Hall conductivity as topological invariant in phase space

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ICNFP 2019
Outlook

History
TKNN
Mathematical Connections
Other invariants

QM in phase space: Weyl-Wigner formalism
A reminder

Wigner-Weyl field theory
Current as topological invariant
Conductivity as topological invariant

Conclusions and Thank You
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,
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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*,
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, 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

\[
\sigma_H = \frac{ie^2}{A_0} \sum_{\epsilon \alpha \beta} \sum_{\epsilon_\alpha \epsilon_\beta} \left( \frac{\partial \hat{H}}{\partial k_\alpha} \right)_{\beta \alpha} \left( \frac{\partial \hat{H}}{\partial k_\beta} \right)_{\alpha \alpha} - \epsilon_\alpha \epsilon_\beta \frac{\partial \hat{H}}{\partial k_\alpha} \left( \frac{\partial \hat{H}}{\partial k_\beta} \right)_{\alpha \alpha},
\]

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

\[
\sigma_H = \frac{ie^2}{2\pi \hbar} \sum_k d^2k \int d^2r \left( \frac{\partial u^*}{\partial k_1} \frac{\partial u}{\partial k_2} - \frac{\partial u^*}{\partial k_2} \frac{\partial u}{\partial k_1} \right)
\]

\[
= \frac{ie^2}{4\pi \hbar} \sum_j df \int d^2r \left( u^* \frac{\partial u}{\partial f_j} - \frac{\partial u^*}{\partial f_j} u \right),
\]

only change by an \( r \)-independent phase factor \( \theta \) 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 \( 2\pi \) times the change in phase around the unit cell and must be an integer multiple of \( 4\pi \).

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 $\mathbf{A}$ over magnetic Brillouin zone

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

(1)

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

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 $\mathbf{A}$ were uniquely defined on the entire torus $T^2$. Non trivial topology makes only integer values possible.

Other invariants

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

**Stability of Fermi surface** is governed by

\[ N_1 = \text{tr} \int_C \frac{dl}{2\pi i} G(p_0, p) \partial_l G^{-1}(p_0, p) \]  \hfill (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)

\[ N_3 = \frac{1}{24\pi^2} \epsilon_{\mu\nu\rho\lambda} \text{tr} \int_S d\Sigma^\mu G^\nu G^{-1} G^\rho G^{-1} G^\lambda G^{-1} \]  \hfill (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

\[ \hat{A} \equiv A(\hat{x}, \hat{p}) \leftrightarrow A_W \equiv A_W(x, p) \]

such that

\[ (\hat{A} \hat{B})_W = A_W \ast B_W, \quad \text{tr} \, \hat{A} = \text{Tr} \, A_W \]
\[ \text{Tr}(A_W \ast B_W) = \text{Tr}(A_W B_W) \]

with some appropriate \(*\) and \(\text{Tr}\).

Weyl 1927, Wigner 1932, Groenewold 1946, Moyal 1949

In infinite space, it is given by

\[ A_W(x, p) = \frac{1}{(2\pi \hbar)^n} \int d^n q \ e^{iqx/\hbar} \langle p + q/2 | \hat{A} | p - q/2 \rangle \]
Wigner-Weyl formalism

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

$$\frac{\partial \rho}{\partial t} = \frac{H \ast \rho - \rho \ast H}{i\hbar} \equiv \{H, \rho\}$$

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

$$\ast = e^{\frac{i\hbar}{2}(\tilde{p}\tilde{x} - \tilde{x}\tilde{p})}$$

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

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

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

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

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

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

\[
\langle p | \hat{W}_{ab}[\psi, \bar{\psi}] | q \rangle = \frac{\psi_b(p)}{\sqrt{2\pi |\mathcal{M}|}} \frac{\bar{\psi}^a(q)}{\sqrt{2\pi |\mathcal{M}|}}.
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\]
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Now variation of partition function is

$$\delta Z = - \int D\bar{\Psi} D\Psi \ e^{-S} \ \text{tr} \left( \hat{W} \delta \hat{Q} \right) = -Z \ \text{tr} \left( \langle \hat{W} \rangle \delta \hat{Q} \right)$$

$$= \int dp dx \ (G_W(x, p) \ast \partial_{p_k} Q_W(x, p) \delta A(x))$$

$$= \int dx \delta A(x) \int dp \ G_W(x, p) \partial_{p_k} Q_W(x, p)$$

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

$$\bar{J}_k \equiv \int dx \langle J_k(x) \rangle = \text{Tr}(G_W \ast \partial_{p_k} Q_W)$$
Current and conductivity

Thus, we have a WW expression for the current

\[ \bar{J}_k = \text{Tr}(G_W \ast \partial_{p_k} Q_W) \]
Current and conductivity

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$$\bar{J}_k = \text{Tr}(G_W \ast \partial_{p_k} G_W^{-1})$$
Current and conductivity

Thus, we have a WW expression for the current

$$\bar{J}_k = \text{Tr}(G_W * \partial_p G_W^{-1})$$

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

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

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

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

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

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

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

and it will be once again a topological invariant.
Conductivity as topological invariant

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

$$\langle J(x) \rangle \equiv \int dp \ G_W(x, p) \partial_{p_k} Q_W(x, p) \approx j^{(0)} + j^{(1)}_i A^i + j^{(2)}_{lm} F^{lm} + \ldots$$
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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 $Q_W$

$$G_W \ast Q_W = 1$$

and it can may be solved iteratively

$$G_W \approx G_W^{(0)} + G_W^{(0)} \ast (\partial_{p_m} Q_W^{(0)} A_m) \ast G_W^{(0)}.$$
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The Groenewold equation connects $G_W$ and $Q_W$

$$G_W * Q_W = 1$$

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

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

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

thus we have

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

where

$$G_{W,m}^{(1)} = G_W^{(0)} \ast \partial_{p_m} Q_W^{(0)} \ast G_W^{(0)}, \quad G_{W,lm}^{(2)} = \frac{i}{2} G_W^{(0)} \ast \partial_{p_l} Q_W^{(0)} \ast G_W^{(0)} \ast \partial_{p_m} Q_W^{(0)} \ast G_W^{(0)}$$
Conductivity as topological invariant

