

# Transverse Thermal Transport due to Magnons : Semiclassical and Linear Response Approaches

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# 1

## Introduction

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Magnons (spin-waves) are low-energy elementary excitations above ordered ground states in spin Hamiltonians. In recent years spin wave band structures have been studied extensively as a view to understanding their topological properties. In particular magnons have been studied as the source of thermal hall effect in insulating magnets [8, 7]. In many insulating magnets like yttrium iron garnet (YIG), it's found that magnon can carry spin information for a prolonged distance with minimal Joule heating. [1]. Furthermore, an accurate and exact control of spin information is needed for being used in spintronics devices.

There are many theoretical [2, 3, 8] and experimental [7] realization of the thermal Hall effect of the magnons. In the Katsura *et al.* paper [8], they have studied a ferromagnet with kagome lattice structure and computed the thermal Hall conductivity using the Kubo-formula. On the other hand, Onose *et al.* [7] have considered a insulating ferromagnet  $\text{Lu}_2\text{V}_2\text{O}_7$  that has a pyrochlore structure with DM interaction and measured the thermal Hall conductivity. However, it has been found in some studies [2, 3] that there are some correction terms coming from the orbital motion of magnons that were overlooked in the earlier calculation of thermal Hall conductivity [8, 7]. One can get these correction terms by using the linear response theory with spatially varying temperature gradient [3]. Also, another approach will be to look at the semiclassical equation of motion for magnons undergoing two types of rotation motion: self-rotation and a motion along the boundary (edge current) similar to the electron cyclotron motion [2]. The only difference will be that unlike electrons magnons don't have charge and instead of Lorentz force the Berry phase coming from the magnon band structure is the reason for these rotational motions.

In this report, we are going to compute the transverse thermal hall conductivity ( $\kappa_{xy}$ ) due to magnons using two different approaches : Semiclassical Theory and Linear Response Theory. In the semiclassical approach, we will use the analogy between electron and magnon equation of motions (EOM) due to which the "Berry Phase" comes there directly [2]. Finally, In the linear response approach, we will include the temperature gradient into the Hamiltonian as a perturbation using the pseudogravitational potential ( $\chi$ ), and then the thermal transport coefficients are calculated as a linear response to  $\chi$  [3, 4], and eventually we get the thermal hall conductivity.

## 1.1 Introduction to Magnons

We know that lattice waves correspond to phonons which are just collective acoustic and optical lattice vibration. Similar to that, spin waves correspond to magnons which are collective magnetic excitations associated to the in-phase precession of the spin moments. In a nutshell, magnons are just low-energy elementary excitations above ordered ground states in spin Hamiltonians. Now, the question that really arises here is that why do we need the Magnons (spin-waves) in the first place. The answer to that is, for ferromagnet they are the exact eigenstates for simple cases and in general good approximation for the exact excitation in both FM and AFM systems to determine low energy thermodynamics. The ferromagnet's spin waves have quadratic dispersion for low  $q$  and antiferromagnet's spin waves have a linear dispersion for low  $q$ .

We know the Holstein-Primakoff transformation,

$$S_i^n = S - b_i^\dagger b_i, \quad S_i^+ = (2S - b_i^\dagger b_i)^{\frac{1}{2}} b_i, \quad S_i^- = b_i^\dagger (2S - b_i^\dagger b_i)^{\frac{1}{2}}$$

Hence, we can write from above that  $a^+ a = S - S_z$ , which means that  $a^+ a$  is roughly the deviation from the order moment. Here,  $S_z$  is the operator for the deviation of the spin along the z-axis. So, when this deviation is much smaller than  $S$ , then the spin-wave theory holds.

In Fig. 1.1, we have a perfectly ordered ferromagnetic ground state, whereas in Fig 1.2, we have a spin state in which each spin has as small transverse component. The orientation of the transverse component of any two spins differ by a small angle.

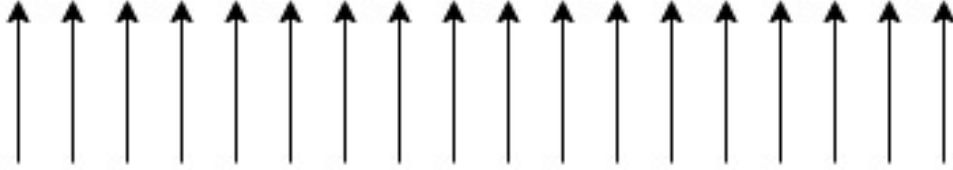


Figure 1.1: Ferromagnetic Ground State

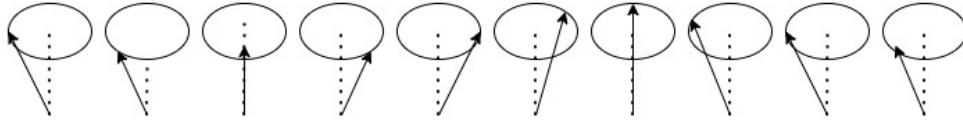


Figure 1.2: Schematic of a spin-wave state

## 1.2 Pyrochlore lattice

The pyrochlore lattice is a face centered lattice and is highly symmetric. The pyrochlore oxides are characterized by the general formula  $A_2B_2O_7$ , where the A-site and B-site form corner-sharing tetrahedral networks that are interpenetrating with each other. The pyrochlore structure causes geometrical frustration due to their 3-D tetrahedral network in many magnetic materials [16]. We are interested in the pyrochlore lattice for  $\kappa_{xy}$  calculations. For instance, the dipolar interaction has been studied as the source of topologically non-trivial band [17] and many oxides in pyrochlore have the dipolar interaction. For the calculation of the transverse thermal hall conductivity ( $\kappa_{xy}$ ) in chapter 2, we are using the DM vectors in the pyrochlore lattice ( $\text{Lu}_2\text{V}_2\text{O}_7$ ) that are determined in [7].

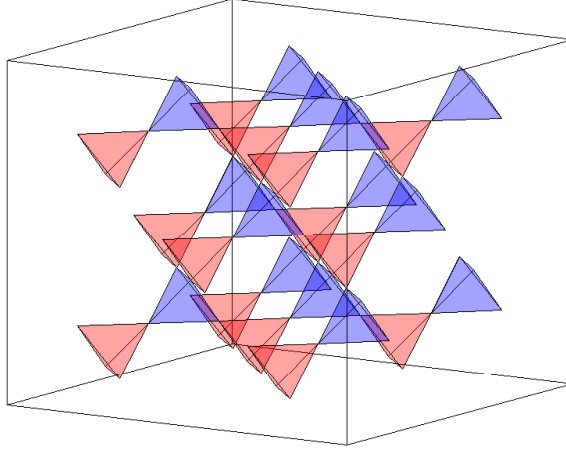


Figure 1.3: The pyrochlore lattice in the (111) axis.

The spin-wave Hamiltonian for the pyrochlore ferromagnet with the DM interaction is given by,

$$H_{eff} = \sum_{\langle ij \rangle} -J \vec{S}_i \cdot \vec{S}_j + \vec{D}_{ij} \cdot (\vec{S}_i \times \vec{S}_j) - g\mu_B \vec{B} \cdot \sum_i \vec{S}_i$$

where,  $J_{ij}$  the exchange integral or coupling constant,  $S_i$  the vanadium(V) spin moment at site  $i$ . and  $\vec{D}_{ij}$  is the DM vector. These  $\vec{D}_{ij}$ 's are highly constrained because of the symmetry of the pyrochlore lattice.

In the next chapter, we will study in detail the thermal Hall effect due to magnons for the pyrochlore ferromagnet with the DM interaction being treated perturbatively and finally, we will obtain the thermal Hall conductivity  $\kappa_{xy}$ .

## 2.1 Spin-wave Hamiltonian

The Dzyaloshinskii-Moriya interaction (DMI) tries to cant the spin because it will reduced the coupling energy ( $E_{DM} < 0$ ). Furthermore, when two spins are perpendicular w.r.t one another then  $E_{DM}$  is minimized. However, the DMI in pyrochlore does not disturb the ferromagnetic ground state for low values of DMI. Hence, spin wave theory can be developed for the same ground states as in the absence of DMI. The spin-wave Hamiltonian for the pyrochlore ferromagnet with the DM interaction :

$$H_{eff} = \sum_{\langle ij \rangle} -J \vec{S}_i \cdot \vec{S}_j + \vec{D}_{ij} \cdot (\vec{S}_i \times \vec{S}_j) - g\mu_B \vec{B} \cdot \sum_i \vec{S}_i \quad (2.1)$$

Here,  $\langle ij \rangle$  denote the nearest neighbor pairs, and  $B = (B_x, B_y, B_z)$  is the magnetic field.

Let's define orthonormal basis  $(\hat{l}, \hat{m}, \hat{n})$  for simplicity such that,

$$\hat{n} = \frac{\vec{B}}{B} \quad \text{with} \quad B = \sqrt{B_x^2 + B_y^2 + B_z^2} \quad (2.2)$$

The DM vector in this basis:

$$\vec{D}_{ij} = (\vec{D}_{ij} \cdot \hat{n})\hat{n} + (\vec{D}_{ij} \cdot \hat{l})\hat{l} + (\vec{D}_{ij} \cdot \hat{m})\hat{m} \quad (2.3)$$

Here, DM vector perpendicular to  $\hat{n}$  does not contribute to the spin-wave Hamiltonian as  $\hat{n}$  is parallel to  $\vec{S}_i \times \vec{S}_j$ . Hence, we have

$$D_{ij}^n = (\vec{D}_{ij} \cdot \hat{n}) \quad (2.4)$$

Let's define the DM vectors in pyrochlore magnets [7]:

$$\vec{D}_{13} = \frac{D}{\sqrt{2}}(-1, 1, 0), \quad \vec{D}_{24} = \frac{D}{\sqrt{2}}(-1, -1, 0), \quad \vec{D}_{43} = \frac{D}{\sqrt{2}}(0, -1, 1), \quad (2.5)$$

$$\vec{D}_{12} = \frac{D}{\sqrt{2}}(0, -1, -1), \quad \vec{D}_{14} = \frac{D}{\sqrt{2}}(1, 0, 1), \quad \vec{D}_{23} = \frac{D}{\sqrt{2}}(1, 0, -1) \quad (2.6)$$

Now using (2.4), (2.5) and (2.6), we can write:

$$\vec{D}_{13} = \frac{D}{\sqrt{2}} \frac{-B_x + B_y}{B} \hat{n}, \quad \vec{D}_{24} = \frac{D}{\sqrt{2}} \frac{-B_x - B_y}{B} \hat{n}, \quad \vec{D}_{43} = \frac{D}{\sqrt{2}} \frac{-B_y + B_z}{B} \hat{n}, \quad (2.7)$$

$$\vec{D}_{12} = \frac{D}{\sqrt{2}} \frac{-B_y - B_z}{B} \hat{n}, \quad \vec{D}_{14} = \frac{D}{\sqrt{2}} \frac{B_x + B_z}{B} \hat{n}, \quad \vec{D}_{23} = \frac{D}{\sqrt{2}} \frac{B_x - B_z}{B} \hat{n} \quad (2.8)$$

Now, we can write

$$H_{eff} = \sum_{\langle ij \rangle} h_{ij} \quad (2.9)$$

The local Hamiltonian  $h_{ij}$  is,

$$\begin{aligned} h_{ij} &= -J\vec{S}_i \cdot \vec{S}_j + \vec{D}_{ij} \cdot \vec{S}_i \times \vec{S}_j - g\mu_B \vec{B} \cdot (\vec{S}_i + \vec{S}_j) \\ &= -J\vec{S}_i \cdot \vec{S}_j + D_{ij}^n (\hat{n} \cdot (\vec{S}_i \times \vec{S}_j)) - g\mu_B B \left( \frac{\vec{B}}{B} \cdot (\vec{S}_i + \vec{S}_j) \right) \\ &= -J\vec{S}_i \cdot \vec{S}_j + D_{ij}^n (\hat{n} \cdot (\vec{S}_i \times \vec{S}_j)) - g\mu_B B (\hat{n} \cdot (\vec{S}_i + \vec{S}_j)) \end{aligned} \quad (2.10)$$

Now,  $\hat{n} \cdot (\vec{S}_i \times \vec{S}_j) = (\vec{S}_i \cdot \hat{l})(\vec{S}_j \cdot \hat{m}) - (\vec{S}_j \cdot \hat{l})(\vec{S}_i \cdot \hat{m})$  and let  $(\vec{S}_i \cdot \hat{v}) = S_i^\nu$ , we get

$$\begin{aligned} h_{ij} &= -J\vec{S}_i \cdot \vec{S}_j + D_{ij}^n (S_i^l S_j^m - S_j^l S_i^m) - g\mu_B B (S_i^n + S_j^n) \\ &= -J(S_i^n S_j^n + S_i^l S_j^l + S_i^m S_j^m) + D_{ij}^n (S_i^l S_j^m - S_j^l S_i^m) - g\mu_B B (S_i^n + S_j^n) \end{aligned} \quad (2.11)$$

Now, we can use the notation,  $S_i^\pm = S_i^l \pm iS_i^m$  to get,

$$\begin{aligned} h_{ij} &= -J(S_i^n S_j^n) - \frac{J}{2}(S_i^+ S_j^- + S_i^- S_j^+) + i\frac{D_{ij}^n}{2}(S_i^+ S_j^- - S_i^- S_j^+) - g\mu_B B (S_i^n + S_j^n) \\ &= -J(S_i^n S_j^n) - \frac{1}{2}(S_i^+ S_j^-)(J - iD_{ij}^n) - \frac{1}{2}(J + iD_{ij}^n)(S_i^- S_j^+) - g\mu_B B (S_i^n + S_j^n) \end{aligned} \quad (2.12)$$

Now let  $J_{ij} = \sqrt{J^2 + (D_{ij}^n)^2}$  and  $\tan\phi_{ij} = \frac{D_{ij}^n}{J}$ , so we get,

$$\begin{aligned} h_{ij} &= -J(S_i^n S_j^n) - \frac{J_{ij}}{2}(S_i^+ S_j^-) \frac{(J - iD_{ij}^n)}{J_{ij}} - \frac{J_{ij}}{2} \frac{(J + iD_{ij}^n)}{J_{ij}} (S_i^- S_j^+) - g\mu_B B (S_i^n + S_j^n) \\ &= -J(S_i^n S_j^n) - \frac{J_{ij}}{2}(S_i^+ S_j^-) e^{-i\phi_{ij}} - \frac{J_{ij}}{2} e^{i\phi_{ij}} (S_i^- S_j^+) - g\mu_B B (S_i^n + S_j^n) \\ &= -J(S_i^n S_j^n) - \frac{J_{ij}}{2} \left( (S_i^+ S_j^-) e^{-i\phi_{ij}} + e^{i\phi_{ij}} (S_i^- S_j^+) \right) - g\mu_B B (S_i^n + S_j^n) \end{aligned} \quad (2.13)$$

Now we can use Holstein-Primakoff transformation,

$$S_i^n = S - b_i^+ b_i, \quad S_i^+ = (2S - b_i^+ b_i)^{\frac{1}{2}} b_i, \quad S_i^- = b_i^+ (2S - b_i^+ b_i)^{\frac{1}{2}} \quad (2.14)$$

Hence, we get

$$\begin{aligned} h_{ij} &= -J((S - b_i^+ b_i)((S - b_j^+ b_j)) - \frac{J_{ij}}{2}(((2S - b_i^+ b_i)^{\frac{1}{2}} b_i)(b_j^+ (2S - b_j^+ b_j)^{\frac{1}{2}})) e^{-i\phi_{ij}} \\ &\quad - \frac{J_{ij}}{2} e^{i\phi_{ij}} (b_i^+ (2S - b_i^+ b_i)^{\frac{1}{2}} (2S - b_j^+ b_j)^{\frac{1}{2}} b_j) - g\mu_B B (S - b_i^+ b_i + S - b_j^+ b_j) \\ \\ h_{ij} &= -J(S^2 - S b_j^+ b_j - S b_i^+ b_i + b_i^+ b_i b_j^+ b_j) - \frac{J_{ij}}{2} (b_j^+ b_i (4S^2 - 2S b_j^+ b_j - 2S b_i^+ b_i + b_i^+ b_i b_j^+ b_j)^{\frac{1}{2}}) e^{-i\phi_{ij}} \\ &\quad - \frac{J_{ij}}{2} e^{i\phi_{ij}} (b_i^+ b_j (4S^2 - 2S b_j^+ b_j - 2S b_i^+ b_i + b_i^+ b_i b_j^+ b_j)^{\frac{1}{2}}) - g\mu_B B (2S - b_i^+ b_i - b_j^+ b_j) \end{aligned}$$



$$h_{ij} = -J(S^2 - Sb_j^\dagger b_j - Sb_i^\dagger b_i + b_i^\dagger b_i b_j^\dagger b_j) - J_{ij}S(b_j^\dagger b_i(1 - \frac{b_j^\dagger b_j}{2S} - \frac{b_i^\dagger b_i}{2S} + \frac{b_i^\dagger b_i b_j^\dagger b_j}{4S^2})^{\frac{1}{2}})e^{-i\phi_{ij}} \\ - J_{ij}Se^{i\phi_{ij}}(b_i^\dagger b_j(1 - \frac{b_j^\dagger b_j}{2S} - \frac{b_i^\dagger b_i}{2S} + \frac{b_i^\dagger b_i b_j^\dagger b_j}{4S^2})^{\frac{1}{2}}) - g\mu_B B(2S - b_i^\dagger b_i - b_j^\dagger b_j)$$

$$\boxed{h_{ij} \approx -JS^2 - g\mu_B B(2S) - J_{ij}S(b_j^\dagger b_i e^{-i\phi_{ij}} + b_i^\dagger b_j e^{i\phi_{ij}}) + (JS + g\mu_B B)(b_i^\dagger b_i + b_j^\dagger b_j)} \quad (2.15)$$

Now, let's write the Hamiltonian in the momentum space by using bosonic operator:

$$b_{\vec{R}+\vec{\delta}_m} = \frac{1}{N} \sum_k e^{-i\vec{k}\cdot(\vec{R}+\vec{\delta}_m)} b_m(\vec{k}) \quad (2.16)$$

Here, N is the total number of unit cells,  $\vec{R}$  denotes the position of the "1 site" in each unit cell, and m = 1, 2, 3, and 4 are the sublattice indices. The vectors  $\vec{\delta}_m$  are given by,

$$\vec{\delta}_1 = \vec{0}, \quad \vec{\delta}_2 = \hat{y} - \hat{z}, \quad \vec{\delta}_3 = \hat{x} + \hat{y}, \quad \vec{\delta}_4 = \hat{x} - \hat{z} \quad (2.17)$$

Now let's use (2.16), so that

$$b_j^\dagger b_i e^{-i\phi_{ij}} + b_i^\dagger b_j e^{i\phi_{ij}} = \frac{1}{N} \sum_{k'} e^{i\vec{k}'\cdot(\vec{R}+\vec{\delta}_{m_2})} b_{m_2}^\dagger(\vec{k}') \frac{1}{N} \sum_k e^{-i\vec{k}\cdot(\vec{R}+\vec{\delta}_{m_1})} b_{m_1}(\vec{k}) e^{-i\phi_{ij}} \\ + \frac{1}{N} \sum_k e^{i\vec{k}\cdot(\vec{R}+\vec{\delta}_{m_1})} b_{m_1}^\dagger(\vec{k}) \frac{1}{N} \sum_{k'} e^{-i\vec{k}'\cdot(\vec{R}+\vec{\delta}_{m_2})} b_{m_2}(\vec{k}') e^{i\phi_{ij}} \quad (2.18) \\ = \frac{1}{N^2} \sum_{kk'} e^{i\vec{k}'\cdot(\vec{R}+\vec{\delta}_{m_2})} e^{-i\vec{k}\cdot(\vec{R}+\vec{\delta}_{m_1})} b_{m_2}^\dagger(\vec{k}') b_{m_1}(\vec{k}) e^{-i\phi_{ij}} \\ + \frac{1}{N^2} \sum_{kk'} e^{i\vec{k}\cdot(\vec{R}+\vec{\delta}_{m_1})} e^{-i\vec{k}'\cdot(\vec{R}+\vec{\delta}_{m_2})} b_{m_1}^\dagger(\vec{k}) b_{m_2}(\vec{k}') e^{i\phi_{ij}}$$

$$b_i^\dagger b_i + b_j^\dagger b_j = \frac{1}{N} \sum_k e^{i\vec{k}\cdot(\vec{R}+\vec{\delta}_{m_1})} b_{m_1}^\dagger(\vec{k}) \frac{1}{N} \sum_{k'} e^{-i\vec{k}'\cdot(\vec{R}+\vec{\delta}_{m_1})} b_{m_1}(\vec{k}') \\ + \frac{1}{N} \sum_k e^{i\vec{k}\cdot(\vec{R}+\vec{\delta}_{m_2})} b_{m_2}^\dagger(\vec{k}) \frac{1}{N} \sum_{k'} e^{-i\vec{k}'\cdot(\vec{R}+\vec{\delta}_{m_2})} b_{m_2}(\vec{k}') \quad (2.19) \\ = \frac{1}{N^2} \sum_{kk'} e^{i\vec{k}\cdot(\vec{R}+\vec{\delta}_{m_1})} e^{-i\vec{k}'\cdot(\vec{R}+\vec{\delta}_{m_1})} b_{m_1}^\dagger(\vec{k}) b_{m_1}(\vec{k}') \\ + \frac{1}{N^2} \sum_{kk'} e^{i\vec{k}\cdot(\vec{R}+\vec{\delta}_{m_2})} e^{-i\vec{k}'\cdot(\vec{R}+\vec{\delta}_{m_2})} b_{m_2}^\dagger(\vec{k}) b_{m_2}(\vec{k}')$$

