Thesis name

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Introduction

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Chapter 1

ValleyHall

1.1 Berry curvature in Gapped graphene

The Hamiltonian for the gapped graphene near the point K_1 and K_2 can be written as

$$H_{K_1} = H_{K_2}^{\dagger} = \begin{bmatrix} \Delta & \hbar v_F(k_x + ik_y) \\ \hbar v_f(k_x - ik_y) & \Delta \end{bmatrix} \tag{1.1}$$

Where Δ is the energy gap and v_F is the Fermi velocity. For ease of notation we are going to work with just H_{K_1} and drop the K_1,[1] and for ease of computation we define $\mathbf{q} = \hbar v_F \mathbf{k}$

$$H = \begin{bmatrix} \Delta & q_x + iq_y \\ q_x - iq_y & \Delta \end{bmatrix} = \sigma_x q_x + \sigma_y q_y + \sigma_z \Delta \equiv \boldsymbol{\sigma} \cdot \mathbf{E} \tag{1.2}$$

Here the enegry vector $\mathbf{E}$ is defined as $\mathbf{E} = (q_x, q_y, \Delta)$. The nice things about it is that $E = |\mathbf{E}| = \sqrt{q_x^2 + q_y^2 + \Delta^2}$ is the positive eigenvalue of the hamiltonian (the negative eigenvalue is just $-E$).
To calculate the Berry curvature we are first going to calculate the Berry connection 2.9, and to calultate the Berry connection we need the eigenvectors which are well known for the Hamiltonian of the form $\boldsymbol{\sigma} \cdot \mathbf{E}$.

$$|+;\theta,\phi\rangle = \begin{bmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{bmatrix} \quad |-;\theta,\phi\rangle = \begin{bmatrix} -e^{-i\phi}\sin\frac{\theta}{2} \\ \cos\frac{\theta}{2} \end{bmatrix} \tag{1.3}$$

Where θ and ϕ are the coordinates of $\mathbf{E}$ in the polar representation

Now we can calculate the Berry connection

$$A_\theta^+ = -A_\theta^- = 0 \quad A_\phi^+ = -A_\phi^- = \sin^2\frac{\theta}{2} \tag{1.4}$$

[1] Don't worry, I'll bring it back if when we'll need it

This means that the Berry curvature is

$$\Omega^+_{\theta\phi} = -\Omega^-_{\theta\phi} = \partial_\theta A^+_\phi = \frac{\sin\theta}{2} \tag{1.5}$$

From now on we are going to work with Ω^+ and we are going to drop the + sign to make the notation lighter.

We want to express Ω in terms of $\mathbf{q}$, however it's more convenient to write it in terms fo $\cos\theta$ and ϕ, so we do a small coordinate transformation

$$\Omega_{\theta\phi} = \frac{\partial\cos\theta}{\partial\theta}\Omega_{\cos(\theta)\phi} \to \Omega_{\cos(\theta)\phi} = \frac{1}{2} \tag{1.6}$$

Now we can easily make the transformation to express Ω in terms of $\mathbf{q}$. The Berry curvature transforms like any other tensor under coordinate transformation, so

$$\Omega_{q_x q_y} = \frac{\partial\cos\theta}{\partial q_x}\frac{\partial\phi}{\partial q_y}\Omega_{\cos(\theta)\phi} + \frac{\partial\phi}{\partial q_x}\frac{\partial\cos\theta}{\partial q_y}\Omega_{\phi\cos(\theta)} \tag{1.7}$$

That can be rewritten as

$$\Omega_{q_x q_y} = \frac{1}{2}\det\left[\frac{\partial(cos\theta,\phi)}{\partial(q_x,q_y)}\right] = \frac{1}{2}\frac{\Delta^2}{q^2E^3}(q_x+q_y-2q) \tag{1.8}$$

And finally we can express it in terms of $\mathbf{k}$

$$\Omega_{k_x k_y} = (\hbar v_F)^2\Omega_{q_x q_y} = \frac{\hbar v_F}{2}\frac{\Delta^2}{k^2E^3}(k_x+k_y-2k) \tag{1.9}$$

Up until now we have worked with the Hamiltonian H_{K_1}, but with the K_1 hidden. The Berry curvature around K_2 is equal, but with opposite sign (figure 1.1) [2]

1.2 Valley-Hall effect

The Hall conductivity σ_{xy} is

$$\sigma_{xy} = \frac{e^2}{\hbar}\int_{\mathbb{R}^2} f[E^+(k)]\Omega^+_{k_x k_y} + f[E^-(k)]\Omega^-_{k_x k_y}\frac{d^2\mathbf{k}}{2\pi} \tag{1.10}$$

Where $f(E) = \left[e^{\beta(E-\mu)}+1\right]^{-1}$ is the Fermi-Dirac distribution, it is applied once for the states with positive energy and once for the states with negative energy.

[2] A short proof for it can be the following: If we send $k_y \to -k_y$ we effectively send $H_{K_1} \to H_{K_2}$.
The berry curvature can be written as $\Omega_{k_x k_y} = i\langle\partial_{k_x}n|\wedge|\partial_{k_y}n\rangle$. By sending $k_y \to -k_y$ we have that $\Omega \to -\Omega$.