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where

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

Finally

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

\[ \langle J_k(x) \rangle \approx F_{lm} \frac{i}{2} \int dp \left( G_W^{(0)} * \partial_p Q_W^{(0)} * G_W^{(0)} * \partial_p Q_W^{(0)} * G_W^{(0)} \cdot \partial_p Q_W^{(0)} \right) \]

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

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

where

\[ \mathcal{N} = \frac{\epsilon_{lmk}}{3!4\pi^2} \int d^3p d^3x \left( G_W^{(0)} * \partial_p Q_W^{(0)} * G_W^{(0)} * \partial_p Q_W^{(0)} * G_W^{(0)} * \partial_p Q_W^{(0)} \right) \]
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then in $2 + 1$D the average conductivity is given by
\[ \bar{\sigma}_H \equiv \int dx \sigma_H(x) = \frac{N}{2\pi} \]
where
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This is a topological invariant, yes!
So, we’ve came to

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

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

$$\bar{\sigma}_H \equiv \int d\chi \sigma_H(\chi) = \frac{\mathcal{N}}{2\pi}$$

where

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

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

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

such that

$$(\hat{A}\hat{B})_W = A_W \ast B_W, \quad \text{tr} \hat{A} = \text{Tr} A_W$$

$$\text{Tr}(A_W \ast B_W) = \text{Tr}(A_W B_W)$$

with some appropriate $\ast$ and Tr.

Weyl 1927, Wigner 1932, Groenewold 1946, Moyal 1949

In infinite space, it is given by

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

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

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

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

\[
\langle p + q/2|\hat{A}|p - q/2\rangle \neq 0 \iff qa \ll 1
\]

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**

\[ \tilde{J}_k = \text{Tr}(G_W \ast \partial_{p_k} G_W^{-1}) \]

**Average conductivity**

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

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

**Coleman theorem analog:** We believe that a proof is ready showing that conductivity \( \sigma_H \) is not renormalized in higher loops.

Possible applications and developments:
- lattice models in non-uniform external EM fields
- under non-uniform strain, etc.
This talk is a report of work in progress, being based on:

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M. Suleymanov, M.A. Zubkov,
*Wigner - Weyl formalism and the propagator of Wilson fermions in the presence of varying external electromagnetic field,*
Current as topological invariant

If we have time, let us check that

$$\delta \bar{J}_k \equiv - \delta \text{Tr} [G_W \ast \partial_{p_k} Q_W] = 0$$

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

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

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

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

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

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

If we have time, let us check that

\[ \delta \bar{J}_k \equiv -\delta \text{Tr} [G_W \ast \partial_{p_k} Q_W] = 0 \]

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

\[ \delta (\text{Tr} [G_W \ast \partial_{p_k} Q_W]) = \text{Tr} \left[ G_W^{(0)} \ast \partial_{p_k} Q_W^{(1)} + G_W^{(1)} \ast \partial_{p_k} Q_W^{(0)} \right] \]

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

\[ \text{Tr} \left[ G_W^{(0)} \ast \partial_{p_k} Q_W^{(1)} - G^{(0)} \ast Q_W^{(1)} \ast G^{(0)} \ast \partial_{p_k} Q_W^{(0)} \right] \]

\[ = \text{Tr} \left[ G^{(0)} \ast \partial_{p_k} Q_W^{(0)} \ast G^{(0)} \ast Q_W^{(1)} - G^{(0)} \ast Q_W^{(1)} \ast G^{(0)} \ast \partial_{p_k} Q_W^{(0)} \right] \]

we integrated by parts(!) and used that \( \partial_{p_l} G_W^{(0)} = -G^{(0)} \ast \partial_{p_l} Q_W^{(0)} \ast G^{(0)} \). Now simple cycling inside the Trace gives zero.
For completeness, let's write it in some other forms

\[
\mathcal{N} = \frac{\epsilon_{lmk}}{3!4\pi^2} \int d^3p d^3x \left( G_W^0 \ast \partial_p l Q_W^0 \ast G_W^0 \ast \partial_m Q_W^0 \ast G_W^0 \ast \partial_k Q_W^0 \right)
\]

\[
= \frac{\epsilon_{lmk}}{3!4\pi^2} \int d^3p d^3x \left( G_W \ast \partial_p l G_W^{-1} \ast G_W \ast \partial_m G_W^{-1} \ast G_W \ast \partial_k G_W^{-1} \right)
\]

\[
= \frac{\epsilon_{lmk}}{3!4\pi^2} \int d^3p d^3x \ \text{tr} \left( G_W \ast \partial_p l G_W^{-1} \ast \partial_m G_W \ast \partial_k G_W^{-1} \right)
\]

Using Weyl representation in momenta space, we can also rewrite

\[
\mathcal{N} = \frac{\epsilon_{abc}}{3!4\pi^2} \int dl \ dk \ dp \ dq \ \text{tr} \left[ G(l, k)(\partial_{ka} + \partial_{pa})Q(k, p)(\partial_{pb} + \partial_{qb})G(p, q)(\partial_{qc} + \partial_{lc})Q(q, l) \right]
\]

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

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

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

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

Thus we will have

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

where one needed to use that

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

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

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