likewise, the energy current density operator $\hat{J}^{(0)}_{Q,\mu}$

(given in eq (B22)) takes a form of ②-34

$$\hat{J}^{(0)}_{Q,\mu} \equiv \frac{i}{4\hbar} \sum_{\mathbb{r},\delta,\delta'} \Psi^{\dagger}(\mathbb{r}) \Big\{ \delta_\mu \hat{H}_\delta \cdot \hat{\sigma}_3 \cdot \hat{H}_{\delta'} + \hat{H}_{\delta'} \cdot \hat{\sigma}_3 \cdot \delta_\mu \hat{H}_\delta \Big\} \Psi(\mathbb{r}+\delta+\delta')$$

$$= \frac{i}{4\hbar} \sum_{\mathbb{k}} \left(\beta^{\dagger}_{\mathbb{k}} \ \beta_{-\mathbb{k}} \right) \cdot \Big\{ \Big(\sum_{\delta} \delta_\mu H_\delta e^{i\mathbb{k}\cdot\delta}\Big) \cdot \sigma_3 \cdot \sum_{\delta'} H_{\delta'} e^{i\mathbb{k}\delta'} + \sum_{\delta'} H_{\delta'} e^{i\mathbb{k}\cdot\delta'} \cdot \sigma_3 \cdot \sum_{\delta} \delta_\mu H_\delta e^{i\mathbb{k}\cdot\delta} \Big\} \cdot \begin{pmatrix} \beta_{\mathbb{k}} \\ \beta^{\dagger}_{-\mathbb{k}} \end{pmatrix}$$

$$= \frac{1}{4\hbar} \sum_{\mathbb{k}} \underbrace{\boxed{\left(\gamma^{\dagger}_{\mathbb{k}} \ \gamma_{-\mathbb{k}} \right)}}_{= \Gamma^{\dagger}_{\mathbb{k}}} \cdot T^{\dagger}_{\mathbb{k}} \cdot \Big\{ \frac{\partial H_{\mathbb{k}}}{\partial k_\mu} \cdot \sigma_3 \cdot H_{\mathbb{k}} + H_{\mathbb{k}} \cdot \sigma_3 \cdot \frac{\partial H_{\mathbb{k}}}{\partial k_\mu} \Big\} \cdot T_{\mathbb{k}} \cdot \underbrace{\boxed{\begin{pmatrix} \gamma_{\mathbb{k}} \\ \gamma^{\dagger}_{-\mathbb{k}} \end{pmatrix}}}_{= \Gamma_{\mathbb{k}}}$$

$\Gamma_{\mathbb{k}}$ ← (2N-component boson vector)

$$= \frac{1}{4} \sum_{\mathbb{k}} \Gamma^{\dagger}_{\mathbb{k}} \cdot T^{\dagger}_{\mathbb{k}} \cdot \underbrace{\Big\{ V_{\mathbb{k},\mu}\, \sigma_3\, H_{\mathbb{k}} + H_{\mathbb{k}}\, \sigma_3\, V_{\mathbb{k},\mu} \Big\}}_{\equiv X_{\mathbb{k},\mu}} T_{\mathbb{k}} \cdot \Gamma_{\mathbb{k}} \qquad \text{(B32)}$$

Substituting Eq (B32) & Eq (B31) into Eq. (B30), we use the Wick's theorem to calculate the imaginary time-ordered function ;

$$P^{T}_{\mu\nu}(\tau) = -\frac{1}{\hbar} \langle T_\tau \{ \hat{J}^{(0)}_{Q,\mu}(\tau) \, \hat{J}^{(0)}_{Q,\nu}(0) \} \rangle_0 .$$

$$= -\frac{1}{16\hbar} \sum_{\mathbb{k},\mathbb{k}'} (T^{\dagger}_{\mathbb{k}} X_{\mathbb{k},\mu} T_{\mathbb{k}})_{ij} \, (T^{\dagger}_{\mathbb{k}'} X_{\mathbb{k}',\nu} T_{\mathbb{k}'})_{lm}$$

$$\times \langle T_\tau \{ \Gamma^{\dagger}_{\mathbb{k},i}(\tau+\eta) \, \Gamma_{\mathbb{k},j}(\tau) \, \Gamma^{\dagger}_{\mathbb{k}',l}(\eta) \, \Gamma_{\mathbb{k}',m}(0) \} \rangle_0$$

$$= -\frac{1}{16\hbar} \sum_{\mathbb{k},\mathbb{k}'} (\;----\;)_{ij} \, (\;----\;)_{lm}$$

$$\times \Big\{ \langle T_\tau \{ \Gamma^{\dagger}_{\mathbb{k},i}(\tau) \, \Gamma^{\dagger}_{\mathbb{k}',l}(0) \} \rangle_0 \langle T_\tau \{ \Gamma_{\mathbb{k},j}(\tau) \, \Gamma_{\mathbb{k}',m}(0) \} \rangle_0$$

$$+ \langle T_\tau \{ \Gamma^{\dagger}_{\mathbb{k},i}(\tau) \, \Gamma_{\mathbb{k}',m}(0) \} \rangle_0 \langle T_\tau \{ \Gamma_{\mathbb{k},j}(\tau) \, \Gamma^{\dagger}_{\mathbb{k}',l}(0) \} \rangle_0$$

$$+ \langle T_\tau \{ \Gamma^{\dagger}_{\mathbb{k},i}(\tau+\eta) \, \Gamma_{\mathbb{k},j}(\tau) \} \rangle_0 \langle T_\tau \{ \Gamma^{\dagger}_{\mathbb{k}',l}(\eta) \, \Gamma_{\mathbb{k}',m}(0) \} \rangle_0 \Big\} \quad \text{—(B33)}$$

where the last term in the { } vanishes under the Fourier transformation in eq. (B30). Or due to $\langle \hat{J}^{(0)}_{Q,\mu} \rangle_0 = \mathrm{Tr}[\rho_0 \hat{J}^{(0)}_{Q,\mu}] = 0$ (it is usually the case).

Note that, for $\tau > 0$, we have,

- $\langle T_\tau \{ \Gamma^{+}_{\mathbb{k},i}(\tau)\, \Gamma^{+}_{\mathbb{k}',l}(0) \} \rangle_0$

$$= e^{\tau \epsilon_{\mathbb{k},i}/\hbar}\, g(\epsilon_{\mathbb{k},i})\, \delta_{\mathbb{k},-\mathbb{k}'}\, (\sigma_+)_{il}$$

$$- e^{-\tau \epsilon_{-\mathbb{k},i-N}/\hbar}\, g(-\epsilon_{-\mathbb{k},i-N})\, \delta_{\mathbb{k},-\mathbb{k}'}\, (\sigma_-)_{il}$$

- $\langle T_\tau \{ \Gamma_{\mathbb{k},j}(\tau)\, \Gamma_{\mathbb{k}',m}(0) \} \rangle_0$

$$= - e^{-\tau \epsilon_{\mathbb{k},j}/\hbar}\, g(-\epsilon_{\mathbb{k},j})\, \delta_{\mathbb{k},-\mathbb{k}'}\, (\sigma_+)_{jm}$$

$$+ e^{\tau \epsilon_{-\mathbb{k},j-N}/\hbar}\, g(\epsilon_{-\mathbb{k},j-N})\, \delta_{\mathbb{k},-\mathbb{k}'}\, (\sigma_-)_{jm}$$

