Thermal Hall conductivity from bulk picture ②

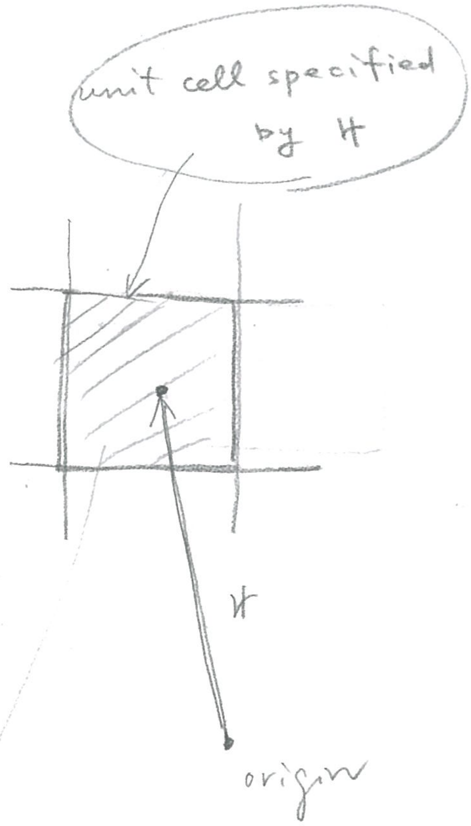
- The following argument is based on (R. Matsumoto, RS, S. Murakami PRB $\underline{89}$ 054420 (2014).)

- To discuss the thermal Hall conductivity, let us define a free boson Hamiltonian more precisely;

$$H = \frac{1}{2} \sum_{R} \psi^{\dagger}(R) \cdot \hat{H}_0 \cdot \psi(R) \qquad \text{— (B1)}$$

where R denotes a unit cell ~~index and $\psi(R)$~~ is a 2N-component vector. N is a number of internal degree of freedom within the unit cell:

$$\psi(R) \equiv \begin{bmatrix} \psi_1(R) \\ \vdots \\ \psi_N(R) \\ \hline \psi_{N+1}(R) \\ \vdots \\ \psi_{2N}(R) \end{bmatrix} \equiv \begin{bmatrix} \beta_1(R) \\ \vdots \\ \beta_N(R) \\ \hline \beta_1^{\dagger}(R) \\ \vdots \\ \beta_N^{\dagger}(R) \end{bmatrix}$$



(within the unit cell, I have N distict boson Degree of freedom (such as sublattice degree of freedom))

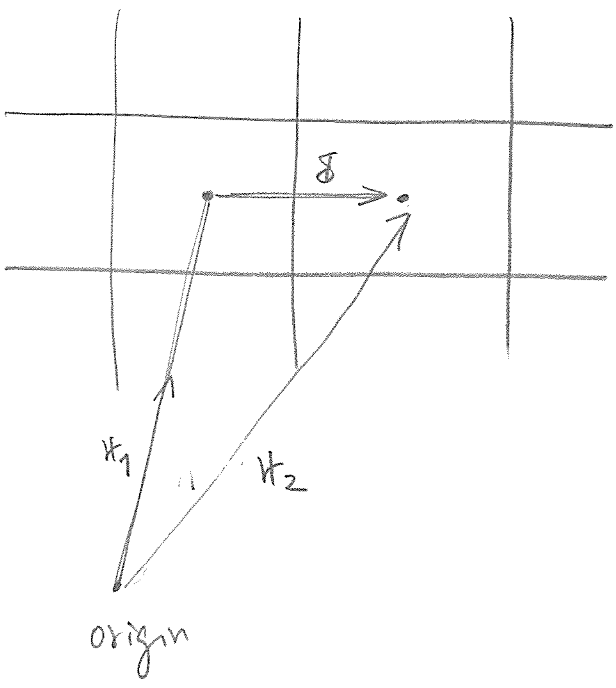
$\hat{H}_0$ is an operator in a sense that it is given by a linear superposition of "translational operators" $e^{i\hat{\mathbf{p}}\cdot\delta}$;

$$\hat{H}_0 \equiv \sum_{\delta} H_\delta \, e^{i\hat{\mathbf{p}}\cdot\delta} \qquad \text{— (B2)}$$

where $\hat{\mathbf{p}}$ is a momentum conjugate to $\mathbf{r}$;

$$e^{i\hat{\mathbf{p}}\cdot\delta} f(\mathbf{r}) = f(\mathbf{r}+\delta) \qquad \text{— (B3)}$$

δ is a spatial vector connecting neighboring unit cells. The summation over δ in eq. (B2)



$\vec{\mathbf{r}}_1 - \vec{\mathbf{r}}_2 = \delta$

is taken over all possible pair of two unit cells between which bosons can transfer.

H_δ is a $2N \times 2N$ matrix (complex-valued). which represents an transfer integral associated with the transfer by δ.

It generally takes a BdG type form;

$$
\hat{H}_\delta = \begin{array}{c|c c}
 & \text{particle} & \text{hole} \\
\hline
\text{particle} & h_\delta & \Delta_\delta \\
\text{hole} & \Delta_\delta^* & h_{-\delta}^t
\end{array} \qquad \text{—(B4)}
$$

from hermitian

with h_δ, Δ_δ being $N \times N$ matrix.

!! $\cdot$ $\beta(x)\cdot(\hat{\Delta}_\delta^*)\cdot\beta(x+\delta)$

$$
+\ \beta^\dagger(x)\cdot(\hat{\Delta}_\delta)\cdot\beta^\dagger(x+\delta)
$$

$$
= (\Delta_\delta^*)_{ij}\,\beta_i(x)\,\beta_j(x+\delta) + (\Delta_\delta)_{ij}\,\beta_i^\dagger(x)\,\beta_j^\dagger(x+\delta).
$$

$$\cdot\ \beta^\dagger(H)\cdot(h_\delta)\cdot\beta(H+\delta)$$

$$+\ \beta(H)\cdot(h^t_{-\delta})\cdot\beta^\dagger(H+\delta)$$

$$= (h_\delta)_{ij}\,\beta_i^\dagger(H)\,\beta_j(H+\delta)$$

$$+ (h_{-\delta})_{ij}\,\beta_j(H)\,\beta_i^\dagger(H+\delta)$$

$$\overset{\curlyvee}{=}\quad 2\,(h_\delta)_{ij}\,\beta_i^\dagger(H)\,\beta_j(H+\delta).$$

under the sum over δ

To set off this factor 2, we put a factor $1/2$ in r.h.s. of eq. (B1).