The spin wave Hamiltonian is,

$$H_{SW} = \sum_{\langle ij \rangle} h_{ij} \quad (2.20)$$

Now using (2.15), (2.18), (2.19) and (2.20), we can write  $H_{SW}$  in k-space,

$$H_{SW} = \sum_{R, m_1, m_2} (-J_{ij}S(\frac{1}{N^2} \sum_{kk'} e^{i\vec{k}'\cdot(\vec{R}+\vec{\delta}_{m_2})} e^{-i\vec{k}\cdot(\vec{R}+\vec{\delta}_{m_1})} b_{m_2}^\dagger(\vec{k}') b_{m_1}(\vec{k}) e^{-i\phi_{m_1 m_2}} + \frac{1}{N^2} \sum_{kk'} e^{i\vec{k}\cdot(\vec{R}+\vec{\delta}_{m_1})} \\ e^{-i\vec{k}'\cdot(\vec{R}+\vec{\delta}_{m_2})} b_{m_1}^\dagger(\vec{k}) b_{m_2}(\vec{k}') e^{i\phi_{m_1 m_2}} + (JS + g\mu_B B)(\frac{1}{N^2} \sum_{kk'} e^{i\vec{k}\cdot(\vec{R}+\vec{\delta}_{m_1})} e^{-i\vec{k}'\cdot(\vec{R}+\vec{\delta}_{m_1})} b_{m_1}^\dagger(\vec{k}) b_{m_1}(\vec{k}') \\ + \frac{1}{N^2} \sum_{kk'} e^{i\vec{k}\cdot(\vec{R}+\vec{\delta}_{m_2})} e^{-i\vec{k}'\cdot(\vec{R}+\vec{\delta}_{m_2})} b_{m_2}^\dagger(\vec{k}) b_{m_2}(\vec{k}')))) \quad (2.21)$$

Now using  $\delta(t - u) = \frac{1}{N^2} \sum_w e^{i(t-u)w}$ , we get

$$H_{SW} = \sum_{k, m_1, m_2} \left( -\frac{J_{ij}}{J} JS(e^{i\vec{k} \cdot \vec{\delta}_{m_2}} e^{-i\vec{k} \cdot \vec{\delta}_{m_1}} b_{m_2}^\dagger(\vec{k}) b_{m_1}(\vec{k}) e^{-i\phi_{m_1 m_2}} + e^{i\vec{k} \cdot \vec{\delta}_{m_1}} e^{-i\vec{k} \cdot \vec{\delta}_{m_2}} b_{m_1}^\dagger(\vec{k}) b_{m_2}(\vec{k}) e^{i\phi_{m_1 m_2}}) + (JS + g\mu_B B)(e^{i\vec{k} \cdot \vec{\delta}_{m_1}} e^{-i\vec{k} \cdot \vec{\delta}_{m_1}} b_{m_1}^\dagger(\vec{k}) b_{m_1}(\vec{k}) + e^{i\vec{k} \cdot \vec{\delta}_{m_2}} e^{-i\vec{k} \cdot \vec{\delta}_{m_2}} b_{m_2}^\dagger(\vec{k}) b_{m_2}(\vec{k})) \right) \quad (2.22)$$

Since  $\cos\phi = \frac{J}{J_{ij}}$ , we have

$$H_{SW} = \sum_{k, m_1, m_2} \left( -( \cos[\phi_{m_1 m_2}] )^{-1} JS(e^{i\vec{k} \cdot \vec{\delta}_{m_2}} e^{-i\vec{k} \cdot \vec{\delta}_{m_1}} b_{m_2}^\dagger(\vec{k}) b_{m_1}(\vec{k}) e^{-i\phi_{m_1 m_2}} + e^{i\vec{k} \cdot \vec{\delta}_{m_1}} e^{-i\vec{k} \cdot \vec{\delta}_{m_2}} b_{m_1}^\dagger(\vec{k}) b_{m_2}(\vec{k}) e^{i\phi_{m_1 m_2}}) + (JS + g\mu_B B)(b_{m_1}^\dagger(\vec{k}) b_{m_1}(\vec{k}) + b_{m_2}^\dagger(\vec{k}) b_{m_2}(\vec{k})) \right) \quad (2.23)$$

From (2.23), we have total 12 pairs namely

$$1 \rightarrow (2, 3, 4), \quad 2 \rightarrow (1, 3, 4), \quad 3 \rightarrow (1, 2, 4), \quad 4 \rightarrow (1, 2, 3) \quad (2.24)$$

Using (2.23) and (2.24) we can write the spin-wave Hamiltonian in momentum space as:

$$\psi^\dagger(\vec{k}) H_{SW} \psi(\vec{k}) \quad (2.25)$$

with  $\psi(\vec{k}) = (b_1(\vec{k}), b_2(\vec{k}), b_3(\vec{k}), b_4(\vec{k}))^T$  and  $H_{SW} = 6JS + 6g\mu_B B - 2JS(\cos\phi_{ij})^{-1} \Lambda(\vec{k}, \phi_{ij})$  where,

$$\Lambda(\vec{k}, \phi_{ij}) = \begin{pmatrix} 0 & e^{-i\phi_{12}} \cos(\vec{k} \cdot \delta_2) & e^{-i\phi_{13}} \cos(\vec{k} \cdot \delta_3) & e^{-i\phi_{14}} \cos(\vec{k} \cdot \delta_4) \\ e^{i\phi_{12}} \cos(\vec{k} \cdot \delta_2) & 0 & e^{-i\phi_{23}} \cos(\vec{k} \cdot (\delta_3 - \delta_2)) & e^{-i\phi_{24}} \cos(\vec{k} \cdot (\delta_4 - \delta_2)) \\ e^{i\phi_{13}} \cos(\vec{k} \cdot \delta_3) & e^{i\phi_{23}} \cos(\vec{k} \cdot (\delta_3 - \delta_2)) & 0 & e^{i\phi_{43}} \cos(\vec{k} \cdot (\delta_3 - \delta_4)) \\ e^{i\phi_{14}} \cos(\vec{k} \cdot \delta_4) & e^{i\phi_{24}} \cos(\vec{k} \cdot (\delta_4 - \delta_2)) & e^{-i\phi_{43}} \cos(\vec{k} \cdot (\delta_3 - \delta_4)) & 0 \end{pmatrix} \quad (2.26)$$

In case of no DM interaction, i.e.,  $\phi_{ij} = 0$ , the eigenvalues can be obtained analytically for  $H_{SW}(\vec{k})$ . The magnon dispersion has two degenerate flat bands at  $\omega = 8JS + g\mu_B B$  and two dispersive bands at  $\omega(\vec{k}) = 6JS + g\mu_B B - 2JS(1 \pm \sqrt{1 + A(\vec{k})})$  with  $A(\vec{k}) = \cos(2k_x) \cos(2k_y) + \cos(2k_y) \cos(2k_z) + \cos(2k_z) \cos(2k_x)$  [15]. Hence, the lowest magnon band is given by  $\omega_1(\vec{k}) = 6JS + g\mu_B B - 2JS(1 + \sqrt{1 + A(\vec{k})})$ . Now, expanding  $\omega_1(\vec{k})$  around  $\vec{k} = \vec{0}$ , we get<sup>1</sup>

$$\boxed{\omega_1(\vec{k}) \sim 2JS|\vec{k}|^2 + g\mu_B B}$$

Now, we will use this limit as the unperturbed limit about which we will develop the linear response theory in the next section.

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<sup>1</sup>We have obtained the magnon dispersion relation for no DMI.

## 2.2 Calculation of Transverse Thermal Hall Conductivity

The TKNN formula for  $\kappa_{xy}$  for non-interacting bosons in the low temperature region is,

$$\kappa_{xy} \simeq -\frac{1}{2T} \text{Im} \int_{BZ} \frac{d^3k}{(2\pi)^3} n_1(\vec{k}) \left\langle \partial_{k_x} u_1(\vec{k}) \left| [H_{SW} + \omega_1(\vec{k})]^2 \right| \partial_{k_y} u_1(\vec{k}) \right\rangle \quad (2.27)$$

Now let's use the identity  $\sum_{m=1}^4 |u_m(\vec{k})\rangle \langle u_m(\vec{k})| = 1$ , we have

$$\begin{aligned} \kappa_{xy} &= -\frac{1}{2T} \text{Im} \int_{BZ} \frac{d^3k}{(2\pi)^3} n_1(\vec{k}) \left\langle \partial_{k_x} u_1(\vec{k}) \left| \sum_{m=1}^4 |u_m(\vec{k})\rangle \langle u_m(\vec{k})| [H_{SW} + \omega_1(\vec{k})]^2 \sum_{m=1}^4 |u_m(\vec{k})\rangle \langle u_m(\vec{k})| \partial_{k_y} u_1(\vec{k}) \right\rangle \right. \\ &= -\frac{1}{2T} \text{Im} \sum_{m=1}^4 \int_{BZ} \frac{d^3k}{(2\pi)^3} n_1(\vec{k}) \left\langle \partial_{k_x} u_1(\vec{k}) \left| u_m(\vec{k}) \right\rangle \langle u_m(\vec{k}) \left| [H_{SW} + \omega_1(\vec{k})]^2 \right| u_m(\vec{k}) \right\rangle \langle u_m(\vec{k}) \left| \partial_{k_y} u_1(\vec{k}) \right\rangle \right. \\ &= -\frac{1}{2T} \sum_{m=2}^4 \int_{BZ} \frac{d^3k}{(2\pi)^3} n_1(\vec{k}) [\omega_m(\vec{k}) + \omega_1(\vec{k})]^2 \text{Im} \left[ \langle \partial_{k_x} u_1(\vec{k}) \left| u_m(\vec{k}) \right\rangle \langle u_m(\vec{k}) \left| \partial_{k_y} u_1(\vec{k}) \right\rangle \right] \end{aligned} \quad (2.28)$$

Here we can remove  $m = 1$  from the summation using the fact that  $|u_1(\vec{k})\rangle$  is normalized :

$$\langle \partial_{k_x} u_1(\vec{k}) \left| u_1(\vec{k}) \right\rangle + \langle u_1(\vec{k}) \left| \partial_{k_x} u_1(\vec{k}) \right\rangle = 0 \quad (2.29)$$

Hence, from (2.29) we can conclude that  $\langle \partial_{k_x} u_1(\vec{k}) \left| u_1(\vec{k}) \right\rangle \langle u_1(\vec{k}) \left| \partial_{k_y} u_1(\vec{k}) \right\rangle$  is real and so  $m=1$  doesn't contribute.

In the low temperature limit, the dominant contribution to the integral in Eq. (2.28) comes from small  $|\vec{k}|$  due to the Bose factor. Hence, In the vicinity of  $\vec{k} = \vec{0}$ , we can write

$$\omega_m(\vec{k}) + \omega_1(\vec{k}) \approx \omega_m(\vec{0}) + \omega_1(\vec{0}) = 8JS + 12g\mu_B B \quad (m = 2, 3, 4) \quad (2.30)$$

Using (2.30) in (2.28), and also using (2.29) in a later step, we get

$$\begin{aligned} \kappa_{xy} &= -\frac{1}{2T} [8JS + 12g\mu_B B]^2 \int_{BZ} \frac{d^3k}{(2\pi)^3} n_1(\vec{k}) \sum_{m=2}^4 \text{Im} \left[ \langle \partial_{k_x} u_1(\vec{k}) \left| u_m(\vec{k}) \right\rangle \langle u_m(\vec{k}) \left| \partial_{k_y} u_1(\vec{k}) \right\rangle \right] \\ &= -\frac{1}{2T} [8JS + 12g\mu_B B]^2 \int_{BZ} \frac{d^3k}{(2\pi)^3} n_1(\vec{k}) \sum_{m=1}^4 \text{Im} \left[ \langle \partial_{k_x} u_1(\vec{k}) \left| u_m(\vec{k}) \right\rangle \langle u_m(\vec{k}) \left| \partial_{k_y} u_1(\vec{k}) \right\rangle \right] \\ &= -\frac{1}{2T} [8JS + 12g\mu_B B]^2 \int_{BZ} \frac{d^3k}{(2\pi)^3} n_1(\vec{k}) \text{Im} \left[ \langle \partial_{k_x} u_1(\vec{k}) \left| \partial_{k_y} u_1(\vec{k}) \right\rangle \right] \end{aligned} \quad (2.31)$$

Now let's define the Berry Curvature (Transverse),

$$F_{xy}(\vec{k}) = -2\text{Im} \left[ \langle \partial_{k_x} u_1(\vec{k}) \left| \partial_{k_y} u_1(\vec{k}) \right\rangle \right] \quad (2.32)$$

Therefore,

$$\kappa_{xy} = \frac{1}{4T} [8JS + 12g\mu_B B]^2 \int_{BZ} \frac{d^3k}{(2\pi)^3} n_1(\vec{k}) F_{xy}(\vec{k}) \quad (2.33)$$

Now to calculate  $F_{xy}(\vec{k})$ , we have to find  $u_1(\vec{k})$  near  $\vec{k} = \vec{0}$  within the first order perturbation in  $\phi_{ij}$ . The perturbed Hamiltonian in the new basis is,

$$H' = -2JSU^\dagger[\Lambda(\vec{k}, \phi_{ij}) - \Lambda(\vec{0}, \phi_{ij} = 0)]U \quad (2.34)$$

Here  $U$  is a unitary matrix such that  $\Lambda(\vec{0}, \phi_{ij} = 0)$  is diagonal. Hence the non-perturbed Hamiltonian is  $H_o = 6JS + 6g\mu_B B - 2JSU^\dagger[\Lambda(\vec{0}, \phi_{ij} = 0)]U$ . The eigenvector is approximated as,<sup>2</sup>

$$|u_1(\vec{k})\rangle \approx \left(1 + \frac{1}{E_o - H_o}(1 - P_o)H'\right) |u_1^{(0)}(\vec{0})\rangle \quad (2.35)$$

Here,  $|u_1^{(0)}(\vec{0})\rangle = (1, 0, 0, 0)^T$ ,  $P_o = |u_1^{(0)}(\vec{0})\rangle \langle u_1^{(0)}(\vec{0})|$ , and  $E_o = \langle u_1^{(0)}(\vec{0}) | H_o | u_1^{(0)}(\vec{0}) \rangle$ . Now in order to calculate the berry curvature, we have find :

$$\partial_y |u_1(\vec{k})\rangle = \frac{-2JS(1 - P_o)}{E_o - H_o} U^\dagger \begin{pmatrix} 0 & -e^{-i\phi_{12}} \frac{\sin(k_y - k_z)}{\cos(\phi_{12})} & -e^{-i\phi_{13}} \frac{\sin(k_x + k_y)}{\cos(\phi_{13})} & 0 \\ -e^{i\phi_{12}} \frac{\sin(k_y - k_z)}{\cos(\phi_{12})} & 0 & 0 & e^{-i\phi_{24}} \frac{\sin(k_x - k_y)}{\cos(\phi_{24})} \\ -e^{i\phi_{13}} \frac{\sin(k_x + k_y)}{\cos(\phi_{13})} & 0 & 0 & -e^{i\phi_{43}} \frac{\sin(k_y + k_z)}{\cos(\phi_{43})} \\ 0 & e^{i\phi_{24}} \frac{\sin(k_x - k_y)}{\cos(\phi_{24})} & -e^{-i\phi_{43}} \frac{\sin(k_y + k_z)}{\cos(\phi_{43})} & 0 \end{pmatrix} U |u_1^{(0)}(\vec{0})\rangle \quad (2.36)$$

$$\partial_x |u_1(\vec{k})\rangle = \frac{-2JS(1 - P_o)}{E_o - H_o} U^\dagger \begin{pmatrix} 0 & 0 & -e^{-i\phi_{13}} \frac{\sin(k_x + k_y)}{\cos(\phi_{13})} & e^{-i\phi_{14}} \frac{\sin(k_z - k_x)}{\cos(\phi_{14})} \\ 0 & 0 & -e^{-i\phi_{23}} \frac{\sin(k_x + k_z)}{\cos(\phi_{23})} & -e^{-i\phi_{24}} \frac{\sin(k_x - k_y)}{\cos(\phi_{24})} \\ -e^{i\phi_{13}} \frac{\sin(k_x + k_y)}{\cos(\phi_{13})} & -e^{i\phi_{23}} \frac{\sin(k_x + k_z)}{\cos(\phi_{23})} & 0 & 0 \\ e^{i\phi_{14}} \frac{\sin(k_z - k_x)}{\cos(\phi_{14})} & -e^{i\phi_{24}} \frac{\sin(k_x - k_y)}{\cos(\phi_{24})} & 0 & 0 \end{pmatrix} U |u_1^{(0)}(\vec{0})\rangle \quad (2.37)$$

Now let's use (2.36) and (2.37) in (2.32),

$$\begin{aligned} F_{xy}(\vec{k}) &= -2Im \left[ \langle \partial_{k_x} u_1(\vec{k}) | \partial_{k_y} u_1(\vec{k}) \rangle \right] \\ &= -2Im \left[ \left( \frac{-2JS(1 - P_o)}{E_o - H_o} \right)^2 \right. \\ &\quad \left. \langle u_1^{(0)}(\vec{0}) | U^\dagger \begin{pmatrix} 0 & 0 & -e^{-i\phi_{13}} \frac{\sin(k_x + k_y)}{\cos(\phi_{13})} & e^{-i\phi_{14}} \frac{\sin(k_z - k_x)}{\cos(\phi_{14})} \\ 0 & 0 & -e^{-i\phi_{23}} \frac{\sin(k_x + k_z)}{\cos(\phi_{23})} & -e^{-i\phi_{24}} \frac{\sin(k_x - k_y)}{\cos(\phi_{24})} \\ -e^{i\phi_{13}} \frac{\sin(k_x + k_y)}{\cos(\phi_{13})} & -e^{i\phi_{23}} \frac{\sin(k_x + k_z)}{\cos(\phi_{23})} & 0 & 0 \\ e^{i\phi_{14}} \frac{\sin(k_z - k_x)}{\cos(\phi_{14})} & -e^{i\phi_{24}} \frac{\sin(k_x - k_y)}{\cos(\phi_{24})} & 0 & 0 \end{pmatrix} U \right. \\ &\quad \left. U^\dagger \begin{pmatrix} 0 & -e^{-i\phi_{12}} \frac{\sin(k_y - k_z)}{\cos(\phi_{12})} & -e^{-i\phi_{13}} \frac{\sin(k_x + k_y)}{\cos(\phi_{13})} & 0 \\ -e^{i\phi_{12}} \frac{\sin(k_y - k_z)}{\cos(\phi_{12})} & 0 & 0 & e^{-i\phi_{24}} \frac{\sin(k_x - k_y)}{\cos(\phi_{24})} \\ -e^{i\phi_{13}} \frac{\sin(k_x + k_y)}{\cos(\phi_{13})} & 0 & 0 & -e^{i\phi_{43}} \frac{\sin(k_y + k_z)}{\cos(\phi_{43})} \\ 0 & e^{i\phi_{24}} \frac{\sin(k_x - k_y)}{\cos(\phi_{24})} & -e^{-i\phi_{43}} \frac{\sin(k_y + k_z)}{\cos(\phi_{43})} & 0 \end{pmatrix} U |u_1^{(0)}(\vec{0})\rangle \right] \end{aligned} \quad (2.38)$$

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<sup>2</sup>Here the method followed by Hosho Katsura et. al for triangular lattice is not valid.

$$F_{xy}(\vec{k}) = -2Im \left[ \left( \frac{-2JS(1-P_o)}{E_o - H_o} \right)^2 \left\langle u_1^{(0)}(\vec{0}) \right| U^\dagger \right. \\ \left. \begin{pmatrix} \left( \frac{\sin(k_x+k_y)}{\cos(\phi_{13})} \right)^2 & e^{i(-\phi_{14}+\phi_{24})} \frac{\sin(k_z-k_x)\sin(k_x-k_y)}{\cos(\phi_{14})\cos(\phi_{24})} & -e^{i(-\phi_{14}+\phi_{43})} \frac{\sin(k_y+k_z)\sin(k_z-k_x)}{\cos(\phi_{14})\cos(\phi_{43})} \\ e^{i(-\phi_{23}+\phi_{13})} \frac{\sin(k_x+k_y)\sin(k_x+k_z)}{\cos(\phi_{14})\cos(\phi_{23})} & -\left( \frac{\sin(k_x-k_y)}{\cos(\phi_{24})} \right)^2 & e^{i(-\phi_{24}-\phi_{43})} \frac{\sin(k_y+k_z)\sin(k_x-k_y)}{\cos(\phi_{43})\cos(\phi_{24})} \\ e^{i(\phi_{12}+\phi_{23})} \frac{\sin(k_x+k_z)\sin(k_y-k_z)}{\cos(\phi_{23})\cos(\phi_{12})} & e^{i(\phi_{13}-\phi_{12})} \frac{\sin(k_y-k_z)\sin(k_x+k_y)}{\cos(\phi_{13})\cos(\phi_{12})} & \left( \frac{\sin(k_x+k_y)}{\cos(\phi_{13})} \right)^2 \\ e^{i(\phi_{24}+\phi_{12})} \frac{\sin(k_x-k_y)\sin(k_y-k_z)}{\cos(\phi_{12})\cos(\phi_{24})} & -e^{i(\phi_{14}-\phi_{12})} \frac{\sin(k_y-k_z)\sin(k_z-k_x)}{\cos(\phi_{14})\cos(\phi_{12})} & -e^{i(-\phi_{13}+\phi_{14})} \frac{\sin(k_x+k_y)\sin(k_z-k_x)}{\cos(\phi_{14})\cos(\phi_{13})} \end{pmatrix} \right. \\ \left. (2.39) \right]$$

$$\begin{aligned} & e^{i(-\phi_{13}+\phi_{43})} \frac{\sin(k_x+k_y)\sin(k_y+k_z)}{\cos(\phi_{43})\cos(\phi_{13})} \\ & e^{i(-\phi_{23}+\phi_{43})} \frac{\sin(k_y+k_z)\sin(k_x+k_z)}{\cos(\phi_{23})\cos(\phi_{43})} \\ & -e^{i(\phi_{23}-\phi_{24})} \frac{\sin(k_x-k_y)\sin(k_x+k_z)}{\cos(\phi_{23})\cos(\phi_{24})} \left. \right] U \left| u_1^{(0)}(\vec{0}) \right\rangle \\ & -\left( \frac{\sin(k_x-k_y)}{\cos(\phi_{24})} \right)^2 \end{aligned}$$