- $\langle T_\tau \{ \Gamma^{+}_{\mathbb{k},i}(\tau)\, \Gamma_{\mathbb{k}',m}(0) \} \rangle_0$

$$= e^{\tau \epsilon_{\mathbb{k},i}/\hbar}\, g(\epsilon_{\mathbb{k},i})\, \delta_{\mathbb{k},\mathbb{k}'} \left(\frac{\sigma_0 + \sigma_3}{2} \right)_{im}$$

$$- e^{-\tau \epsilon_{-\mathbb{k},i-N}/\hbar}\, g(-\epsilon_{-\mathbb{k},i-N})\, \delta_{\mathbb{k},\mathbb{k}'} \left(\frac{\sigma_0 - \sigma_3}{2} \right)_{im}$$

$$\cdot \langle T_\tau \{ \Gamma_{\mathbb{k},j}(\tau)\, \Gamma^\dagger_{\mathbb{k}',l}(0) \} \rangle_0$$

$$= -e^{-\tau \epsilon_{\mathbb{k},j}/\hbar}\, g(-\epsilon_{\mathbb{k},j})\, \delta_{\mathbb{k},\mathbb{k}'} \left(\frac{\sigma_0+\sigma_3}{2}\right)_{jl}$$

$$+ e^{\tau \epsilon_{-\mathbb{k},j-N}/\hbar}\, g(\epsilon_{-\mathbb{k},j-N})\, \delta_{\mathbb{k},\mathbb{k}'} \left(\frac{\sigma_0-\sigma_3}{2}\right)_{jl}.$$

where $\sigma_+ = \frac{1}{2}(\sigma_1 + i\sigma_2) = \left(\begin{array}{c|c} 0 & \mathbb{1}_{N\times N} \\ \hline 0 & 0 \end{array}\right)$

$$\sigma_- = \frac{1}{2}(\sigma_1 - i\sigma_2) = \left(\begin{array}{c|c} 0 & 0 \\ \hline \mathbb{1}_{N\times N} & 0 \end{array}\right)$$

$$\frac{\sigma_0+\sigma_3}{2} = \left(\begin{array}{c|c} \mathbb{1}_{N\times N} & 0 \\ \hline 0 & 0 \end{array}\right), \quad \frac{\sigma_0-\sigma_3}{2} = \left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & \mathbb{1}_{N\times N} \end{array}\right)$$

$$g(\epsilon) = \frac{1}{e^{\beta\epsilon}-1}$$

Noting that

$$\left\{\begin{array}{l} \sigma_1 T_{-k} \sigma_1 = T^*_{\mathbb{k}} \quad \text{(apart from a trivial U(1) phase DOF)} \\ \sigma_1 \hat{H}_{-k} \sigma_1 = H^*_k \\ \sigma_1 V_{-k,\mu} \sigma_1 = -V^*_{-k,\mu} \\ \sigma_1 X_{k,\mu} \sigma_1 = X^*_{-k,\mu} = X^\dagger_{-k,\mu} \end{array}\right.$$

$$\Rightarrow \quad T^\dagger_{-k} X_{-k,\mu} T_{-k} = \sigma_1 \left(T^\dagger_k X_{k,\mu} T_k\right)^T \sigma_1$$

Using these, we can show that the first term and the second term in the { } of eq. (B33) are identical to each other;

$$P^{T}_{\mu\nu}(\tau) = \frac{1}{8\hbar}\sum_{\mathbb{k}} (T^{\dagger}_{\mathbb{k}} X_{\mathbb{k},\mu} T_{\mathbb{k}})_{ij} (T^{\dagger}_{\mathbb{k}} X_{\mathbb{k},\nu} T_{\mathbb{k}})_{lm}$$

$$\times \Big\{ e^{\tau(\epsilon_{k,i}-\epsilon_{k,j})/\hbar} g(\epsilon_{k,i}) g(-\epsilon_{k,j}) \left(\frac{\sigma_0+\sigma_3}{2}\right)_{jl} \left(\frac{\sigma_0+\sigma_3}{2}\right)_{mi}$$

$$- e^{\tau(\epsilon_{k,i}+\epsilon_{-k,j-N})/\hbar} g(\epsilon_{k,i}) g(\epsilon_{-k,j-N}) \left(\frac{\sigma_0-\sigma_3}{2}\right)_{jl} \left(\frac{\sigma_0+\sigma_3}{2}\right)_{mi}$$

$$- e^{-\tau(\epsilon_{-k,i-N}+\epsilon_{k,j})/\hbar} g(-\epsilon_{-k,i-N}) g(-\epsilon_{k,j}) \left(\frac{\sigma_0+\sigma_3}{2}\right)_{jl} \left(\frac{\sigma_0-\sigma_3}{2}\right)_{mi}$$

$$+ e^{-\tau(\epsilon_{-k,i-N}-\epsilon_{-k,j-N})/\hbar} g(-\epsilon_{-k,i-N}) g(\epsilon_{-k,j-N}) \left(\frac{\sigma_0-\sigma_3}{2}\right)_{jl} \left(\frac{\sigma_0-\sigma_3}{2}\right)_{mi} \Big\} \quad \text{—(B34)}$$

Taking the Fourier transform with respect to the imaginary time with

$$\cdot \frac{1}{\hbar}\int_0^{\beta\hbar} e^{[i\Omega + (\epsilon_1 - \epsilon_2)/\hbar]\tau} d\tau \; g(\epsilon_1)\, g(-\epsilon_2)$$

$$= \frac{1}{i\Omega\hbar + (\epsilon_1 - \epsilon_2)} \left[g(\epsilon_1) - g(\epsilon_2) \right]$$

---

we obtain

$$P^T_{\mu\nu}(i\Omega) = \frac{1}{8} \sum_{\mathbb{k}} \sum_{i,j=1}^{N}$$

$$\Big\{ \frac{g(\epsilon_{k,i}) - g(\epsilon_{k,j})}{i\Omega\hbar + (\epsilon_{k,i} - \epsilon_{k,j})} (T_k^\dagger X_{k,\mu} T_k)_{ij} (T_k^\dagger X_{k,\nu} T_k)_{ji}$$

$$- \frac{g(\epsilon_{k,i}) - g(-\epsilon_{-k,j})}{i\Omega\hbar + (\epsilon_{k,i} + \epsilon_{-k,j})} (T_k^\dagger X_{k,\mu} T_k)_{i,j+N} (T_k^\dagger X_{k,\nu} T_k)_{j+N,i}$$

$$- \frac{g(-\epsilon_{-k,i}) - g(\epsilon_{k,j})}{i\Omega\hbar - (\epsilon_{-k,i} + \epsilon_{k,j})} (T_k^\dagger X_{k,\mu} T_k)_{i+N,j} (T_k^\dagger X_{k,\nu} T_k)_{j,i+N}$$

$$+ \frac{g(-\epsilon_{-k,i}) - g(-\epsilon_{-k,j})}{i\Omega\hbar - (\epsilon_{-k,i} - \epsilon_{-k,j})} (T_k^\dagger X_{k,\mu} T_k)_{i+N,j+N} (T_k^\dagger X_{k,\nu} T_k)_{j+N,i+N} \Big\}$$

— (B35)

Taking $i\Omega \to \omega + i\delta$ and taking the DC limit in (B28), we finally obtain

$$\lim_{\omega \to 0} J^{0}_{\theta,\mu}(\omega) = \frac{i\hbar}{8} \sum_{\mathbb{k}} \sum_{i,j=1}^{N}$$

$$\Bigg\{ \frac{g(\epsilon_{k,i}) - g(\epsilon_{k,j})}{(\epsilon_{k,i} - \epsilon_{k,j})^2} (T_k^\dagger X_{k,\mu} T_k)_{ij} (T_k^\dagger X_{k,\nu} T_k)_{ji}$$

$$- \frac{g(\epsilon_{k,i}) - g(-\epsilon_{-k,j})}{(\epsilon_{k,i} + \epsilon_{-k,j})^2} (T_k^\dagger X_{k,\mu} T_k)_{i,j+N} (T_k^\dagger X_{k,\nu} T_k)_{j+N,i}$$

$$- \frac{g(-\epsilon_{-k,i}) - g(\epsilon_{k,j})}{(\epsilon_{-k,i} + \epsilon_{k,j})^2} (T_k^\dagger X_{k,\mu} T_k)_{i+N,j} (T_k^\dagger X_{k,\nu} T_k)_{j,i+N}$$

$$+ \frac{g(-\epsilon_{-k,i}) - g(-\epsilon_{-k,j})}{(\epsilon_{-k,i} - \epsilon_{-k,j})^2} (T_k^\dagger X_{k,\mu} T_k)_{i+N,j+N} (T_k^\dagger X_{k,\nu} T_k)_{j+N,i+N} \Bigg\}$$