Note that, the hermiteness of H in combination with translational symmetry requires

$$H_\delta^\dagger = H_{-\delta} \qquad \text{— (B5)}$$

$\because$

$$\psi^\dagger(H)\cdot(H_\delta)\cdot\psi(H+\delta)$$

$$+\ \psi^\dagger(H)\cdot(H_{-\delta})\cdot\psi(H-\delta)$$

$$= (H_\delta)_{ij}\, \psi_i^\dagger(\mathbf{r})\, \psi_j(\mathbf{r}+\delta)$$

$$+ (H_{-\delta})_{ij}\, \psi_i^\dagger(\mathbf{r})\, \psi_j(\mathbf{r}-\delta)$$

where the hermitian conjugate of the first term should be the same as the 2nd term under the summation over $\mathbf{r}$;

$$\left((H_\delta)_{ij}\, \psi_i^\dagger(\mathbf{r})\, \psi_j(\mathbf{r}+\delta) \right)^\dagger$$

$$= (H_\delta)^*_{ij}\, \psi_j^\dagger(\mathbf{r}+\delta)\, \psi_i(\mathbf{r})$$

$$\overset{\mathbf{r}}{=} (H_\delta)^*_{ij}\, \psi_j^\dagger(\mathbf{r})\, \psi_i(\mathbf{r}-\delta)$$

under the sum over $\mathbf{r}$.

Note also that the Hamiltonian has the generic particle-hole symmetry;

$$\sigma_1 \cdot H_\delta \cdot \sigma_1 = H^t_{-\delta} \quad \text{— (B6)}$$

where

$$\sigma_1 = \begin{array}{c} \begin{array}{cc} \overbrace{\quad\quad}^{\text{particle}} & \overbrace{\quad\quad}^{\text{hole}} \end{array} \\ \left(\begin{array}{c|c} \Phi & \mathbb{1}_{N\times N} \\ \hline \mathbb{1}_{N\times N} & \Phi \end{array} \right) \end{array} \begin{array}{l} \\ \} \; p \\ \} \; h. \end{array}$$

$\because$

$$\underline{\psi^\dagger(r)} \cdot (H_\delta) \cdot \psi(r+\delta)$$

$$= \psi(r) \cdot \sigma_1 \cdot (H_\delta) \cdot \sigma_1 \cdot \psi^\dagger(r+\delta)$$

$$= \psi^\dagger(r+\delta) \cdot (\sigma_1 \cdot H_\delta \cdot \sigma_1)^t \cdot \psi(r)$$

To make the r.h.s. to be same as

$\psi^\dagger(r) \cdot \hat{H}_{-\delta} \cdot \psi(r-\delta)$ under $\sum_r$,

we have

$$\sigma_1 H_\delta \cdot \sigma_1 = \hat{H}^t_{-\delta}.$$

In the following, we often use the following commutation relations of boson, which are all identical to one another:

$$\left[\Psi_i(k),\ \Psi_j^{\dagger}(k')\right] = (\hat{\sigma}_3)_{ij}\ \delta_{k,k'}$$

where

$$(\sigma_3) \equiv \begin{array}{cc} \begin{array}{cc} \overbrace{\qquad\quad}^{p} & \overbrace{\qquad\quad}^{h} \end{array} & \\ \left(\begin{array}{c|c} \mathbb{1}_{N\times N} & \\ \hline & -\mathbb{1}_{N\times N} \end{array}\right) & \begin{array}{l} \}\, p \\ \}\, h \end{array} \end{array}$$

$$\left[\Psi_i^{\dagger}(k),\ \Psi_j^{\dagger}(k')\right] \qquad \text{— (B7)}$$

$$= (\sigma_1)_{im}\left[\Psi_m(k),\ \Psi_j^{\dagger}(k')\right]$$

$$= -i(\sigma_2)_{ij}\ \delta_{k,k'}$$

$$\left[\Psi_i(k),\ \Psi_j(k')\right]$$

$$= \left[\Psi_i(k),\ \Psi_m^{\dagger}(k')\right](\sigma_1)_{mj}$$

$$= i(\sigma_2)_{ij}\ \delta_{k,k'}.$$

with

$$(\sigma_2) \equiv \begin{array}{cc} \begin{array}{cc} \overbrace{\qquad\quad}^{p} & \overbrace{\qquad\quad}^{h} \end{array} & \\ \left(\begin{array}{c|c} & -i\,\mathbb{1}_{N\times N} \\ \hline i\,\mathbb{1}_{N\times N} & \end{array}\right) & \begin{array}{l} \}\, p \\ \}\, h \end{array} \end{array}$$

- With this Hamiltonian in mind, let us consider an effect of temperature gradient.

$$T(\mathbf{r}) \equiv \frac{T}{1 + \chi(\mathbf{r})}$$ ($\chi(\mathbf{r})$ is called pseudo gravitational potential). 1 corresponds to the non-perturbed part and $\chi(\mathbf{r})$ describes the finite spatial gradient.

- For simplicity, let us assume that the temperature gradient is sufficiently small, such that the temperature within each unit cell can be regarded as constant.

In such case, the statistical density operator in the presence of the temperature gradient may be given as (let's take k_B to be unit)

$$e^{-\frac{H}{T}} \longrightarrow e^{-\frac{1}{2}\sum_{\mathbf{r}} \frac{\hat{h}(\mathbf{r})}{T(\mathbf{r})}}$$

$$\begin{cases} H = \frac{1}{2}\sum_{\mathbf{r}} \hat{h}_{\mathbf{r}} \\ \hat{h}_{\mathbf{r}} = \psi^{\dagger}(\mathbf{r}) \cdot \hat{H}_0 \cdot \psi(\mathbf{r}) \end{cases}$$

$$= e^{-\frac{1}{2}\sum_{\#} \frac{(1+\chi(\#))}{T} \cdot \hat{h}(\#)}$$

$$\equiv e^{-\frac{1}{T}(\hat{H}+\hat{F})} \quad -(B8)$$

where

$$\hat{H} = \frac{1}{2}\sum_{\#} \hat{h}(\#) \quad \text{non-perturbed part}$$

$$\hat{F} \overset{?}{=} \frac{1}{2}\sum_{\#} \chi(\#)\,\hat{h}(\#) \ : \ \text{perturbatation.}$$

due to the temperature gradient.