The Unitary matrix U is given by,

$$U = \begin{pmatrix} 1 & -1 & -1 & -1 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$$

$$F_{xy}(\vec{k}) = -2Im \left[ \left( \frac{-2JS(1-P_o)}{E_o - H_o} \right)^2 \begin{pmatrix} 1 & 1 & 1 & 1 \end{pmatrix} \right. \\ \left. \begin{pmatrix} \left( \frac{\sin(k_x+k_y)}{\cos(\phi_{13})} \right)^2 + e^{i(-\phi_{14}+\phi_{24})} \frac{\sin(k_z-k_x)\sin(k_x-k_y)}{\cos(\phi_{14})\cos(\phi_{24})} - e^{i(-\phi_{14}+\phi_{43})} \frac{\sin(k_y+k_z)\sin(k_z-k_x)}{\cos(\phi_{14})\cos(\phi_{43})} \\ + e^{i(-\phi_{13}+\phi_{43})} \frac{\sin(k_x+k_y)\sin(k_y+k_z)}{\cos(\phi_{43})\cos(\phi_{13})} \\ e^{i(-\phi_{23}+\phi_{13})} \frac{\sin(k_x+k_y)\sin(k_x+k_z)}{\cos(\phi_{14})\cos(\phi_{23})} - \left( \frac{\sin(k_x-k_y)}{\cos(\phi_{24})} \right)^2 + e^{i(-\phi_{24}-\phi_{43})} \frac{\sin(k_y+k_z)\sin(k_x-k_y)}{\cos(\phi_{43})\cos(\phi_{24})} \\ + e^{i(-\phi_{23}+\phi_{43})} \frac{\sin(k_y+k_z)\sin(k_x+k_z)}{\cos(\phi_{23})\cos(\phi_{43})} \\ e^{i(\phi_{12}+\phi_{23})} \frac{\sin(k_x+k_z)\sin(k_y-k_z)}{\cos(\phi_{23})\cos(\phi_{12})} + e^{i(\phi_{13}-\phi_{12})} \frac{\sin(k_y-k_z)\sin(k_x+k_y)}{\cos(\phi_{13})\cos(\phi_{12})} + \left( \frac{\sin(k_x+k_y)}{\cos(\phi_{13})} \right)^2 \\ - e^{i(\phi_{23}-\phi_{24})} \frac{\sin(k_x-k_y)\sin(k_x+k_z)}{\cos(\phi_{23})\cos(\phi_{24})} \\ e^{i(\phi_{24}+\phi_{12})} \frac{\sin(k_x-k_y)\sin(k_y-k_z)}{\cos(\phi_{12})\cos(\phi_{24})} - e^{i(\phi_{14}-\phi_{12})} \frac{\sin(k_y-k_z)\sin(k_z-k_x)}{\cos(\phi_{14})\cos(\phi_{12})} - e^{i(-\phi_{13}+\phi_{14})} \frac{\sin(k_x+k_y)\sin(k_z-k_x)}{\cos(\phi_{14})\cos(\phi_{13})} \\ - \left( \frac{\sin(k_x-k_y)}{\cos(\phi_{24})} \right)^2 \end{pmatrix} \right] \quad (2.40)$$

$$\begin{aligned}
F_{xy}(\vec{k}) = & -2Im \left[ \left( \frac{-2JS(1-P_o)}{E_o - H_o} \right)^2 \left( \frac{\sin(k_x + k_y)}{\cos(\phi_{13})} \right)^2 + e^{i(-\phi_{14} + \phi_{24})} \frac{\sin(k_z - k_x)\sin(k_x - k_y)}{\cos(\phi_{14})\cos(\phi_{24})} \right. \\
& - e^{i(-\phi_{14} + \phi_{43})} \frac{\sin(k_y + k_z)\sin(k_z - k_x)}{\cos(\phi_{14})\cos(\phi_{43})} + e^{i(-\phi_{13} + \phi_{43})} \frac{\sin(k_x + k_y)\sin(k_y + k_z)}{\cos(\phi_{43})\cos(\phi_{13})} \\
& + e^{i(-\phi_{23} + \phi_{13})} \frac{\sin(k_x + k_y)\sin(k_x + k_z)}{\cos(\phi_{14})\cos(\phi_{23})} - \left( \frac{\sin(k_x - k_y)}{\cos(\phi_{24})} \right)^2 + e^{i(-\phi_{24} - \phi_{43})} \frac{\sin(k_y + k_z)\sin(k_x - k_y)}{\cos(\phi_{43})\cos(\phi_{24})} \\
& + e^{i(-\phi_{23} + \phi_{43})} \frac{\sin(k_y + k_z)\sin(k_x + k_z)}{\cos(\phi_{23})\cos(\phi_{43})} + e^{i(\phi_{12} + \phi_{23})} \frac{\sin(k_x + k_z)\sin(k_y - k_z)}{\cos(\phi_{23})\cos(\phi_{12})} \\
& + e^{i(\phi_{13} - \phi_{12})} \frac{\sin(k_y - k_z)\sin(k_x + k_y)}{\cos(\phi_{13})\cos(\phi_{12})} + \left( \frac{\sin(k_x + k_y)}{\cos(\phi_{13})} \right)^2 - e^{i(\phi_{23} - \phi_{24})} \frac{\sin(k_x - k_y)\sin(k_x + k_z)}{\cos(\phi_{23})\cos(\phi_{24})} \\
& e^{i(\phi_{24} + \phi_{12})} \frac{\sin(k_x - k_y)\sin(k_y - k_z)}{\cos(\phi_{12})\cos(\phi_{24})} - e^{i(\phi_{14} - \phi_{12})} \frac{\sin(k_y - k_z)\sin(k_z - k_x)}{\cos(\phi_{14})\cos(\phi_{12})} \\
& \left. - e^{i(-\phi_{13} + \phi_{14})} \frac{\sin(k_x + k_y)\sin(k_z - k_x)}{\cos(\phi_{14})\cos(\phi_{13})} - \left( \frac{\sin(k_x - k_y)}{\cos(\phi_{24})} \right)^2 \right]
\end{aligned} \tag{2.41}$$

Expanding this in terms of  $\phi_{ij}$  and  $k_\alpha$ , we get

$$F_{xy}(\vec{k}) \approx \frac{2\phi_{12} + \phi_{13} - \phi_{24}}{16} (k_x^2 + k_y^2 + 2k_z^2) + \dots \tag{2.42}$$

Now let's consider the  $\phi$  terms from (2.42),

$$2\phi_{12} + \phi_{13} - \phi_{24} \tag{2.43}$$

Now we know  $\tan\phi_{ij} = \frac{D_{ij}^n}{J} \approx \phi_{ij}$ , we get<sup>3</sup>

$$2\phi_{12} + \phi_{13} - \phi_{24} = 2\frac{D_{12}^n}{J} + \frac{D_{13}^n}{J} - \frac{D_{24}^n}{J} \tag{2.44}$$

Now using (2.7) and (2.8) in (2.44), we get

$$\begin{aligned}
2\phi_{12} + \phi_{13} - \phi_{24} &= 2\frac{D}{\sqrt{2}J} \frac{-B_y - B_z}{B} + \frac{D}{\sqrt{2}J} \frac{-B_x + B_y}{B} - \frac{D}{\sqrt{2}J} \frac{-B_x - B_y}{B} \\
&= \frac{D}{\sqrt{2}J} \left( \frac{-2B_y - 2B_z - B_x + B_y + B_x + B_y}{B} \right) \\
&= \frac{D}{\sqrt{2}J} \left( \frac{-2B_z}{B} \right)
\end{aligned} \tag{2.45}$$

Therefore,

$$F_{xy}(\vec{k}) \approx \left( \frac{D}{16\sqrt{2}J} \left( \frac{-2B_z}{B} \right) \right) (k_x^2 + k_y^2 + 2k_z^2) \tag{2.46}$$

Since  $n_z = \frac{B_z}{B}$ , we have

$$F_{xy}(\vec{k}) \approx -\frac{D}{8\sqrt{2}J} n_z (k_x^2 + k_y^2 + 2k_z^2) \tag{2.47}$$

---

<sup>3</sup>This is because we are treating the DMI perturbatively.

Now using (2.33), we can get the transverse thermal hall conductivity,

$$\begin{aligned}\kappa_{xy} &\approx \frac{1}{4T} [8JS + 12g\mu_B B]^2 \int_{BZ} \frac{d^3k}{(2\pi)^3} n_1(\vec{k}) \left[ -\frac{D}{8\sqrt{2}J} n_z(k_x^2 + k_y^2 + 2k_z^2) \right] \\ &= -n_z \frac{D}{8\sqrt{2}J} \frac{[8JS + 12g\mu_B B]^2}{4T} \int_{BZ} \frac{d^3k}{(2\pi)^3} n_1(\vec{k}) (k_x^2 + k_y^2 + 2k_z^2)\end{aligned}\quad (2.48)$$

Here,  $n_1(\vec{k}) = \frac{1}{e^{\beta\omega_1(\vec{k})} - 1} = \frac{1}{e^{\beta(2JS|\vec{k}|^2 + g\mu_B B)} - 1}$ . Therefore,

$$\kappa_{xy} = -n_z \frac{D}{8\sqrt{2}J} \frac{[8JS + 12g\mu_B B]^2}{4T} \int_{BZ} \frac{d^3k}{(2\pi)^3} \frac{1}{e^{\beta(2JS|\vec{k}|^2 + g\mu_B B)} - 1} (k_x^2 + k_y^2 + 2k_z^2) \quad (2.49)$$

Now changing the integration from over the BZ to over all  $\vec{k}$ , we have

$$\begin{aligned}\kappa_{xy} &= -n_z \frac{D}{8\sqrt{2}J} \frac{[8JS + 12g\mu_B B]^2}{4T} \int_0^\infty \frac{4\pi k^2 dk}{(2\pi)^3} \frac{1}{e^{\beta(2JS|\vec{k}|^2 + g\mu_B B)} - 1} (k_x^2 + k_y^2 + 2k_z^2) \\ &= -n_z \frac{D}{8\sqrt{2}J} \frac{[8JS + 12g\mu_B B]^2}{4T} \times 4\pi \int_0^\infty \frac{dk}{(2\pi)^3} \frac{\frac{4}{3}k^4}{e^{\beta(2JS|\vec{k}|^2 + g\mu_B B)} - 1}\end{aligned}\quad (2.50)$$

Now in order to solve (2.50), we will do a change of variable  $t = 2\beta JS k^2$  such that :

$$\begin{aligned}dk &= \frac{dt}{4\beta JS k} \\ k &= \left(\frac{t}{2\beta JS}\right)^{\frac{1}{2}}\end{aligned}\quad (2.51)$$

Using (2.51) in (2.50), we get

$$\kappa_{xy} = -n_z \frac{D}{16\sqrt{2}J} \frac{[8JS + 12g\mu_B B]^2 T^{\frac{3}{2}}}{6\pi^2 (2JS)^{\frac{5}{2}}} \int_0^\infty dt \frac{t^{\frac{3}{2}}}{e^{(t + \beta g\mu_B B)} - 1} \quad (2.52)$$

Now, we know the integral formula for the polylogarithm :

$$\int_0^\infty dt \frac{t^s}{e^{t-\mu} - 1} = \Gamma(s+1) Li_{1+s}(e^\mu) \quad (2.53)$$

Here,  $\Gamma(x)$  is the Euler gamma function and  $Li_n(z)$  is the polylogarithm. Now, Using (2.53) in (2.52), we get:

$$\kappa_{xy} = -n_z \frac{D}{16\sqrt{2}J} \frac{[8JS + 12g\mu_B B]^2 T^{\frac{3}{2}}}{6\pi^2 (2JS)^{\frac{5}{2}}} \Gamma\left(\frac{5}{2}\right) Li_{1+s}(e^{-\beta g\mu_B B}) \quad (2.54)$$

Here, we have  $\Gamma(\frac{5}{2}) = \frac{3\sqrt{\pi}}{4}$ , hence,

$$\boxed{\kappa_{xy} = -n_z \frac{D}{16\sqrt{2}J} \frac{[4JS + 6g\mu_B B]^2 T^{\frac{3}{2}}}{2\pi^{3/2} (2JS)^{\frac{5}{2}}} Li_{1+s}(e^{-\beta g\mu_B B})} \quad (2.55)$$

It can be clearly seen that the transverse thermal conductivity in (2.55) is dependent only on the z-component of magnetic field not on x and y component. So, we can conclude that the transverse thermal conductivity( $\kappa_{\alpha\beta}$ ) is non-zero if calculated in the plane perpendicular to that of magnetic field( $B_\gamma$ ) provided that  $B_\gamma$  component is non-zero. Hence, it is due to the special Hamiltonian that we are considering that the transverse components of B do not contribute. The role of DM interaction in the transverse thermal conductivity being non-zero is very clear from (2.42) as its absence means  $\phi_{ij} = 0$ . Now, how its presence leads to non-zero transverse thermal conductivity( $\kappa_{xy}$ ) is very clear by the calculation from (2.43) to (2.47). The DM interaction is also playing a very important role here because it gives rise to the phase factors which are responsible for non-zero Berry curvature.

In this chapter, we have calculated the thermal Hall conductivity  $\kappa_{xy}$  using the spin-wave Hamiltonian for the pyrochlore ferromagnet with the DM interaction being treated perturbatively. In the next chapter, we will use the semiclassical approach to compute  $\kappa_{xy}$  in analogy with the electron system to find the overlooked correction term in (2.55) which is coming from the orbital motions of magnons [2].



# 3

## Transverse Thermal Transport due to Magnons: Semiclassical Approach

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### 3.1 Semiclassical Theory for Electron

The semiclassical theory tells about the reaction of the electrons to an externally applied electric and magnetic field which varies slowly over the dimensions of the corresponding wave packet [5]. The delicacy of the semiclassical theory which is making it intricate is the fact that the periodic potential of the lattice changes over dimensions which are small in comparison to the spread of the wave packet, and hence can't be treated classically. Therefore, the semiclassical theory is partially classical, i.e, the externally applied fields are classically treated, but not the periodic field.

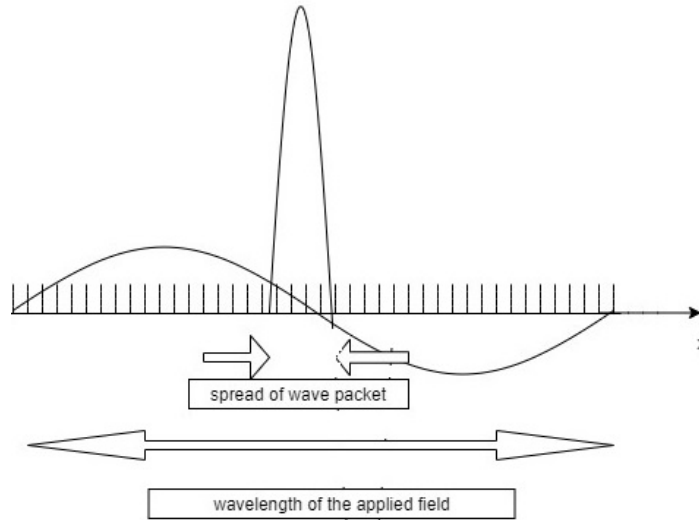


Figure 3.1: Schematic showing that the spread of the wave packet of electron is much smaller than the length scale of the applied field.

The main objective of the semiclassical theory is to connect the band structure with the transport properties. The theory is widely used to study transport properties from a provided band structure and also to infer the characteristics of the band structure with the help of the observed transport properties.

Now, we will derive the semiclassical equation of motions using a well-localised wave packet in a Bloch band.

### 3.2 Wave packet in a Bloch band

Let's consider a wave packet which is well localised around the  $(r_c, k_c)$  in the phase space:

$$|W_n\rangle = \int dk a_n(k, t) |\phi_{nk}\rangle \quad (3.1)$$

where  $|\phi_{nk}\rangle$  is the Bloch wave function with the band index  $n$  and  $a_n(k, t)$  is a function localized around  $k_c$ . It is chosen such that:

$$\bullet \quad \int dk |a_n(k, t)|^2 = 1, \quad (3.2)$$

$$\bullet \quad \int dk |a_n(k, t)|^2 k = k_c, \quad (3.3)$$

and  $|W_n\rangle$  satisfies,

$$\langle W_n | \hat{r} | W_n \rangle = r_c \quad (3.4)$$

Let's define  $\phi_{nk}(r) = u_n(k, r)e^{ik \cdot r}$ , so that we have,

$$\frac{\partial \phi_{nk}}{\partial k} = (ir)e^{ik \cdot r} u_n(k, r) + e^{ik \cdot r} \frac{\partial u_n(k, r)}{\partial k} \quad (3.5)$$

Hence,

$$(ir)\phi_{nk}(r) = \frac{\partial \phi_{nk}}{\partial k} - e^{ik \cdot r} \frac{\partial u_n(k, r)}{\partial k} \quad (3.6)$$

Finally, we get

$$\hat{r}\phi_{nk}(r) = -i \frac{\partial \phi_{nk}}{\partial k} + ie^{ik \cdot r} \frac{\partial u_n(k, r)}{\partial k} \quad (3.7)$$

So, we can write (3.4) as :

$$\begin{aligned} \langle W_n | \hat{r} | W_n \rangle &= \int dk' \int dk \langle \phi_{n'k'} | a_{n'}^*(k', t) \hat{r} a_n(k, t) | \phi_{nk} \rangle \\ &= \int dk' \int dk a_{n'}^*(k', t) a_n(k, t) \langle \phi_{n'k'} | \hat{r} | \phi_{nk} \rangle \\ &= \int dk' \int dk a_{n'}^*(k', t) a_n(k, t) \langle \phi_{n'k'} | (-i \frac{\partial | \phi_{nk} \rangle}{\partial k} + ie^{ik \cdot r} \frac{\partial | u_n(k, r) \rangle}{\partial k}) \\ &= \int dk' \int dk a_{n'}^*(k', t) a_n(k, t) \left[ -i \frac{\partial}{\partial k} (\langle \phi_{n'k'} | \phi_{nk} \rangle) + \langle u_{n'}(k', r) | e^{i(k-k') \cdot r} i \frac{\partial}{\partial k} | u_n(k, r) \rangle \right] \end{aligned} \quad (3.8)$$

Since  $\langle u_{n'}(k', r) | e^{i(k-k') \cdot r} i \frac{\partial}{\partial k} | u_n(k, r) \rangle = \delta(k - k') \langle u_n(k, r) | i \frac{\partial}{\partial k} | u_n(k, r) \rangle$ , we have,

$$\langle W_n | \hat{r} | W_n \rangle = \int dk' \int dk a_{n'}^*(k', t) a_n(k, t) \left[ (-i \frac{\partial}{\partial k}) \delta(k - k') + \delta(k - k') \langle u_n(k, r) | i \frac{\partial}{\partial k} | u_n(k, r) \rangle \right] \quad (3.9)$$

Now,

$$\int dt f(t) \frac{\partial}{\partial t} (\delta(t - t')) = -f'(t') \quad (3.10)$$

Hence,

$$\langle W_n | \hat{r} | W_n \rangle = \int dk \left[ a_n^*(k, t) (i \frac{\partial}{\partial k}) a_n(k, t) + |a_n(k, t)|^2 \langle u_n(k, r) | i \frac{\partial}{\partial k} | u_n(k, r) \rangle \right] = \mathbf{r}_c \quad (3.11)$$

Now, let  $a_n(k, t) = |a_n(k, t)|e^{-i\gamma(k, t)}$ , so that

$$\begin{aligned}
\int dk a_n^*(k, t) \left( i \frac{\partial}{\partial k} \right) a_n(k, t) &= \int dk |a_n(k, t)| e^{i\gamma(k, t)} \left( i \frac{\partial (|a_n(k, t)| e^{-i\gamma(k, t)})}{\partial k} \right) \\
&= \int dk |a_n(k, t)| e^{i\gamma(k, t)} \left( i \frac{\partial (|a_n(k, t)|)}{\partial k} e^{-i\gamma(k, t)} + |a_n(k, t)| e^{-i\gamma(k, t)} \frac{\partial \gamma(k, t)}{\partial k} \right) \\
&= \int dk |a_n(k, t)| e^{i\gamma(k, t)} \left( i \frac{\partial (|a_n(k, t)|)}{\partial k} e^{-i\gamma(k, t)} \right) + \int dk |a_n(k, t)|^2 \frac{\partial \gamma(k, t)}{\partial k} \\
&= i \int dk |a_n(k, t)| \frac{\partial (|a_n(k, t)|)}{\partial k} + \int dk |a_n(k, t)|^2 \frac{\partial \gamma(k, t)}{\partial k} \\
&= \frac{i}{2} \frac{\partial}{\partial k} \left( \int dk |a_n(k, t)|^2 \right) + \int dk |a_n(k, t)|^2 \frac{\partial \gamma(k, t)}{\partial k} \\
&= \int dk |a_n(k, t)|^2 \frac{\partial \gamma(k, t)}{\partial k}
\end{aligned} \tag{3.12}$$

So finally,

$$\langle W_n | \hat{r} | W_n \rangle = \int dk |a_n(k, t)|^2 \left[ \frac{\partial \gamma(k, t)}{\partial k} + \langle u_n(k, r) | i \frac{\partial}{\partial k} | u_n(k, r) \rangle \right] \tag{3.13}$$