$$\times C_\nu$$

Since

$$T_k^\dagger X_{k,\mu} T_k = T_k^\dagger V_{k,\mu} T_k \sigma_3 \hat{E}_{d,k} + \hat{E}_{d,k} \sigma_3 T_k^\dagger V_{k,\mu} T_k \qquad \text{(B 36)}$$

we have

- $(T_k^\dagger X_{k,\mu} T_k)_{ij} (T_k^\dagger X_{k,\nu} T_k)_{ji}$

$$= (\epsilon_{k,i} + \epsilon_{k,j})^2 (T_k^\dagger V_{k,\mu} T_k)_{ij} (T_k^\dagger V_{k,\nu} T_k)_{ji}$$

$$\cdot \quad (T_k^\dagger X_{k,\mu} T_k)_{i,j+N} (T_k^\dagger X_{k,\nu} T_k)_{j+N,i}$$

$$= (\epsilon_{k,i} - \epsilon_{-k,j})^2 (T_k^\dagger V_{k,\mu} T_k)_{i,j+N} \times (T_k^\dagger V_{k,\nu} T_k)_{j+N,i}$$

$$\cdot \quad (T_k^\dagger X_{k,\mu} T_k)_{i+N,j+N} (T_k^\dagger X_{k,\nu} T_k)_{j+N,i+N}$$

$$= (\epsilon_{-k,i} + \epsilon_{-k,j})^2 (T_k^\dagger V_{k,\mu} T_k)_{i+N,j+N} \times (T_k^\dagger V_{k,\nu} T_k)_{j+N,i+N}$$

with $i, j = 1, \cdots, N$. Using these, we finally have the "Kubo-contribution" to the energy current (i.e. the 2nd term of Eq (B-23)) ;

$$\lim_{\omega \to 0} J^0_{Q,\mu}(\omega) = \frac{i\hbar}{8} \sum_{k} \sum_{i,j=1}^{N}$$

$$\times \Big\{ \frac{g(\epsilon_{k,i}) - g(\epsilon_{k,j})}{(\epsilon_{k,i} - \epsilon_{k,j})^2} (\epsilon_{k,i} + \epsilon_{k,j})^2 (T_k^\dagger V_{k,\mu} T_k)_{ij} (T_k^\dagger V_{k,\nu} T_k)_{j,i}$$

$$- \frac{g(\epsilon_{k,i}) - g(-\epsilon_{-k,j})}{(\epsilon_{k,i} + \epsilon_{-k,j})^2} (\epsilon_{k,i} - \epsilon_{-k,j})^2 (T_k^\dagger V_{k,\mu} T_k)_{i,j+N} (T_k^\dagger V_{k,\nu} T_k)_{j+N,i}$$

$$- \frac{g(-\epsilon_{-k,i}) - g(\epsilon_{k,j})}{(\epsilon_{-k,i} + \epsilon_{k,j})^2} (\epsilon_{-k,i} - \epsilon_{k,j})^2 (T_k^\dagger V_{k,\mu} T_k)_{i+N,j} (T_k^\dagger V_{k,\nu} T_k)_{j,i+N}$$

$$+ \frac{g(-\epsilon_{-k,i}) - g(-\epsilon_{-k,j})}{(\epsilon_{-k,i} - \epsilon_{-k,j})^2} (\epsilon_{-k,i} + \epsilon_{-k,j})^2 (T_k^\dagger V_{k,\mu} T_k)_{i+N,j+N} (\cdots \nu \cdots)_{j+N,i+N} \Big\}$$

$\times$ CV

For later convenience, let us decompose this into the following two;

$(\nabla_\nu \chi)$.

$$\lim_{\omega \to 0} \overset{\circ}{J}_{Q,\mu}(\omega) \equiv \left(S^{(1)}_{\mu\nu} + S^{(2)}_{\mu\nu} \right) c_\nu$$

with

$$
\begin{aligned}
S^{(1)}_{\mu\nu} + S^{(2)}_{\mu\nu} = \frac{i\hbar}{8} \sum_{k} \sum_{i,j=1}^{N}
\times \Bigg\{ & \frac{g(\epsilon_i) - g(\epsilon_j)}{(\epsilon_i - \epsilon_j)^2} \left\{ (\epsilon_i - \epsilon_j)^2 + 4\epsilon_i \epsilon_j \right\} (\cdot\mu\cdot)_{ij} (\cdot\nu\cdot)_{ji} \\
- & \frac{g(\epsilon_i) - g(-\bar{\epsilon}_j)}{(\epsilon_i + \bar{\epsilon}_j)^2} \left\{ (\epsilon_i + \bar{\epsilon}_j)^2 - 4\epsilon_i \bar{\epsilon}_j \right\} (\cdot\mu\cdot)_{i,j+N} (\cdot\nu\cdot)_{j+N,i} \\
- & \frac{g(-\bar{\epsilon}_i) - g(\epsilon_j)}{(\bar{\epsilon}_i + \epsilon_j)^2} \left\{ (\bar{\epsilon}_i + \epsilon_j)^2 - 4\bar{\epsilon}_i \epsilon_j \right\} (\cdot\mu\cdot)_{i+N,j} (\cdot\nu\cdot)_{j,i+N} \\
+ & \frac{g(-\bar{\epsilon}_i) - g(-\bar{\epsilon}_j)}{(\bar{\epsilon}_i - \bar{\epsilon}_j)^2} \left\{ (\bar{\epsilon}_i - \bar{\epsilon}_j)^2 + 4\bar{\epsilon}_i \bar{\epsilon}_j \right\} (\cdot\mu\cdot)_{i+N,j+N} (\cdot\nu\cdot)_{j+N,i+N} \Bigg\}
\end{aligned}
\quad -(B37)
$$

$\downarrow S^{(2)}_{\mu\nu}$ $\qquad \downarrow S^{(1)}_{\mu\nu}$

(where we use the following notation

$\bar{\epsilon}_i \Leftarrow \epsilon_{-k,i}$, $\epsilon_i \Leftarrow \epsilon_{k,i}$.

Each of these two can be further simplified into

$$S_{\mu\nu}^{(2)} = \frac{i\hbar}{8} \sum_{\mathbb{k}} \sum_{i,j=1}^{N} \Big\{ g(\epsilon_i) (\cdot\mu\cdot)_{ij} (\cdot\nu\cdot)_{ji}$$

$$- g(\epsilon_i) (\cdot\cdot\mu\cdot\cdot)_{i,j+N} (-\nu-)_{j+N,i}$$

$$- g(-\bar{\epsilon}_i) (\cdot\cdot\mu\cdot\cdot)_{i+N,j} (-\nu-)_{j,i+N}$$

$$+ g(-\bar{\epsilon}_i) (\cdot\cdot\mu\cdot\cdot)_{i+N,j+N} (\cdot\cdot\nu\cdot\cdot)_{j+N,i+N} \Big\} \qquad (B38)$$

$$- (\mu \Leftrightarrow \nu) \Big\}$$

$$S_{\mu\nu}^{(1)} = \frac{i\hbar}{2} \sum_{\mathbb{k}} \sum_{i,j=1}^{2N} g\left((\sigma_3 \hat{E}_{d,k})_{ii}\right) \times$$

$$\left\{ (T_k^{\dagger} V_\mu T_k)_{ij} \frac{(\hat{E}_{d,k})_{ii} (\hat{E}_{d,k})_{jj}}{\left((\sigma_3 \hat{E}_{d,k})_{ii} - (\sigma_3 \hat{E}_{d,k})_{jj}\right)^2} (\hat{T}_k^{\dagger} V_\nu T_k)_{ji}\right.$$

$$\left. - (\nu \Leftrightarrow \mu) \right\} \qquad \text{— (B39)}$$

Note that we can exclude in Eq (B38, B39) those terms with $i=j$. This is because the corresponding terms in eq (B35) reduce to zero with finite $i\Omega$.