Remark that $\hat{h}(\#)$ contains a hopping term which describes a boson transfer between different unit cells with different temperature;

$$\hat{h}(\#) = \sum_{\delta} \psi^{\dagger}(\#) \cdot H_{\delta} \cdot \psi(\# + \delta) \quad (B9)$$

where

$$\chi(\#) \neq \chi(\# + \delta)$$

As such, it is more symmetric to redefine $\hat{F}$

in the following way:

$$\hat{F} \overset{?}{=} \frac{1}{2} \sum_{H} \chi(H)\, \psi^{\dagger}(H) \cdot \hat{H}_0 \cdot \psi(H)$$

$$\rightarrow \frac{1}{4} \sum_{H} \psi^{\dagger}(H) \left\{ \hat{H}_0\, \chi(H) + \chi(H)\, \hat{H}_0 \right\} \psi(H)$$

$$= \frac{1}{4} \sum_{H} \sum_{\delta} \psi^{\dagger}(H) \left\{ H_{\delta} \cdot \chi(H+\delta) + \chi(H)\, H_{\delta} \right\} \psi(H+\delta)$$

— (B10)

In summary, we have rewrite a temperature gradient ("statistical" force) into a perturbed Hamiltonian $\hat{F}$ ("dynamical" force)

$$e^{-\frac{1}{T}(\hat{H} + \hat{F})}$$

(perturbatation which represents a temperature gadient)

zero-th order part

(temperature before the temperature gradient is introduced)

- Since we are interested only in the linear response w.r.t. spatial gradient of temperature, we regard $\chi(H)$ to be small (or precisely $\chi(H) = C_\mu H_\mu$ and regard C_μ to be small).

- Within the linear order in $\chi(H)$ (or C_μ), we may rewrite our total Hamiltonian as

$$H_T = \hat{H} + \hat{F}$$

$$\tilde{\Psi}^\dagger(H)$$

$$= \frac{1}{2} \sum_H \underbrace{\left(1 + \frac{\chi_H}{2}\right) \Psi^\dagger(H)}_{= \tilde{\Psi}^\dagger(H)} \cdot \hat{H}_0 \cdot \left(1 + \frac{\chi_H}{2}\right) \Psi(H)$$

$$\stackrel{d}{\equiv} \frac{1}{2} \sum_H \tilde{\Psi}^\dagger(H) \cdot \hat{H}_0 \cdot \tilde{\Psi}(H) \quad -(B11)$$

- Observing this, one can easily define an energy density at H, say $h_T(H)$, as

$$\hat{h}_T(H) \equiv \frac{1}{2} \tilde{\Psi}^\dagger(H) \cdot \hat{H}_0 \cdot \tilde{\Psi}(H) \quad (B12)$$

- Thermal conductivities are nothing but an energy current induced by the temperature gradient.

- To define the energy current, let us use a continuity equation of energy, which relates the energy density $\hat{h}_T(\boldsymbol{r})$ with an energy current density $\hat{\boldsymbol{j}}_Q(\boldsymbol{r})$;

$$\boxed{\frac{\partial}{\partial t}\hat{h}_T(\boldsymbol{r}) + \nabla_{\boldsymbol{r}}\cdot\hat{\boldsymbol{j}}_Q(\boldsymbol{r}) = 0} \quad \text{—(B13)}$$

By calculating $\frac{\partial}{\partial t}\hat{h}_T(\boldsymbol{r}) = \frac{i}{\hbar}\left[\hat{H}_T, \hat{h}_T(\boldsymbol{r})\right]$, we can get $\hat{\boldsymbol{j}}_Q(\boldsymbol{r})$ up to the first order in $\chi(\boldsymbol{r})$:

To this end, ②-13

$$\dot{h}_T(\mathsf{H}) = \frac{i}{2\hbar}\left[\hat{H}_T,\ \tilde{\Psi}^\dagger(\mathsf{H})\cdot\hat{H}_0\cdot\tilde{\Psi}(\mathsf{H})\right]$$

$$= \frac{i}{4\hbar}\left\{\left[\hat{H}_T,\ \tilde{\Psi}^\dagger(\mathsf{H})\cdot\hat{H}_0\cdot\tilde{\Psi}(\mathsf{H})\right] - \left[\tilde{\Psi}^\dagger(\mathsf{H})\cdot\hat{H}_0\cdot\tilde{\Psi}(\mathsf{H}),\ \hat{H}_T\right]\right\} \quad \text{(B 13)}$$

hermite conjugate

where

$$\left[\hat{H}_T,\ \tilde{\Psi}^\dagger(\mathsf{H})\cdot\hat{H}_0\cdot\tilde{\Psi}(\mathsf{H})\right]$$

$$= \left[\hat{H}_T,\ \tilde{\Psi}_i^\dagger(\mathsf{H})\right][H_\delta]_{ij}\,\tilde{\Psi}_j(\mathsf{H}+\delta)$$

$$+ \tilde{\Psi}_i^\dagger(\mathsf{H})\,[H_\delta]_{ij}\left[\hat{H}_T,\ \tilde{\Psi}_j(\mathsf{H}+\delta)\right] \quad \text{(B 14)}$$

Note that

$$\left[\hat{H}_T,\ \tilde{\Psi}_i^\dagger(\mathsf{H})\right]$$

$$= \frac{1}{2}\sum_{\mathsf{H}',\delta'}[H_{\delta'}]_{\ell m}\left[\tilde{\Psi}_\ell^\dagger(\mathsf{H}')\,\tilde{\Psi}_m(\mathsf{H}'+\delta'),\ \tilde{\Psi}_i^\dagger(\mathsf{H})\right]$$

$$= \frac{1}{2}\sum_{\mathsf{H}',\delta'}[H_{\delta'}]_{\ell m}\Big\{\tilde{\Psi}_\ell^\dagger(\mathsf{H}')\left[\tilde{\Psi}_m(\mathsf{H}'+\delta'),\ \tilde{\Psi}_i^\dagger(\mathsf{H})\right]$$

$$+ \left[\tilde{\Psi}_\ell^\dagger(\mathsf{H}'),\ \tilde{\Psi}_i^\dagger(\mathsf{H})\right]\tilde{\Psi}_m(\mathsf{H}'+\delta')\Big\}$$

