}, \boldsymbol{p}) = \sum_{j=1}^{M} e^{\mathrm{i}\boldsymbol{p}\boldsymbol{b}^{(j)}} \sum_{\boldsymbol{y} \in \mathcal{O}_{1/2}^{(j)}} t^{(j)}(\boldsymbol{y}) \mathcal{F}(\boldsymbol{x} - \boldsymbol{y}), \qquad \mathcal{F}(\boldsymbol{x}) = \frac{1}{|\mathcal{M}|} \int_{\mathcal{M}} d\boldsymbol{q}\, e^{\mathrm{i}\boldsymbol{q}\boldsymbol{x}}$$

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$$H^{(j)}_{21,W}(\boldsymbol{x},\boldsymbol{p})\Big|_{\boldsymbol{x}\in\mathcal{O}^{(j)}_{1/2}} = e^{\mathrm{i}\boldsymbol{p}\boldsymbol{b}^{(j)}}\, t^{(j)}(\boldsymbol{x})$$

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$$H^{(j)}_{21,W}(\boldsymbol{x},\boldsymbol{p})\Big|_{\boldsymbol{x}\in\mathcal{O}^{(j)}_{1/2}} = e^{\mathrm{i}\boldsymbol{p}\boldsymbol{b}^{(j)}} t^{(j)}(\boldsymbol{x})$$

To introduce the EM field we need to use *translation operators*, i.e.

$$t^{(j)}(\boldsymbol{x}) \to t^{(j)}(\boldsymbol{x})e^{-\mathrm{i}A^{(j)}(\boldsymbol{x})}$$

as a short notation we introduced

$$A^{(j)}(\boldsymbol{x}) = \int_{\boldsymbol{x}-\boldsymbol{b}^{(j)}/2}^{\boldsymbol{x}+\boldsymbol{b}^{(j)}/2} \boldsymbol{A}(\boldsymbol{y})d\boldsymbol{y}.$$

Weyl symbol of Dirac Operator with EM

We obtain thus the Dirac operator symbol

$$Q_W = \sum_{j=1}^{M} Q_W^{(j)}$$

where

$$Q_W^{(j)}(\boldsymbol{x},\boldsymbol{p})\Big|_{\boldsymbol{x}\in\mathcal{O}_{1/2}^{(j)}} = \begin{pmatrix} \mathrm{i}\omega/M & -t^{(j)}(\boldsymbol{x})\, e^{\mathrm{i}(\boldsymbol{p}\boldsymbol{b}^{(j)}-A^{(j)}(\boldsymbol{x}))} \\ -t^{(j)}(\boldsymbol{x})\, e^{-i(\boldsymbol{p}\boldsymbol{b}^{(j)}-A^{(j)}(\boldsymbol{x}))} & \mathrm{i}\omega/M \end{pmatrix}$$

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For both $t^{(j)}$ and $\boldsymbol{A}$ that do not vary significantly at the distances of order of lattice spacing we may use above expression for arbitrary values of $\boldsymbol{x}$.

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For both $t^{(j)}$ and $\boldsymbol{A}$ that do not vary significantly at the distances of order of lattice spacing we may use above expression for arbitrary values of $\boldsymbol{x}$.
As before

$$A^{(j)}(\boldsymbol{x}) = \int_{\boldsymbol{x}-\boldsymbol{b}^{(j)}/2}^{\boldsymbol{x}+\boldsymbol{b}^{(j)}/2} \boldsymbol{A}(\boldsymbol{y})d\boldsymbol{y}.$$

Elastic deformations

Strained graphene at $x_3 = 0$ is described by new coordinates y_k

$$y_k(\boldsymbol{x}) = x_k + u_k(\boldsymbol{x}), \qquad y_3(\boldsymbol{x}) = u_3(\boldsymbol{x})$$

The displacements have three components $u_a(\boldsymbol{x})$. Induced metric is

$$g_{ik} = \delta_{ik} + 2u_{ik}, \quad u_{ik} = \frac{1}{2}\Big(\partial_i u_k + \partial_k u_i + \partial_i u_a \partial_k u_a\Big), \quad a = 1,2,3, \quad i,k = 1,2.$$