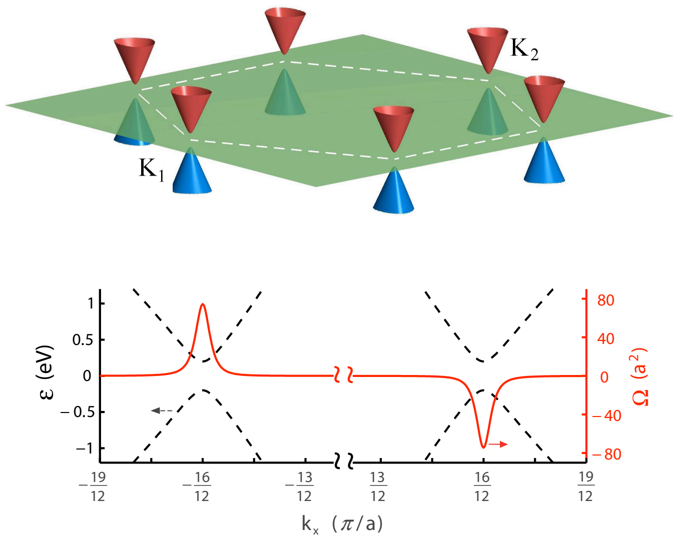

Figure 1.1: In the top panel are displayed the Energy bands in 2D. In the bottom panel with the dotted line are displayed a section of the energy bands, and with the continuous red line the Berry curvature.

We are going to analyze the system at low temperatures ($k_\beta T \ll 1$), so our Fermi-Dirac distribution can be considered like a step-function.

First let's integrate the conductivity for the positive energies and drop the $+$ sign to make the notation lighter.

$$\int_{\mathbb{R}^2} f[E(k)]\Omega_{k_x k_y} dk_x dk_y = \int_{\mathbb{R}^2} f[E(q)]\Omega_{q_x q_y} dq_x dq_y \approx$$

$$\approx \int_0^{2\pi} \int_0^{q_F} \frac{1}{2} \frac{\Delta^2}{q^2 E^3}(q_x + q_y - 2q) q dq d\theta =$$

$$= -2\pi\Delta^2 \int_0^{q_f} \frac{dq}{E^2} = -2\pi\Delta^2 \int_0^{q_f} \frac{dq}{(\Delta^2 + q^2)^{3/2}} = -\frac{2\pi q_F}{\sqrt{\Delta^2 + q_F^2}}$$

And now we express it in terms of the chemical potential μ [3]

$$\int_{\mathbb{R}^2} f[E(k)]\Omega_{k_x k_y} dk_x dk_y \approx -2\pi \frac{\sqrt{\mu^2 - \Delta^2}}{\mu} \theta(\mu - \Delta) \tag{1.11}$$

The $\theta(\mu - \Delta)$ is there to make sure that if no states are inside the Fermi-Dirac the integral is zero. One thing to notice is that if you have $\mu \gg \Delta$ (aka. all states in the band are occupied) then the integral is equal to -2π.

[3] Here we can use interchangeably μ and E_F

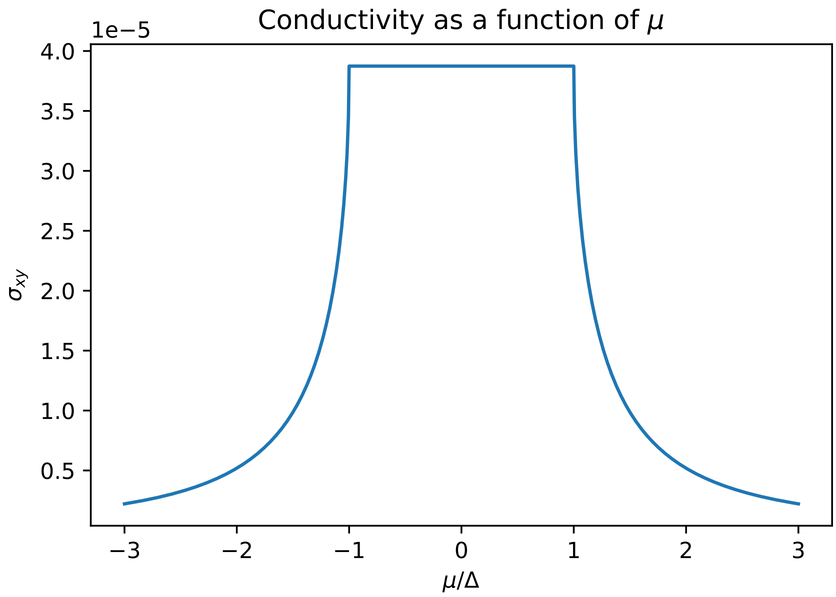

Figure 1.2: Here is shown $\sigma_{xy}(\mu)$ (eq. 1.12). Notice how, when $\mu \in [-\Delta, \Delta]$ then $\sigma_{xy} = \frac{e^2}{2\pi\hbar}$

The integral of the lower band is very similar. By the end equation of the conductivity 1.10 becomes

$$\sigma_{xy}(\mu) = -\frac{e^2}{2\pi\hbar}\left[\frac{\sqrt{\mu^2 - \Delta^2}}{\mu}\theta(\mu^2 - \Delta^2) - \theta(\mu - \Delta)\right] \tag{1.12}$$