For those with $i \neq j$, we can use followings

$$\boxed{\begin{aligned}
&\cdot\ (\hat{T}_k^{\dagger}\, \hat{V}_{k,\mu}\, \hat{T}_k)_{ij} = \frac{1}{\hbar}\left(\hat{T}_k\, \frac{\partial \hat{H}_k}{\partial k_\mu} \cdot \hat{T}_k \right)_{ij} \\
&\qquad = \frac{1}{\hbar}\left[(\hat{\sigma}_3 \hat{E}_{d,k})_{ii} - (\hat{\sigma}_3 \hat{E}_{d,k})_{jj} \right] \\
&\qquad\quad \times \left(\frac{\partial \hat{T}_k^{\dagger}}{\partial k_\mu}\, \hat{\sigma}_3\, \hat{T}_k \right)_{ij} \\
&\cdot\ (\hat{T}_k^{\dagger}\, \hat{V}_{k,\nu}\, \hat{T}_k)_{ji} = \frac{1}{\hbar}\left[(\hat{\sigma}_3 \hat{E}_{d,k})_{ii} - (\hat{\sigma}_3 \hat{E}_{d,k})_{jj} \right] \\
&\qquad\quad \times \left(\hat{T}_k^{\dagger} \cdot \hat{\sigma}_3 \cdot \frac{\partial \hat{T}_k}{\partial k_\nu} \right)_{ji}
\end{aligned}}$$

— (B 39)'

so that (B 39) reduces to .

$$S^{(1)}_{\mu\nu} = \frac{i}{2\hbar} \sum_{k} \sum_{i,j=1}^{2N} g\left((\sigma_3 \hat{E}_{d,k})_{ii} \right) (\hat{E}_{d,k})_{ii} \times$$

$$\times \left\{ \left(\frac{\partial \hat{T}_k^{\dagger}}{\partial k_\mu}\, \sigma_3\, \hat{T}_k \right)_{ij} (\hat{E}_{d,k})_{jj} \left(\hat{T}_k^{\dagger} \cdot \hat{\sigma}_3\, \frac{\partial \hat{T}_k}{\partial k_\nu} \right)_{ji} - (\mu \leftrightarrow \nu) \right\}$$

$$\neq \frac{i}{2\hbar} \sum_{k} \sum_{i=1}^{2N} g\left((\sigma_3 \hat{E}_{d,k})_{ii} \right) (\hat{E}_{d,k})_{ii} \times$$

$$\sigma_3 H_k \sigma_3 = T_k E_{d,k} T_k^{\dagger}$$

$$\times \left\{ \left(\frac{\partial \hat{T}_k^{\dagger}}{\partial k_\mu}\, \hat{H}_k\, \frac{\partial \hat{T}_k}{\partial k_\nu} \right)_{ii} - (\mu \leftrightarrow \nu) \right\}$$

$$S_{\mu\nu}^{(1)} = \frac{i}{2\hbar} \int_{-\infty}^{+\infty} d\eta \; \eta \, g(\eta) \times$$

$$\left\{ \mathrm{Tr}\left[\delta(\eta - \hat{\sigma}_3 \hat{E}_{d,k}) \, \sigma_3 \frac{\partial \hat{T}_k^{\dagger}}{\partial k_\mu} \hat{H}_k \frac{\partial \hat{T}_k}{\partial k_\nu} \right] - (\mu \leftrightarrow \nu) \right\} \quad \text{—(B40)}$$

where the Trace (Tr) is over the 2N-dim vector space on which $\hat{H}_k$ are applied.

To summarize so far, the Kubo-contribution to the thermal transport coefficient has been calculated;

$$\delta\langle \hat{J}_{Q,\mu}(t) \rangle_F = \mathrm{Tr}[\hat{\rho}_0 \hat{J}_{Q,\mu}^{(1)}] \quad \text{(B 23)}$$

$$+ \frac{i}{\hbar} \int_{-\infty}^{t} dt' \, \mathrm{Tr}[\hat{\rho}_0 [\hat{F}_H(t'), \hat{J}_{Q,\mu,H}^{(0)}(t)]]$$

$$= \langle \hat{J}_{Q,\mu}^{(1)} \rangle_0$$

"Kubo contribution"

$$+ (S_{\mu\nu}^{(1)} + S_{\mu\nu}^{(2)}) c_\nu \quad \text{—(B 40)'}$$

where $S_{\mu\nu}^{(1,2)}$ are given in eq.(B38) & (B40). respectively.

The remaining quantity to be evaluated is an ②-46

equilibrium expectation value of the first order in X_H of the energy current operator;

$$\mathrm{Tr}\left[\hat{\rho}_0 \hat{J}^{(1)}_{\theta,\mu}\right] = \langle J^{(1)}_{\theta,\mu} \rangle_0 = ?$$

where the first order in X_H of the energy current operator is given in eq.(B22):

$$\hat{J}^{(1)}_{\theta,\mu} = -c_\nu \frac{i\hbar}{8} \sum_{H} \Psi^\dagger(H) \left\{ \hat{V}_\mu \hat{\sigma}_3 \hat{V}_\nu - \hat{V}_\nu \hat{\sigma}_3 \hat{V}_\mu \right\} \Psi(H)$$

$$+ c_\nu \frac{1}{8} \sum_{H} \Psi^\dagger(H) \left\{ (\hat{r}_\nu \hat{V}_\mu \hat{\sigma}_3 + 3\hat{V}_\mu \hat{\sigma}_3 \hat{r}_\nu) \cdot \hat{H}_0 + \hat{H}_0 \cdot (3\hat{r}_\nu \hat{\sigma}_3 \hat{V}_\mu + \hat{\sigma}_3 \hat{V}_\mu \hat{r}_\nu) \right\} \Psi(H) \quad \text{(B41)}$$

Correspondingly, we have two contribution to

$$\langle J^{(1)}_{\theta,\mu} \rangle_0 = M^{(2)}_{\mu\nu} c_\nu + M^{(1)}_{\mu\nu} c_\nu$$

with

$$M_{\mu\nu}^{(2)} \triangleq -\frac{i\hbar}{8}\left\langle \sum_{t} \Psi^{\dagger}(t)\left\{\hat{V}_{\mu}\hat{\sigma}_3\hat{V}_{\nu}-\hat{V}_{\nu}\hat{\sigma}_3\hat{V}_{\mu}\right\}\Psi(t)\right\rangle_0$$

$$= -\frac{i\hbar}{8}\sum_{\mathbb{k}}\langle \Gamma^{\dagger}_{\mathbb{k},i}\,\Gamma_{\mathbb{k},j}\rangle_0 \times$$

$$\left(\left(T^{\dagger}_{\mathbb{k}}\hat{V}_{\mathbb{k},\mu}\hat{\sigma}_3\hat{V}_{\mathbb{k},\nu}T_{\mathbb{k}}\right)_{ij} - (\mu\leftrightarrow\nu)\right)$$

$$= -\frac{i\hbar}{8}\sum_{\mathbb{k}}\sum_{i=1}^{N}$$

$$\Big\{ g(\epsilon_{\mathbb{k},i})\left(\hat{T}^{\dagger}_{\mathbb{k}}\hat{V}_{\mathbb{k},\mu}\hat{\sigma}_3\hat{V}_{\mathbb{k},\nu}T_{\mathbb{k}}\right)_{ii}$$

$$- g(-\epsilon_{-\mathbb{k},i})\left(\hat{T}^{\dagger}_{\mathbb{k}}\hat{V}_{\mathbb{k},\mu}\hat{\sigma}_3\hat{V}_{\mathbb{k},\nu}T_{\mathbb{k}}\right)_{i+N,i+N}$$

$$- (\mu\leftrightarrow\nu)\Big\}$$

$$\neq -S_{\mu\nu}^{(2)} \quad (\text{see Eq. (B38)}). \tag{B42}$$

$$\hat{\sigma}_3 = T_k\hat{\sigma}_3 T_k^{\dagger}$$

Namely $M_{\mu\nu}^{(2)}$ cancels with $S_{\mu\nu}^{(2)}$ in (B40)!

$$M_{\mu\nu}^{(1)} \stackrel{\Delta}{\equiv} \frac{1}{8} \Big\langle \sum_{H} \Psi^{\dagger}(H) \Big\{ \underline{\underline{(\hat{r}_\nu \hat{V}_\mu \hat{\sigma}_3 + 3\hat{V}_\mu \hat{\sigma}_3 \hat{r}_\nu)}} \hat{H}_0$$

$$+ \hat{H}_0 \underline{\underline{(3\hat{r}_\nu \hat{\sigma}_3 \hat{V}_\mu + \hat{\sigma}_3 \hat{V}_\mu \hat{r}_\nu)}} \Big\} \Psi(H) \Big\rangle_0 . \qquad \text{(B43)}$$

- Unlike $M_{\mu\nu}^{(2)}$, $M_{\mu\nu}^{(1)}$ contain the position operator $(\hat{r}_\nu)$, which, by itself, is ill-defined in the Hilbert space with the periodic boundary condition.