$$= \frac{1}{2}\sum_{\mathsf{H}',\delta'}[H_{\delta'}]_{\ell m}\Big\{\tilde{\Psi}_\ell^\dagger(\mathsf{H}')\,[\sigma_3]_{mi}\left(1+\frac{x_{\mathsf{H}}}{2}\right)^2\delta_{\mathsf{H}'+\delta',\mathsf{H}}$$

$$+ (-i\sigma_2)_{\ell i}\left(1+\frac{x_{\mathsf{H}}}{2}\right)^2\delta_{\mathsf{H}',\mathsf{H}}\,\tilde{\Psi}_m(\mathsf{H}'+\delta')\Big\}$$

where we use

$$[\tilde{\Psi}_i(H), \tilde{\Psi}^\dagger_j(H')] = (\sigma_3)_{ij}\, \delta_{H,H'} \left(1 + \frac{x_H}{2}\right)^2$$

$$[\tilde{\Psi}^\dagger_i(H), \tilde{\Psi}^\dagger_j(H')] = (-i\sigma_2)_{ij}\, \delta_{H,H'} \left(1 + \frac{x_H}{2}\right)^2$$

Using (B5) & (B6), we can rewrite the first term of eq (B14) as

$$\sum_{\delta} [\hat{H}_T, \tilde{\Psi}^\dagger_i(H)]\, [H_\delta]_{ij}\, \tilde{\Psi}_j(H+\delta)$$

$$= \frac{1}{2} \sum_{\delta,\delta'} \tilde{\Psi}^\dagger_l(H-\delta')\, [H_{\delta'}\sigma_3]_{li} \left(1 + \frac{x_H}{2}\right)^2 [H_\delta]_{ij}\, \tilde{\Psi}_j(H+\delta)$$

$$+ \frac{1}{2} \sum_{\delta,\delta'} \underbrace{\tilde{\Psi}_m(H+\delta')}_{=\tilde{\Psi}^\dagger_n(H+\delta')[\sigma_1]_{nm}}\, [H_{\delta'}]_{lm}\, (\underbrace{-i\sigma_2}_{=\sigma_1\cdot\sigma_3})_{li} \left(1 + \frac{x_H}{2}\right)^2 \times [H_\delta]_{ij}\, \tilde{\Psi}_j(H+\delta)$$

$$= \cdots\cdots$$

$$+ \frac{1}{2} \sum_{\delta,\delta'} \tilde{\Psi}^\dagger_n(H+\delta')\, [\underbrace{\sigma_1 H^t_{\delta'} \cdot \sigma_1}_{=H_{-\delta'}} \sigma_3]_{ni} \left(1 + \frac{x_H}{2}\right)^2 \times [H_\delta]_{ij}\, \tilde{\Psi}_j(H+\delta)$$

$$\neq \sum_{\delta,\delta'} \tilde{\Psi}^{\dagger}_{l}(H-\delta')\,[H_{\delta'}\cdot\sigma_3]_{li}\left(1+\frac{X_H}{2}\right)^2 [H_\delta]_{ij}\,\tilde{\Psi}_j(H+\delta$$

under the sum over δ, δ'

②-15

(B15)

Likewise, the 2nd term in eq. (B14) can be also calculated as

$$\sum_{\delta} \tilde{\Psi}^{\dagger}_i(H)\,[H_\delta]_{ij}\,[\hat{H}_T, \tilde{\Psi}_j(H+\delta)]$$

$$= -\sum_{\delta,\delta'} \tilde{\Psi}^{\dagger}_i(H)\,[H_{\delta'}\sigma_3]_{ij}\left(1+\frac{X_{H+\delta'}}{2}\right)^2 [H_\delta]_{jl}\,\tilde{\Psi}_l(H+\delta+\delta'$$

$$= \underset{\sim}{-}\left(\text{the first term in eq. (B14)}\right)\Big|_{H\to H+\delta'} \qquad \text{— (B16)}$$

Thus, regarding $|\delta'|$ as an infinitesimally small, we can rewrite (B14) into a spatival divergence of a vector field $\mathbb{f}_\Theta(H)$

$$(\text{B14}) = -\nabla_H\cdot\mathbb{f}_\Theta(H)$$

where

$$f_{\Theta,\mu}(H) = -\sum_{\delta,\delta'} \tilde{\Psi}^{\dagger}_{l}(H+\delta')\,[\delta'_\mu H_{-\delta'}\cdot\sigma_3]_{li}\left(1+\frac{X_H}{2}\right)^2$$

$$\times [H_\delta]_{ij}\,\tilde{\Psi}_i(H+\delta)$$

Noting that $H_\delta^\dagger = H_{-\delta}$ ((B 5)), we can rewrite this vector field in a compact form,

$$f_{Q,\mu}(x) = -i\hbar \left(\hat{V}_\mu \cdot \tilde{\Psi}(x)\right)^\dagger \cdot \sigma_3 \left(1 + \frac{X_x}{2}\right)^2 \cdot \hat{H}_0 \cdot \tilde{\Psi}(x) \quad \text{— (B 18)}$$

where

$$\hat{V}_\mu \equiv \frac{i}{\hbar} \sum_\delta \delta_\mu H_\delta e^{i\hat{p}\cdot\delta}$$

$$= \frac{1}{i\hbar}\left[\hat{x}_\mu, \hat{H}_0\right] \quad \text{— (B 19)}$$

(velocity operator)

Then, substituting (B 18), (B 17) into (B 13)′, we finally have

$$\dot{h}_T(x) = -\nabla_x \cdot \left\{ \frac{1}{4}\left(\hat{V}\cdot\tilde{\Psi}(x)\right)^\dagger \cdot \sigma_3 \left(1+\frac{X_x}{2}\right)^2 \cdot \hat{H}_0 \cdot \tilde{\Psi}(x) \right.$$

$$\left. + \frac{1}{4} \tilde{\Psi}^\dagger(x) \cdot \hat{H}_0 \left(1+\frac{X_x}{2}\right)^2 \cdot \sigma_3 \cdot \hat{V} \cdot \tilde{\Psi}(x) \right\}$$