Therefore, we have

$$\boxed{\mathbf{r}_c = \frac{\partial \gamma(k_c, t)}{\partial k_c} + \langle u_n(k_c, r_c) | i \frac{\partial}{\partial k_c} | u_n(k_c, r_c) \rangle} \tag{3.14}$$

### 3.3 Equations of motion

Let's for simplicity assume the presence of EM fields, the Hamiltonian is then,

$$H = \frac{(p + eA(r, t))^2}{2m} + V(r) - e\phi(r) \tag{3.15}$$

Here,  $V(r)$  is the periodic lattice potential and  $A(r)$  and  $\phi(r)$  are the EM potentials. Now if the length scale of perturbations is larger in comparison with the spread of the wave packet, then the approximate Hamiltonian can be obtained by linearizing the perturbation about wave packet center  $r_c$ ,

$$H = \frac{[p + eA(r_c, t) + e(A(r, t) - A(r_c, t))]^2}{2m} + V(r) - e\phi(r_c) - (e\phi(r) - e\phi(r_c)) \tag{3.16}$$

$$H \approx \left[ \frac{[p + eA(r_c, t)]^2}{2m} + V(r) - e\phi(r_c) \right] + \left[ \frac{e}{2m} [e(A(r, t) - A(r_c, t)) \cdot p + h.c] - eE \cdot (r - r_c) \right] \tag{3.17}$$

$$H \approx H_c + \Delta H \tag{3.18}$$

Now, the effect of  $A(r_c)$  (assume uniform) is to add a phase to the unperturbed eigenstates. Hence,

$$|W(r, k)\rangle = e^{-ie/\hbar A(r_c, t) \cdot r} |W_n(r, k)\rangle \tag{3.19}$$

The effective Lagrangian is given by,

$$L(r_c, k_c, \dot{r}_c, \dot{k}_c) = \langle W | i \frac{\partial}{\partial t} | W \rangle - \langle W | H | W \rangle \quad (3.20)$$

Here, the first term is given by,

$$\begin{aligned} \langle W | i \frac{\partial}{\partial t} | W \rangle &= \langle W_n | e \dot{A}(r_c, t) \cdot r | W_n \rangle + \int dk a_n^*(k, t) i \hbar \frac{\partial}{\partial t} a_n(k, t) \\ &= e \dot{A}(r_c, t) \cdot r_c + \int dk |a_n(k, t)|^2 \frac{\partial}{\partial t} \gamma(k, t) \\ &= e \dot{A}(r_c, t) \cdot r_c + \hbar \frac{\partial}{\partial t} \gamma(k_c, t) \end{aligned} \quad (3.21)$$

Now the second term is given by,

$$\begin{aligned} \langle W | H | W \rangle &\approx \langle W | (H_c + \Delta H) | W \rangle \\ &= \langle W | H_c | W \rangle + \langle W | \Delta H | W \rangle \\ &= E(k_c) + \langle W | \Delta H | W \rangle \\ &= \epsilon(k_c) \end{aligned} \quad (3.22)$$

The Lagrangian calculation using (3.20), (3.21) and (3.22),

$$L = e \dot{A}(r_c, t) \cdot r_c + \hbar \frac{\partial}{\partial t} \gamma(k_c, t) - \epsilon(k_c) \quad (3.23)$$

Now, we have,

$$\frac{d[A(r_c, t) \cdot r_c]}{dt} = \dot{A}(r_c, t) \cdot r_c + A(r_c, t) \cdot \dot{r}_c \quad (3.24)$$

$$\frac{d\gamma_c(k_c, t)}{dt} = \frac{\partial \gamma_c(k_c, t)}{\partial k_c} \cdot \dot{k}_c + \frac{\partial \gamma_c(k_c, t)}{\partial t} \quad (3.25)$$

Using (3.24) and (3.25) in (3.23), we get

$$L = e \frac{d[A(r_c, t) \cdot r_c]}{dt} - e A(r_c, t) \cdot \dot{r}_c + \hbar \frac{d\gamma_c(k_c, t)}{dt} - \hbar \frac{\partial \gamma_c(k_c, t)}{\partial k_c} \cdot \dot{k}_c - \epsilon(k_c) \quad (3.26)$$

Now let's use (3.14) to get,

$$L = e \frac{d[A(r_c, t) \cdot r_c]}{dt} - e A(r_c, t) \cdot \dot{r}_c + \hbar \frac{d\gamma_c(k_c, t)}{dt} - \hbar (r_c - F(k_c)) \cdot \dot{k}_c - \epsilon(k_c) \quad (3.27)$$

Also, we can write,

$$\frac{d(r_c \cdot k_c)}{dt} = \dot{r}_c \cdot k_c + r_c \cdot \dot{k}_c \quad (3.28)$$

So finally,

$$L = e \frac{d[A(r_c, t) \cdot r_c]}{dt} - e A(r_c, t) \cdot \dot{r}_c + \hbar \frac{d\gamma_c(k_c, t)}{dt} - \hbar \frac{d(r_c \cdot k_c)}{dt} + \hbar (\dot{r}_c \cdot k_c) + \hbar F(k_c) \cdot \dot{k}_c - \epsilon(k_c) \quad (3.29)$$

Now neglecting the total time derivative in the above expression, since it doesn't affect the EOM, we get (dropping c):

$$\boxed{L = -e A(r, t) \cdot \dot{r} + \hbar (\dot{r} \cdot k) + \hbar F(k) \cdot \dot{k} - \epsilon(k)} \quad (3.30)$$

Here,  $\epsilon(k) = E(k) + \langle W | \Delta H | W \rangle$ , and

$$F(k) = i \langle u_n(k, r) | \frac{\partial}{\partial k} | u_n(k, r) \rangle \quad (3.31)$$

Now the Berry curvature is,

$$\Omega(k) = \nabla \times F(k) \quad (3.32)$$

Now using the Euler-Lagrange equation, let's get the EOM,

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{k}} \right) - \frac{\partial L}{\partial k} = 0 \quad (3.33)$$

$$\hbar F(\dot{k}) - \hbar \frac{\partial F(k)}{\partial k} \cdot \dot{k} + \frac{\partial \epsilon(k)}{\partial k} - \hbar \dot{r} = 0 \quad (3.34)$$

$$\dot{r} = \frac{\partial \epsilon(k)}{\hbar \partial k} - \frac{\partial F(k)}{\partial k} \cdot \dot{k} + F(\dot{k}) \quad (3.35)$$

Since,

$$\dot{k} \times \Omega(k) = \dot{k} \times (\nabla \times F(k)) = \dot{k} \cdot \frac{\partial F(k)}{\partial k} - F(\dot{k}) \quad (3.36)$$

Hence,

$$\boxed{\dot{r} = \frac{\partial \epsilon(k)}{\hbar \partial k} - \dot{k} \times \Omega(k)} \quad (3.37)$$

Similarly, we have

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{r}} \right) - \frac{\partial L}{\partial r} = 0 \quad (3.38)$$

$$\hbar \dot{k} - e \dot{A}(r, t) + e \frac{\partial A(r, t)}{\partial r} = 0 \quad (3.39)$$

$$\boxed{\hbar \dot{k} = e \dot{A}(r, t) - e \frac{\partial A(r, t)}{\partial r}} \quad (3.40)$$

### 3.4 Semiclassical Theory for Magnons

In the approach used by Katsura *et al.*[8] and Y Onose *et al.*[7], they have overlooked the correction term coming from the orbital motions of magnons which is considered by Matsumoto *et al.* [2] in the semiclassical approach. They have used the analogy between magnon and electron EOM due to which the ‘‘Berry Phase’’ comes here directly. They have considered that magnons undergo two types of rotation motion: self-rotation and a motion along the boundary (edge current) similar to the electron cyclotron motion. The only difference will be that unlike electrons magnons don't have charge and instead of Lorentz force the Berry phase coming from the magnon band structure is the reason for these rotational motions.

#### 3.4.1 Semiclassical Approach to Calculating $k_{xy}$

We got the following semiclassical EOM in the previous calculation :

$$\dot{r} = \frac{\partial \epsilon_n(k)}{\hbar \partial k} - \dot{k} \times \Omega_n(k) \quad (3.41)$$

$$\hbar \dot{k} = -\Delta U(r) \quad (3.42)$$

In the equation (3.42), we have replaced the Lorentz force term with the gradient of the confining potential  $U(r)$  that exists only near the boundary of sample. It's done because magnons unlike electrons don't have charge, and also here Berry phase coming from magnon band structure is the one causing the rotational motions.

Now let's have a look at the edge current of magnons near the edge of the samples due to the anomalous velocity term :

$$-\dot{\mathbf{k}} \times \Omega_n(k) = \frac{\Delta U(r)}{\hbar} \times \Omega_n(k) \quad (3.43)$$

Now, the magnon edge current for edge along y-direction is given by summing (3.43) over all occupied states,

$$I_y = \int_a^b dx \frac{1}{v} \sum_{n,k} \rho(\epsilon_{nk} + U(r)) \left[ \frac{\Delta U(r)}{\hbar} \times \Omega_n(k) \right]_y \quad (3.44)$$

Here,

$$\left[ \frac{\Delta U(r)}{\hbar} \times \Omega_n(k) \right]_y = -\frac{\partial U(r)}{\hbar \partial x} \Omega_{n,z}(k) \quad (\text{Only due to } \partial_x U(r)) \quad (3.45)$$

Using (3.45) in (3.44), we get

$$\begin{aligned} I_y &= \int_a^b dx \frac{1}{v} \sum_{n,k} \rho(\epsilon_{nk} + U(r)) \left[ -\frac{\partial U(r)}{\hbar \partial x} \Omega_{n,z}(k) \right] \\ &= - \int_a^b dU(r) \left[ \frac{1}{\hbar v} \sum_{n,k} \rho(\epsilon_{nk} + U(r)) \Omega_{n,z}(k) \right] \end{aligned} \quad (3.46)$$

Let  $\epsilon_{nk} + U(r) = \epsilon$ , then  $dU(r) = d\epsilon$ . Then,

$$I_y = -\frac{1}{\hbar v} \sum_{n,k} \int_{\epsilon_{nk}}^{\infty} d\epsilon \rho(\epsilon) \Omega_{n,z}(k) \quad (3.47)$$

In order to get (3.47), we have chosen  $x=a$  (inside) and  $x=b$  (outside) such that  $U(a)=0$  and  $U(b)=\infty$ ,  $v$  is the area of the sample and  $\rho(\epsilon)$  is the Bose-Einstein function.

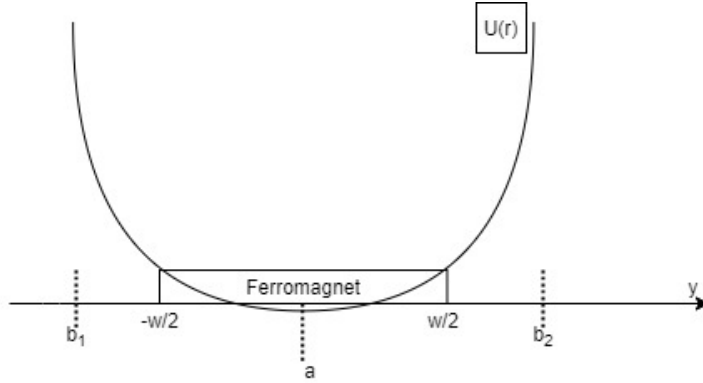


Figure 3.2: Ferromagnet coordinate that is used for the calculation of the edge current. Here,  $U(r)$  is the confining potential.

Now, Let's say that the chemical potential  $\mu$  or the temperature changes spatially. In that case, the thermal Hall effect will take place. The reason for this is the non-cancellation of the magnon edge current between one edge and the opposite edge due to which a net current will pop up. Now, we will calculate the thermal transport coefficients. Let's consider the edge current in the x-direction, with small temperature gradient in the y-direction, and the coordinate system is set as shown in Fig 3.2. So  $w$  is the width of the system and  $a, b_1, b_2$  are such that  $U(a)=0$ ,  $U(b_1)=U(b_2)=\infty$ , and  $b_1 < -w/2 < a < w/2 < b_2$ . Now, we can get the current density by integrating the local current density  $j_x(y)$ , and dividing it by the width of the system :

$$j_x = \frac{1}{w} \int_{b_1}^{b_2} dy j_x(y) = \frac{1}{w} \int_{b_1}^a dy j_x(y) + \frac{1}{w} \int_a^{b_2} dy j_x(y) \quad (3.48)$$

Now, we defined  $j_x(y)$  as follows:

$$j_x(y) = \frac{1}{\hbar V} \sum_{n,k} \rho[\epsilon_{nk} + U(r); T(y)] \frac{\partial U(r)}{\partial y} \Omega_{n,z}(k) \quad (3.49)$$

The above quantity is non-zero if  $\frac{\partial U(r)}{\partial y} \neq 0$  which implies that  $y \sim \pm w/2$ . Now, at these points:

$$\rho[\epsilon_{nk} + U(r); T(y)] \approx \begin{cases} \rho[\epsilon_{nk} + U(r); T(\frac{w}{2})] & (y \sim w/2) \\ \rho[\epsilon_{nk} + U(r); T(-\frac{w}{2})] & (y \sim -w/2) \end{cases} \quad (3.50)$$

Putting (3.50) and (3.49) in (3.48), we get:

$$\begin{aligned} j_x &= \frac{1}{w} \int_{b_1}^a dy \left[ \frac{1}{\hbar V} \sum_{n,k} \rho[\epsilon_{nk} + U(r); T(-\frac{w}{2})] \frac{\partial U(r)}{\partial y} \Omega_{n,z}(k) \right] \\ &\quad + \frac{1}{w} \int_a^{b_2} dy \left[ \frac{1}{\hbar V} \sum_{n,k} \rho[\epsilon_{nk} + U(r); T(\frac{w}{2})] \frac{\partial U(r)}{\partial y} \Omega_{n,z}(k) \right] \end{aligned} \quad (3.51)$$

Now, Let's take  $\epsilon_{nk} + U(r) = \epsilon$ , then  $dU(r) = d\epsilon$ . Then,

$$\begin{aligned} j_x &= \frac{1}{w} \frac{1}{\hbar V} \left[ \sum_{n,k} \int_{-\infty}^{\epsilon_{nk}} d\epsilon [\rho[\epsilon; T(-\frac{w}{2})] \Omega_{n,z}(k)] + \sum_{n,k} \int_{\epsilon_{nk}}^{\infty} d\epsilon [\rho[\epsilon; T(\frac{w}{2})] \Omega_{n,z}(k)] \right] \\ &= \frac{1}{w} \frac{1}{\hbar V} \sum_{n,k} \int_{\epsilon_{nk}}^{\infty} d\epsilon \times \left[ -\rho[\epsilon; T(-\frac{w}{2})] + \rho[\epsilon; T(\frac{w}{2})] \right] \Omega_{n,z}(k) \\ &= \frac{\partial}{\partial y} \left[ \frac{1}{\hbar V} \sum_{n,k} \int_{\epsilon_{nk}}^{\infty} d\epsilon \rho[\epsilon; T(y)] \Omega_{n,z}(k) \right] \end{aligned} \quad (3.52)$$

In the similar way, we can get the edge current along y-direction with the temperature gradient in the x-direction to be:

$$j_y = -\frac{\partial}{\partial x} \left[ \frac{1}{\hbar V} \sum_{n,k} \int_{\epsilon_{nk}}^{\infty} d\epsilon \rho[\epsilon; T(x)] \Omega_{n,z}(k) \right] \quad (3.53)$$

Now, combining (3.52) and (3.53), if T varies well slowly spatially, then we can write:

$$j = \nabla \times \frac{1}{\hbar V} \sum_{n,k} \int_{\epsilon_{nk}}^{\infty} d\epsilon \rho(\epsilon) \Omega_n(k) \quad (3.54)$$

Similarly, we can write the energy current from edge current density as:

$$j_E = \nabla \times \frac{1}{\hbar V} \sum_{n,k} \int_{\epsilon_{nk}}^{\infty} d\epsilon \epsilon \rho(\epsilon) \Omega_n(k) \quad (3.55)$$

Using (3.54) and (3.55), we can get various transverse transport coefficients. For example, if again we have a temperature gradient in the y-direction, then we can write the edge current and energy current as follows:

$$(j_x)^{\nabla T} = T \left[ \partial_y \left( \frac{1}{T} \right) \right] \sum_{n,k} \int_{\epsilon_{nk}}^{\infty} d\epsilon \frac{\epsilon - \mu}{\hbar V} \left( \frac{d\rho}{d\epsilon} \right) \Omega_{n,z}(k) \quad (3.56)$$

$$(j_E)_x^{\nabla T} = T \left[ \partial_y \left( \frac{1}{T} \right) \right] \sum_{n,k} \int_{\epsilon_{nk}}^{\infty} d\epsilon \frac{\epsilon(\epsilon - \mu)}{\hbar V} \left( \frac{d\rho}{d\epsilon} \right) \Omega_{n,z}(k) \quad (3.57)$$

Here, we have used the following:

$$\partial_y \rho(\epsilon) = \partial_y \left( \frac{1}{e^{\frac{\epsilon - \mu}{k_B T(y)}} - 1} \right) = \frac{-1}{(e^{\frac{\epsilon - \mu}{k_B T(y)}} - 1)^2} \times e^{\frac{\epsilon - \mu}{k_B T(y)}} \times \frac{(\epsilon - \mu)}{k_B} \times \left[ \partial_y \left( \frac{1}{T} \right) \right] \quad (3.58)$$

Now, let's use the following:

$$\frac{d\rho}{d\epsilon} = \frac{-1}{(e^{\frac{\epsilon - \mu}{k_B T(y)}} - 1)^2} \times e^{\frac{\epsilon - \mu}{k_B T(y)}} \times \frac{1}{k_B T(y)} \quad (3.59)$$

Putting (3.59) in (3.58), we get:

$$\partial_y \rho(\epsilon) = T \left[ \partial_y \left( \frac{1}{T} \right) \right] (\epsilon - \mu) \frac{d\rho}{d\epsilon} \quad (3.60)$$

So, we have used (3.60) to get (3.56) and (3.57). In the similar way, we can get these for the chemical potential gradient in the y-direction:

$$(j_x)^{\nabla \mu} = -(\partial_y \mu) \sum_{n,k} \int_{\epsilon_{nk}}^{\infty} d\epsilon \frac{1}{\hbar V} \left( \frac{d\rho}{d\epsilon} \right) \Omega_{n,z}(k) \quad (3.61)$$

$$(j_E)_x^{\nabla \mu} = -(\partial_y \mu) \sum_{n,k} \int_{\epsilon_{nk}}^{\infty} d\epsilon \frac{\epsilon}{\hbar V} \left( \frac{d\rho}{d\epsilon} \right) \Omega_{n,z}(k) \quad (3.62)$$

Now, let's define a heat current as  $j_Q \equiv j_E - \mu j$  and also the linear response of the magnon current and heat current is written as:<sup>1</sup>

$$j = L_{11}[-\nabla U - \nabla \mu] + L_{12} \left[ T \nabla \left( \frac{1}{T} \right) \right] \quad (3.63)$$

$$j_Q = L_{21}[-\nabla U - \nabla \mu] + L_{22} \left[ T \nabla \left( \frac{1}{T} \right) \right] \quad (3.64)$$

Now using (3.56), (3.57), (3.61) and (3.62), we can get the transverse transport coefficients  $L_{ij}^{xy}$ :

$$L_{11}^{xy} = \frac{1}{\hbar V} \sum_{n,k} \int_{\epsilon_{nk}}^{\infty} d\epsilon \left( \frac{d\rho}{d\epsilon} \right) \Omega_{n,z}(k) \quad (3.65)$$

$$L_{12}^{xy} = \frac{1}{\hbar V} \sum_{n,k} \int_{\epsilon_{nk}}^{\infty} d\epsilon (\epsilon - \mu) \left( \frac{d\rho}{d\epsilon} \right) \Omega_{n,z}(k) \quad (3.66)$$

$$L_{21}^{xy} = \frac{1}{\hbar V} \sum_{n,k} \int_{\epsilon_{nk}}^{\infty} d\epsilon (\epsilon - \mu) \left( \frac{d\rho}{d\epsilon} \right) \Omega_{n,z}(k) \quad (3.67)$$

$$L_{22}^{xy} = \frac{1}{\hbar V} \sum_{n,k} \int_{\epsilon_{nk}}^{\infty} d\epsilon (\epsilon - \mu)^2 \left( \frac{d\rho}{d\epsilon} \right) \Omega_{n,z}(k) \quad (3.68)$$

We can combine (3.65), (3.66), (3.67) and (3.68) to write:

$$L_{ij}^{xy} = -\frac{1}{\hbar V \beta q} \sum_{n,k} \Omega_{n,z}(k) c_q(\rho_n) \quad (3.69)$$

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<sup>1</sup>This is directly taken from G.D. Mahan, *Many Body Physics*, pg.-179.



