Lecture 16 (27 February 2009)

Transport coefficients, cont.

Recall:

$$\begin{aligned}
\mathcal{L} &= [H,\,\cdot\,] && \rho = \text{ equilibrium density matrix} \\
\mathcal{L}_{\text{per}} &= \mathcal{L} + \vec{\lambda}\cdot\vec{\delta}\,, && \vec{\delta} = (\delta_1,\dots,\delta_n) \quad \text{commuting derivations:} \quad [\delta_i,\delta_j] = 0 \\
& && \vec{\lambda} = (\lambda_1,\dots,\lambda_n) \quad \text{complex constants}
\end{aligned}$$

Given the perturbation $\vec{\lambda}\cdot\vec{\delta}$ of $\mathcal{L}$ there is a response: $\langle\vec{\delta}H\rangle_{\text{per}} = \tau(\rho_{\text{per}}\vec{\delta}H)$, according to our philosophy.

Hypothesis:

$$\rho_{\text{per}} = \text{“}\lim_{t\to\infty}\text{”}\,\mathrm{e}^{it\mathcal{L}_{\text{per}}}(\rho)$$

equation of motion

very often must be regularized

Assumptions:

1) $\tau\circ\delta = 0$

   Then

$$\begin{aligned}
\langle\vec{\delta}H\rangle_{\text{per}} &= \tau(\rho_{\text{per}}\vec{\delta}H) = \lim_{t\to\infty}\tau(\mathrm{e}^{it\mathcal{L}_{\text{per}}}(\rho)\vec{\delta}\cdot\vec{H}) \\
&\qquad \text{(formally, } \tau(\mathcal{L}_{\text{per}}(\rho)A) = -\tau(\rho\mathcal{L}_{\text{per}}(A))\text{)} \\
(*) \qquad &= \lim_{t\to\infty}\tau(\rho\mathrm{e}^{-it\mathcal{L}_{\text{per}}}\vec{\delta}\cdot\vec{H})
\end{aligned}$$

2) Bold assumption: use the Dyson expansion for $\mathrm{e}^{-it\mathcal{L}_{\text{per}}}$

$$(*) \underset{\text{power series in }\lambda}{\overset{\text{Dyson}}{=}} \tau(\rho\,\vec{\delta}\cdot\vec{H}) + \underbrace{\lim_{t\to\infty}\tau\left(\rho\int_{\substack{s_0,s_1\geq 0\\ s_0+s_1=1}}\mathrm{e}^{-is_0\mathcal{L}}\vec{\lambda}\cdot\vec{\delta}\mathrm{e}^{-is_1\mathcal{L}}\vec{\delta}\vec{H}\right)}_{1^{\text{st}}\text{ order term}} + \mathcal{O}(\lambda^2)$$

λ^0-term; mostly $= 0$

translate this thing

3) 1^{st} order term. Assumption: $\mathcal{O}(\lambda^2)$ is really negligible.

$\langle \vec{\delta} H \rangle_{\text{per}} = \sigma^\delta \vec{\lambda}$ (σ^δ is a matrix; a tensor in the case of the higher order terms.)

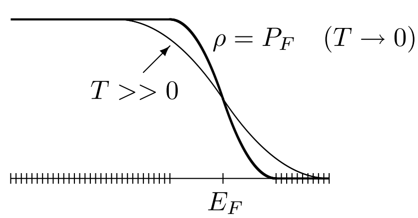
where

$$\sigma^\delta_{\nu\mu} = \lim_{t\to\infty} \overbrace{\tau\left(\rho \int_0^t \mathrm{e}^{-i(t-s_1)\mathcal{L}} \delta_\mu \mathrm{e}^{-is_1\mathcal{L}} \delta_\nu H\right) \mathrm{d}s_1}^{\sigma_{\nu\mu}(t)}$$

is the tensor of transport coefficients in the 1^{st} order approximation (higher orders; higher order tensors). We have:

$$\begin{aligned} \sigma_{\nu\mu}(t) &= \tau\left(\underbrace{\mathrm{e}^{i(t-s_1)\mathcal{L}}(\rho)}_{=\rho \text{ by invariance}} \, \delta_\mu \int_0^t \mathrm{e}^{-s_1\mathcal{L}} \delta_\nu H \mathrm{d}s_1 \right) \\ &\overset{7}{=} \tau\left(-\delta_\mu(\rho) \int_0^t \mathrm{e}^{-is\mathcal{L}} \delta_\nu H \mathrm{d}s \right) \end{aligned}$$

Now *a priori* there is a singularity if $t \to \infty$ in case $\delta_\nu \notin \operatorname{Ker} \mathcal{L}^\perp$. Suppose that the temperature T is very low and the Fermi energy $E_F \in \operatorname{Gap}(H)$. Hence $\rho = P_F =$ the spectral projection of H to states below the Fermi energy:



Remark. If $p = p^2$ and δ is any derivation:

$$\begin{aligned} &\delta(p^2) = p\delta(p) + \delta(p)p\,, \text{ and} \\ &\quad || \\ &\delta(p) = p\delta(p) + p^\perp\delta(p) \quad (p^\perp = 1 - p) \\ &\quad || \\ &\delta(p) = \delta(p)p + \delta(p)p^\perp \quad \text{(ditto)} \\ \Leftrightarrow\ &\delta(p)p = p^\perp\delta(p) \text{ and } p\delta(p) = \delta(p)p^\perp \end{aligned}$$

$(*)$ put this together $\overset{8}{\Rightarrow} \delta(p) = p\delta(p)p^\perp + p^\perp\delta(p)p$

[7]Using the fact that δ_μ is a derivation and that τ is invariant under δ.