- However, $\{\ \ \}$ in $M_{\mu\nu}^{(1)}$ turns out to be rewritten into an operator which is well-defined in the Hilbert space with the p.b.c.

- To see this, we follow the Smřčka and Středa method.

To this end, we first rewrite $\Psi(H)$ in terms of Γ_{k} (see (B31)).

$$\Psi(\mathbb{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbb{k}} e^{i\mathbb{k}\cdot\mathbb{r}}\, \hat{T}_{\mathbb{k}} \cdot \Gamma_{\mathbb{k}} \qquad \text{②-49}$$

$\Psi(\mathbb{r})$: 2N-component vector.

$\Gamma_{\mathbb{k}}$: 2N vector field

$e^{i\mathbb{k}\cdot\mathbb{r}}\hat{T}_{\mathbb{k}} \equiv \hat{t}_{\mathbb{k}}(\mathbb{r})$: 2N×2N paraunitary matrix

$$[\hat{\sigma}_3, \hat{r}_\nu] = 0.$$

$$M^{(1)}_{\mu\nu} = \frac{1}{8}\sum_{\mathbb{k},\mathbb{k}'}\sum_{i,j=1}^{2N} \langle \Gamma^{\dagger}_{\mathbb{k},i}\Gamma_{\mathbb{k}',j}\rangle_0$$

$$\times \sum_{\mathbb{r}} \Big(t^{\dagger}_{\mathbb{k}}(\mathbb{r})\cdot\big\{(\hat{r}_\nu \hat{V}_\mu \hat{\sigma}_3 + 3\hat{V}_\mu \hat{r}_\nu \hat{\sigma}_3)\cdot \hat{H}_0$$

$$+ \hat{H}_0\cdot(3\hat{\sigma}_3 \hat{r}_\nu \hat{V}_\mu + \hat{\sigma}_3 \hat{V}_\mu \hat{r}_\nu)\big\}\cdot t_{\mathbb{k}'}(\mathbb{r})\Big)_{ij}$$

$$= \frac{1}{8}\sum_{\mathbb{k}}\sum_{i=1}^{2N} (\sigma_3)_{ii}\, g\big((\sigma_3 \hat{E}_{d,k})_{ii}\big)$$

$$\times \sum_{\mathbb{r}} \Big(t^{\dagger}_{\mathbb{k}}(\mathbb{r})\cdot\big\{(\hat{r}_\nu \hat{V}_\mu \hat{\sigma}_3 + 3\hat{V}_\mu \hat{r}_\nu \hat{\sigma}_3)\cdot \hat{H}_0$$

$$+ \hat{H}_0\cdot(3\hat{\sigma}_3 \hat{r}_\nu \hat{V}_\mu + \hat{\sigma}_3 \hat{V}_\mu \hat{r}_\nu)\big\}\cdot t_{\mathbb{k}}(\mathbb{r})\Big)_{ii}$$

Note that

$$\begin{cases} \hat{H}_0\cdot t_{\mathbb{k}}(\mathbb{r}) = \sigma_3\, t_{\mathbb{k}}(\mathbb{r})\cdot(\sigma_3 \hat{E}_{d,k}) \\ t^{\dagger}_{\mathbb{k}}(\mathbb{r})\cdot \hat{H}_0 = (\sigma_3 \hat{E}_{d,k})\cdot t^{\dagger}_{\mathbb{k}}(\mathbb{r})\cdot \sigma_3 \end{cases}$$

$$M_{\mu\nu}^{(1)} = \frac{1}{2} \sum_{\mathbb{k}} \sum_{i=1}^{2N} (E_{d,k})_{ii}\, g\left((\sigma_3 \hat{E}_{d,k})_{ii}\right)$$

$$\times \sum_{\mathbb{H}} \left(t_{\mathbb{k}}^{\dagger}(\mathbb{H}) \cdot (\hat{r}_\nu \hat{V}_\mu + \hat{V}_\mu \hat{r}_\nu) \cdot t_{\mathbb{k}}(\mathbb{H}) \right)_{ii}$$

(B-44)

Noting that

$$\sum_{\mathbb{k}} t_{\mathbb{k}}(\mathbb{H}) \cdot \hat{\sigma}_3 \cdot t_{\mathbb{k}}^{\dagger}(\mathbb{H}') = \hat{\sigma}_3\, \delta_{\mathbb{H},\mathbb{H}'}$$

(B-46)

we can rewrite $M_{\mu\nu}^{(1)}$ as follows;

$$M_{\mu\nu}^{(1)} = \frac{1}{2} \int_{-\infty}^{+\infty} d\eta\, \eta\, g(\eta) \times$$

$$\mathrm{tr}\left[\hat{\sigma}_3 (\hat{r}_\nu \hat{V}_\mu + \hat{V}_\mu \hat{r}_\nu)\, \delta(\eta - \sigma_3 \hat{H}_0) \right]$$

(B-45)

where the trace (tr) is taken not only over the sublattice and particle-hole index but also over the unit cell index ($\mathbb{H}$)

(tr ≠ Tr)

To see the indentity between (B-44) & (B-45), use (B-46) for $\hat{\sigma}_3$ in eq.(B-45);

(r.h.s) of (B-45)

$$= \frac{1}{2}\int_{-\infty}^{+\infty} \eta\, g(\eta) \times$$

$$\mathrm{tr}\left[\sum_{\mathbb{K}} t_{\mathbb{K}} \cdot \sigma_3 \cdot t_{\mathbb{K}}^{\dagger} (\hat{r}_\nu \hat{V}_\mu + \hat{V}_\mu \hat{r}_\nu) \times \delta(\eta - \sigma_3 \hat{H}_0) \right]$$

$$= \frac{1}{2}\sum_{\mathbb{K}} \int_{-\infty}^{+\infty} \eta\, g(\eta) \times$$

$$\sum_{H} \mathrm{Tr}\left[\hat{\sigma}_3 \cdot t_{\mathbb{K}}^{\dagger}(H) \cdot (\hat{r}_\nu \hat{V}_\mu + \hat{V}_\mu \hat{r}_\nu) \cdot t_{\mathbb{K}}(H) \times \delta(\eta - (\sigma_3 \hat{E}_{d,k}) \right]$$

where we use

$$\delta(\eta - \sigma_3 \hat{H}_0)\, \hat{t}_{\mathbb{K}} = \hat{t}_{\mathbb{K}}\, \delta(\eta - \sigma_3 \hat{E}_{d,k})$$

Taking the integral over η, we have the r.h.s. of (B-44). ▨

We further make the integrand in Eq(B45) into an antisymmetric form with respect μ and ν:

$$tr\left[\hat{\sigma}_3\left(\hat{r}_\nu \hat{V}_\mu + \hat{V}_\mu \hat{r}_\nu\right)\delta(\eta - \sigma_3 \hat{H}_0)\right]$$

$$\overset{\curlyvee}{=} tr\left[\left\{\hat{\sigma}_3 \hat{r}_\nu \hat{V}_\mu + \frac{1}{i\hbar}\left(\hat{r}_\mu \sigma_3 \hat{H}_0 - \sigma_3 \hat{H}_0 \hat{r}_\mu\right)\hat{r}_\nu\right\} \times \delta(\eta - \sigma_3 \hat{H}_0)\right]$$