To be fear we only calculated σ_{xy} for the electrons in the valley K_1, the conductivity for the other valley is just $-\sigma_{xy}$. So, putting it all together, we have

$$\sigma_{K_i,xy}(\mu) = (-1)^i\frac{e^2}{2\pi\hbar}\left[\frac{\sqrt{\mu^2 - \Delta^2}}{\mu}\theta(\mu^2 - \Delta^2) - \theta(\mu - \Delta)\right] \tag{1.13}$$

However in most cases it's safe to assume that the chemical potential is inside the energy gap, so equation 1.13 becomes

$$\sigma_{K_i,xy} = (-1)^{i+1}\frac{e^2}{2\pi\hbar} \tag{1.14}$$

1.3 Non-local Charge transport

If we apply a voltage V in two opposite points of a strip of a ohmic material of width W and infinite lenght, and we see a current that flows from one

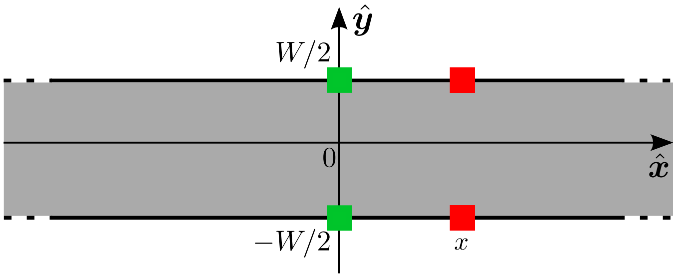

Figure 1.3: Representation of the strip

point to another figure 1.3.
Clearly the current isn't completely localized along the axis that unites the two injection points, and so does the voltage difference.
If we probe the voltage from two different points with an offset of x from the injection points and we divide it by the total current between the contacts we see that

$$\frac{V(x)}{I} = \frac{2\rho}{\pi} \ln \left| \coth\left(\frac{\pi x}{2W}\right) \right| \tag{1.15}$$

Where ρ is the resistivity. Don't worry later on there is the proof of this equation.

However, two-dimentional material like gapped graphene [1–3] and transition metal dichalcogenides [4–6], don't obey this equation. This is because theese materials display the Valley Hall effect we talked about previously (inserire reference a sezione).

Non-local transport can be a useful tool to probe the existance of anomalous Hall effect [7–12]

1.4 Theory of non local charge transport

The charges inside the material get pushed around from the electrochemical potential ψ_K

$$\psi_K(\mathbf{r}) = V(\mathbf{r}) - \frac{1}{e}\mu_K[n_{K_1}(\mathbf{r}), n_{K_2}(\mathbf{r}), T] \tag{1.16}$$

Where ϕ is the electrical potential, and $\mu_K = \frac{\partial}{\partial n_K} F[n_{K_1}(\mathbf{r}), n_{K_2}(\mathbf{r}), T]$ is the chemical potential of the material and F is the free energy.

The current generated from this potential in the valley K_α in the $i-$th direction is

$$-eJ_{K_\alpha,i}(\mathbf{r}) = \sum_{j,b} \underbrace{-\sigma_{K_\alpha K_\beta,ij}}_{\text{conductivity}} \partial_j \psi_{K_\beta}(\mathbf{r}) \tag{1.17}$$

From now we are going to set $T \approx 0$[4] and ignore intervalley scattering, so if $K_\alpha \neq K_\beta$ $\sigma_{K_\alpha K_\beta,ij} = 0$, also because of this the free energy can be written as the sum of the two Free energies

$$F(n_{K_1}, n_{K_2}) = F_1(n_{K_1}(\mathbf{r})) + F_2(n_{K_2}(\mathbf{r})) \tag{1.18}$$

And so the chemical potential of a given valley depend only on the number of electron in the same valley

$$\mu_\alpha(n_{K_\alpha}(\mathbf{r})) = \frac{\partial}{\partial n_{K_\alpha}} F(n_{K_0}, n_{K_1}) = \frac{\partial}{\partial n_{K_\alpha}} F_\alpha(n_{K_\alpha}(\mathbf{r})) \tag{1.19}$$

This simplifies the trasport equation in

$$-e\mathbf{J}_{K_\alpha}(\mathbf{r}) = \sigma_{K_\alpha}(\mathbf{r}) \nabla \psi_{K_\alpha}(\mathbf{r}) \tag{1.20}$$

Where σ_{K_α} is the following matrix

$$\sigma_{K_\alpha} = \begin{bmatrix} \sigma_{K_\alpha K_\alpha,xx} & \sigma_{K_\alpha K_\alpha,xy} \\ -\sigma^*_{K_\alpha K_\alpha,xy} & \sigma_{K_\alpha K_\alpha,xx} \end{bmatrix}$$

Now we need to write the gradient electrochemical potential $\nabla\psi(\mathbf{r})$

$$\nabla\psi_{K_\alpha}(\mathbf{r}) = \nabla V(\mathbf{r}) - \frac{1}{e} \frac{\partial}{\partial n_{K_\alpha}} \mu_\alpha(n_{K_\alpha}(\mathbf{r})) \nabla n_{K_\alpha} \tag{1.21}$$

