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.

$$
\begin{aligned}
\sigma_{\mu\nu} &= \frac{e^2\hbar}{4\pi V}\mathrm{Tr}\left[\hat{v}_\nu\hat{G}_+\hat{v}_\mu\left(\hat{G}_+-\hat{G}_-\right)-\hat{v}_\nu\left(\hat{G}_+-\hat{G}_-\right)\hat{v}_\mu\hat{G}_-\right] \qquad (1)\\
&+\frac{e^2\hbar}{4\pi V}\mathrm{Tr}\left[\left(\hat{G}_+-\hat{G}_-\right)\left(\hat{r}_\mu\hat{v}_\nu-\hat{r}_\nu\hat{v}_\mu\right)\right]\\
&= \sigma^I_{\mu\nu}+\sigma^{II}_{\mu\nu} \qquad (2)
\end{aligned}
$$

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

$$
\hat{G}_\pm = \mp\frac{2\mathrm{i}}{\sqrt{1-E^2}}\sum_m g_m \mathrm{e}^{\pm\mathrm{i}m\arccos(E)}T_m\left(\hat{H}\right) \qquad (3)
$$

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

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

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

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

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

$$
\begin{aligned}
\sigma^I_{\mu\nu} &= \frac{e^2\hbar}{4\pi V}\mathrm{Tr}\left[\hat{v}_\nu\hat{G}_+\hat{v}_\mu\left(\hat{G}_+-\hat{G}_-\right)-\hat{v}_\nu\left(\hat{G}_+-\hat{G}_-\right)\hat{v}_\mu\hat{G}_-\right] \qquad (7)\\
&= \frac{e^2\hbar}{4\pi V}\mathrm{Tr}\Bigg[\hat{v}_\nu\left(-\frac{2\mathrm{i}}{\sqrt{1-E^2}}\sum_m g_m\mathrm{e}^{\mathrm{i}m\arccos(E)}T_m\left(\hat{H}\right)\right)\hat{v}_\mu\left(-\frac{4\mathrm{i}}{\sqrt{1-E^2}}\sum_n g_n T_n(E)T_n\left(\hat{H}\right)\right)-\hat{v}_\nu\left(-\frac{4\mathrm{i}}{\sqrt{1-E^2}}\sum_m g_m T_m(E)T_m\left(\right.\right. \qquad (8)\\
&= \frac{2e^2\hbar}{\pi V\left(1-E^2\right)}\mathrm{Tr}\Bigg[-\hat{v}_\nu\left(\sum_m g_m\mathrm{e}^{\mathrm{i}m\arccos(E)}T_m\left(\hat{H}\right)\right)\hat{v}_\mu\left(\sum_n g_n T_n(E)T_n\left(\hat{H}\right)\right)+\hat{v}_\nu\left(\sum_m g_m T_m(E)T_m\left(\hat{H}\right)\right)\hat{v}_\mu\left(\sum_m g_n\mathrm{e}^{-\mathrm{i}n\arccos}\right. \qquad (9)
\end{aligned}
$$

employing stochastic evaluation of traces

$$
\mathrm{Tr}\left[\hat{O}\right] \approx \sum_r \langle r|\,\hat{O}\,|r\rangle \qquad (10)
$$

$$
\begin{aligned}
\sigma^I_{\mu\nu} &= \frac{2e^2\hbar}{\pi V\left(1-E^2\right)}\sum_r\Bigg[\langle r|\,\hat{v}_\nu\left(\sum_m g_m T_m(E)T_m\left(\hat{H}\right)\right)\hat{v}_\mu\left(\sum_m g_n\mathrm{e}^{-\mathrm{i}n\arccos(E)}T_n\left(\hat{H}\right)\right)|r\rangle-\langle r|\,\hat{v}_\nu\left(\sum_m g_m\mathrm{e}^{\mathrm{i}m\arccos(E)}T_m\left(\hat{H}\right)\right)\hat{v}_\mu\left(\right. \qquad (11)\\
&= \frac{2e^2\hbar}{\pi V\left(1-E^2\right)}\sum_r\left[\langle\alpha r|\,\beta r\rangle-\langle\gamma r|\,\delta r\rangle\right] \qquad (12)
\end{aligned}
$$

with

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

$$
|\beta r\rangle = \hat{v}_\mu\left(\sum_m g_n\mathrm{e}^{-\mathrm{i}n\arccos(E)}T_n\left(\hat{H}\right)\right)|r\rangle \qquad (14)
$$

$$
\langle\gamma r| = \langle r|\,\hat{v}_\nu\left(\sum_m g_m\mathrm{e}^{\mathrm{i}m\arccos(E)}T_m\left(\hat{H}\right)\right) \qquad (15)
$$

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

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

$$
\begin{aligned}
\sigma^{II}_{\mu\nu} &= \frac{e^2\hbar}{4\pi V}\mathrm{Tr}\left[\left(\hat{G}_+ - \hat{G}_-\right)\left(\hat{r}_\mu\hat{v}_\nu - \hat{r}_\nu\hat{v}_\mu\right)\right] = && (17)\\
&= -\frac{\mathrm{i}e^2\hbar}{\pi V\sqrt{1-E^2}}\mathrm{Tr}\left[\left(\sum_m g_m T_m(E) T_m\left(\hat{H}\right)\right)\left(\hat{r}_\mu\hat{v}_\nu - \hat{r}_\nu\hat{v}_\mu\right)\right] && (18)\\
&= -\frac{\mathrm{i}e^2\hbar}{\pi V\sqrt{1-E^2}}\sum_r\left[\langle r|\left(\sum_m g_m T_m(E) T_m\left(\hat{H}\right)\right)\left(\hat{r}_\mu\hat{v}_\nu - \hat{r}_\nu\hat{v}_\mu\right)|r\rangle\right] && (19)\\
&= -\frac{\mathrm{i}e^2\hbar}{\pi V\sqrt{1-E^2}}\sum_r\langle Ar|\,r\rangle && (20)
\end{aligned}
$$

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