

Kubo-Streda formula for KPM based evaluation of the Hall conductivity

Below I compile a short derivation for the Hall conductivity suitable for single energy KPM calculations.

Let us start from Eq. 1.56-1.58 of Jan Mrozek's PhD thesis.

$$\sigma_{\mu\nu} = \frac{e^2\hbar}{4\pi V} \text{Tr} \left[\hat{v}_\nu \hat{G}_+ \hat{v}_\mu (\hat{G}_+ - \hat{G}_-) - \hat{v}_\nu (\hat{G}_+ - \hat{G}_-) \hat{v}_\mu \hat{G}_- \right] \quad (1)$$

$$\begin{aligned} &+ \frac{e^2\hbar}{4\pi V} \text{Tr} \left[(\hat{G}_+ - \hat{G}_-) (\hat{r}_\mu \hat{v}_\nu - \hat{r}_\nu \hat{v}_\mu) \right] \\ &= \sigma_{\mu\nu}^I + \sigma_{\mu\nu}^{II} \end{aligned} \quad (2)$$

Taking in to account the Chebyshev expansion of the Green's function

$$\hat{G}_\pm = \mp \frac{2i}{\sqrt{1-E^2}} \sum_m g_m e^{\pm im \arccos(E)} T_m(\hat{H}) \quad (3)$$

and also (see e.g. Tatiana G. Rappoport's supplementary)

$$\delta(E - H) = -\frac{1}{2\pi i} (\hat{G}_+ - \hat{G}_-) \quad (4)$$

$$\delta(E - \hat{H}) = \frac{2}{\pi\sqrt{1-E^2}} \sum_m g_m T_m(E) T_m(\hat{H}), \quad (5)$$

$$(\hat{G}_+ - \hat{G}_-) = -\frac{4i}{\sqrt{1-E^2}} \sum_m g_m T_m(E) T_m(\hat{H}) \quad (6)$$

where g_m are smoothing kernels of the Chebyshev expansion (e.g. Jackson). We have for the first contribution

$$\sigma_{\mu\nu}^I = \frac{e^2\hbar}{4\pi V} \text{Tr} \left[\hat{v}_\nu \hat{G}_+ \hat{v}_\mu (\hat{G}_+ - \hat{G}_-) - \hat{v}_\nu (\hat{G}_+ - \hat{G}_-) \hat{v}_\mu \hat{G}_- \right] \quad (7)$$

$$= \frac{e^2\hbar}{4\pi V} \text{Tr} \left[\hat{v}_\nu \left(-\frac{2i}{\sqrt{1-E^2}} \sum_m g_m e^{im \arccos(E)} T_m(\hat{H}) \right) \hat{v}_\mu \left(-\frac{4i}{\sqrt{1-E^2}} \sum_n g_n T_n(E) T_n(\hat{H}) \right) - \hat{v}_\nu \left(-\frac{4i}{\sqrt{1-E^2}} \sum_n g_n T_n(E) T_n(\hat{H}) \right) \hat{v}_\mu \left(-\frac{2i}{\sqrt{1-E^2}} \sum_m g_m e^{im \arccos(E)} T_m(\hat{H}) \right) \right] \quad (8)$$

$$= \frac{2e^2\hbar}{\pi V (1-E^2)} \text{Tr} \left[-\hat{v}_\nu \left(\sum_m g_m e^{im \arccos(E)} T_m(\hat{H}) \right) \hat{v}_\mu \left(\sum_n g_n T_n(E) T_n(\hat{H}) \right) + \hat{v}_\nu \left(\sum_m g_m T_m(E) T_m(\hat{H}) \right) \hat{v}_\mu \left(\sum_n g_n e^{in \arccos(E)} T_n(\hat{H}) \right) \right] \quad (9)$$

employing stochastic evaluation of traces

$$\text{Tr}[\hat{O}] \approx \sum_r \langle r | \hat{O} | r \rangle \quad (10)$$

$$\sigma_{\mu\nu}^I = \frac{2e^2\hbar}{\pi V(1-E^2)} \sum_r \left[\langle r | \hat{v}_\nu \left(\sum_m g_m T_m(E) T_m(\hat{H}) \right) \hat{v}_\mu \left(\sum_m g_m e^{-in \arccos(E)} T_n(\hat{H}) \right) | r \rangle - \langle r | \hat{v}_\nu \left(\sum_m g_m \right. \right. \quad (11)$$

$$\left. \left. = \frac{2e^2\hbar}{\pi V(1-E^2)} \sum_r [\langle \alpha r | \beta r \rangle - \langle \gamma r | \delta r \rangle] \right] \quad (12)$$

with

$$\langle \alpha r | = \langle r | \hat{v}_\nu \left(\sum_m g_m T_m(E) T_m(\hat{H}) \right) \quad (13)$$

$$| \beta r \rangle = \hat{v}_\mu \left(\sum_m g_m e^{-in \arccos(E)} T_n(\hat{H}) \right) | r \rangle \quad (14)$$

$$\langle \gamma r | = \langle r | \hat{v}_\nu \left(\sum_m g_m e^{im \arccos(E)} T_m(\hat{H}) \right) \quad (15)$$

$$| \delta r \rangle = \hat{v}_\mu \left(\sum_n g_n T_n(E) T_n(\hat{H}) \right) | r \rangle \quad (16)$$

The above might be organized a bit more intelligently :) The other contribution is somewhat simpler

$$\sigma_{\mu\nu}^{II} = \frac{e^2\hbar}{4\pi V} \text{Tr} \left[\left(\hat{G}_+ - \hat{G}_- \right) (\hat{r}_\mu \hat{v}_\nu - \hat{r}_\nu \hat{v}_\mu) \right] = \quad (17)$$

$$= -\frac{ie^2\hbar}{\pi V\sqrt{1-E^2}} \text{Tr} \left[\left(\sum_m g_m T_m(E) T_m(\hat{H}) \right) (\hat{r}_\mu \hat{v}_\nu - \hat{r}_\nu \hat{v}_\mu) \right] \quad (18)$$

$$= -\frac{ie^2\hbar}{\pi V\sqrt{1-E^2}} \sum_r \left[\langle r | \left(\sum_m g_m T_m(E) T_m(\hat{H}) \right) (\hat{r}_\mu \hat{v}_\nu - \hat{r}_\nu \hat{v}_\mu) | r \rangle \right] \quad (19)$$

$$= -\frac{ie^2\hbar}{\pi V\sqrt{1-E^2}} \sum_r \langle Ar | r \rangle \quad (20)$$

$$\langle Ar | = \langle r | \left(\sum_m g_m T_m(E) T_m(\hat{H}) \right) (\hat{r}_\mu \hat{v}_\nu - \hat{r}_\nu \hat{v}_\mu) \quad (21)$$