Comparing this with the postulated energy conservation equation (B.13), we obtain the energy current density operator;

$$\hat{\mathring{J}}_{Q,\mu}(H) \equiv \frac{1}{4}\left(\hat{V}_\mu\cdot\tilde{\Psi}(H)\right)^\dagger\cdot\sigma_3\left(1+\frac{x_H}{2}\right)^2\cdot\hat{H}_0\cdot\tilde{\Psi}(H) + \frac{1}{4}\tilde{\Psi}^\dagger(H)\cdot H_0\cdot\sigma_3\left(1+\frac{x_H}{2}\right)^2\cdot\hat{V}_\mu\cdot\tilde{\Psi}(H) \quad \text{(B20)}$$

Accordingly, the energy current operator takes form of

$$\hat{J}_{Q,\mu} = \frac{1}{4}\boxed{\sum_H}\tilde{\Psi}^\dagger(H)\cdot\left\{\hat{V}_\mu\cdot\hat{\sigma}_3\cdot\left(1+\frac{x_H}{2}\right)^2\cdot\hat{H}_0 + \hat{H}_0\cdot\sigma_3\cdot\left(1+\frac{x_H}{2}\right)^2\cdot\hat{V}_\mu\right\}\cdot\tilde{\Psi}(H) \quad \text{(B21)}$$

(Note that this expression is correct only up to the first order in x_H, because so are H_T and $h_T(H)$ given in (B11) & (B12) respectively)

summation over volume

Since we are interested in the energy current induced by the temperature gradient, up to the first order in the gradient (χ_{H} or c_μ), let us further examine 0th and 1st order in χ_{H} ($\equiv c_\mu r_\mu$) of the energy current.

$$\hat{J}_{\Theta,\mu} = \hat{J}^{(0)}_{\Theta,\mu} + \hat{J}^{(1)}_{\Theta,\mu} + o(c_\mu^2) \quad \text{—(B 21)}$$

$$\hat{J}^{(0)}_{\Theta,\mu} \equiv \frac{1}{4}\sum_{H} \Psi^{\dagger}(H)\cdot\left\{\hat{V}_\mu \hat{\sigma}_3 \hat{H}_0 + \hat{H}_0 \hat{\sigma}_3 \hat{V}_\mu\right\}\cdot\Psi(H)$$

$$\text{—(B 22)}$$

$$\hat{J}^{(1)}_{\Theta,\mu} \equiv c_\nu \cdot \frac{1}{8}\sum_{H} \Psi^{\dagger}(H)\left\{\hat{r}_\nu \hat{V}_\mu \hat{\sigma}_3 \hat{H}_0\right.$$

$$+ 2\hat{V}_\mu \hat{\sigma}_3 \underline{\hat{r}_\nu \hat{H}_0} + \hat{V}_\mu \hat{\sigma}_3 \underline{\hat{H}_0 \hat{r}_\nu}$$

$$\left. + \underline{\hat{r}_\nu \hat{H}_0 \hat{\sigma}_3} \hat{V}_\mu + 2\hat{H}_0 \underline{\hat{\sigma}_3 \hat{r}_\nu} \hat{V}_\mu + \hat{H}_0 \hat{\sigma}_3 \hat{V}_\mu \hat{r}_\nu\right\}\Psi(H)$$

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

= (continued to the next page)

$$= C_V \frac{1}{8} \sum_{H} \Psi^{\dagger}(H) \left\{ \hat{V}_{\mu} \cdot \hat{\sigma}_3 \cdot [\hat{H}_0, \hat{r}_{\nu}] - [\hat{H}_0, \hat{r}_{\nu}] \cdot \hat{\sigma}_3 \cdot \hat{V}_{\mu} \right\} \Psi(H)$$

$$+ C_V \cdot \frac{1}{8} \sum_{H} \Psi^{\dagger}(H) \left\{ (\hat{r}_{\nu} \hat{V}_{\mu} \hat{\sigma}_3 + 3 \hat{V}_{\mu} \sigma_3 \hat{r}_{\nu}) \hat{H}_0 + \hat{H}_0 \cdot (3 \hat{r}_{\nu} \cdot \sigma_3 \cdot \hat{V}_{\mu} + \sigma_3 \hat{V}_{\mu} \hat{r}_{\nu}) \right\} \cdot \Psi(H) \quad \text{—(B22)}$$

- Armed with the expression for the energy current $\hat{J}_Q$ (B20 – B22) & for the dynamical force $\hat{F}$ which is equivalent to the temperature gradient (B10), we will henceforth evaluate the linear response of $\hat{J}_Q$ with respect to $\hat{F}$ using the linear response theory.

- Consider that the system is equilibriated with temperature T at time $t' = -\infty$.

- At $t' = -\infty + \varepsilon$, the system is disconnected from the bath, while the dynamical force $\hat{F}$ is <u>adiabatically</u> introduced during $t' = (-\infty, t)$.
- The expectation value of $\hat{J}_{Q,\mu}$ at $t' = t$ is then given up to the linear order in χ_H (or c_μ) as follows;

$$\left\langle \hat{J}_{Q,\mu}(t) \right\rangle_F = \left\langle \hat{J}_{Q,\mu} \right\rangle_{F=0} + \frac{i}{\hbar}\int_{-\infty}^{t} dt' \, \mathrm{Tr}\left[\hat{\rho}_0 \, \hat{F}_H(t'), \hat{J}_{Q,\mu,H}(t) \right] + O(c_\mu^2)$$

where

$$\begin{cases} \langle \cdots \rangle_{F=0} = \mathrm{Tr}\left[\hat{\rho}_0 \cdots \right] \\ \hat{\rho}_0 = \dfrac{e^{-\beta H}}{\mathrm{Tr}\left[e^{-\beta H} \right]} \quad \text{without } \hat{F} \\ \hat{A}_H(s) = e^{iHs/\hbar} \, \hat{A} \, e^{-iHs/\hbar} \end{cases}$$

◎ Noting that $\hat{J}_{Q,\mu}$ itself contains the 1st order in X_H (or c_ν) as in eq. (B.22), we can see that the linear contribution of $\langle \hat{J}_{Q,\mu}(t) \rangle_F$ comprises of two parts ;

$$\delta \langle \hat{J}_{Q,\mu}(t) \rangle_F = \mathrm{Tr}[\hat{\rho}_0 \hat{J}^{(1)}_{Q,\mu}] + \frac{i}{\hbar}\int_{-\infty}^{t} dt' \, \mathrm{Tr}[\hat{\rho}_0 [\hat{F}_H(t'), \hat{J}^{(0)}_{Q,\mu,H}(t)]] + o(c_\mu^2) \quad \text{(B-23)}$$

(Here we retain only the first order in c_μ ;

$$\delta \langle \hat{J}_{Q,\mu}(t) \rangle_F \equiv \langle \hat{J}_{Q,\mu}(t) \rangle_F - \langle \hat{J}^{(0)}_{Q,\mu} \rangle_{F=0}$$)

- The first term is nothing but the equiliribium expectation value of $\hat{J}^{(1)}_{\Theta,\mu}$, a part of energy current operator which exists only in the presence of the external field $\hat{F}$.