From equation INSERIRE REFERENCE A EQUAZIONE we can write for gapped Dirac hamiltonians that VERIFICARE SE VALE ANCHE PER BILAYER GRAPHENE

$$\frac{\partial \mu_{K_\alpha}}{\partial n_{K_\alpha}} = \frac{\pi}{\sqrt{2\pi|n| + \Delta^2}} + \Delta\delta(n) \approx \frac{\pi}{\Delta} + \Delta\delta(n) \quad \forall\alpha$$

In this equation we assumed that there are very few charge carries, so $\frac{n}{\Delta^2} \approx 0$. We can shorten the equation 1.21 by defining

$$e^2 D_{K_\alpha,ij} = \sigma_{K_\alpha,ij} \frac{\partial \mu_\alpha}{\partial n_{K_\alpha}} [n_{K_\alpha}(\mathbf{r})] \tag{1.22}$$

So equation 1.20 becomes

$$-eJ_{K_\alpha,i}(\mathbf{r}) = \sigma_{K_\alpha,ij} E_j(\mathbf{r}) - eD_{K_\alpha,ij} \partial_j n_{K_\alpha}(\mathbf{r}) \tag{1.23}$$

or, written in matrix form

$$-e\mathbf{J}_{K_\alpha}(\mathbf{r}) = \sigma_{K_\alpha} \mathbf{E}(\mathbf{r}) - eD_{K_\alpha} \nabla n_{K_\alpha}(\mathbf{r}) \tag{1.24}$$

Where σ_{K_α} and $-eD_{K_\alpha}$ are matrices.

[4] A more precise statement is that the thermal De Broglie wavelenght λ_T must be much larger than the average distance between the electrons. We are not going into the math here, but if you want to calculate it, keep in mind that the dispersion relation is relativistic, so the formula of λ_T is going to be a bit different

1.4.1 Re-writing the equations in terms of charge current and valley current

Measuring the currents in different valley can be cumbersome, however measuring the charge current $\mathbf{J}_c = \mathbf{J}_{K_1} + \mathbf{J}_{K_2}$ is straightforward, and for mathematical convenience we also define the valley current $\mathbf{J}_v = \mathbf{J}_{K_1} - \mathbf{J}_{K_2}$.

Since we no longer describe the currents in terms of their valley index, but on the sum and the difference of what happens at the different valleys, we are going to reparametrize also the other quantities in the same fashion.

$$\begin{cases} \sigma_c = \sigma_{K_1} + \sigma_{K_2} = 2\sigma_{xx}\delta_{ij} \\ \sigma_v = \sigma_{K_1} - \sigma_{K_2} = \sigma_v = 2\sigma_{xy}\epsilon_{ij} \end{cases} \tag{1.25}$$

The term $-eD_{K_\alpha}\nabla n_{K_\alpha}(\mathbf{r})$ is a little harder to traslate. First off we are going to impose the local charge conservation

$$n(\mathbf{r}) = n_{K_0} + n_{K_1} \approx 0$$

and so

$$n_v(\mathbf{r}) = n_{K_1} - n_{K_2} = 2n_{K_1} = -2n_{K_2} \tag{1.26}$$

Now let's do the sum of the $D_{K_\alpha}\nabla n_{K_\alpha}(\mathbf{r})$ terms to write them in terms of charge and valleys degrees of freedom

$$D_{K_1}\nabla n_{K_1} + D_{K_2}\nabla n_{K_2} = (D_{K_1} - D_{K_2})\nabla n_v(\mathbf{r})/2$$

$$D_{K_1} - D_{K_2} = \sigma\frac{\partial\mu_1}{\partial n_{K_1}} - \sigma^T\frac{\partial\mu_2}{\partial n_{K_2}}$$

since $\mu_v = 2\mu_1 = -2\mu_2$ and $n_v = 2n_{K_1} = -2n_{K_2}$

$$D_{K_1} - D_{K_2} = \frac{1}{e^2}(\sigma - \sigma^T)\frac{\partial\mu_v}{\partial n_v} = \frac{2}{e^2}\sigma_v\frac{\partial\mu_v}{\partial n_v}$$

so I define

$$D_{cv} = \frac{2}{e^2}\sigma_v\frac{\partial\mu_v}{\partial n_v} \approx \frac{2}{e^2}\frac{\pi}{\Delta}\sigma_v$$

so we get that

$$D_{K_1}\nabla n_{K_1} + D_{K_2}\nabla n_{K_2} = D_{cv}n_v$$

Putting it all together we have that

$$\mathbf{J}_c(\mathbf{r}) = \sigma_c\mathbf{E}(\mathbf{r}) + eD_{cv}\nabla n_v(\mathbf{r})$$

Writing all the indices

$$J_{c,i} = \sum_j \sigma_{c,xx}\delta_{ij}E_i + D_{cv,xy}\epsilon_{ij}\partial_j n_v \tag{1.27}$$

so we can rewrite them as

$$\mathbf{J}_c = \sigma_{c,xx}\mathbf{E}_i + D_{cv,xy}\nabla \times n_v \tag{1.28}$$

where $\sigma_{c,xx}$ and $D_{cv,xy}$ are scalars.