Elastic deformations change the spatial hopping parameters

$$t^{(j)}(\boldsymbol{x}) = t\left(1 - \beta u_{ik}(\boldsymbol{x}) b_i^{(j)} b_k^{(j)}\right).$$

here β is the Gruneisen parameter. We imply that $\beta|u_{ij}| \ll 1$.
For arbitrarily varying field u we obtain the following expression for Q_W:

$$Q_W = \mathrm{i}\omega - t\sum_{j=1}^{3}\left(1 - \beta u_{ik}(\boldsymbol{x}) b_i^{(j)} b_k^{(j)}\right)\begin{pmatrix} 0 & e^{\mathrm{i}(\boldsymbol{p}\boldsymbol{b}^{(j)} - A^{(j)}(\boldsymbol{x}))} \\ e^{-\mathrm{i}(\boldsymbol{p}\boldsymbol{b}^{(j)} - A^{(j)}(\boldsymbol{x}))} & 0 \end{pmatrix}$$

Conclusions? Not yet

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

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

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

Thus, we need to obtain Weyl symbol of Dirac operator and of its inverse

$$Q_W(\boldsymbol{x}, \boldsymbol{p}), \qquad G_W(\boldsymbol{x}, \boldsymbol{p})$$

$$\boldsymbol{Q} \equiv \boldsymbol{G}^{-1} = \mathrm{i}\omega - \boldsymbol{H}.$$

Kubo formula revisited

Using Kubo formula for $\sigma = \mathcal{N}/2\pi$

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

We decompose the coordinates x_1, x_2 in relative coordinates ξ_i (with bounded values) and center coordinates X_i (the unbounded part)

$$\hat{x}_1 = \hat{\xi}_1 + \hat{X}_1, \qquad \hat{x}_2 = \hat{\xi}_2 + \hat{X}_2 \tag{1}$$

Quite naturally we then come to (in Landau gauge $\mathcal{H} \equiv \mathcal{H}(\xi_1, \xi_2)$)

$$\begin{aligned}\mathcal{N} &= -\frac{2\mathrm{i}\,(2\pi)^3}{8\pi^2\,\mathcal{A}} \sum_{n,k} \epsilon_{ij}\,\theta(-\mathcal{E}_n)\theta(\mathcal{E}_k)\,\frac{\langle n|[\mathcal{H},\hat{\xi}_i]|k\rangle\,\langle k|[\mathcal{H},\hat{\xi}_j]|n\rangle}{(\mathcal{E}_k-\mathcal{E}_n)^2}_{A=0} \\ &= \frac{2\mathrm{i}\pi}{\mathcal{A}} \sum_n \Big[\langle n|[\hat{\xi}_1,\hat{\xi}_2]|n\rangle\Big]_{A=0}\theta(-\mathcal{E}_n) = -\frac{2\mathrm{i}\pi}{\mathcal{A}\,B}\sum_n \langle n|n\rangle\theta(-\mathcal{E}_n).\end{aligned} \tag{2}$$

Assuming that we have two good quantum numbers, $|n\rangle \to |p_2, m\rangle$

$$\mathcal{N} = -\frac{(2\pi)}{\mathcal{A}} \sum_m \int \frac{dp_2 L}{2\pi} \frac{1}{B} \theta(-\mathcal{E}_m(p_2)) = N \,\mathrm{sign}(-B)$$

In conventional systems number of occupied levels, N, is counted from the neutrality point. In graphene there are deeply lying levels with large negative Chern numbers, effectively rendering the sum to go from the zero energy.
D. Sheng, et al., 2006. Y. Hatsugai, et al., 2006.

However, our approximation is probably valid only up to $|E_F| \sim t$, i.e. in-between the innermost van Hove singularities, and we cannot count deep lying levels. Their contribution is known – it cancels precisely that of $\mathcal{N}/(2\pi)$ at the half filling, $\sigma_{xy}^{(0)} = \mathcal{N}^{(0)}/(2\pi)$. Finally,

$$\sigma_{xy} = \frac{\mathcal{N}}{2\pi} - \sigma_{xy}^{(0)} = \frac{N'}{2\pi}\mathrm{sign}(-B) \qquad (3)$$

where N' is counted from the half filling.

Conclusions, finally

Topological invariants in the Wigner-Weyl formalism, applicable to non-uniform $\mathbb{Z}_2$ lattices

Total current

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

Average conductivity

$$\bar{\sigma}_H = \frac{\mathcal{N} - \mathcal{N}(0)}{2\pi}$$

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

Both valid in graphene with (slowly) varying external fields and non-uniform mechanical strain.

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