Here, for  $i,j=1,2$ , we have

$$c_q(\rho_n) = \int_{\epsilon_{nk}}^{\infty} d\epsilon [\beta(\epsilon - \mu)]^q \left(-\frac{d\rho}{d\epsilon}\right) \quad (3.70)$$

Now, we know

$$\rho = \frac{1}{e^{\beta(\epsilon - \mu)} - 1} \quad (3.71)$$

Hence, we can write using (3.71):

$$\begin{aligned} \frac{\rho + 1}{\rho} &= e^{\beta(\epsilon - \mu)} \\ \text{or} \quad \beta(\epsilon - \mu) &= \log\left(\frac{1 + \rho}{\rho}\right) \end{aligned} \quad (3.72)$$

Now, using (3.72) in (3.70), we get

$$c_q(\rho_n) = \int_0^{\rho_n} dt \left(\log\left(\frac{1+t}{t}\right)\right)^q \quad (3.73)$$

Here,  $q = i + j - 2$ , and  $\rho_n \equiv \rho(\epsilon_{nk})$ . Now, using (3.73), we have

$$c_0(\rho) = \rho \quad (3.74)$$

$$c_1(\rho) = (1 + \rho) \log(1 + \rho) - \rho \log(\rho) \quad (3.75)$$

$$\begin{aligned} c_2(\rho) &= \int_0^{\rho} dt \left(\log\left(\frac{1+t}{t}\right)\right)^2 \\ &= (1 + \rho) \left(\log \frac{1 + \rho}{\rho}\right)^2 - (\log \rho)^2 - 2Li_2(-\rho) \end{aligned} \quad (3.76)$$

In (3.76),  $Li_2(z)$  is the polylogarithm function. Now, finally we obtain the transverse thermal Hall conductivity in a clean limit by using (3.69) in the following:

$$\kappa_{xy} = \frac{L_{22}^{xy}}{T} \quad (3.77)$$

$$\kappa_{xy} = \frac{2k_B^2 T}{\hbar V} \sum_{n,k} c_2(\rho_n) \text{Im} \left\langle \frac{\partial u_n}{\partial k_x} \middle| \frac{\partial u_n}{\partial k_y} \right\rangle \quad (3.78)$$

Hence, it can be clearly seen that there are additional terms coming in the transverse thermal Hall conductivity ( $\kappa_{xy}$ ) as compared to the calculation done in chapter 2 [7, 8]. The reason for this is that in the previous calculation, we overlooked the orbital motion of the magnons. In order to understand this in more detail, we will look at the linear response approach to magnons system in analogy with electron system in the next chapter.

# 4

## Transverse Thermal Transport due to magnons: Linear Response Approach

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### 4.1 Non-interacting boson Hamiltonian

The non-interacting boson Hamiltonian is given by:

$$H = \frac{1}{2} \int dr \ \psi^\dagger(r) H_o \psi(r) \quad (4.1)$$

Here,  $H_o$  is an arbitrary  $2N \times 2N$  Hermite matrix,  $\psi^\dagger = [\alpha_1^\dagger(r), \dots, \alpha_N^\dagger(r), \alpha_1(r), \dots, \alpha_N(r)]$ ,  $\alpha_i^\dagger(r)$  and  $\alpha_i(r)$  ( $1 \leq i \leq N$ ) are the bosonic creation and annihilation operator,  $[\alpha_i(r), \alpha_j^\dagger(r')] = \delta_{rr'} \delta_{ij}$  and  $N$  is the number of bosons in a unit cell.

### 4.2 Perturbation through temperature gradient

We know in the normal linear response theory to an external field, the field enters the Hamiltonian in the form of perturbation. In the case of temperature gradient, it does not affect the Hamiltonian but the Boltzmann factor  $e^{\frac{-H}{k_B T}}$ , where  $H$  is a Hamiltonian and  $k_B$  is the Boltzmann constant. Now, the temperature gradient is,

$$T(r) = T_o[1 - \chi(r)] \quad (4.2)$$

where  $T_o$  is a constant and  $\chi$  is a space-dependent small parameter. Now, Let's put  $T(r)$  in the Boltzmann factor:

$$e^{\frac{-H}{k_B T(r)}} = e^{\frac{-H}{k_B T_o(1-\chi(r))}} \simeq e^{\frac{-(1+\chi(r))H}{k_B T_o}} \quad (4.3)$$

Hence,  $\chi H$  can be seen as a perturbation to the Hamiltonian due to the temperature gradient. Hence, the perturbing field from the temperature gradient is:

$$H_p = \frac{1}{4} \int dr \ \psi^\dagger(r) (H_o \chi + \chi H_o) \psi(r) \quad (4.4)$$

The total Hamiltonian can be written as :

$$H_T = H + H_p \quad (4.5)$$

$$H_T = \frac{1}{2} \int dr \ \psi^\dagger(r) H_o \psi(r) + \frac{1}{4} \int dr \ \psi^\dagger(r) (H_o \chi + \chi H_o) \psi(r) \quad (4.6)$$

$$H_T = \frac{1}{2} \int dr \ \psi^\dagger(r) (H_o + \frac{1}{2} (H_o \chi + \chi H_o)) \psi(r) \quad (4.7)$$

Since  $\chi$  is small, we can write :

$$\begin{aligned}
H_o + \frac{1}{2}(H_o\chi + \chi H_o) &\simeq H_o + \frac{1}{2}(H_o\chi + \chi H_o) + \frac{\chi^2}{4}H_o \\
&= H_o(1 + \frac{\chi}{2}) + \frac{\chi H_o}{2}(1 + \frac{\chi}{2}) \\
&= (H_o + \frac{\chi H_o}{2})(1 + \frac{\chi}{2}) \\
&= (1 + \frac{\chi}{2})H_o(1 + \frac{\chi}{2})
\end{aligned} \tag{4.8}$$

Since  $\chi$  is small, the total Hamiltonian is rewritten as:

$$H_T = \frac{1}{2} \int dr \ (1 + \frac{\chi}{2})\psi^\dagger(r)H_o(1 + \frac{\chi}{2})\psi(r) \tag{4.9}$$

### 4.3 Computation of thermal current operator

We know from the continuity equation,

$$\frac{\partial \rho_T}{\partial t} + \nabla \cdot j^Q(r) = 0 \tag{4.10}$$

Here,  $\rho_T = (1 + \frac{\chi}{2})\psi^\dagger(r)H_o(1 + \frac{\chi}{2})\psi(r)$  is an energy density and  $j^Q(r)$  is a thermal current density operator. Now for simplicity, Let's consider a lattice model whose Hamiltonian is as (4.1):

$$H = \frac{1}{2} \int dr \ \psi^\dagger(r)H_o\psi(r) \tag{4.11}$$

where,

$$H_o = \sum_{\delta} H_{\delta} e^{ip \cdot \delta} \tag{4.12}$$

$$H_{\delta} = \begin{pmatrix} h_{\delta} & \Delta_{\delta} \\ \Delta_{\delta}^* & h_{-\delta}^t \end{pmatrix} \tag{4.13}$$

$$\psi_i(r) = \begin{cases} \alpha_i(r) & (i = 1, \dots, N) \\ \alpha_{i-N}^\dagger(r) & (i = N + 1, \dots, 2N) \end{cases} \tag{4.14}$$

Also,  $[\alpha_i(r), \alpha_i^\dagger(r')] = \delta_{rr'}\delta_{ij}$  and  $N$  is the number of bosons in a unit cell. The  $h_{\delta}$  and  $\Delta_{\delta}$  are the hopping terms between sites apart by  $\delta$  with a translation operator:

$$e^{ip \cdot \delta} \alpha_i(r) = \alpha_i(r + \delta) \tag{4.15}$$

$H_o$  is a Hermitian operator, which means

$$H_o = H_o^\dagger \tag{4.16}$$

$$\sum_{\delta} H_{\delta} e^{ip \cdot \delta} = \sum_{\delta} H_{\delta}^\dagger e^{-ip \cdot \delta} \tag{4.17}$$

Now multiplying both sides by  $e^{ip \cdot \delta'}$  and integrating over  $p$ , we get :

$$\int H_{\delta} e^{ip(\delta + \delta')} dp = \int H_{\delta'}^\dagger e^{ip(-\delta + \delta')} dp \tag{4.18}$$

$$H_{\delta} \delta(\delta + \delta') = H_{\delta'}^\dagger \delta(\delta - \delta') \tag{4.19}$$

$$H_{-\delta} = H_{\delta'}^\dagger \tag{4.20}$$

The following commutation relation for (4.14) :

$$[\psi_i(r), \psi_j^\dagger(r')] = (\sigma_3)_{ij} \delta_{r,r'} \quad (4.21)$$

$$[\psi_i^\dagger(r), \psi_j^\dagger(r')] = -i(\sigma_2)_{ij} \delta_{r,r'} \quad (4.22)$$

$$[\psi_i(r), \psi_j(r')] = i(\sigma_2)_{ij} \delta_{r,r'} \quad (4.23)$$

where,

$$\sigma_2 = \begin{pmatrix} 0 & -i1_{N \times N} \\ i1_{N \times N} & 0 \end{pmatrix} \quad (4.24)$$

$$\sigma_3 = \begin{pmatrix} 1_{N \times N} & 0 \\ 0 & -1_{N \times N} \end{pmatrix} \quad (4.25)$$

$$\begin{aligned} \sigma_1 H_\delta \sigma_1 &= \begin{pmatrix} 0 & -i1_{N \times N} \\ i1_{N \times N} & 0 \end{pmatrix} \begin{pmatrix} h_\delta & \Delta_\delta \\ \Delta_\delta^* & h_{-\delta}^t \end{pmatrix} \begin{pmatrix} 0 & -i1_{N \times N} \\ i1_{N \times N} & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & -i1_{N \times N} \\ i1_{N \times N} & 0 \end{pmatrix} \begin{pmatrix} i\Delta_{gN \times N} & -ih_{\delta N \times N} \\ ih_{-\delta N \times N}^t & -i\Delta_{\delta N \times N}^* \end{pmatrix} \\ &= \begin{pmatrix} h_{-\delta N \times N}^t & -\Delta_{\delta N \times N}^* \\ -\Delta_{-\delta N \times N} & h_{\delta N \times N} \end{pmatrix} \\ &= \begin{pmatrix} h_{-\delta N \times N} & \Delta_{-\delta N \times N} \\ \Delta_{-\delta N \times N}^* & h_{\delta N \times N}^t \end{pmatrix}^t \\ &= H_{-\delta}^t \end{aligned} \quad (4.26)$$

The total Hamiltonian under a potential  $\chi$  is,

$$H_T = \sum_r \rho_T(r) \quad (4.27)$$

where,

$$\rho_T(r) = \frac{1}{2} \tilde{\psi}^\dagger(r) H_o \psi(r) \quad (4.28)$$

with  $\tilde{\psi}(r) = (1 + \frac{\chi}{2})\psi(r)$ .

Now, we know from the Ehrenfest Theorem,

$$\frac{dA}{dt} = \frac{i}{\hbar} [H, A] \quad (4.29)$$

Hence, we have

$$\begin{aligned} \dot{\rho}_T(r) &= \frac{i}{\hbar} [H_T, \rho_T(r)] = \frac{i}{\hbar} [H_T, \frac{1}{2} \tilde{\psi}^\dagger(r) H_o \psi(r)] = \frac{i}{2\hbar} [H_T, \tilde{\psi}^\dagger(r)] H_o \psi(r) + \frac{i}{2\hbar} \tilde{\psi}^\dagger(r) [H_T, H_o \psi(r)] \\ \dot{\rho}_T(r) &= \frac{i}{2\hbar} [\sum_{r'} \frac{1}{2} \tilde{\psi}^\dagger(r') H_o \psi(r'), \tilde{\psi}^\dagger(r)] H_o \psi(r) + \frac{i}{2\hbar} \tilde{\psi}^\dagger(r) [\sum_{r'} \frac{1}{2} \tilde{\psi}^\dagger(r') H_o \psi(r'), H_o \psi(r)] \\ \dot{\rho}_T(r) &= \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r') [H_o \psi(r'), \tilde{\psi}^\dagger(r)] H_o \psi(r) + \frac{i}{4\hbar} \sum_{r'} [\tilde{\psi}^\dagger(r'), \tilde{\psi}^\dagger(r)] H_o \psi(r') H_o \psi(r) + \\ &\quad \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r) \tilde{\psi}^\dagger(r') [H_o \psi(r'), H_o \psi(r)] + \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r) [\tilde{\psi}^\dagger(r'), H_o \psi(r)] H_o \psi(r') \end{aligned} \quad (4.30)$$

$$\begin{aligned}
\dot{\rho}_T(r) = & \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r') H_o[\psi(\tilde{r}'), \tilde{\psi}^\dagger(r)] H_o\psi(\tilde{r}) + \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r') [H_o, \tilde{\psi}^\dagger(r)] \psi(\tilde{r}') H_o\psi(\tilde{r}) + \\
& \frac{i}{4\hbar} \sum_{r'} (-i\sigma_2) \delta_{rr'} (1 + \frac{\chi(r)}{2})^2 H_o\psi(\tilde{r}') H_o\psi(\tilde{r}) + \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r) \tilde{\psi}^\dagger(r') H_o\psi(\tilde{r}') H_o\psi(\tilde{r}) \\
& - \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r) \tilde{\psi}^\dagger(r') H_o\psi(\tilde{r}) H_o\psi(\tilde{r}') + \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r) H_o[\tilde{\psi}^\dagger(r'), \psi(\tilde{r})] H_o\psi(\tilde{r}') \\
& + \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r) [\tilde{\psi}^\dagger(r'), H_o] \psi(\tilde{r}) H_o\psi(\tilde{r}')
\end{aligned} \tag{4.31}$$

Now let's open the commutation of the last term in (4.31) so that its first term cancels out with the fifth term of (4.31) and second term cancels out with the first term of second term in (4.31).

$$\begin{aligned}
\dot{\rho}_T(r) = & \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r') H_o[\psi(\tilde{r}'), \tilde{\psi}^\dagger(r)] H_o\psi(\tilde{r}) + \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r') H_o\tilde{\psi}^\dagger(r) \psi(\tilde{r}') H_o\psi(\tilde{r}) \\
& - \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r') \tilde{\psi}^\dagger(r) H_o\psi(\tilde{r}') H_o\psi(\tilde{r}) + \frac{i}{4\hbar} \sum_{r'} (-i\sigma_2) \delta_{rr'} (1 + \frac{\chi(r)}{2})^2 H_o\psi(\tilde{r}') H_o\psi(\tilde{r}) \\
& + \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r) \tilde{\psi}^\dagger(r') H_o\psi(\tilde{r}') H_o\psi(\tilde{r}) - \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r) \tilde{\psi}^\dagger(r') H_o\psi(\tilde{r}) H_o\psi(\tilde{r}') + \\
& \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r) H_o[\tilde{\psi}^\dagger(r'), \psi(\tilde{r})] H_o\psi(\tilde{r}') + \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r) \tilde{\psi}^\dagger(r') H_o\psi(\tilde{r}) H_o\psi(\tilde{r}') \\
& - \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r) H_o\tilde{\psi}^\dagger(r') \psi(\tilde{r}) H_o\psi(\tilde{r}')
\end{aligned} \tag{4.32}$$

$$\begin{aligned}
\dot{\rho}_T(r) = & \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r') H_o[\psi(\tilde{r}'), \tilde{\psi}^\dagger(r)] H_o\psi(\tilde{r}) + \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r') H_o\tilde{\psi}^\dagger(r) \psi(\tilde{r}') H_o\psi(\tilde{r}) \\
& - \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r') \tilde{\psi}^\dagger(r) H_o\psi(\tilde{r}') H_o\psi(\tilde{r}) + \frac{i}{4\hbar} \sum_{r'} (-i\sigma_2) \delta_{rr'} (1 + \frac{\chi(r)}{2})^2 H_o\psi(\tilde{r}') H_o\psi(\tilde{r}) \\
& + \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r) \tilde{\psi}^\dagger(r') H_o\psi(\tilde{r}') H_o\psi(\tilde{r}) + \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r) H_o[\tilde{\psi}^\dagger(r'), \psi(\tilde{r})] H_o\psi(\tilde{r}') \\
& - \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r) H_o\tilde{\psi}^\dagger(r') \psi(\tilde{r}) H_o\psi(\tilde{r}')
\end{aligned} \tag{4.33}$$

Now let's use the commutation relations in (4.21) and (4.22):

$$\tilde{\psi}^\dagger(r') \tilde{\psi}^\dagger(r) = -i(\sigma_2) (1 + \frac{\chi(r)}{2})^2 \delta_{rr'} + \tilde{\psi}^\dagger(r) \tilde{\psi}^\dagger(r') \tag{4.34}$$

Putting (4.34) in (4.33), we get :

$$\begin{aligned}
\dot{\rho}_T(r) = & \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r') H_o(\sigma_3 \delta_{rr'}) (1 + \frac{\chi(r)}{2})^2 H_o\psi(\tilde{r}) + \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r') H_o\tilde{\psi}^\dagger(r) \psi(\tilde{r}') H_o\psi(\tilde{r}) \\
& + \frac{i}{4\hbar} \sum_{r'} (i\sigma_2) \delta_{rr'} (1 + \frac{\chi(r)}{2})^2 H_o\psi(\tilde{r}') H_o\psi(\tilde{r}) + \frac{i}{4\hbar} \sum_{r'} (-i(\sigma_2) (1 + \frac{\chi(r)}{2})^2 \delta_{rr'}) H_o\psi(\tilde{r}') H_o\psi(\tilde{r}) \\
& + \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r) H_o(-\sigma_3 \delta_{rr'}) (1 + \frac{\chi(r)}{2})^2 H_o\psi(\tilde{r}') - \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r) H_o\tilde{\psi}^\dagger(r') \psi(\tilde{r}) H_o\psi(\tilde{r}')
\end{aligned} \tag{4.35}$$

$$\begin{aligned}
\dot{\rho}_T(r) = & \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r') H_o(\sigma_3 \delta_{rr'}) (1 + \frac{\chi(r)}{2})^2 H_o\psi(\tilde{r}) + \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r') H_o\tilde{\psi}^\dagger(r) \psi(\tilde{r}') H_o\psi(\tilde{r}) \\
& + \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r) H_o(-\sigma_3 \delta_{rr'}) (1 + \frac{\chi(r)}{2})^2 H_o\psi(\tilde{r}') - \frac{i}{4\hbar} \sum_{r'} \tilde{\psi}^\dagger(r) H_o\tilde{\psi}^\dagger(r') \psi(\tilde{r}) H_o\psi(\tilde{r}')
\end{aligned} \tag{4.36}$$

Since the last two terms are the h.c of the first two and applying  $\delta_{rr'}$ , we can write :

$$\dot{\rho}_T(r) = \frac{i}{4\hbar} \tilde{\psi}^\dagger(r) H_o(\sigma_3) (1 + \frac{\chi(r)}{2})^2 H_o \tilde{\psi}(r) + \frac{i}{4\hbar} \tilde{\psi}^\dagger(r) H_o \tilde{\psi}^\dagger(r) \tilde{\psi}(r) H_o \tilde{\psi}(r) + h.c \quad (4.37)$$

Since  $H_o = H_o^\dagger$ , the h.c of the second term in (4.37) is,

$$I^\dagger = \left( \frac{i}{4\hbar} \tilde{\psi}^\dagger(r) H_o \tilde{\psi}^\dagger(r) \tilde{\psi}(r) H_o \tilde{\psi}(r) \right)^\dagger = -\frac{i}{4\hbar} \tilde{\psi}^\dagger(r) H_o \tilde{\psi}^\dagger(r) \tilde{\psi}(r) H_o \tilde{\psi}(r) = -I \quad (4.38)$$

Using (4.38) in (4.37) , we get

$$\dot{\rho}_T(r) = \frac{i}{4\hbar} \tilde{\psi}^\dagger(r) H_o(\sigma_3) (1 + \frac{\chi(r)}{2})^2 H_o \tilde{\psi}(r) + h.c \quad (4.39)$$

Now, let's use our  $H_o$  from (4.12) and also the fact that  $H_o = H_o^\dagger$  :

$$\dot{\rho}_T(r) = \frac{i}{4\hbar} \tilde{\psi}^\dagger(r) \sum_{\delta} H_{\delta}^t e^{-ip \cdot \delta} (\sigma_3) (1 + \frac{\chi(r)}{2})^2 \sum_{\delta'} H_{\delta'} e^{ip \cdot \delta'} \tilde{\psi}(r) + h.c \quad (4.40)$$

$$\dot{\rho}_T(r) = \frac{i}{4\hbar} \sum_{\delta\delta'} \tilde{\psi}^\dagger(r) H_{\delta}^t e^{-ip \cdot \delta} (\sigma_3) (1 + \frac{\chi(r)}{2})^2 H_{\delta'} e^{ip \cdot \delta'} \tilde{\psi}(r) + h.c \quad (4.41)$$

Now let's use (4.15) :

$$\begin{aligned} \dot{\rho}_T(r) = \frac{i}{4\hbar} \sum_{\delta\delta'} \tilde{\psi}^\dagger(r) H_{\delta}^t e^{-ip \cdot \delta} (\sigma_3) (1 + \frac{\chi(r)}{2})^2 H_{\delta'} \tilde{\psi}(r + \delta') + \frac{i}{4\hbar} \sum_{r'} \sum_{\delta\delta'} \tilde{\psi}^\dagger(r') H_{\delta} e^{ip \cdot \delta} \tilde{\psi}^\dagger(r) \tilde{\psi}(r') H_{\delta'} \tilde{\psi}(r + \delta') \\ + h.c \end{aligned} \quad (4.42)$$

We have,

$$e^{ip \cdot \delta} \tilde{\psi}(r) = \tilde{\psi}(r + \delta) \quad (4.43)$$

Now taking conjugate both sides of (4.43),

$$\tilde{\psi}^\dagger(r) e^{-ip \cdot \delta} = \tilde{\psi}^\dagger(r + \delta) \quad (4.44)$$

Using (4.44) in (4.42), we get

$$\dot{\rho}_T(r) = \frac{i}{4\hbar} \sum_{\delta\delta'} \tilde{\psi}^\dagger(r + \delta) H_{\delta}^t (\sigma_3) (1 + \frac{\chi(r)}{2})^2 H_{\delta'} \tilde{\psi}(r + \delta') + h.c \quad (4.45)$$

$$\dot{\rho}_T(r) = \frac{i}{4\hbar} \sum_{\delta\delta'} (H_{\delta} \tilde{\psi}(r + \delta))^\dagger (\sigma_3) (1 + \frac{\chi(r)}{2})^2 H_{\delta'} \tilde{\psi}(r + \delta') + h.c \quad (4.46)$$

Now, let's Taylor expand (4.46) till first order, we get

$$\dot{\rho}_T(r) = \frac{i}{4\hbar} \sum_{\delta\delta'} \sum_{\nu=x,y} \nabla_{\nu} \left[ \delta_{\nu} (H_{\delta} \tilde{\psi}(r + \delta))^\dagger (\sigma_3) (1 + \frac{\chi(r)}{2})^2 H_{\delta'} \tilde{\psi}(r + \delta') + h.c \right] \quad (4.47)$$