And now the difference of the $D_{K_\alpha}\nabla n_{K_\alpha}(\mathbf{r})$ terms to write them in terms of charge and valleys degrees of freedom

$$D_{K_0}\nabla n_{K_0} - D_{K_1}\nabla n_{K_1} = (D_{K_0} + D_{K_1})\nabla n_v(\mathbf{r})/2$$

and with some calculations done in a similar fashion to the one we use to calculate $\mathbf{J}_c$ we have that

$$D_v = \frac{1}{2}(D_{K_0} + D_{K_1}) = \frac{1}{e^2}\sigma_c\frac{\partial \mu_c}{\partial n_c}$$

so, in matrix form

$$\mathbf{J}_v(\mathbf{r}) = \sigma_v\mathbf{E}(\mathbf{r}) + eD_v\nabla n_v(\mathbf{r}) \tag{1.29}$$

which can be re-written as

$$J_{v,i}(\mathbf{r}) = \sum_j \sigma_{c,xy}\epsilon_{ij}E_j(\mathbf{r}) + eD_{v,xx}\delta_{ij}\partial_j n_v(\mathbf{r}) \tag{1.30}$$

where $\sigma_{c,xy}$ and $D_{v,xx}$ are scalars

1.4.2 Laplace equation

Now that we have the charge and valley currents differential equations we calculate the laplacians to solve them. Let's start from the equation for the charge currents 1.28

$$\nabla \cdot \mathbf{J}_c = \nabla \cdot (\sigma_c\mathbf{E}) + eD_{cv,xx}\nabla \cdot (\nabla \times n_v) \tag{1.31}$$

Inside the material the are no sources of charge current, so $\nabla \cdot \mathbf{J}_c =$, and the divergence of a rotor is zero, so $\nabla \cdot (\nabla \times n_v) = 0$. This means that inside the material

$$\boxed{\nabla^2 V(x, y) = 0} \tag{1.32}$$

So, to be able to solve the laplace equation we just need to impose the boundary conditions that the current is injected in a single point at $x = 0$ along the $\hat{\mathbf{y}}$ direction.

$$-e\mathbf{J}_c(x, \pm W/2) = I\delta(x)\hat{\mathbf{y}}$$

If we put it in equation 1.31 we get

$$\boxed{I\delta(x) = \sigma_{c,xx}\partial_y V(x, \pm W/2) - eD_{cv,xy}\partial_x n_v(x, \pm W/2)} \tag{1.33}$$

Now let's calculate the laplacian for the valley current equation 1.30

$$\nabla \cdot \mathbf{J}_v = \nabla \times (\sigma_{c,xy}\mathbf{E}) + e\nabla \cdot (D_{v,xx}\nabla n_v) \tag{1.34}$$

Now, lets analyze all the terms one by one

- For the continuity equation we have that $\nabla \cdot \mathbf{J}_v = \frac{\partial}{\partial t} n_v$, since intervalley scattering is zero, this should be zero, but why don't add it back now? so we say that it decays exponentially $\frac{\partial}{\partial t} n_v = -\frac{1}{\tau_v} n_v$
- $e\nabla \cdot (D_{v,xx}\nabla n_v)$ is really nothing special, inside the material $D_{v,xx}$ is constsant so in the end it is equal to $eD_{v,xx}\nabla^2 n_v$
- $\nabla \times (\sigma_{c,xy}\mathbf{E})$ is equal to zero inside the material, but on the edge can be non-zero because $\sigma_{c,xy}$ changes form inside to the outside

In the end we get that

$$eD_{v,xx}\nabla^2 n_v = -\frac{1}{\tau_v} n_v - \nabla \times (\sigma_{c,xy}\mathbf{E}) \tag{1.35}$$

This means that at the equilibrium $n_v \neq 0$ only if you are were $\nabla \times (\sigma_{c,xy}\mathbf{E}) \neq 0$, and this is only true along the edge, so we we'll have to worry about this term only in the boundary conditions, So

$$\boxed{\left[\nabla^2 - \frac{1}{\tau_v D_{v,xx}}\right] n_v(\mathbf{r}) = 0} \tag{1.36}$$

The boundary condition is simply that the valley current doesn't exit the material, so

$$J_{v,y}(x, \pm W/2) = 0 \tag{1.37}$$

putting it into the differential equation for J_v (eq 1.30) we get

$$\boxed{\sigma_{v,xy}\partial_x V(x, \pm W/2) + eD_{v,xx}\partial_y n_v(x, \pm W/2) = 0} \tag{1.38}$$

All the boxed equations we wrote in the in this section enable us to completely solve the system. For convenience let's write the m in a single system of equations

$$\begin{cases} \nabla^2 V(x, y) = 0 \\ \left[\nabla^2 - \frac{1}{\tau_v D_{v,xx}}\right] n_v(\mathbf{r}) = 0 \\ I\delta(x) = \sigma_{c,xx}\partial_y V(x, \pm W/2) - eD_{cv,xy}\partial_x n_v(x, \pm W/2) \\ \sigma_{v,xy}\partial_x V(x, \pm W/2) + eD_{v,xx}\partial_y n_v(x, \pm W/2) = 0 \end{cases} \tag{1.39}$$

From the third equation in the system above we can see that $V(x, y)$ is even along the $\hat{\mathbf{x}}$ axis and odd along the $\hat{\mathbf{y}}$ axis.
From the fourth equation we can see that n_v has the opposite parity to V, so it's odd along the $\hat{\mathbf{x}}$ axis and even along the $\hat{\mathbf{y}}$ axis.