The result marked $(*)$ is an extremely important algebraic calculation.

Suppose that we have an eigenbasis of H by $\{\psi_i\}_i$ (perhaps generalized eigenvectors). Then

$$\tau\left(\delta_\mu(P_F)\int_0^t \mathrm{e}^{-is\mathcal{L}}\delta_\nu H \mathrm{d}s\right) = \sum_{i,j}\underbrace{\langle\psi_i \mid \delta_\mu P_F \mid \psi_j\rangle}_{X_{ij}}\langle\psi_j \mid \int_0^t \mathrm{e}^{-is\mathcal{L}}\delta_\nu H \mid \psi_i\rangle$$

where $X_{ij} = 0$ if both ψ_i and ψ_j belong to either $\operatorname{Im} P_F$ or its orthogonal complement

Notes are incomplete from here,

$$\langle\psi_j \mid H\delta_\nu H \mid \psi_i\rangle - \langle\psi_j \mid \delta_\nu(H)H \mid \psi_i\rangle$$

$$H|\psi_i\rangle = E_i|\psi_i\rangle$$

$$\Rightarrow |E_i - E_j| \geq |\tilde{E}_1 - \tilde{E}_0|$$

to here

So

$$\langle\psi_j|\int_0^t \mathrm{e}^{-is\mathcal{L}}\delta_\nu|\psi_i\rangle\mathrm{d}s = \int_0^t \mathrm{e}^{-is(E_j-E_i)}\mathrm{d}s\,\langle\psi_j \mid \delta_\nu H \mid \psi_i\rangle$$

$$\begin{aligned}\lim_{t\to\infty}\int_0^t \mathrm{e}^{-is\omega}\mathrm{d}s &= \text{FT of the Heaviside function}\\ &= \underbrace{PV\left(\frac{1}{i\omega}\right)}_{\text{principal value}} + \frac{\pi}{2}\delta(\omega) \text{ in the distribution space}\end{aligned}$$

Hence

$$\frac{1}{i(E_j - E_i)}\langle\psi_j \mid \delta_\nu H \mid \psi_i\rangle = \frac{1}{i}\langle\psi_j \mid \mathcal{L}^{-1}\delta_\nu H \mid \psi_i\rangle$$

Drawing everything together,

Proposition. $\sigma^\delta_{\nu\mu} = -\frac{1}{i}\tau\left(\delta_\mu(P_F)\mathcal{L}^{-1}\delta_\nu H\right)$

not at all invertible so need P_F

[8] $\delta(p) = p(p\delta(p)) + p^\perp(p^\perp\delta(p)) = p\delta(p)p^\perp + p^\perp\delta(p)p$

Using the extremely important $(*)$ twice (as well as commuting properties of $\mathcal{L}$ with the projections),

$$-\frac{1}{i}\tau\left(\delta_\mu(P_F)\mathcal{L}^{-1}\delta_\nu H\right) = -\frac{1}{i}\tau\left(P_F\delta_\mu(P_F)P_F^\perp\mathcal{L}^{-1}\delta_\nu H + P_F^\perp\delta_\mu(P_F)P_F\mathcal{L}^{-1}\delta_\nu H\right)$$
$$= -\frac{1}{i}\tau\left(P_F\delta_\mu(P_F)P_F^\perp\mathcal{L}^{-1}(\delta_\nu(H))P_F + P_F^\perp\delta_\mu(P_F)P_F\mathcal{L}^{-1}(\delta_\nu(H))P_F^\perp\right)$$

Lemma.

$$P_F^\perp\mathcal{L}^{-1}(\delta_\nu(H))P_F = -P_F^\perp\delta_\nu(P_F)P_F$$
$$\text{and } P_F\mathcal{L}^{-1}(\delta_\nu(H))P_F^\perp = P_F\delta_\nu(P_F)P_F^\perp$$

Proof. Apply $\mathcal{L}$ to right-hand side:

$$\mathcal{L}\left(P_F^\perp\delta_\nu(P_F)P_F\right) = P_F^\perp\underbrace{[H,\delta_\nu(P_F)]}_{\substack{\delta_\nu[H,P_F]-[\delta_\nu(H),P_F] \\ =0-[\delta_\nu(H),P_F]}}P_F \text{ (commutator in } H \text{ commutes with } (\delta_\nu H))$$
$$= -P_F^\perp[\delta_\nu(H),P_F]P_F$$
$$= -P_F^\perp\delta_\nu(H)P_F$$

This proves the first equality. The second is proved in the same sort of way. □

Final result:

Proposition. $\sigma^\delta_{\nu\mu} = -i\tau\left(P_F\delta_\mu(P_F)\delta_\nu(P_F) - \delta_\nu(P_F)\delta_\mu(P_F)\right)$

This is a non-commutative Chern character!!!