Now from (4.10) and (4.47), we get

$$j_\nu^Q(r) = -\frac{i}{4\hbar} \sum_{\delta\delta'} \left[ \delta_\nu (H_\delta \tilde{\psi}(r+\delta))^\dagger (\sigma_3) \left(1 + \frac{\chi(r)}{2}\right)^2 H_{\delta'} \tilde{\psi}(r+\delta') + h.c \right] \quad (4.48)$$

Now, also we know the velocity operator is given by,

$$V_\nu = \frac{1}{i\hbar} [x_\nu, H_o] \quad (4.49)$$

We know the identity,

$$[x_i, F(p)] = i\hbar \frac{\partial F}{\partial p_i} \quad (4.50)$$

Hence,

$$V_\nu = \frac{\partial H_o}{\partial p_\nu} = \frac{\partial \sum_\delta H_\delta e^{ip_\nu \delta_\nu}}{\partial p_\nu} = \frac{i}{\hbar} \sum_\delta \delta_\nu H_\delta e^{ip_\nu \delta_\nu} \quad (4.51)$$

Using (4.15) in (4.48), we have

$$j_\nu^Q(r) = -\frac{i}{4\hbar} \sum_{\delta\delta'} \left[ \delta_\nu (H_\delta e^{ip \cdot \delta} \tilde{\psi}(r))^\dagger (\sigma_3) \left(1 + \frac{\chi(r)}{2}\right)^2 H_{\delta'} e^{ip \cdot \delta'} \tilde{\psi}(r) + h.c \right] \quad (4.52)$$

$$j_\nu^Q(r) = \frac{1}{4} \left[ \left( \frac{i}{\hbar} \sum_\delta \delta_\nu H_\delta e^{ip \cdot \delta} \tilde{\psi}(r) \right)^\dagger (\sigma_3) \left(1 + \frac{\chi(r)}{2}\right)^2 \left( \sum_{\delta'} H_{\delta'} e^{ip \cdot \delta'} \tilde{\psi}(r) + h.c \right) \right] \quad (4.53)$$

Using (4.51) and (4.12), we get

$$j_\nu^Q(r) = \frac{1}{4} \left[ (V_\nu \tilde{\psi}(r))^\dagger (\sigma_3) \left(1 + \frac{\chi(r)}{2}\right)^2 H_o \tilde{\psi}(r) + h.c \right] \quad (4.54)$$

$$j_\nu^Q(r) = \frac{1}{4} \left[ \tilde{\psi}^\dagger(r) V_\nu (\sigma_3) \left(1 + \frac{\chi(r)}{2}\right)^2 H_o \tilde{\psi}(r) + \tilde{\psi}^\dagger(r) H_o \left(1 + \frac{\chi(r)}{2}\right)^2 (\sigma_3) V_\nu \tilde{\psi}(r) \right] \quad (4.55)$$

$$j_\nu^Q(r) = \frac{1}{4} \tilde{\psi}^\dagger(r) \left[ V_\nu (\sigma_3) \left(1 + \frac{\chi(r)}{2}\right)^2 H_o + H_o \left(1 + \frac{\chi(r)}{2}\right)^2 (\sigma_3) V_\nu \right] \tilde{\psi}(r) \quad (4.56)$$

Since  $\tilde{\psi}(r) = (1 + \frac{\chi}{2})\psi(r)$ , we have

$$\boxed{j_\nu^Q(r) = \frac{1}{4} \psi^\dagger(r) \left[ 1 + \frac{\chi(r)}{2} \right] \left[ V_\nu (\sigma_3) \left(1 + \frac{\chi(r)}{2}\right)^2 H_o + H_o \left(1 + \frac{\chi(r)}{2}\right)^2 (\sigma_3) V_\nu \right] \left[ 1 + \frac{\chi(r)}{2} \right] \psi(r)} \quad (4.57)$$

Now, let's expand (4.57) using the relation  $\chi(r) = r \cdot \nabla \chi$ ,

$$j_\nu^Q(r) = \frac{1}{4} \psi^\dagger(r) \left[ 1 + \frac{r \cdot \nabla \chi}{2} \right] \left[ V_\nu (\sigma_3) \left(1 + \frac{r \cdot \nabla \chi}{2}\right)^2 H_o + H_o \left(1 + \frac{r \cdot \nabla \chi}{2}\right)^2 (\sigma_3) V_\nu \right] \left[ 1 + \frac{r \cdot \nabla \chi}{2} \right] \psi(r) \quad (4.58)$$

$$\begin{aligned}
j_\nu^Q(r) = \frac{1}{4}\psi^\dagger(r) & \left[ V_\nu(\sigma_3)H_o + V_\nu(\sigma_3)\left(\frac{r \cdot \nabla \chi}{2}\right)^2 H_o + V_\nu \sigma_3 (r \cdot \nabla \chi) H_o + H_o \sigma_3 V_\nu + H_o \left(\frac{r \cdot \nabla \chi}{2}\right)^2 \sigma_3 V_\nu \right. \\
& + H_o (r \cdot \nabla \chi) \sigma_3 V_\nu + \left(\frac{r \cdot \nabla \chi}{2}\right) V_\nu (\sigma_3) H_o + \left(\frac{r \cdot \nabla \chi}{2}\right) V_\nu (\sigma_3) \left(\frac{r \cdot \nabla \chi}{2}\right)^2 H_o + \left(\frac{r \cdot \nabla \chi}{2}\right) V_\nu (\sigma_3) (r \cdot \nabla \chi) H_o \\
& + \left(\frac{r \cdot \nabla \chi}{2}\right) H_o (\sigma_3) V_\nu + \left(\frac{r \cdot \nabla \chi}{2}\right) H_o \left(\frac{r \cdot \nabla \chi}{2}\right)^2 (\sigma_3) V_\nu + \left(\frac{r \cdot \nabla \chi}{2}\right) H_o (r \cdot \nabla \chi) (\sigma_3) V_\nu + V_\nu (\sigma_3) H_o \left(\frac{r \cdot \nabla \chi}{2}\right) \\
& + V_\nu (\sigma_3) \left(\frac{r \cdot \nabla \chi}{2}\right)^2 H_o \left(\frac{r \cdot \nabla \chi}{2}\right) + V_\nu \sigma_3 (r \cdot \nabla \chi) H_o \left(\frac{r \cdot \nabla \chi}{2}\right) + H_o \sigma_3 V_\nu \left(\frac{r \cdot \nabla \chi}{2}\right) + H_o \left(\frac{r \cdot \nabla \chi}{2}\right)^2 \sigma_3 V_\nu \\
& \left(\frac{r \cdot \nabla \chi}{2}\right) + H_o (r \cdot \nabla \chi) \sigma_3 V_\nu \left(\frac{r \cdot \nabla \chi}{2}\right) + \left(\frac{r \cdot \nabla \chi}{2}\right) V_\nu (\sigma_3) H_o \left(\frac{r \cdot \nabla \chi}{2}\right) + \left(\frac{r \cdot \nabla \chi}{2}\right) V_\nu (\sigma_3) \left(\frac{r \cdot \nabla \chi}{2}\right)^2 H_o \left(\frac{r \cdot \nabla \chi}{2}\right) \\
& + \left(\frac{r \cdot \nabla \chi}{2}\right) V_\nu (\sigma_3) (r \cdot \nabla \chi) H_o \left(\frac{r \cdot \nabla \chi}{2}\right) + \left(\frac{r \cdot \nabla \chi}{2}\right) H_o (\sigma_3) V_\nu \left(\frac{r \cdot \nabla \chi}{2}\right) + \left(\frac{r \cdot \nabla \chi}{2}\right) H_o \left(\frac{r \cdot \nabla \chi}{2}\right)^2 (\sigma_3) V_\nu \left(\frac{r \cdot \nabla \chi}{2}\right) \\
& \left. + \left(\frac{r \cdot \nabla \chi}{2}\right) H_o (r \cdot \nabla \chi) (\sigma_3) V_\nu \left(\frac{r \cdot \nabla \chi}{2}\right) \right] \psi(r)
\end{aligned} \tag{4.59}$$

Since, we are only interested in terms upto linear order in  $\chi$ :

$$\begin{aligned}
j_\nu^Q(r) = \frac{1}{4}\psi^\dagger(r) & \left[ V_\nu \sigma_3 H_o + H_o \sigma_3 V_\nu \right] \psi(r) + \frac{1}{4}\psi^\dagger(r) \left[ V_\nu \sigma_3 (r \cdot \nabla \chi) H_o + H_o (r \cdot \nabla \chi) \sigma_3 V_\nu + \right. \\
& \left. \left(\frac{r \cdot \nabla \chi}{2}\right) V_\nu (\sigma_3) H_o + \left(\frac{r \cdot \nabla \chi}{2}\right) H_o (\sigma_3) V_\nu + V_\nu (\sigma_3) H_o \left(\frac{r \cdot \nabla \chi}{2}\right) + H_o \sigma_3 V_\nu \left(\frac{r \cdot \nabla \chi}{2}\right) \right] \psi(r)
\end{aligned} \tag{4.60}$$

Now, let's look at this commutation relation:

$$\begin{aligned}
[x_\mu \nabla_\mu \chi, H_o] &= x_\mu [\nabla_\mu \chi, H_o] + [x_\mu, H_o] \nabla_\mu \chi \\
&= [x_\mu, H_o] \nabla_\mu \chi \\
&= i\hbar V_\mu \nabla_\mu \chi
\end{aligned} \tag{4.61}$$

Now lets use (4.61) in (4.60):

$$\begin{aligned}
j_\nu^Q(r) = \frac{1}{4}\psi^\dagger(r) & \left[ V_\nu \sigma_3 H_o + H_o \sigma_3 V_\nu \right] \psi(r) + \frac{1}{4}\psi^\dagger(r) \left[ V_\nu \sigma_3 (i\hbar V_\mu \nabla_\mu \chi + H_o (x_\mu \nabla_\mu \chi)) + \right. \\
& ((x_\mu \nabla_\mu \chi) H_o - V_\mu \nabla_\mu \chi) \sigma_3 V_\nu + \left(\frac{x_\mu \nabla_\mu \chi}{2}\right) V_\nu (\sigma_3) H_o + \left(\frac{x_\mu \nabla_\mu \chi}{2}\right) H_o (\sigma_3) V_\nu + V_\nu (\sigma_3) H_o \left(\frac{x_\mu \nabla_\mu \chi}{2}\right) + \\
& \left. H_o \sigma_3 V_\nu \left(\frac{x_\mu \nabla_\mu \chi}{2}\right) \right] \psi(r)
\end{aligned} \tag{4.62}$$

$$\begin{aligned}
j_\nu^Q(r) = \frac{1}{4}\psi^\dagger(r) & \left[ V_\nu \sigma_3 H_o + H_o \sigma_3 V_\nu \right] \psi(r) + \frac{i\hbar}{4} (\nabla_\mu \chi) \psi^\dagger(r) \left[ V_\nu \sigma_3 V_\mu - V_\mu \sigma_3 V_\nu \right] \psi(r) + \\
& \frac{1}{8} (\nabla_\mu \chi) \left[ \psi^\dagger(r) (x_\mu V_\nu \sigma_3 + 3V_\mu \sigma_3 x_\mu) H_o \psi(r) + \psi^\dagger(r) H_o (3x_\mu \sigma_3 V_\nu + \sigma_3 V_\mu x_\mu) \psi(r) \right]
\end{aligned} \tag{4.63}$$

Hence, we can divide (4.63) into two parts  $j_{0,\nu}^Q(r)$  which is independent of  $\nabla \chi$ , and the other one  $j_{1,\nu}^Q(r)$  which is linear in  $\nabla \chi$ .

$$j_{0,\nu}^Q(r) = \frac{1}{4}\psi^\dagger(r) \left[ V_\nu \sigma_3 H_o + H_o \sigma_3 V_\nu \right] \psi(r) \tag{4.64}$$

$$\begin{aligned}
j_{1,\nu}^Q(r) = \frac{i\hbar}{4} (\nabla_\mu \chi) \psi^\dagger(r) & \left[ V_\nu \sigma_3 V_\mu - V_\mu \sigma_3 V_\nu \right] \psi(r) + \frac{1}{8} (\nabla_\mu \chi) \left[ \psi^\dagger(r) (x_\mu V_\nu \sigma_3 + 3V_\mu \sigma_3 x_\mu) H_o \psi(r) \right. \\
& \left. + \psi^\dagger(r) H_o (3x_\mu \sigma_3 V_\nu + \sigma_3 V_\mu x_\mu) \psi(r) \right]
\end{aligned} \tag{4.65}$$



Now, we can write the Fourier transform of the total thermal current:

$$J_{1,\nu}^Q = \int dr j_{1,\nu}^Q(r) = \frac{1}{4} \sum_k \psi_k^\dagger \left[ V_{k,\nu} \sigma_3 H_k + H_k \sigma_3 V_{k,\nu} \right] \psi_k \quad (4.66)$$

$$\begin{aligned} j_{1,\nu}^Q = & \frac{i\hbar}{4} (\nabla_\mu \chi) \sum_k \psi_k^\dagger \left[ V_{k,\nu} \sigma_3 V_{k,\mu} - V_{k,\mu} \sigma_3 V_{k,\nu} \right] \psi_k + \frac{1}{8} (\nabla_\mu \chi) \sum_k \left[ \psi_k^\dagger (x_\mu V_{k,\nu} \sigma_3 + 3V_{k,\mu} \sigma_3 x_\mu) H_k \psi_k \right. \\ & \left. + \psi_k^\dagger H_k (3x_\mu \sigma_3 V_{k,\nu} + \sigma_3 V_{k,\mu} x_\mu) \psi_k \right] \end{aligned} \quad (4.67)$$

Here,  $V_{k,\nu} = \sum_\delta \frac{i}{\hbar} \delta_\nu H_\delta e^{ik \cdot \delta} = \frac{1}{\hbar} \frac{\partial H_k}{\partial k_\nu}$  and

$$\psi_{i,k} = \begin{cases} \alpha_{i,k} & (i = 1, \dots, N) \\ \alpha_{i-N,-k}^\dagger & (i = N+1, \dots, 2N) \end{cases} \quad (4.68)$$

In order for the Hamiltonian to be diagonalized, we define paraunitary<sup>1</sup> matrix  $T_k$ :

$$H = \frac{1}{2} \sum_k (\gamma_k^\dagger \gamma_{-k}) \epsilon_k \begin{pmatrix} \gamma_k \\ \gamma_{-k}^\dagger \end{pmatrix} \quad (4.69)$$

where,  $\begin{pmatrix} \gamma_k \\ \gamma_{-k}^\dagger \end{pmatrix} = T_k^{-1} \begin{pmatrix} \alpha_k \\ \alpha_{-k}^\dagger \end{pmatrix}$  and  $\epsilon_k = T_k^\dagger H_k T_k$ . Therefore, using (4.68) we can write

$$\psi_{i,k} = \sum_{n=1}^N (T_k)_{i,n} \gamma_{nk} + \sum_{n=1}^N (T_k)_{i,n+N} \gamma_{n,-k}^\dagger \quad (4.70)$$

$$\psi_{i,k}^\dagger = \sum_{n=1}^N (T_k^\dagger)_{n,i} \gamma_{nk}^\dagger + \sum_{n=1}^N (T_k^\dagger)_{n+N,i} \gamma_{n,-k} \quad (4.71)$$

## 4.4 Calculation of thermal transport coefficient

The thermal transport coefficients as calculated by J.M. Luttinger under the effect of a pseudo-gravitational potential is,

$$\langle J_\nu^Q \rangle = L_{\nu\mu} \left( T \nabla_\mu \frac{1}{T} - \nabla_\mu \chi \right) \quad (4.72)$$

where  $L_{\nu\mu}$  is the thermal transport coefficient and  $\langle . \rangle$  is the thermal and quantum mechanical average.

Now,

$$\langle J_\nu^Q \rangle = \langle J_{0,\nu}^Q \rangle + \langle J_{1,\nu}^Q \rangle \quad (4.73)$$

where,

$$\langle J_{0,\nu}^Q \rangle = -S_{\nu\mu} \nabla_\mu \chi \quad (4.74)$$

$$\langle J_{1,\nu}^Q \rangle = -M_{\nu\mu} \nabla_\mu \chi \quad (4.75)$$

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<sup>1</sup>It's an extension of a unitary matrix when the matrix entries are Laurent polynomials [1].

#### 4.4.1 Calculation of $S_{\nu\mu}$

Now  $S_{\nu\mu}$  is given by,<sup>2</sup>

$$S_{\nu\mu} = -\frac{\delta \langle J_{0,\nu}^Q \rangle}{\delta \partial_\mu \chi} = -\lim_{\Omega \rightarrow 0} \frac{P_{\nu\mu}^R(\Omega) - P_{\nu\mu}^R(0)}{i\Omega} \quad (4.76)$$

Here,  $P_{\nu\mu}^R(\Omega)$  is the retarded current-current correlation function, and is given by,<sup>3</sup>

$$P_{\nu\mu}^R(\Omega) = P_{\nu\mu}(i\Omega \rightarrow \Omega + i0) \quad (4.77)$$

such that

$$P_{\nu\mu}(i\Omega) = -\int_0^\beta d\tau e^{i\Omega\tau} \langle T_\tau J_{o,\nu}^Q(\tau) J_{o,\mu}^Q(0) \rangle \quad (4.78)$$

Here,  $J_{o,\nu}^Q(\tau) = e^{\tau H} J_{o,\nu}^Q e^{-\tau H}$ . Now, using (4.66) we have

$$P_{\nu\mu}(i\Omega) = -\frac{1}{16} \int_0^\beta d\tau e^{i\Omega\tau} \sum_{k,k'} \langle T_\tau [e^{(\tau'+\tau)H} \psi_k^\dagger e^{-(\tau'+\tau)H} X_{k,\nu} e^{(\tau'+\tau)H} \psi_k e^{-(\tau'+\tau)H} e^{\tau'H} \psi_{k'}^\dagger e^{-\tau'H} X_{k',\mu} e^{\tau'H} \psi_{k'} e^{-\tau'H}] \rangle \quad (4.79)$$

$$P_{\nu\mu}(i\Omega) = -\frac{1}{16} \int_0^\beta d\tau e^{i\Omega\tau} \sum_{k,k'} \langle T_\tau [\psi_k^\dagger(\tau + \tau') X_{k,\nu} \psi_k(\tau + \tau') \psi_{k'}^\dagger(\tau') X_{k',\mu} \psi_{k'}(\tau')] \rangle \quad (4.80)$$

$$P_{\nu\mu}(i\Omega) = -\frac{1}{16} \int_0^\beta d\tau e^{i\Omega\tau} \sum_{k,k'} \sum_{\alpha,\beta,\gamma,\delta} \langle T_\tau [\psi_k^\dagger(\tau + \tau') |\phi_\alpha\rangle \langle\phi_\alpha| X_{k,\nu} |\phi_\beta\rangle \langle\phi_\beta| \psi_k(\tau + \tau') \psi_{k'}^\dagger(\tau') |\phi_\gamma\rangle \langle\phi_\gamma| X_{k',\mu} |\phi_\delta\rangle \langle\phi_\delta| \psi_{k'}(\tau')] \rangle \quad (4.81)$$

Now, using Wick's Theorem, we get

$$P_{\nu\mu}(i\Omega) = -\frac{1}{16} \int_0^\beta d\tau e^{i\Omega\tau} \sum_{k,k'} (X_{k,\nu})_{\alpha,\beta} (X_{k',\mu})_{\gamma,\delta} [\langle T_\tau \psi_{\alpha,k}^\dagger(\tau + \tau') \psi_{\delta,k'}(\tau') \rangle \langle T_\tau \psi_{\beta,k}(\tau + \tau') \psi_{\gamma,k'}^\dagger(\tau') \rangle + \langle T_\tau \psi_{\alpha,k}^\dagger(\tau + \tau') \psi_{\gamma,k'}^\dagger(\tau') \rangle \langle T_\tau \psi_{\beta,k}(\tau + \tau') \psi_{\delta,k'}(\tau') \rangle + \langle T_\tau \psi_{\alpha,k}^\dagger(\tau + \tau') \psi_{\beta,k}(\tau + \tau') \rangle \langle T_\tau \psi_{\gamma,k'}^\dagger(\tau') \psi_{\delta,k'}(\tau') \rangle] \quad (4.82)$$

Here,  $X_{k,\nu} = V_{k,\nu} \sigma_3 H_k + H_k \sigma_3 V_{k,\nu}$  and  $\Omega = \frac{2\pi n}{\beta}$  = Matsubara Frequency. The last term in (82) does not contribute as it vanishes over the integral on  $\tau$ . Now let's look at the terms in (4.82) using (4.70) and (4.71)<sup>4</sup>:

$$\langle T_\tau \psi_{\alpha,k}^\dagger(\tau + \tau') \psi_{\delta,k'}(\tau') \rangle = \langle T_\tau [e^{(\tau+\tau')H} [\sum_{n=1}^N (T_k^\dagger)_{n,\alpha} \gamma_{nk}^\dagger + \sum_{n=1}^N (T_k^\dagger)_{n+N,\alpha} \gamma_{n,-k}] e^{-\tau H} [\sum_{m=1}^N (T_{k'})_{\delta,m} \gamma_{mk'} + \sum_{m=1}^N (T_{k'})_{\delta,m+N} \gamma_{m,-k'}^\dagger] e^{-\tau' H}] \rangle \quad (4.83)$$

$$\langle T_\tau \psi_{\alpha,k}^\dagger(\tau + \tau') \psi_{\delta,k'}(\tau') \rangle = \langle T_\tau [e^{(\tau+\tau')H} [\sum_{n=1}^N (T_k^\dagger)_{n,\alpha} \gamma_{nk}^\dagger] e^{-\tau H} [\sum_{m=1}^N (T_{k'})_{\delta,m} \gamma_{mk'}] e^{-\tau' H} + e^{(\tau+\tau')H} [\sum_{n=1}^N (T_k^\dagger)_{n+N,\alpha} \gamma_{n,-k}] e^{-\tau H} [\sum_{m=1}^N (T_{k'})_{\delta,m+N} \gamma_{m,-k'}^\dagger] e^{-\tau' H}] \rangle \quad (4.84)$$

<sup>2</sup>The Kubo-Greenwood contribution to  $L_{\nu\mu}$

<sup>3</sup>This is directly taken from G.D. Mahan, *Many-Body Physics*, Pg-165.