To be able to solve it we first have to do a fourier transform over the $\hat{\mathbf{x}}$ direction. The first two equations of eq 1.39 become

$$\begin{cases} (\partial_y^2 - k^2)V(k, y) = 0 \\ \left[\partial_y^2 - \omega^2(k)\right]n_v(k, y) = 0 \end{cases} \tag{1.40}$$

And the solutions that respect the symmetries we talked about earlier are

$$V(k, y) = V(k)\sinh(ky) \qquad n_v(k, y) = n_v(k)\cosh[\omega(k)y] \tag{1.41}$$

However we still don't know what are $V(k)$ and $n_v(k)$, to obtain them we have to plug the equations above in the last two equations of 1.39

$$\begin{cases} \sigma_{c,xx}k\cosh(kw/2)V(k) - eD_{cv,xy}ik\cosh(\omega W/2)n_v(k) = I \\ -\sigma_{v,xy}ik\sinh(kw/2)V(k) - eD_{v,xx}\omega(k)\sinh(\omega W/2)n_v(k) = 0 \end{cases} \tag{1.42}$$

This system of equation is linear in $V(k)$ and $n_v(k)$, so it can be written in this form

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}\begin{bmatrix} V \\ n_v \end{bmatrix} = \begin{bmatrix} I \\ 0 \end{bmatrix} \tag{1.43}$$

And the inverse is simply

$$\begin{bmatrix} V \\ n_v \end{bmatrix} = \frac{I}{AD - BC}\begin{bmatrix} D \\ -C \end{bmatrix} \tag{1.44}$$

Since we want only care to calculate the voltage we only need to evaluate

$$V = \frac{I}{A - \frac{BC}{D}}$$

wich turns out to be equal to

$$V(k) = \frac{I}{\sigma_c}\frac{\omega(k)/k}{\sinh(kW/2)}\left\{\frac{\omega(k)}{\tanh(kW/2)} + \frac{k\tan^2(\theta_{VH})}{\tanh[\omega(k)W/2]}\right\}^{-1} \tag{1.45}$$

We can plug it into equation 1.41 and evaluate it at $y = \pm W/2$

$$V(k, \pm W/2) = V(k)\sinh(\pm kW/2) = \frac{I\omega}{\sigma_c k}\left\{\dots\right\}^{-1} \tag{1.46}$$

Where the terms inside the curly brakets are the same from the previous equation (1.45).
Finally we can calculate the non-local resistance

$$R_{NL}(k) = \frac{V(k, W/2) - V(k, -W/2)}{I} \tag{1.47}$$

Which is equal to

$$R_{NL}(k) = \frac{2\omega(k)}{k\sigma_c}\left\{\frac{\omega(k)}{\tanh(kW/2)} + \frac{k\tan^2(\theta_{VH})}{\tanh[\omega(k)W/2]}\right\}^{-1} \tag{1.48}$$

1.5 Study of R_{NL}

Unfortunately 1.48 doesn't have an analytic Fourier transform. If there are no topological effect, so $\tan(\theta_{VH}) = 0$, it can be solved analytically.

$$R_{NL}(x) = \frac{2}{\sigma_c}\int_{-\infty}^{+\infty} \frac{\tanh(kW/2)}{k}\frac{dk}{2\pi} = -\frac{2\rho}{\pi}\ln\left|\tanh\left(\frac{\pi x}{2W}\right)\right| \tag{1.49}$$

This is the purely ohmic nonlocal signal that we have talked about in 1.15.

However if we are going to explore topological materials we cannot set $\tan(\theta_{VH}) = 0$, rhis means that we'll have to explore equation 1.48 in regimes where it is approximately equal to a function that admits an analytic Fourier transform.

Let's look at the graph of the $R_{NL}(k)$ before doing any approximations: As you can see from the figure 1.4 if $W \gg l_v$ we have a single bell like function with the width of the bell being $\approx 1/W$. If $W \ll l_v$ we have a double-bell function, where the first bell has a height of 1 and a width of $1/l_v$, and the second one has a shorter height. To evaluate the precise height we just need to set $l_v^{-1} \ll k \ll W^{-1}$ in equation 1.48, this gives us ,

$$R_{NL}(l_v^{-1} \ll k \ll W^{-1}) \approx \frac{R_{xx}}{1 + \tan^2(\theta_{VH})} \tag{1.50}$$

Where $R_{xx} = \frac{W}{\sigma_{xx}}$

So, if we have $l_v \ll W$ or $\tan(\theta_{VH}) \ll 1$ (or both) we have a single bell structure. Incidentally these are the conditions to NOT have topological effects, so the less visible the double bell is, the less visible the topological effects are. We'll also see later how one of the bell represents the ohmic nonlocal signal, while the other represents the topological nonlocal signal.