- Meanwhile, the second term is a usual linear response contribution associated with $\hat{J}^{(0)}_{\Theta,\mu}$, a part of energy current operator which exists even with the external field $\hat{F}$.

- One may compare this with electric current in superconductor, which comprises of the so-called diamagnetic current and paramagnetic current.

$$\mathring{j}_\mu(t) = \mathring{j}_\mu^{(0)}(t) + \mathring{j}_\mu^{(1)}(t)$$

$$\begin{cases} \mathring{j}_\mu^{(0)}(t) \equiv \dfrac{i\hbar e}{2m}\left(\psi_\alpha^\dagger(t)\, \nabla_\mu \psi_\alpha(t) - \left(\nabla_\mu \psi_\alpha^\dagger(t)\right) \psi_\alpha(t) \right) \\ \mathring{j}_\mu^{(1)}(t) \equiv -\dfrac{e^2}{mc} \underbrace{A_\mu}_{\text{external vector potential}} \psi_\alpha^\dagger(t)\, \psi_\alpha(t) \end{cases}$$

- Thereby, the equilibrium expectation value of $\mathring{j}_\mu^{(1)}(t)$ is called as the diamagnetic current, while the usual linear response associated with $\mathring{j}_\mu^{(0)}$ corresponds to the paramagnetic current.

- In eq(B-23), the first term in the r.h.s. formally corresponds to the diamagnetic current in superconductor, while the 2nd term in the r.h.s. corresponds to the paramagnetic current in SC.

- As we will see below, both of these two have finite contributions to the thermal Hall conductivity.

2-24

- Let us begin with the "paramagnetic part" (the 2nd term in eq (B.-23).)

It is given by a retarded correlation fuction between $\hat{F}$ and $\hat{J}^{(0)}_{Q,\mu}$.

- $\hat{J}^{(0)}_{Q,\mu}$ is given by a symmetrized product between an velocity operator and energy density, $\hat{V}_\mu$ and $\hat{H}_0$ respectively.

- On the one hand, $\hat{F}$ (dynamical force) is given by a symmetrized product between an position operator ($x_H = C_\nu H_\nu$) and H_0.

- As we know, the position operator is an ill-defined operator in the Hilbert space with the periodic boundary conditions.

- As such, we follow the standard Kubo's trick to relate this with a correlation between $\frac{d\hat{F}}{dt}$ and $\hat{J}^{(0)}_{Q,\mu}$.

- Namely, consider $\hat{F}$ as a time-dependent field ($\hat{F} \to \hat{F} e^{-i\omega t'}$), we have.

$$\delta_0 \langle \hat{J}_{Q,\mu}(t) \rangle_F = \frac{i}{\hbar} \int_{-\infty}^{t} dt' \, \mathrm{Tr}\left[\hat{\rho}_0 \left[\hat{F}_H(t'), \hat{J}^{(0)}_{Q,\mu,H}(t) \right]\right]$$

$$\equiv e^{-i\omega t} \, J^{0}_{Q,\mu}(\omega) \quad \text{— (B 24)}$$

where

$$J^{0}_{Q,\mu}(\omega) = \frac{i}{\hbar} \int_0^{+\infty} dt' \, e^{i\omega t'} \underbrace{\mathrm{Tr}\left[\hat{\rho}_0 \left[\hat{F}_H(-t'), \hat{J}^{(0)}_{Q,\mu}\right]\right]}_{= X^{(0)}_{\mu}(t')}$$

$$\overset{d}{\equiv} \frac{i}{\hbar} \int_0^{+\infty} dt' \, e^{i\omega t'} X^{(0)}_{\mu}(t')$$

$$= \frac{i}{\hbar}\int_0^{+\infty} dt' \, \frac{1}{i\omega}\frac{de^{i\omega t'}}{dt'} \, X_\mu^{(0)}(t')$$ ②-26

$$= \frac{i}{\hbar}\left[\frac{1}{i\omega} e^{i\omega t'} X_\mu^{(0)}(t')\right]_{t'=0}^{t'=+\infty}$$

$$- \frac{i}{\hbar}\int_0^{+\infty} \frac{1}{i\omega} e^{i\omega t'}\left(\frac{d}{dt'} X_\mu^{(0)}(t')\right) dt'.$$

Assuming that $\underline{X_\mu^{(0)}(t'=+\infty)}$ vanishes,

we have

$$= \frac{i}{\hbar}\left[-\frac{X_\mu^{(0)}(0)}{i\omega} - \int_0^{+\infty} \frac{e^{i\omega t}}{i\omega}\frac{dX_\mu^{(0)}(t)}{dt} dt\right]$$

$$= -\frac{i}{\hbar}\int_0^{+\infty} \frac{e^{i\omega t} - 1}{i\omega}\frac{dX_\mu^{(0)}(t)}{dt} dt \,.$$ (B24)'

$\frac{dX_\mu^{(0)}(t)}{dt}$ is nothing but a correlation function

between $\frac{d\hat{F}}{dt}$ and $J_{Q,\mu}^{(0)}$:

$$\frac{dX_{\mu}^{(0)}(t)}{dt} = -\mathrm{Tr}\left[\hat{\rho}_0 \left[\frac{d\hat{F}_H}{dt}, \hat{J}^{(0)}_{Q,\mu}(t)\right]\right]$$

$$= \mathrm{Tr}\left[\hat{\rho}_0 \left[\hat{J}^{(0)}_{Q,\mu}(t), \frac{d\hat{F}_H}{dt}\right]\right] \quad \text{—(B25)}$$