$\hat{V}_\mu = \frac{1}{i\hbar}[\hat{r}_\mu, \hat{H}_0]$

$$\overset{\curlyvee}{=} tr\left[\left\{\hat{\sigma}_3 \hat{r}_\nu \hat{V}_\mu - \hat{r}_\mu \frac{1}{i\hbar}[\hat{r}_\nu, \sigma_3 \hat{H}_0]\right\}\delta(\eta - \sigma_3 \hat{H}_0)\right]$$

$\sigma_3 \hat{H}_0$ commutes with $\delta(\eta - \sigma_3 \hat{H}_0)$

$$\overset{\curlyvee}{=} tr\left[\sigma_3\left(\hat{r}_\nu \hat{V}_\mu - \hat{r}_\mu \hat{V}_\nu\right)\delta(\eta - \sigma_3 \hat{H}_0)\right]$$

$[\sigma_3, r_\nu] = 0$

Equivalently, we have

$$M_{\mu\nu}^{(1)} = \frac{1}{2}\int_{-\infty}^{+\infty} d\eta\, \eta\, g(\eta) \times tr\left[\hat{\sigma}_3\left(\hat{r}_\nu \hat{V}_\mu - \hat{r}_\mu \hat{V}_\nu\right)\delta(\eta - \sigma_3 \hat{H}_0)\right] \quad \text{(B-46)}$$

We follow the Smrčka and Středa, to introduce following two functions.

$$A_{\mu\nu}(\eta) \triangleq i\,\mathrm{tr}\Big[\sigma_3 \hat{V}_\mu \frac{d\hat{G}^+}{d\eta} \sigma_3 \hat{V}_\nu \delta(\eta - \sigma_3 \hat{H}_0)$$

$$- \sigma_3 \hat{V}_\mu \delta(\eta - \sigma_3 \hat{H}_0) \sigma_3 \hat{V}_\nu \frac{d\hat{G}^-}{d\eta}\Big] \quad \text{—(B47)}$$

$$B_{\mu\nu}(\eta) \triangleq i\,\mathrm{tr}\Big[\sigma_3 \hat{V}_\mu \hat{G}^+ \sigma_3 \hat{V}_\nu \delta(\eta - \sigma_3 \hat{H}_0)$$

$$- \sigma_3 \hat{V}_\mu \delta(\eta - \sigma_3 \hat{H}_0) \sigma_3 \hat{V}_\nu \hat{G}^-\Big] \quad \text{—(B48)}$$

where the retarded and advanced Green's function $G^\pm$ are defined as

$$G^\pm \triangleq [\eta \pm i0 - \hat{\sigma}_3 \hat{H}_0]^{-1} \quad \text{—(B49)}$$

We can relate these two functions with Eq. (B-46) as follows;

②-54

$$A_{\mu\nu}(\eta) - \frac{1}{2}\frac{dB_{\mu\nu}(\eta)}{d\eta} = -\frac{1}{2\hbar}\mathrm{tr}\left[\sigma_3(\hat{r}_\nu\hat{V}_\mu - \hat{r}_\mu\hat{V}_\nu)\frac{d}{d\eta}\delta(\eta-\sigma_3\hat{H}_0)\right] \quad \text{(B50)}$$

Smrčka–Středa formula.

where we used (See J. Phys. C. 10 2153 (1997))

$$\begin{cases} \hat{G}^+ - \hat{G}^- = -2\pi i\,\delta(\eta - \sigma_3\hat{H}_0) \\ \hat{V}_\mu = \frac{i}{\hbar}\left[\hat{r}_\mu, \sigma_3(\hat{G}^\pm)^{-1}\right] \end{cases} \quad \text{(B51)}$$

Using this formula, (B-46) is given only by the velocity operator;

$$M^{(1)}_{\mu\nu} = -\hbar\int_{-\infty}^{+\infty} d\eta\,\eta\,g(\eta)\int_{-\infty}^{\eta} d\tilde{\eta}\left(A_{\mu\nu}(\tilde{\eta}) - \frac{1}{2}\frac{dB_{\mu\nu}(\tilde{\eta})}{d\tilde{\eta}}\right) \quad \text{(B-52)}$$

Since $A_{\mu\nu}(\eta)$ and $B_{\mu\nu}(\eta)$ are given only by the velocity operator (not by the position operator), we can readily find its Fourier representation;

$A_{\mu\nu,\mathbb{k}}(\eta)$

$$A_{\mu\nu}(\eta) = i\sum_{\mathbb{k}} \mathrm{Tr}\Big[\hat{\sigma}_3 \hat{V}_{\mathbb{k},\mu} \frac{d\hat{G}^{+}_{\mathbb{k}}}{d\eta} \hat{\sigma}_3 \hat{V}_{\mathbb{k},\nu}\, \delta(\eta - \hat{\sigma}_3 \hat{H}_{\mathbb{k}}) - \hat{\sigma}_3 \hat{V}_{\mathbb{k},\mu}\, \delta(\eta - \hat{\sigma}_3 \hat{H}_{\mathbb{k}})\, \hat{\sigma}_3 \hat{V}_{\mathbb{k},\nu} \frac{d\hat{G}^{-}_{\mathbb{k}}}{d\eta}\Big] \quad \text{—(B53)}$$

$$B_{\mu\nu}(\eta) = i\sum_{\mathbb{k}} \mathrm{Tr}\Big[\hat{\sigma}_3 \hat{V}_{\mathbb{k},\mu} \hat{G}^{+}_{\mathbb{k}} \hat{\sigma}_3 \hat{V}_{\mathbb{k},\nu}\, \delta(\eta - \hat{\sigma}_3 \hat{H}_{\mathbb{k}}) - \hat{\sigma}_3 \hat{V}_{\mathbb{k},\mu}\, \delta(\eta - \hat{\sigma}_3 \hat{H}_{\mathbb{k}})\, \hat{\sigma}_3 \hat{V}_{\mathbb{k},\nu} \hat{G}^{-}_{\mathbb{k}}\Big] \quad \text{—(B54)}$$

$B_{\mu\nu,\mathbb{k}}(\eta)$

where

$$\hat{G}^{\pm}_{\mathbb{k}} = \left[\eta \pm i0 - \hat{\sigma}_3 \hat{H}_{\mathbb{k}}\right]^{-1} \quad \text{—(B55)}$$

and the trace (Tr) here is taken only over the sublattice and particle-hole indices.

Thus, both $A_{\mu\nu,\mathbb{k}}(\eta)$ and $B_{\mu\nu,\mathbb{k}}(\eta)$ are given by an $\mathbb{k}$-derivative of the para-unitary transformation;

$$A_{\mu\nu,\mathbb{k}}(\eta) = -i \,\mathrm{Tr}\Big[T_{\mathbb{k}}\, \sigma_3\, T_{\mathbb{k}}^{\dagger} \cdot V_{\mathbb{k},\mu} \frac{1}{(\eta + i0 - \sigma_3 \hat{H}_{\mathbb{k}})^2}$$

$$\times\, T_{\mathbb{k}}\, \sigma_3\, T_{\mathbb{k}}^{\dagger} \cdot V_{\mathbb{k},\nu}\, \delta(\eta - \sigma_3 \hat{H}_{\mathbb{k}}) \Big]$$

$$+ i\, \mathrm{Tr}\Big[T_{\mathbb{k}}\, \sigma_3\, T_{\mathbb{k}}^{\dagger} \cdot V_{\mathbb{k},\mu}\, \delta(\eta - \sigma_3 \hat{H}_{\mathbb{k}})$$

$$\times\, T_{\mathbb{k}}\, \sigma_3\, T_{\mathbb{k}}^{\dagger} \cdot V_{\mathbb{k},\nu} \frac{1}{(\eta - i0 - \sigma_3 \hat{H}_{k})^2} \Big].$$

$$= -i \sum_{n,m=1}^{2N} (T_{\mathbb{k}}^{\dagger} V_{\mathbb{k},\mu} T_{\mathbb{k}})_{nm} \frac{(\sigma_3)_{mm}}{\big((\sigma_3 \hat{E}_{d,k})_{nn} - (\sigma_3 \hat{E}_{d,k})_{mm} + i0\big)^2}$$

$$\times\, (T_{\mathbb{k}}^{\dagger} V_{\mathbb{k},\nu} T_{\mathbb{k}})_{mn}\, \delta\big(\eta - (\sigma_3 \hat{E}_{d,k})_{nn}\big)\, (\sigma_3)_{nn}$$

$$+ i \sum_{n,m=1}^{2N} (T_{\mathbb{k}}^{\dagger} V_{\mathbb{k},\nu} T_{\mathbb{k}})_{nm} \frac{(\sigma_3)_{mm}}{\big((\sigma_3 E_{d,k})_{nn} - (\sigma_3 \hat{E}_{d,k})_{mm} - i0\big)^2}$$

$$\times\, (T_{\mathbb{k}}^{\dagger} V_{\mathbb{k},\mu} T_{\mathbb{k}})_{mn}\, \delta\big(\eta - (\sigma_3 \hat{E}_{d,k})_{nn}\big)\, (\sigma_3)_{nn}$$

where n, m denote the energy band index (including particle-hole index). Those terms with $n=m$ vanish because of a cancellation between the first term and the second term.