Let's start by exploring $k \ll l_v^{-1}, W^{-1}$. This will tell us how the function behaves for $x \gg l_v, W$. In this regime

$$\omega(k) \approx \frac{1}{l_v}\left[1 + \frac{(kl_v)^2}{2}\right] \qquad \coth(kW/2) \approx \frac{2}{kW} + \frac{kW}{6} \tag{1.51}$$

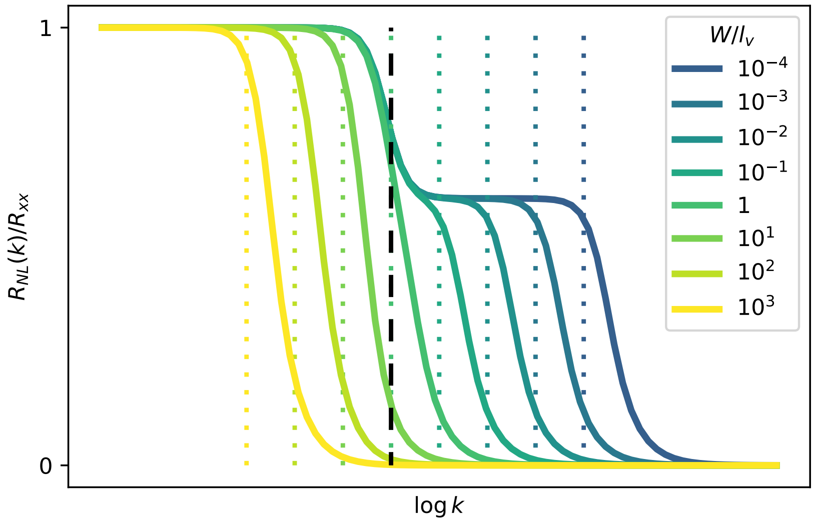

Figure 1.4: $R_{NK}(k)$ for several values of W/l_v. The dashed black line represents where $k = 1/l_v$, the colored dashed line represents where $k = 1/W$

Plugging this into equation 1.48 we have that $R_{NL}(k) \approx$

$$\frac{2}{\sigma_c}\frac{1}{l_v k}\left[\frac{1}{l_v}\left(1+\frac{k^2 l_v^2}{2}\right)\left(\frac{2}{kW}+\frac{kW}{6}\right)+\frac{k\tan^2(\theta_{VH})}{\tanh(W/2l_v)}+o(k^2)\right]^{-1} \tag{1.52}$$

With some mathematical manipulation it can be shown that it is equal to

$$R_{NL}(k \ll l_v^{-1}, W^{-1}) = \frac{W}{\sigma_c}\frac{1}{1+L_v^2 k^2} + o(k^3) \tag{1.53}$$

where the renormalized valley diffusion length L_v^2 is

$$L_v^2 = l_v^2 + \frac{W^2}{12} + \frac{l_v W}{2}\frac{\tan^2(\theta_{VH})}{\tanh(W/2l_v)} \tag{1.54}$$

Now we do the Fourier transform of equation 1.53 ignoring the $o(k^3)$ term to get the behavior of $R_{NL}(x \gg l_v, W)$

$$R_{NL}(x \gg l_v, W) = \mathcal{F}^{-1} R_{NL}(k \ll l_v^{-1}, W^{-1}) \tag{1.55}$$

That is equal to

$$\frac{W}{\sigma_c}\int_{-\infty}^{+\infty}\frac{1}{1+L_v^2 k^2}\frac{dk}{2\pi} = \frac{W\rho}{2L_v}e^{-\frac{|x|}{L_v}} \tag{1.56}$$

So,

$$R_{NL}(x \gg l_v, W) = \frac{W\rho}{2L_v} e^{-\frac{|x|}{L_v}} \tag{1.57}$$

Now we are going to study what happens for $k \gg l_v^{-1}$, in this case $\omega(k) \approx k$, So

$$R_{NL}(k \gg l_v^{-1}) = \frac{2}{\sigma_c} \frac{\tanh}{k} \left(\frac{kW}{2} \right) \frac{1}{1 + \tan^2(\theta_{VH})} \tag{1.58}$$

it's Fourier transform is

$$R_{NL}(x \ll l_v) = -\frac{2}{\pi \sigma_c} \frac{1}{1 + \tan^2(\theta_{VH})} \ln \left| \tanh \left(\frac{\pi x}{2W} \right) \right| \tag{1.59}$$

This last equation is $1 + \tan^2(\theta_{VH})$ smaller to the one for the purely ohmic nonlocal signal (eq. 1.49)