Like in the electric conductivity, $\frac{d\hat{F}_H}{dt}$ is given by the energy current operator up to the leading order ;

$$\frac{d\hat{F}}{dt} = \frac{i}{\hbar}\left[\hat{H}, \hat{F}\right]$$

$$= \frac{i}{\hbar}\left[\hat{H}, \hat{H}_T\right]$$

$$= \frac{i}{2\hbar} \sum_{r} \left[\hat{H}, \tilde{\Psi}^{\dagger}(r)\cdot\hat{H}_0\cdot\tilde{\Psi}(r)\right] \quad \text{—(B26)}$$

where

$$\left[\hat{H}, \tilde{\Psi}^{\dagger}(r)\cdot H_0\cdot\tilde{\Psi}(r)\right]$$

$$= \sum_{\delta} \left[\hat{H}, \tilde{\Psi}^{\dagger}_i(r)\right] [H_\delta]_{ij}\, \tilde{\Psi}_j(r+\delta) + \tilde{\Psi}^{\dagger}_i(r)\, [H_\delta]_{ij} \left[\hat{H}, \tilde{\Psi}_j(r+\delta)\right] \quad \text{(B27)}$$

Noting again that

$$[\hat{H}, \tilde{\Psi}_i^\dagger(H)]$$

$$= \frac{1}{2} \sum_{H', \delta'} [H_{\delta'}]_{lm} [\Psi_l^\dagger(H') \Psi_m(H'+\delta'), \tilde{\Psi}_i^\dagger(H)]$$

$$= \frac{1}{2} \sum_{H', \delta'} [H_{\delta'}]_{lm} \Big\{ \Psi_l^\dagger(H') [\sigma_3]_{mi} \left(1 + \frac{\chi_H}{2}\right) \delta_{H'+\delta', H}$$

$$+ (-i\sigma_2)_{li} \left(1 + \frac{\chi_H}{2}\right) \delta_{H', H} \Psi_m(H'+\delta') \Big\}$$

where we use

$$[\Psi_i(H), \tilde{\Psi}_j^\dagger(H')] = (\sigma_3)_{ij} \delta_{H,H'} \left(1 + \frac{\chi_H}{2}\right)$$

Using eq.(B6), we can rewrite the first term of eq.(B27) as

$$\sum_\delta [\hat{H}, \tilde{\Psi}_i^\dagger(H)] [H_\delta]_{ij} \tilde{\Psi}_j(H+\delta)$$

$$= \sum_{\delta, \delta'} \Psi_l^\dagger(H-\delta') [H_{\delta'} \cdot \sigma_3]_{li} \left(1 + \frac{\chi_H}{2}\right) [H_\delta]_{ij} \tilde{\Psi}_j(H+\delta)$$

Likewise, the 2nd term of eq.(B27) is calculated as

$$\sum_\delta \tilde{\Psi}_i^\dagger(H) [H_\delta]_{ij} [\hat{H}, \tilde{\Psi}_j(H+\delta)]$$

$$= - \sum_{\delta, \delta'} \tilde{\Psi}_i^\dagger(H) [H_{\delta'} \cdot \sigma_3]_{ij} \left(1 + \frac{\chi_{H+\delta'}}{2}\right) [H_\delta]_{jl} \Psi_l(H+\delta+\delta$$

Thus, we have

$$\frac{d\hat{F}}{dt} = \frac{i}{2\hbar}\left\{ \sum_{k} \Psi^{\dagger}(k)\cdot \hat{H}_0 \cdot \hat{\sigma}_3 \left(1+\frac{\chi_k}{2}\right)\cdot \hat{H}_0 \cdot \tilde{\Psi}(k) - \sum_{k} \tilde{\Psi}^{\dagger}(k)\cdot \hat{H}_0\cdot\hat{\sigma}_3\left(1+\frac{\chi_k}{2}\right)\cdot \hat{H}_0 \cdot \Psi(k) \right\}$$

$$\underset{\chi_k = c_\nu k_\nu}{=} \frac{i}{2\hbar}\sum_{k}\Psi^{\dagger}(k)\cdot\left\{ \hat{H}_0\cdot\hat{\sigma}_3\left(1+\frac{c_\nu r_\nu}{2}\right)\cdot \hat{H}_0\left(1+\frac{c_\nu r_\nu}{2}\right) - \left(1+\frac{c_\nu r_\nu}{2}\right)\cdot \hat{H}_0\cdot\hat{\sigma}_3\left(1+\frac{c_\nu r_\nu}{2}\right)\cdot\hat{H}_0 \right\}\Psi(k)$$

$$= \frac{i}{4\hbar}\sum_{k}\Psi^{\dagger}(k)\cdot\left\{ [\hat{H}_0, \hat{r}_\nu]\,\hat{\sigma}_3\,\hat{H}_0 + \hat{H}_0\cdot\sigma_3\cdot[\hat{H}_0, \hat{r}_\nu]\right\}\Psi(k)\cdot c_\nu$$

$\hat{V}_\nu$

$$= \frac{1}{4}\sum_{k}\Psi(k)\left\{\hat{V}_\nu\cdot\sigma_3\cdot\hat{H}_0 + \hat{H}_0\,\sigma_3\,\hat{V}_\nu\right\}\Psi(k)c_\nu$$

$$= c_\nu\,\hat{J}^{(0)}_{Q,\nu} + o(c_\nu^2)$$

Substituting this into (B25), we see that $\frac{dX^{(0)}_\mu(t)}{dt}$ is nothing but a correlation function of energy current $\hat{J}^{(0)}_{Q,\mu}$!

$$\frac{d X_\mu^{(0)}(t)}{dt} = \mathrm{Tr}[\hat{\rho}_0 [\hat{J}^{(0)}_{\theta,\mu}(t), \hat{J}^{(0)}_{\theta,\nu}]] \, c\nu$$

- From eq (B24)', we have

(B28)

$$J^0_{\theta,\mu}(\omega) = \frac{P^R_{\mu\nu}(\omega) - P^R_{\mu\nu}(\omega=0)}{i\omega} \, c\nu$$

$\nabla_\nu X$

where $P^R_{\mu\nu}(\omega)$ is a Fourier transform of a retarded correlation function of energy current density:

$$\begin{cases} P^R_{\mu\nu}(\omega) \equiv \int_{-\infty}^{+\infty} e^{i\omega t} P^R_{\mu\nu}(t)\, dt \\ P^R_{\mu\nu}(t) \equiv -\frac{i}{\hbar}\theta(t)\,\mathrm{Tr}[\hat{\rho}_0 [\hat{J}^{(0)}_{\theta,\mu}(t), \hat{J}^{(0)}_{\theta,\nu}]] \end{cases} \quad \text{(B29)}$$