- For those terms with $n \neq m$, we use (B-39)$'$ again to rewrite $A_{\mu\nu,\mathbb{k}}(\eta)$ as follows;

$$A_{\mu\nu,\mathbb{k}}(\eta) = -\frac{i}{\hbar^2}\Big\{\mathrm{Tr}\Big[\hat{\sigma}_3\,\delta(\eta-\sigma_3\hat{E}_{d,k})\times\left(\frac{\partial T_{\mathbb{k}}^\dagger}{\partial k_\mu}\cdot\sigma_3\,T_{\mathbb{k}}\right)\cdot\sigma_3\cdot\left(T_{\mathbb{k}}^\dagger\cdot\sigma_3\frac{\partial T_{\mathbb{k}}}{\partial k_\nu}\right)\Big]-(\mu\leftrightarrow\nu)\Big\}$$

$$= -\frac{i}{\hbar^2}\Big\{\mathrm{Tr}\Big[\hat{\sigma}_3\,\delta(\eta-\sigma_3\hat{E}_{d,k})\frac{\partial T_{\mathbb{k}}^\dagger}{\partial k_\mu}\sigma_3\frac{\partial T_{\mathbb{k}}}{\partial k_\nu}\Big]-(\mu\leftrightarrow\nu)\Big\} \quad \text{— (B 56)}$$

- For $B_{\mu\nu,\mathbb{k}}(\eta)$, the situation becomes a little subtle (for me) and needs some remarks.

$B_{\mu\nu,\mathbb{k}}(\eta)$

$$= i \sum_{n,m=1}^{2N} (T_{\mathbb{k}}^{\dagger} V_{\mathbb{k},\mu} T_{\mathbb{k}})_{nm} \frac{(\sigma_3)_{mm}}{((\sigma_3 E_{d,\mathbb{k}})_{nn} - (\sigma_3 E_{d,\mathbb{k}})_{mm} + i\delta)}$$

$$\times (T_{\mathbb{k}}^{\dagger} V_{\mathbb{k},\nu} T_{\mathbb{k}})_{mn} \, \delta(\eta - (\sigma_3 E_{d,\mathbb{k}})_{nn}) \, (\sigma_3)_{nn}$$

$$- i \sum_{n,m=1}^{2N} (T_{\mathbb{k}}^{\dagger} V_{\mathbb{k},\nu} T_{\mathbb{k}})_{nm} \frac{(\sigma_3)_{mm}}{((\sigma_3 E_{d,\mathbb{k}})_{nn} - (\sigma_3 E_{d,\mathbb{k}})_{mm} - i\delta)}$$

$$\times (T_{\mathbb{k}}^{\dagger} V_{\mathbb{k},\mu} T_{\mathbb{k}})_{mn} \, \delta(\eta - (\sigma_3 E_{d,\mathbb{k}})_{nn}) \, (\sigma_3)_{nn}$$

For those terms with $n = m$, we use

$$(T_{\mathbb{k}}^{\dagger} V_{\mathbb{k},\mu} T_{\mathbb{k}})_{nn} = \begin{cases} \dfrac{1}{\hbar} \dfrac{\partial \epsilon_{\mathbb{k},n}}{\partial k_\mu} & (n = 1, \cdots, N) \\[2ex] \dfrac{1}{\hbar} \dfrac{\partial \epsilon_{-\mathbb{k},n}}{\partial k_\mu} & (n = N+1, \cdots, 2N) \end{cases}$$

, to obtain

$$\frac{2}{\delta \hbar^2} \left\{ \sum_{n=1}^{N} \frac{\partial \epsilon_{\mathbb{k},n}}{\partial k_\mu} \frac{\partial \epsilon_{\mathbb{k},n}}{\partial k_\nu} \delta(\eta - \epsilon_{\mathbb{k},n}) + \sum_{n=N+1}^{2N} \frac{\partial \epsilon_{-\mathbb{k},n}}{\partial k_\mu} \frac{\partial \epsilon_{-\mathbb{k},n}}{\partial k_\nu} \delta(\eta + \epsilon_{-\mathbb{k},n}) \right\}$$

- physically speaking, δ (small quantity) corresponds to an inverse of life time of quasi-particle boson (τ), so that it takes a following form;

$$\frac{2\tau}{\hbar^2}\cdot\left\{\sum_{n=1}^{N}\frac{\partial\epsilon_{\mathbb{k},n}}{\partial k_\mu}\cdot\frac{\partial\epsilon_{\mathbb{k},n}}{\partial k_\nu}\,\delta(\eta-\epsilon_{\mathbb{k},n})\right.$$
$$\left.+\sum_{n=N+1}^{2N}\frac{\partial\epsilon_{-\mathbb{k},n}}{\partial k_\mu}\cdot\frac{\partial\epsilon_{-\mathbb{k},n}}{\partial k_\nu}\,\delta(\eta+\epsilon_{-\mathbb{k},n})\right\}$$

- For $\mu\neq\nu$ (Hall conductivity), this contribution always vanishes after the integration over momentum $\mathbb{k}$ (at least) for any systems I can imagine.*

Thus we ignore this in the following.

• For those terms with $n \neq m$, we use eq (B-39') to rewrite $B_{\mu\nu,\mathbb{k}}(\eta)$ as follows;

$$B_{\mu\nu,\mathbb{k}}(\eta) = \frac{i}{\hbar^2}\Big\{ \mathrm{Tr}\Big[\sigma_3\, \delta(\eta - \sigma_3 \hat{E}_{d,k}) \times \left(\frac{\partial T_k^\dagger}{\partial k_\mu} \sigma_3 T_k \right) \sigma_3 (\eta - \sigma_3 \hat{E}_{d,k}) \left(T_k^\dagger \sigma_3 \frac{\partial T_k}{\partial k_\nu} \right) \Big] - (\mu \leftrightarrow \nu) \Big\} \quad -(B57).$$

• Eq. (B56) suggests the following identity;

$$\int_{-\infty}^{+\infty} d\eta \left(A_{\mu\nu,\mathbb{k}}(\eta) - \frac{1}{2} \frac{d B_{\mu\nu,\mathbb{k}}(\eta)}{d\eta} \right)$$

$$= \int_{-\infty}^{+\infty} d\eta\, A_{\mu\nu,\mathbb{k}}(\eta)$$

$$= -\frac{i}{\hbar^2}\left\{ \mathrm{Tr}\left[\sigma_3 \frac{\partial T_{\mathbb{k}}^\dagger}{\partial k_\mu} \sigma_3 \frac{\partial T_{\mathbb{k}}}{\partial k_\nu} \right] - (\mu \leftrightarrow \nu) \right\}$$

$$= 0 \quad (\text{see } \ldots\ldots) \quad -(B58)$$

Using (B-58), we can rewrite (B-52) as follows;

$$M^{(1)}_{\mu\nu} = \hbar \sum_{\mathbb{k}} \left(\int_0^{+\infty} d\eta \int_\eta^{\infty} d\tilde{\eta} + \int_{-\infty}^{0} d\eta \int_\eta^{-\infty} d\tilde{\eta} \right)$$

$$\times\ \eta\, g(\eta) \left(A_{\mu\nu,\mathbb{k}}(\tilde{\eta}) - \frac{1}{2} \frac{d B_{\mu\nu,\mathbb{k}}(\tilde{\eta})}{d\tilde{\eta}} \right)$$