<sup>4</sup>Here, I have used the approach taught by Dr. V Ravi Chandra in the Many Body Physics course.

$$\begin{aligned}
\langle T_\tau \psi_{\alpha,k}^\dagger(\tau + \tau') \psi_{\delta,k'}(\tau') \rangle &= \langle [\sum_{n=1}^N \sum_{m=1}^N (T_k^\dagger)_{n,\alpha} (T_{k'})_{\delta,m} \gamma_{nk}^\dagger [e^{-\tau H} \gamma_{mk'}]] \rangle e^{\tau E_o} + \\
&\quad \langle [\sum_{n=1}^N \sum_{m=1}^N (T_k^\dagger)_{n+N,\alpha} (T_{k'})_{\delta,m+N} \gamma_{n,-k} [e^{-\tau H} \gamma_{m,-k'}^\dagger]] \rangle e^{\tau E_o} \\
&= \langle [\sum_{n=1}^N \sum_{m=1}^N (T_k^\dagger)_{n,\alpha} (T_{k'})_{\delta,m} \gamma_{nk}^\dagger \gamma_{mk'}] \rangle e^{-\tau(E_o - E_{m,k'})} e^{\tau E_o} + \\
&\quad \langle [\sum_{n=1}^N \sum_{m=1}^N (T_k^\dagger)_{n+N,\alpha} (T_{k'})_{\delta,m+N} \gamma_{n,-k} \gamma_{m,-k'}^\dagger] \rangle e^{-\tau(E_o + E_{m,-k'})} e^{\tau E_o}
\end{aligned} \tag{4.85}$$

Now using  $\langle \gamma_{nk}^\dagger \gamma_{mk} \rangle = \delta_{n,m} g(E_{nk})$  and  $\langle \gamma_{nk} \gamma_{mk}^\dagger \rangle = -\delta_{n,m} g(-E_{nk})$ , we get

$$\begin{aligned}
\langle T_\tau \psi_{\alpha,k}^\dagger(\tau + \tau') \psi_{\delta,k'}(\tau') \rangle &= \sum_{n=1}^N \sum_{m=1}^N (T_k^\dagger)_{n,\alpha} (T_{k'})_{\delta,m} \delta_{nm} \delta_{kk'} g(E_{mk}) e^{\tau E_{m,k'}} - \\
&\quad \sum_{n=1}^N \sum_{m=1}^N (T_k^\dagger)_{n+N,\alpha} (T_{k'})_{\delta,m+N} \delta_{nm} \delta_{kk'} g(-E_{m,-k}) e^{-\tau E_{m,-k'}} \\
&= \sum_{n=1}^N (T_k^\dagger)_{n,\alpha} (T_k)_{\delta,n} g(E_{nk}) e^{\tau E_{n,k}} - \sum_{n=1}^N (T_k^\dagger)_{n+N,\alpha} (T_k)_{\delta,n+N} g(-E_{n,-k}) e^{-\tau E_{n,-k}}
\end{aligned} \tag{4.86}$$

Here,  $g(E) = \frac{1}{e^{\beta E} - 1}$ . Now let's compute the other term:

$$\begin{aligned}
\langle T_\tau \psi_{\beta,k}(\tau + \tau') \psi_{\gamma,k'}^\dagger(\tau') \rangle &= \langle T_\tau [e^{(\tau+\tau')H} [\sum_{n=1}^N (T_k)_{\beta,n} \gamma_{nk} + \sum_{n=1}^N (T_k)_{\beta,n+N} \gamma_{n,-k}^\dagger] e^{-\tau H} [\sum_{m=1}^N (T_{k'}^\dagger)_{m,\gamma} \gamma_{mk'}^\dagger + \\
&\quad \sum_{m=1}^N (T_{k'}^\dagger)_{m+N,\gamma} \gamma_{m,-k'}] e^{-\tau' H}] \rangle \\
&= \langle T_\tau [e^{(\tau+\tau')H} [\sum_{n=1}^N (T_k)_{\beta,n} \gamma_{nk}] e^{-\tau H} [\sum_{m=1}^N (T_{k'}^\dagger)_{m,\gamma} \gamma_{mk'}^\dagger] e^{-\tau' H} + \\
&\quad e^{(\tau+\tau')H} [\sum_{n=1}^N (T_k)_{\beta,n+N} \gamma_{n,-k}^\dagger] e^{-\tau H} [\sum_{m=1}^N (T_{k'}^\dagger)_{m+N,\gamma} \gamma_{m,-k'}] e^{-\tau' H}] \rangle \\
&= \langle [\sum_{n=1}^N \sum_{m=1}^N (T_k)_{\beta,n} (T_{k'}^\dagger)_{m,\gamma} \gamma_{nk} [e^{-\tau H} \gamma_{mk'}^\dagger]] \rangle e^{\tau E_o} + \\
&\quad \langle [\sum_{n=1}^N \sum_{m=1}^N (T_k)_{\beta,n+N} (T_{k'}^\dagger)_{m+N,\gamma} \gamma_{n,-k}^\dagger [e^{-\tau H} \gamma_{m,-k'}]] \rangle e^{\tau E_o} \\
&= \langle [\sum_{n=1}^N \sum_{m=1}^N (T_k)_{\beta,n} (T_{k'}^\dagger)_{m,\gamma} \gamma_{nk} \gamma_{mk'}^\dagger] \rangle e^{-\tau(E_o + E_{mk'})} e^{\tau E_o} + \\
&\quad \langle [\sum_{n=1}^N \sum_{m=1}^N (T_k)_{\beta,n+N} (T_{k'}^\dagger)_{m+N,\gamma} \gamma_{n,-k}^\dagger \gamma_{m,-k'}] \rangle e^{-\tau(E_o - E_{m,-k'})} e^{\tau E_o}
\end{aligned} \tag{4.87}$$

$$\begin{aligned}
\langle T_\tau \psi_{\beta,k}(\tau + \tau') \psi_{\gamma,k'}^\dagger(\tau') \rangle &= - \sum_{n=1}^N \sum_{m=1}^N (T_k)_{\beta,n} (T_k^\dagger)_{m,\gamma} \delta_{nm} \delta_{kk'} g(-E_{mk}) e^{-\tau E_{mk}} + \\
&\quad \sum_{n=1}^N \sum_{m=1}^N (T_k)_{\beta,n+N} (T_k^\dagger)_{m+N,\gamma} \delta_{nm} \delta_{kk'} g(E_{m,-k'}) e^{\tau E_{m,-k'}} \\
&= - \sum_{n=1}^N (T_k)_{\beta,n} (T_k^\dagger)_{n,\gamma} g(-E_{nk}) e^{-\tau E_{nk}} + \sum_{n=1}^N (T_k)_{\beta,n+N} (T_k^\dagger)_{n+N,\gamma} g(E_{n,-k}) e^{\tau E_{n,-k}}
\end{aligned} \tag{4.88}$$

Now let's use (4.88) and (4.86) in (4.82),

$$\begin{aligned}
P_{\nu\mu}(i\Omega) &= -\frac{1}{16} \int_0^\beta d\tau e^{i\Omega\tau} \sum_k (X_{k,\nu})_{\alpha,\beta} (X_{k,\mu})_{\gamma,\delta} \left[ \sum_{n=1}^N (T_k^\dagger)_{n,\alpha} (T_k)_{\delta,n} g(E_{nk}) e^{\tau E_{n,k}} - \right. \\
&\quad \sum_{n=1}^N (T_k^\dagger)_{n+N,\alpha} (T_k)_{\delta,n+N} g(-E_{n,-k}) e^{-\tau E_{n,-k}} \left. \times \left[ - \sum_{m=1}^N (T_k)_{\beta,m} (T_k^\dagger)_{m,\gamma} g(-E_{mk}) e^{-\tau E_{mk}} + \right. \right. \\
&\quad \left. \left. \sum_{m=1}^N (T_k)_{\beta,m+N} (T_k^\dagger)_{m+N,\gamma} g(E_{m,-k}) e^{\tau E_{m,-k}} \right] \right]
\end{aligned} \tag{4.89}$$

$$\begin{aligned}
P_{\nu\mu}(i\Omega) &= -\frac{1}{16} \int_0^\beta d\tau e^{i\Omega\tau} \sum_k (X_{k,\nu})_{\alpha,\beta} (X_{k,\mu})_{\gamma,\delta} \left[ - \sum_{n,m=1}^N (T_k^\dagger)_{n,\alpha} (T_k)_{\delta,n} g(E_{nk}) (T_k)_{\beta,m} (T_k^\dagger)_{m,\gamma} g(-E_{mk}) \right. \\
&\quad e^{\tau(E_{n,k}-E_{mk})} + \sum_{n,m=1}^N (T_k^\dagger)_{n,\alpha} (T_k)_{\delta,n} g(E_{nk}) (T_k)_{\beta,m+N} (T_k^\dagger)_{m+N,\gamma} g(E_{m,-k}) e^{\tau(E_{n,k}+E_{m,-k})} \\
&\quad + \sum_{n,m=1}^N (T_k^\dagger)_{n+N,\alpha} (T_k)_{\delta,n+N} g(-E_{n,-k}) (T_k)_{\beta,m} (T_k^\dagger)_{m,\gamma} g(-E_{mk}) e^{-\tau(E_{n,-k}+E_{mk})} \\
&\quad \left. - \sum_{n,m=1}^N (T_k^\dagger)_{n+N,\alpha} (T_k)_{\delta,n+N} g(-E_{n,-k}) (T_k)_{\beta,m+N} (T_k^\dagger)_{m+N,\gamma} g(E_{m,-k}) e^{\tau(E_{m,-k}-E_{n,-k})} \right]
\end{aligned} \tag{4.90}$$

Now let's look at the type of integral we have above,

$$I = \int_0^\beta d\tau e^{i\Omega\tau} e^{\tau E} = \left[ \frac{e^{(i\Omega+E)\tau}}{i\Omega+E} \right]_0^\beta = \frac{e^{(i\Omega+E)\beta} - 1}{i\Omega+E} = \frac{e^{i(2\pi n)} e^{E\beta} - 1}{i\Omega+E} = \frac{e^{E\beta} - 1}{i\Omega+E} \tag{4.91}$$

Hence using (4.91), we get

$$\begin{aligned}
P_{\nu\mu}(i\Omega) &= -\frac{1}{16} \sum_k \sum_{n,m=1}^N [-g(E_{nk})g(-E_{mk}) \left( \frac{e^{(E_{n,k}-E_{mk})\beta} - 1}{i\Omega + E_{n,k} - E_{mk}} \right) (T_k^\dagger X_{k,\nu} T_k)_{nm} (T_k^\dagger X_{k,\mu} T_k)_{mn} \\
&\quad + g(E_{nk})g(E_{m,-k}) \left( \frac{e^{(E_{n,k}+E_{m,-k})\beta} - 1}{i\Omega + E_{n,k} + E_{m,-k}} \right) (T_k^\dagger X_{k,\nu} T_k)_{n,m+N} (T_k^\dagger X_{k,\mu} T_k)_{m+N,n} \\
&\quad + g(-E_{n,-k})g(-E_{mk}) \left( \frac{e^{-(E_{n,-k}+E_{mk})\beta} - 1}{i\Omega - (E_{n,-k} + E_{mk})} \right) (T_k^\dagger X_{k,\nu} T_k)_{n+N,m} (T_k^\dagger X_{k,\mu} T_k)_{m,n+N} \\
&\quad - g(-E_{n,-k})g(E_{m,-k}) \left( \frac{e^{(E_{m,-k}-E_{n,-k})\beta} - 1}{i\Omega + E_{m,-k} - E_{n,-k}} \right) (T_k^\dagger X_{k,\nu} T_k)_{n+N,m+N} (T_k^\dagger X_{k,\mu} T_k)_{m+N,n+N}]
\end{aligned} \tag{4.92}$$

Hence, putting (4.92) in (4.76), we get the first term contribution to the thermal transport coefficients ( $L_{\nu\mu}$ ). Also using the following:

•

$$\begin{aligned} g(E_{nk}) - g(E_{mk}) &= \frac{1}{e^{\beta E_{nk}} - 1} - \frac{1}{e^{\beta E_{mk}} - 1} \\ &= \frac{e^{\beta E_{mk}} - e^{\beta E_{nk}}}{(e^{\beta E_{nk}} - 1)(e^{\beta E_{mk}} - 1)} \\ &= g(E_{nk})g(E_{mk})(e^{\beta E_{mk}} - e^{\beta E_{nk}}) \end{aligned} \quad (4.93)$$

So that we have,

$$g(E_{nk})g(E_{mk}) = \frac{g(E_{nk}) - g(E_{mk})}{(e^{\beta E_{mk}} - e^{\beta E_{nk}})} \quad (4.94)$$

•  $X_{k,\nu} = V_{k,\nu}\sigma_3 H_k + H_k\sigma_3 V_{k,\nu}$

Now before using (4.94) and putting (4.92) in (4.76), let's have these terms:

•

$$\begin{aligned} (T_k^\dagger X_{k,\nu} T_k)_{nm} &= (T_k^\dagger)_{n\alpha} (V_{k,\nu}\sigma_3 H_k + H_k\sigma_3 V_{k,\nu})_{\alpha\beta} (T_k)_{\beta m} \\ &= [(T_k^\dagger)_{n\alpha} (V_{k,\nu})_{\alpha\beta} (T_k)_{\beta m}] (\sigma_3)_{mm} [T_k^\dagger H_k T_k]_{mm} \\ &\quad + [T_k^\dagger H_k T_k]_{nn} (\sigma_3)_{nn} [(T_k^\dagger)_{n\alpha} (V_{k,\nu})_{\alpha\beta} (T_k)_{\beta m}] \\ &= (E_{mk} + E_{nk}) (T_k^\dagger V_{k,\nu} T_k)_{nm} \end{aligned} \quad (4.95)$$

•

$$\begin{aligned} (T_k^\dagger X_{k,\nu} T_k)_{n,m+N} &= (T_k^\dagger)_{n\alpha} (V_{k,\nu}\sigma_3 H_k + H_k\sigma_3 V_{k,\nu})_{\alpha\beta} (T_k)_{\beta,m+N} \\ &= [(T_k^\dagger)_{n\alpha} (V_{k,\nu})_{\alpha\beta} (T_k)_{\beta,m+N}] (\sigma_3)_{m+N,m+N} [T_k^\dagger H_k T_k]_{m+N,m+N} \\ &\quad + [T_k^\dagger H_k T_k]_{m,n} (\sigma_3)_{n,n} [(T_k^\dagger)_{n\alpha} (V_{k,\nu})_{\alpha\beta} (T_k)_{\beta,m+N}] \\ &= (-E_{m,-k} + E_{nk}) (T_k^\dagger V_{k,\nu} T_k)_{n,m+N} \end{aligned} \quad (4.96)$$

•

$$\begin{aligned} (T_k^\dagger X_{k,\nu} T_k)_{n+N,m} &= (T_k^\dagger)_{n+N,\alpha} (V_{k,\nu}\sigma_3 H_k + H_k\sigma_3 V_{k,\nu})_{\alpha\beta} (T_k)_{\beta,m} \\ &= [(T_k^\dagger)_{n+N,\alpha} (V_{k,\nu})_{\alpha\beta} (T_k)_{\beta,m}] (\sigma_3)_{m,m} [T_k^\dagger H_k T_k]_{m,m} \\ &\quad + [T_k^\dagger H_k T_k]_{n+N,n+N} (\sigma_3)_{n+N,n+N} [(T_k^\dagger)_{n+N,\alpha} (V_{k,\nu})_{\alpha\beta} (T_k)_{\beta,m}] \\ &= (E_{mk} - E_{n,-k}) (T_k^\dagger V_{k,\nu} T_k)_{n+N,m} \end{aligned} \quad (4.97)$$

•

$$\begin{aligned} (T_k^\dagger X_{k,\nu} T_k)_{n+N,m+N} &= (T_k^\dagger)_{n+N,\alpha} (V_{k,\nu}\sigma_3 H_k + H_k\sigma_3 V_{k,\nu})_{\alpha\beta} (T_k)_{\beta,m+N} \\ &= [(T_k^\dagger)_{n+N,\alpha} (V_{k,\nu})_{\alpha\beta} (T_k)_{\beta,m+N}] (\sigma_3)_{m+N,m+N} [T_k^\dagger H_k T_k]_{m+N,m+N} \\ &\quad + [T_k^\dagger H_k T_k]_{n+N,n+N} (\sigma_3)_{n+N,n+N} [(T_k^\dagger)_{n+N,\alpha} (V_{k,\nu})_{\alpha\beta} (T_k)_{\beta,m+N}] \\ &= (-E_{m,-k} - E_{n,-k}) (T_k^\dagger V_{k,\nu} T_k)_{n+N,m+N} \end{aligned} \quad (4.98)$$

Eq. (4.93) can also be written as :

$$\begin{aligned}
g(E_{nk}) - g(E_{mk}) &= g(E_{nk})g(E_{mk})(e^{\beta E_{mk}} - e^{\beta E_{nk}}) \\
&= g(E_{nk}) \frac{1}{e^{\beta E_{mk}} - 1} (e^{\beta E_{mk}} - e^{\beta E_{nk}}) \\
&= g(E_{nk}) \frac{-e^{\beta E_{mk}}}{e^{\beta E_{mk}} - 1} (e^{\beta(E_{nk}-E_{mk})} - 1) \\
&= g(E_{nk})g(-E_{mk})(e^{\beta(E_{nk}-E_{mk})} - 1)
\end{aligned} \tag{4.99}$$

Now using (4.95), (4.96), (4.97), (4.98) and (4.99) in (4.92), and then putting it in (4.76), we get the following expression for  $S_{\nu\mu}$  :

$$\begin{aligned}
S_{\nu\mu} &= -\frac{i}{8} \sum_k \sum_{n,m=1}^N \left[ \frac{g(E_{nk}) - g(E_{mk})}{(E_{nk} - E_{mk})^2} (E_{nk} + E_{mk})^2 (T_k^\dagger V_{k,\nu} T_k)_{nm} (T_k^\dagger V_{k,\mu} T_k)_{mn} \right. \\
&\quad - \frac{g(E_{nk}) - g(-E_{m,-k})}{(E_{nk} - E_{m,-k})^2} (E_{nk} - E_{m,-k})^2 (T_k^\dagger V_{k,\nu} T_k)_{n,m+N} (T_k^\dagger V_{k,\mu} T_k)_{m+N,n} \\
&\quad - \frac{g(-E_{n,-k}) - g(E_{mk})}{(E_{n,-k} + E_{mk})^2} (E_{n,-k} - E_{mk})^2 (T_k^\dagger V_{k,\nu} T_k)_{n+N,m} (T_k^\dagger V_{k,\mu} T_k)_{m,n+N} \\
&\quad \left. + \frac{g(-E_{n,-k}) - g(-E_{m,-k})}{(E_{n,-k} - E_{m,-k})^2} (E_{n,-k} + E_{m,-k})^2 (T_k^\dagger V_{k,\nu} T_k)_{n+N,m+N} (T_k^\dagger V_{k,\mu} T_k)_{m+N,n+N} \right]
\end{aligned} \tag{4.100}$$

#### 4.4.2 Calculation of $M_{\nu\mu}$

The second term contribution to the thermal transport coefficients, i.e.  $M_{\nu\mu}$  is coming from the orbital motion of magnons. The  $M_{\nu\mu}$  is given by,

$$M_{\nu\mu} = -\frac{\delta \langle J_{1,\nu}^Q \rangle}{\delta \partial_\mu \chi} \tag{4.101}$$

Now using (4.67), we have

$$\begin{aligned}
M_{\nu\mu} &= \frac{i\hbar}{4} \sum_k \langle \psi_k^\dagger (V_{k,\nu} \sigma_3 V_{k,\mu} - V_{k,\mu} \sigma_3 V_{k,\nu}) \psi_k \rangle - \frac{1}{8} \sum_k \left[ \langle \psi_k^\dagger (x_\mu V_{k,\nu} \sigma_3 + 3V_{k,\mu} \sigma_3 x_\mu) H_k \psi_k \rangle \right. \\
&\quad \left. + \langle \psi_k^\dagger H_k (3x_\mu \sigma_3 V_{k,\nu} + \sigma_3 V_{k,\mu} x_\mu) \psi_k \rangle \right]
\end{aligned} \tag{4.102}$$

Now using (4.70), (4.71), and  $\langle \gamma_{nk}^\dagger \gamma_{mk} \rangle = \delta_{n,m} g(E_{nk})$  and  $\langle \gamma_{nk} \gamma_{mk}^\dagger \rangle = -\delta_{n,m} g(-E_{nk})$ , we get

$$\begin{aligned}
M_{\nu\mu} &= -\frac{i\hbar}{4} \sum_{n,m=1}^N \sum_k [g(E_{nk}) (T_k^\dagger V_{k,\nu} T_k)_{nm} (T_k^\dagger V_{k,\mu} T_k)_{mn} - [g(E_{nk}) (T_k^\dagger V_{k,\nu} T_k)_{n,m+N} (T_k^\dagger V_{k,\mu} T_k)_{m+N,n} \\
&\quad - [g(-E_{n,-k}) (T_k^\dagger V_{k,\nu} T_k)_{n+N,m} (T_k^\dagger V_{k,\mu} T_k)_{m,n+N} + [g(-E_{n,-k}) (T_k^\dagger V_{k,\nu} T_k)_{n+N,m+N} (T_k^\dagger V_{k,\mu} T_k)_{m+N,n+N}] \\
&\quad + (\nu \leftrightarrow \mu) - \frac{1}{2} \sum_{n=1}^N \sum_k [(T_k^\dagger (x_\mu V_{k,\nu} + V_{k,\nu} x_\mu) T_k)_{nn} E_{nk} g(E_{nk}) + (T_k^\dagger (x_\mu V_{k,\nu} + V_{k,\nu} x_\mu) T_k)_{n+N,n+N} \\
&\quad \quad \quad E_{n,-k} g(-E_{n,-k})]
\end{aligned} \tag{4.103}$$

## 4.5 Calculation of Thermal Transport Coefficient ( $L_{\nu\mu}$ )

We know, the total thermal transport coefficient is given by,

$$L_{\nu\mu} = S_{\nu\mu} + M_{\nu\mu} \quad (4.104)$$

Now, we will divide the coefficients into two parts:

$$\begin{aligned} S_{\nu\mu} &= S_{\nu\mu}^{(1)} + S_{\nu\mu}^{(2)} \\ M_{\nu\mu} &= M_{\nu\mu}^{(1)} + M_{\nu\mu}^{(2)} \end{aligned} \quad (4.105)$$

Here,  $S_{\nu\mu}^{(2)} + M_{\nu\mu}^{(2)}$  cancels out and hence only the remaining terms are left to calculate. Now, we will use the following relation to decompose  $S_{\nu\mu}$ :

$$(E_{nk} \pm E_{mk})^2 = (E_{nk} \mp E_{mk})^2 \pm 4E_{nk}E_{mk} \quad (4.106)$$

The first term in (4.106) corresponds to  $S_{\nu\mu}^{(2)}$  and second term corresponds to  $S_{\nu\mu}^{(1)}$ .