- Following the standard field theory treatment, we can relate this retarded function with the imaginary time-ordered correlation function via the Lehmann representation.

$$P^{R}_{\mu\nu}(\omega) = P^{T}_{\mu\nu}(i\omega_n = \omega + i\delta) \quad \text{—(B29)}$$

where the imaginary time ordered function is given by

$$\left\{\begin{aligned} P^{T}_{\mu\nu}(i\omega_n) &\equiv \int_0^{\beta\hbar} d\tau\, e^{i\omega_n \tau} P^{T}_{\mu\nu}(\tau) \\ P^{T}_{\mu\nu}(\tau) &\equiv -\frac{1}{\hbar}\,\mathrm{Tr}\left[\hat{\rho}_0\, T_\tau \left\{ \hat{J}^{(0)}_{Q,\mu}(\tau)\, \hat{J}^{(0)}_{Q,\nu} \right\}\right]. \end{aligned}\right. \quad \text{(B30)}$$

with

$$A(\tau) \equiv e^{\tau H/\hbar}\, \hat{A}\, e^{-\tau H/\hbar}$$

and $i\omega_n = \dfrac{2n\pi}{\beta\hbar}$ (Matsubara frequency).

- Therefore, to obtain the ("Kubo-contribution" to "paramagnetic" part of) the energy current (i.e. the 2nd term of Eq. (B-23)), we have only to calculate Eq. (B30) and replace $i\omega_n = \omega + i\delta$, to take the static limit $(\omega \to 0)$.

- The calculation of Eq. (B30) is straightforward, because it is just a free boson system in a clean limit. ② -32

- By taking the Fourier transformation, we rewrite the energy current operator $\hat{J}^{(0)}_{Q,\mu}$ in the basis which diagonalizes the Hamiltonian $\hat{H}$.

- Suppose that $\hat{H}$ is diagonalized;

$$\hat{H} = \frac{1}{2}\sum_{\mathbb{H},\delta} \Psi^{\dagger}(\mathbb{H}) \cdot H_{\delta} \cdot \Psi(\mathbb{H}+\delta)$$

N×N diagonal

N-component

$$= \frac{1}{2}\sum_{\mathbb{k}} (\gamma^{\dagger}_{\mathbb{k}}, \gamma_{-\mathbb{k}}) \cdot \begin{pmatrix} E_{d,\mathbb{k}} & \\ & E_{d,-\mathbb{k}} \end{pmatrix} \begin{pmatrix} \gamma_{\mathbb{k}} \\ \gamma^{\dagger}_{-\mathbb{k}} \end{pmatrix} \quad \text{—(B31)}$$

where

N-component

$$\Psi(\mathbb{H}) = \begin{pmatrix} \beta(\mathbb{H}) \\ \beta^{\dagger}(\mathbb{H}) \end{pmatrix} = \frac{1}{\sqrt{V}}\sum_{\mathbb{k}} e^{i\mathbb{k}\cdot\mathbb{H}} \begin{pmatrix} \beta_{\mathbb{k}} \\ \beta^{\dagger}_{-\mathbb{k}} \end{pmatrix}$$

volume (or number of unit cell)

$$\begin{pmatrix} \beta_{\mathbb{k}} \\ \beta^{\dagger}_{-\mathbb{k}} \end{pmatrix} = T_{\mathbb{k}} \cdot \begin{pmatrix} \gamma_{\mathbb{k}} \\ \gamma^{\dagger}_{-\mathbb{k}} \end{pmatrix}$$

$\Gamma_{\mathbb{k}}$

—(B31)'

- $$T_{\mathbb{k}}^{\dagger} \cdot H_{\mathbb{k}} \cdot T_{\mathbb{k}} = \begin{pmatrix} \hat{E}_{k} & \\ & \hat{E}_{-k} \end{pmatrix} \equiv \hat{E}_{d,k}$$

- $$\hat{E}_{k} = \begin{pmatrix} \epsilon_{1,k} & & \\ & \ddots & \\ & & \epsilon_{N,k} \end{pmatrix}, \quad \hat{E}_{-k} = \begin{pmatrix} \epsilon_{1,-k} & & \\ & \ddots & \\ & & \epsilon_{N,-k} \end{pmatrix}$$

- $$H_{\mathbb{k}} = \sum_{\delta} H_{\delta} e^{i \mathbb{k} \cdot \delta}$$

For later convenience, note that the velocity operator $\hat{V}_{\mu}$ is given as follows in this basis

$$\sum_{\mathbb{r}} \Psi^{\dagger}(\mathbb{r}) \cdot \hat{V}_{\mu} \cdot \Psi(\mathbb{r})$$

$$= \frac{i}{\hbar} \sum_{\mathbb{r}, \delta} \delta_{\mu} \, \Psi^{\dagger}(\mathbb{r}) \cdot H_{\delta} \cdot \Psi(\mathbb{r}+\delta)$$

$$= \frac{1}{\hbar} \sum_{\mathbb{k}} \left(\beta_{\mathbb{k}}^{\dagger} \; \beta_{-\mathbb{k}} \right) \cdot \underbrace{\frac{\partial H_{\mathbb{k}}}{\partial \mathbb{k}_{\mu}}}_{= \left(\sum_{\delta} i \delta_{\mu} H_{\delta} e^{i \mathbb{k} \cdot \delta} \right)} \cdot \begin{pmatrix} \beta_{\mathbb{k}} \\ \beta_{-\mathbb{k}}^{\dagger} \end{pmatrix}$$

$$= \frac{1}{\hbar} \sum_{\mathbb{k}} \left(\gamma_{\mathbb{k}}^{\dagger} \cdot \gamma_{-\mathbb{k}} \right) \underbrace{T_{\mathbb{k}}^{\dagger} \cdot \frac{\partial H_{k}}{\partial k_{\mu}} \cdot T_{k}}_{\equiv \hat{V}_{\mathbb{k},\mu}} \begin{pmatrix} \gamma_{\mathbb{k}} \\ \gamma_{-\mathbb{k}}^{\dagger} \end{pmatrix}$$