Since

$$\boxed{\begin{aligned} \int_0^{\infty} d\eta \int_\eta^{\infty} d\tilde{\eta} &= \int_0^{+\infty} d\tilde{\eta} \int_0^{\tilde{\eta}} d\eta \\ \int_{-\infty}^{0} d\eta \int_\eta^{-\infty} d\tilde{\eta} &= \int_{-\infty}^{0} d\tilde{\eta} \int_0^{\tilde{\eta}} d\eta \end{aligned}}$$

$$M^{(1)}_{\mu\nu} = \hbar \sum_{\mathbb{k}} \int_{-\infty}^{+\infty} d\tilde{\eta} \left(A_{\mu\nu,\mathbb{k}}(\tilde{\eta}) - \frac{1}{2} \frac{d B_{\mu\nu,\mathbb{k}}(\tilde{\eta})}{d\tilde{\eta}} \right)$$

$$\times \int_0^{\tilde{\eta}} d\eta\ \eta\, g(\eta)$$

Taking integral by part for the second term, we finally reach the following for $M^{(1)}_{\mu\nu}$;

$M_{\mu\nu}^{(1)}$

$$= -\frac{i}{\hbar}\sum_{\mathbb{k}}\int_{-\infty}^{+\infty} d\tilde{\eta}\ \mathrm{Tr}\left[\sigma_3\,\delta(\tilde{\eta}-\sigma_3\hat{E}_{d,k})\frac{\partial T_k^{\dagger}}{\partial k_\mu}\sigma_3\frac{\partial T_k}{\partial k_\nu}\right]$$

$$\times\int_0^{\tilde{\eta}}\eta\, g(\eta)\, d\eta$$

$$+\frac{i}{2\hbar}\sum_{\mathbb{k}}\int_{-\infty}^{+\infty} d\tilde{\eta}\ \mathrm{Tr}\Big[\sigma_3\,\delta(\tilde{\eta}-\sigma_3\hat{E}_{d,k})\ \times$$

$$\left(\frac{\partial T_k^{\dagger}}{\partial k_\mu}\sigma_3 T_k\right)\sigma_3(\tilde{\eta}-\sigma_3\hat{E}_{d,k})\left(\hat{T}_k^{\dagger}\cdot\sigma_3\frac{\partial\hat{T}_k}{\partial k_\nu}\right)\Big]\tilde{\eta}\, g(\tilde{\eta})$$

$$-(\mu\leftrightarrow\nu). \qquad -\ (B-59)$$

To summarize, we have

$$\langle J_{\Theta,\mu}^{(1)}\rangle_0 = M_{\mu\nu}^{(2)}c_\nu + M_{\mu\nu}^{(1)}c_\nu$$

where $M_{\mu\nu}^{(1,2)}$ are given in Eq (B42) and (B59) respectively.

Combining this with the Kubo contribution in Eq. (B40)' and Eq. (B40), we finally have the total energy current induced by the temperature gradient;

$$\delta\langle \hat{J}_{Q,\mu}(t)\rangle_F = \left(M^{(1)}_{\mu\nu} + \cancel{M^{(2)}_{\mu\nu}}\right) c_\nu + \left(S^{(1)}_{\mu\nu} + \cancel{S^{(2)}_{\mu\nu}}\right) c_\nu$$

cancel each other (see Eq.(B42))

(B40)
(B59)

$$\not\equiv \left\{ -\frac{i}{2\hbar}\sum_{\mathbb{k}} \int_{-\infty}^{+\infty} d\tilde{\eta}\, \mathrm{Tr}\left[\sigma_3\, \delta(\tilde{\eta}-\sigma_3 \hat{E}_{d,k}) \frac{\partial T^\dagger_{\mathbb{k}}}{\partial k_\mu}\sigma_3 \frac{\partial T_{\mathbb{k}}}{\partial k_\nu}\right] \times \left(2\int_0^{\tilde{\eta}} \eta\, g(\eta)\, d\eta - \tilde{\eta}^2 g(\tilde{\eta})\right) - (\mu \leftrightarrow \nu)\right\} c_\nu$$

$$= \left\{ \frac{i}{2\hbar}\sum_{\mathbb{k}} \int_{-\infty}^{+\infty} d\tilde{\eta}\, \mathrm{Tr}\left[\sigma_3\, \delta(\tilde{\eta}-\sigma_3 \hat{E}_{d,\mathbb{k}}) \frac{\partial T^\dagger_{\mathbb{k}}}{\partial k_\mu}\sigma_3 \frac{\partial T_{\mathbb{k}}}{\partial k_\nu}\right] \times \left(\int_0^{\tilde{\eta}} \eta^2 \frac{dg(\eta)}{d\eta} d\eta\right) - (\mu \leftrightarrow \nu)\right\} c_\nu$$

$$= \frac{1}{2\hbar} \sum_{\mathbb{k}} \sum_{n=1}^{2N} \int_0^{(\hat{\sigma}_3 \hat{E}_{d,k})_{nn}} \eta^2 \frac{dg(\eta)}{d\eta} d\eta \, \Omega^{\mu\nu}_{n\mathbb{k}} \, c_\nu$$

---

with

$$\Omega^{\mu\nu}_{n\mathbb{k}} \equiv i\epsilon_{\mu\nu} \left(\hat{\sigma}_3 \frac{\partial T^\dagger_{\mathbb{k}}}{\partial k_\mu} \hat{\sigma}_3 \frac{\partial T_{\mathbb{k}}}{\partial k_\nu} \right)_{nn}$$

Noting that

$$\left(\begin{array}{c} \Omega^{\mu\nu}_{n+N,\mathbb{k}} = -\Omega^{\mu\nu}_{n,-\mathbb{k}} \\ \int_0^{-\epsilon} \eta^2 \frac{dg(\eta)}{d\eta} d\eta = -\int_0^{\epsilon} \eta^2 \frac{dg(\eta)}{d\eta} d\eta \end{array} \right)$$

one can show that the hole contribution ($n = N+1, \cdots, 2N$) is identical to the particle contribution ($n = 1, \cdots, N$)

$$\delta \langle \hat{J}_{Q,\mu}(t) \rangle_F = \frac{1}{\hbar} \sum_{\mathbb{k}} \sum_{n=1}^{N} \int_0^{\epsilon_{n,\mathbb{k}}} \eta^2 \frac{dg(\eta)}{d\eta} d\eta \, \Omega^{\mu\nu}_{n\mathbb{k}} \, c_\nu$$

$$= \frac{(k_B T)^2}{\hbar} \sum_{\mathbb{k}} \sum_{n=1}^{N} \left(c_2 [g(\epsilon_{n,\mathbb{k}})] - \frac{\pi^2}{3} \right) \Omega^{\mu\nu}_{n\mathbb{k}} \, c_\nu$$

where

$$C_2[X] \equiv \int_0^X \left[\ln\left(\frac{1+t}{t}\right)\right]^2 dt .$$

The thermal Hall conductivity $\kappa_{\mu\nu}$

energy current density

$$\underbrace{j_{Q,\mu}}_{\#\ \frac{1}{V}\langle \hat{J}_{Q,\mu}(t)\rangle_F} = \kappa_{\mu\nu} \nabla_\nu T$$

$$T(\mathbb{r}) = \frac{T}{1+X(\mathbb{r})}$$

$$- T \underbrace{\nabla_\nu X}_{c_\nu}$$

$$T(\mathbb{r}) = T - TX(\mathbb{r})$$

Thus, the thermal Hall conductivity $\kappa_{\mu\nu}$ is given by

$$\boxed{\kappa_{\mu\nu} = \frac{k_B^2 T}{\hbar V} \sum_{\mathbb{k}} \sum_{n=1}^{N} \left(C_2[g(\epsilon_{n,\mathbb{k}})] - \frac{\pi^2}{3} \right) \Omega_{n,\mathbb{k}}^{\mu\nu}}$$