Similarly, we can also decompose  $M_{\nu\mu}$ , where  $M_{\nu\mu}^{(1)}$  is the term containing  $T_k^\dagger(x_\mu V_{k,\nu} + V_{k,\nu}x_\mu)T_k$  in (4.103). One can easily see using the above information in (4.100) and (4.103) that  $S_{\nu\mu}^{(2)} + M_{\nu\mu}^{(2)} = 0$  and hence  $L_{\nu\mu} = S_{\nu\mu}^{(1)} + M_{\nu\mu}^{(1)}$ . Now, we can write the remaining  $S_{\nu\mu}^{(1)}$  and  $M_{\nu\mu}^{(1)}$  as follows:

$$S_{\nu\mu}^{(1)} = -\frac{i}{2} \sum_{n,m=1}^{2N} \sum_k \left( (T_k^\dagger V_{k,\nu} T_k)_{nm} \left[ \frac{(\epsilon_k)_{nn} \epsilon_k}{((\sigma_3 \epsilon)_{nn} - \epsilon_k \sigma_3)^2} \right]_{mm} (T_k^\dagger V_{k,\mu} T_k)_{mn} \right) [g(\sigma \epsilon_k)]_{nn} - (\nu \leftrightarrow \mu) \quad (4.107)$$

Here,  $\epsilon_k = T_k^\dagger H_k T_k = \begin{pmatrix} E_k & \\ & E_{-k} \end{pmatrix}$ , where

$$E_k = \begin{pmatrix} E_{1k} & & & \\ & \ddots & & \\ & & \ddots & \\ & & & E_{Nk} \end{pmatrix} \quad (4.108)$$

Also, the term  $\left[ \frac{(\epsilon_k)_{nn} \epsilon_k}{((\sigma_3 \epsilon)_{nn} - \epsilon_k \sigma_3)^2} \right]_{mm} = \left[ \frac{E_{nk} E_{m,-k}}{(E_{nk} + E_{m,-k})^2} \right]_{mm}$  for  $1 \leq n \leq N$  and  $N+1 \leq m \leq 2N$ .

Now, we can write (4.107) by introducing  $\delta(\eta - \sigma_3 \epsilon_k)$  and changing summation over n with trace as it's just the sum of the diagonal elements, we get:

$$\begin{aligned} S_{\nu\mu}^{(1)} &= -\frac{i}{2} \sum_k \int_{-\infty}^{\infty} \eta g(\eta) \text{Tr} \left[ \delta(\eta - \sigma_3 \epsilon_k) \sigma_3 \left[ T_k^\dagger V_{k,\nu} T_k \frac{\epsilon_k}{(\eta - \sigma_3 \epsilon_k)^2} T_k^\dagger V_{k,\mu} T_k \right] \right] d\eta - (\nu \leftrightarrow \mu) \\ &= -\frac{i}{2} \sum_k \int_{-\infty}^{\infty} \eta g(\eta) \text{Tr} \left[ \delta(\eta - \sigma_3 \epsilon_k) \sigma_3 \frac{\partial T_k^\dagger}{\partial k_\nu} H_k \frac{\partial T_k}{\partial k_\mu} \right] d\eta - (\nu \leftrightarrow \mu) \end{aligned} \quad (4.109)$$

In (4.109), we have used  $T_k^\dagger \sigma_3 T_k = \sigma_3$  and  $T_k^{-1} f(\sigma_3 H_k) T_k = f(\sigma_3 \epsilon_k)$ , where  $f(x)$  is an arbitrary function.

$$\begin{aligned}
M_{\nu\mu}^{(1)} &= -\frac{1}{2} \sum_{n=1}^{2N} \sum_k [T_k^\dagger (x_\mu V_{k,\nu} + V_{k,\nu} x_\mu) T_k \epsilon_k g(\sigma_3 \epsilon) k]_{nn} \\
&= -\frac{1}{2} \sum_k \int_{-\infty}^{\infty} \eta g(\eta) \text{Tr} [\sigma_3 (x_\mu V_{k,\nu} - x_\nu V_{k,\mu}) \delta(\eta - \sigma_3 H_k)] d\eta
\end{aligned} \tag{4.110}$$

Here, we are done with  $S_{\nu\mu}^{(1)}$  calculation, but  $M_{\nu\mu}^{(1)}$  has to be calculate further to express it in terms of the spin-wave dispersion  $E_{nk}$  and paraunitary matrix  $T_k$ . We can get  $M_{\nu\mu}^{(1)}$  following the Smrčka and Strěda approach :<sup>5</sup>[12]

$$\begin{aligned}
M_{\nu\mu}^{(1)} &= i \sum_k \int_{-\infty}^{\infty} d\tilde{\eta} \text{Tr} [\delta(\tilde{\eta} - \sigma_3 \epsilon_k) \sigma_3 \frac{\partial T_k^\dagger}{\partial k_\nu} \sigma_3 \frac{\partial T_k}{\partial k_\mu}] \cdot \int_0^{\tilde{\eta}} \eta g(\eta) d\eta \\
&\quad - \frac{i}{2} \sum_k \int_{-\infty}^{\infty} d\tilde{\eta} \text{Tr} \left[ \delta(\tilde{\eta} - \sigma_3 \epsilon_k) \sigma_3 \frac{\partial T_k^\dagger}{\partial k_\nu} \sigma_3 (\tilde{\eta} - \sigma_3 H_k) \frac{\partial T_k}{\partial k_\mu} \right] \tilde{\eta} g(\tilde{\eta}) - (\nu \leftrightarrow \mu)
\end{aligned} \tag{4.111}$$

Finally, from ((4.109) and (4.111), we get the total thermal transport coefficient  $L_{\nu\mu}$ :

$$\begin{aligned}
L_{\nu\mu} &= S_{\nu\mu}^{(1)} + M_{\nu\mu}^{(1)} \\
&= \frac{i}{2} \sum_k \int_{-\infty}^{\infty} d\tilde{\eta} \text{Tr} \left[ \delta(\tilde{\eta} - \sigma_3 \epsilon_k) \sigma_3 \frac{\partial T_k^\dagger}{\partial k_\nu} \sigma_3 \frac{\partial T_k}{\partial k_\mu} \right] \left[ 2 \int_0^{\tilde{\eta}} \eta g(\eta) d\eta - \tilde{\eta}^2 g(\tilde{\eta}) \right] - (\nu \leftrightarrow \mu)
\end{aligned} \tag{4.112}$$

Now, we can write:

$$\frac{d}{d\eta} (\eta^2 g(\eta)) = 2\eta g(\eta) + \eta^2 \frac{dg(\eta)}{d\eta} \tag{4.113}$$

Also, the Berry curvature in momentum space is given by [13],

$$\Omega_{nk} = i\epsilon_{\nu\mu} \left[ \sigma_3 \frac{\partial T_k^\dagger}{\partial k_\nu} \sigma_3 \frac{\partial T_k}{\partial k_\mu} \right] \tag{4.114}$$

Now, using (4.114) and (4.113) in (4.112), we get:

$$L_{\nu\mu} = -\frac{1}{2} \sum_k \sum_{n=1}^{2N} \int_0^{(\sigma_3 \epsilon_k)_{nn}} \eta^2 \frac{dg(\eta)}{d\eta} d\eta \Omega_{nk} - (\nu \leftrightarrow \mu) \tag{4.115}$$

The integral in (4.115) is similar to (3.70). Hence, using the result of (3.76), and adding and subtracting  $c_2(\infty) = \frac{\pi^2}{3}$ , we get:

$$L_{\nu\mu} = -\sum_k \sum_{n=1}^N (k_B T)^2 \left[ c_2(g(E_{nk}) - \frac{\pi^2}{3}) \right] \Omega_{nk} \tag{4.116}$$

In the clean limit, the thermal hall conductivity ( $\kappa_{xy}$ ) is,

$$\kappa_{xy} = -\frac{k_B^2 T}{\hbar V} \sum_k \sum_{n=1}^N \left[ c_2(g(E_{nk}) - \frac{\pi^2}{3}) \right] \Omega_{nk} \tag{4.117}$$

Here,  $c_2(x)$  is given by (3.76). The result obtained in (4.117) is similar to the one obtained in the semiclassical approach (3.78). In both the approaches, we are getting the correction terms coming from the orbital motion of magnons which were missed in the initial calculation (2.55).

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<sup>5</sup>For detailed derivation, one can see A.1



# 5

## Future Work

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We have looked at the two approaches for calculating the transverse thermal hall conductivity ( $\kappa_{xy}$ ) due to magnons : the semiclassical and linear response approaches . We have learned that there are extra correction terms coming from the orbital motion of magnons ( $M_{\nu\mu}$ ) for both the cases [2, 3] that were initially overlooked in (2.55) [7, 8]. We also derive the semiclassical EOM for the magnon wave packet in analogy with the electron system. Here, we saw that there is an extra anomalous velocity term which is coming in the semiclassical EOM due to which the Berry phase comes in directly in contrast to the calculation done in Section 2.2. Also, we saw here that the spatial variation of the chemical potential  $\mu$  or the temperature causes the thermal Hall effect. The reason for which is the non-cancellation of the magnon edge current between one edge and the opposite edge due to which a net current will emerge. Eventually, we are obtaining the thermal hall conductivity ( $\kappa_{xy}$ ) by comparing with the well defined heat current [6]. In the linear response approach, we obtained the thermal current operator and thermal transport coefficient ( $L_{\nu\mu}$ ) by incorporating the spatially varying temperature gradient as perturbation using the psuedogravitational potential [4]. Then finally using the Smrčka and Strěda approach [12], we got the transverse thermal hall conductivity ( $\kappa_{xy}$ ) in accordance with the semiclassical approach. Now, for the future work, we will try to incorporate dipolar interaction instead of the DMI and try to look if the existing  $A_2B_2O_7$  pyrochlores have any favourable regime which we can explore. Also, we will understand how the dipolar interaction give rise to the topologically non-trivial band structures.

## References

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# A

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## A.1 Smrčka and Strěda Approach

They have defined two functions  $A_{\nu\mu}(\eta)$  and  $B_{\nu\mu}(\eta)$  as:

$$A_{\nu\mu}(\eta) = iTr \left[ \sigma_3 V_{k,\nu} \frac{dG^+}{d\eta} \sigma_3 V_{k,\mu} \delta(\eta - \sigma_3 H_k) - \sigma_3 V_{k,\mu} \delta(\eta - \sigma_3 H_k) \sigma_3 V_{k,\mu} \frac{dG^-}{d\eta} \right] \quad (\text{A.1})$$

$$B_{\nu\mu}(\eta) = iTr [\sigma_3 V_{k,\nu} G^+ \sigma_3 V_{k,\mu} \delta(\eta - \sigma_3 H_k) - \sigma_3 V_{k,\mu} \delta(\eta - \sigma_3 H_k) \sigma_3 V_{k,\mu} G^-] \quad (\text{A.2})$$

Here this  $G^\pm$  is defined as :

$$G^\pm = \frac{1}{\eta \pm i0 - \sigma_3 H_k} \quad (\text{A.3})$$

Now, these functions have the following identity :

$$A_{\nu\mu}(\eta) - \frac{1}{2} \frac{B_{\nu\mu}(\eta)}{d\eta} = \frac{1}{4\pi} Tr [\sigma_3 V_{k,\nu} (G^+)^2 \sigma_3 V_{k,\mu} G^+ - \sigma_3 V_{k,\nu} (G^-)^2 \sigma_3 V_{k,\mu} G^-] - (\nu \leftrightarrow \mu) \quad (\text{A.4})$$

Now, we will use the relation  $V_{k,\nu} = i[x_\nu, \sigma_3 (G^\pm)^{-1}]$  to get the following:

$$\begin{aligned} A_{\nu\mu}(\eta) - \frac{1}{2} \frac{B_{\nu\mu}(\eta)}{d\eta} &= \frac{i}{4\pi} Tr [x_\nu G^+ \sigma_3 V_{k,\mu} G^+ - x_\nu (G^+)^2 \sigma_3 V_{k,\mu} - x_\nu G^- \sigma_3 V_{k,\mu} G^- + x_\nu (G^-)^2 \sigma_3 V_{k,\mu}] \\ &\quad - (\nu \leftrightarrow \mu) \\ &= \frac{1}{4\pi i} Tr [x_\nu ((G^+)^2 - (G^-)^2) \sigma_3 V_{k,\mu}] - (\nu \leftrightarrow \mu) \\ &= -\frac{1}{2} Tr [\sigma_3 (x_\mu V_{k,\nu} - x_\nu V_{k,\mu}) \frac{d}{d\eta} \delta(\eta - \sigma_3 H_k)] \end{aligned} \quad (\text{A.5})$$

In (A.5), we have used the following:

$$G^+ - G^- = -2\pi i \delta(\eta - \sigma_3 H_k) \quad (\text{A.6})$$

Now, let's integrate (A.5) to get,

$$Tr [\sigma_3 (x_\mu V_{k,\nu} - x_\nu V_{k,\mu}) \delta(\eta - \sigma_3 H_k)] = 2 \int_\eta^\infty d\tilde{\eta} \left[ A_{\nu\mu}(\tilde{\eta}) - \frac{1}{2} \frac{B_{\nu\mu}(\tilde{\eta})}{d\tilde{\eta}} \right] \quad (\text{A.7})$$

Now, we will use the following identity to be able to use (A.7) in (4.110),

$$\int_{-\infty}^{\infty} d\tilde{\eta} \left[ A_{\nu\mu}(\tilde{\eta}) - \frac{1}{2} \frac{B_{\nu\mu}(\tilde{\eta})}{d\tilde{\eta}} \right] = i \int_{-\infty}^{\infty} Tr \left[ \sigma_3 V_{k,\nu} \frac{dG^+}{d\tilde{\eta}} \sigma_3 V_{k,\mu} \delta(\tilde{\eta} - \sigma_3 H_k) - \sigma_3 V_{k,\mu} \delta(\tilde{\eta} - \sigma_3 H_k) \sigma_3 V_{k,\mu} \frac{dG^-}{d\tilde{\eta}} \right] \quad (\text{A.8})$$

Now, using (A.3) and writing Trace in the summation form, we get,

$$\begin{aligned} \int_{-\infty}^{\infty} d\tilde{\eta} \left[ A_{\nu\mu}(\tilde{\eta}) - \frac{1}{2} \frac{B_{\nu\mu}(\tilde{\eta})}{d\tilde{\eta}} \right] &= i \int_{-\infty}^{\infty} \sum_{n=1}^{2N} (\sigma_3)_{nn} \delta[\tilde{\eta} - (\sigma_3 \epsilon_k)_{nn}] \left[ T_k^\dagger V_{k,\nu} T_k \frac{1}{[(\sigma_3 \epsilon_k)_{nn} - \sigma_3 \epsilon_k]^2} \sigma_3 T_k^\dagger V_{k,\mu} T_k \right] \\ &\quad - (\nu \leftrightarrow \mu) \\ &= -i \int_{-\infty}^{\infty} Tr \left[ \delta(\tilde{\eta} - \sigma_3 \epsilon_k) \sigma_3 \frac{\partial T_k^\dagger}{\partial k_\nu} \sigma_3 \frac{\partial T_k^\dagger}{\partial k_\mu} \right] d\tilde{\eta} - (\nu \leftrightarrow \mu) \end{aligned} \quad (\text{A.9})$$

Now, since the Berry curvature in the momentum space is defined by (4.114), we have,

$$\int_{-\infty}^{\infty} d\tilde{\eta} \left[ A_{\nu\mu}(\tilde{\eta}) - \frac{1}{2} \frac{B_{\nu\mu}(\tilde{\eta})}{d\tilde{\eta}} \right] = - \sum_{n=1}^{2N} \Omega_{nk} \quad (\text{A.10})$$

Now, the Berry curvature satisfies the following sum rule :

$$\begin{aligned} \sum_{n=1}^{2N} \Omega_{nk} &= i Tr \left[ \sigma_3 \frac{\partial T_k^\dagger}{\partial k_\nu} \sigma_3 \frac{\partial T_k}{\partial k_\mu} - (\nu \leftrightarrow \mu) \right] \\ &= i Tr \left[ \sigma_3 \frac{\partial T_k^\dagger}{\partial k_\nu} \sigma_3 T_k \sigma_3 T_k^\dagger \sigma_3 \frac{\partial T_k}{\partial k_\mu} - (\nu \leftrightarrow \mu) \right] \end{aligned} \quad (\text{A.11})$$

Now using the cyclic permutation property of the Trace, we get

$$\begin{aligned} \sum_{n=1}^{2N} \Omega_{nk} &= -i Tr \left[ \sigma_3 T_k^\dagger \sigma_3 \frac{\partial T_k}{\partial k_\nu} \sigma_3 \frac{\partial T_k^\dagger}{\partial k_\mu} \sigma_3 T_k - (\nu \leftrightarrow \mu) \right] \\ &= - \sum_{n=1}^{2N} \Omega_{nk} = 0 \end{aligned} \quad (\text{A.12})$$

Using the result in (A.7) and (A.12), we can write the following:

$$Tr[\sigma_3(x_\mu V_{k,\nu} - x_\nu V_{k,\mu})\delta(\eta - \sigma_3 H_k)] = -2 \int_{-\infty}^{\eta} d\tilde{\eta} \left[ A_{\nu\mu}(\tilde{\eta}) - \frac{1}{2} \frac{B_{\nu\mu}(\tilde{\eta})}{d\tilde{\eta}} \right] \quad (\text{A.13})$$

Hence, using (A.13) along with (4.110), we get  $M_{\nu\mu}^{(1)}$  in the form mentioned in (4.111).

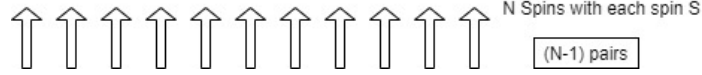
## A.2 Semiclassical approach to the ferromagnetic chain

The Heisenberg Hamiltonian for the ferromagnet is given by,

$$H = - \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j \quad (\text{A.14})$$

where,  $J_{ij}$  is the exchange integral or coupling constant. Also,  $J_{ij} > 0$  means parallel spin alignment and  $J_{ij} < 0$  means anti-parallel spin alignment.

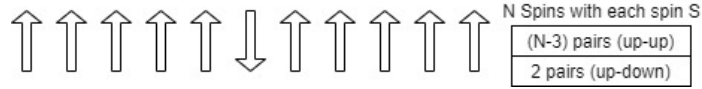
Now, suppose we have a 1-D ferromagnetic chain in the lowest energy configuration ( $J > 0$ ) :



The exchange energy associated with this chain assuming only nearest neighbour coupling is given by :

$$E_{exchange} = -JS^2(N - 1)$$

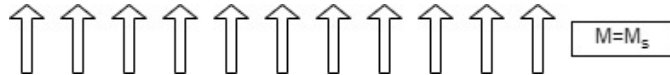
Now, let's say I want to make an excitation or increase the energy of the system. In order to do that we flip just one spin, i.e,



The exchange energy for the above configuration is :

$$\begin{aligned} E_{exchange} &= -JS^2(N - 3) + 2JS^2 \times 2 \\ &= -JS^2(N - 1) + 4JS^2 \end{aligned}$$

Now, suppose we have a perfectly ferromagnetic configuration:



Now, keeping the number of spins same, we make any two neighbouring spins slightly canted w.r.t each other such that,



The magnetization for the above set-up is zero (one complete cycle) which means that it's a highly energetic state from the mean field perspective as  $E = -\vec{M} \cdot \vec{B}$ . But looking at the exchange interaction energy between any two neighbouring spins keeping in mind that the spins are slightly tilted w.r.t one another, we have

$$\begin{aligned} E_{plane} &= -J\hat{S}_1 \cdot \hat{S}_2 \\ &= -JS^2 \cos\theta \\ &\approx -JS^2 \end{aligned}$$

Hence, the energy of the system is actually quite small, but the mean field theory says that it's energy is really high. Actually what we have done is we have taken the configuration with one spin down and spread this spin flip over the entire chain. This kind of configuration is called spin-wave (magnon).