Now let's see how these equations fear in practice As you can see from

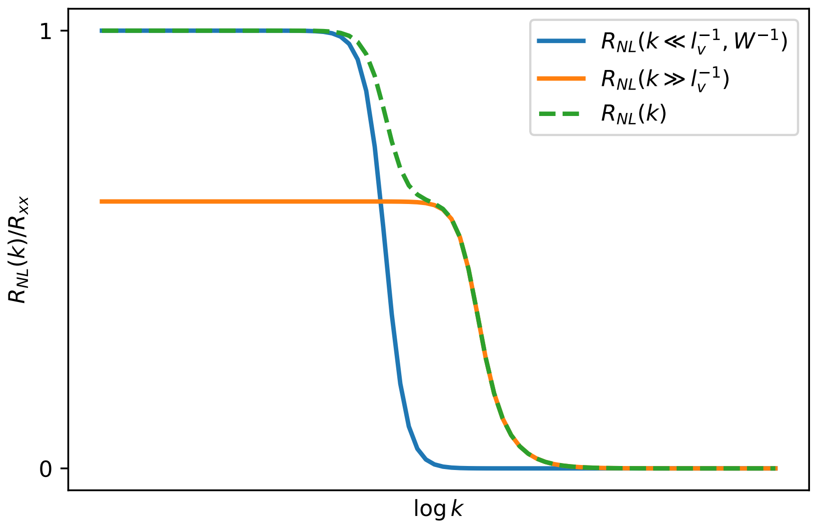

Figure 1.5: For this example $l_v = 20W$

figure 1.5 the two approximations work pretty well, except in the neighborhood where $k \approx l_v^{-1}$. But what we really care about is $R_{NL}(x)$.
If we plot $R_{NL}(x \gg l_v, W)$ (eq. 1.55) and $R_{NL}(x \ll l_v)$ (eq. 1.57) alongside the numerical Fourier transform of $R_{NL}(k)$ 1.48 we get figure 1.6

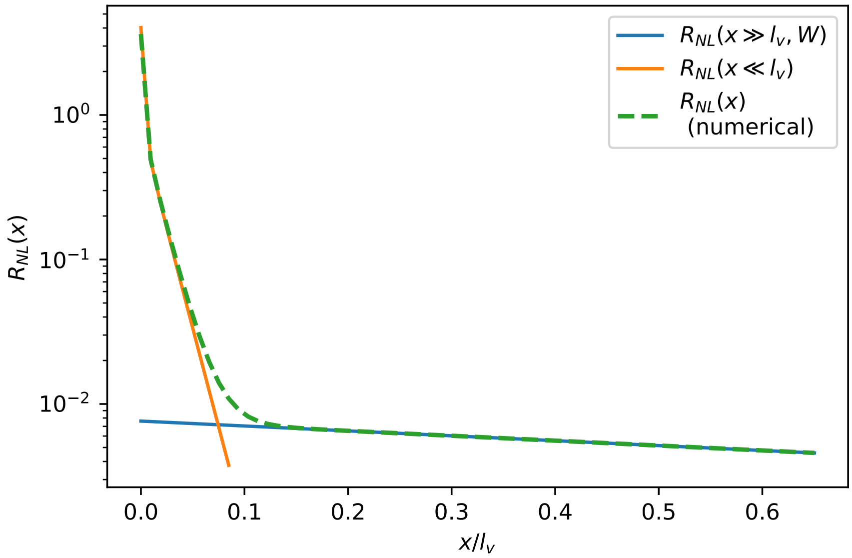

Figure 1.6: The parameters for this graph are exactly the same for the previous graph (figure 1.5)

1.5.1 Improving the approximation

We can do better than this! By combining the two approximations it's possible to have a single equation that is very accurate for k far from l_v^{-1} ($(k - l_v^{-1})^2 \gg 1$), but it ends up being reasonably good for $k \approx l_v^{-1}$ as well. Since the Fourier transform is linear, the idea is to find the linear combination of the two approximation that best approximates the $R_{NL}(k)$.

$$R_{NL}(k) \approx \alpha R_{NL}(k \ll l_v^{-1}, W^{-1}) + \beta R_{NL}(k \gg l_v^{-1})$$

Where α and β are the coefficient to be determined.
Since we only need to evaluate two variables, we only need to evaluate the expression above in two different points. The most reasonable points to choose are $k = 0$ and $k = +\infty$, since they are the points where the approximations work better. For doing the calculations it's best to write out the two approximations

$$R_{NL}(k) \approx \alpha \frac{W}{\sigma_c} \frac{1}{1 + L_v^2 k^2} + \beta \frac{2}{\sigma_c} \frac{\tanh}{k} \left(\frac{kW}{2} \right) \frac{1}{1 + \tan^2(\theta_{VH})}$$

The term that is multiplied by β for $k \to +\infty$ is an increasingly precise estimate of $R_{NL}(k)$, and it dominates over the term that is multiplied by alpha, so $\beta = 1$.

If we set $k = 0$ we have that

$$R_{xx} = \alpha R_{xx} + \frac{R_{xx}}{1 + \tan^2(\theta_{VH})}$$

So, $\alpha = \left[1 + \tan^{-2}(\theta_{VH})\right]^{-1}$. Putting it all together we define the resulting approximation

$$\boxed{\tilde{R}_{NL}(k) \equiv \frac{R_{xx}}{1 + L_v^2 k^2} \frac{1}{1 + \tan^{-2}(\theta_{VH})} + \frac{2}{\sigma_c} \frac{\tanh}{k} \left(\frac{kW}{2}\right) \frac{1}{1 + \tan^2(\theta_{VH})}} \tag{1.60}$$

And if we plot the approximation $\tilde{R}_{NL}(k)$ alongside the actual values of $R_{NL}(k)$ we can see that they are remarkably similar (figure 1.7)

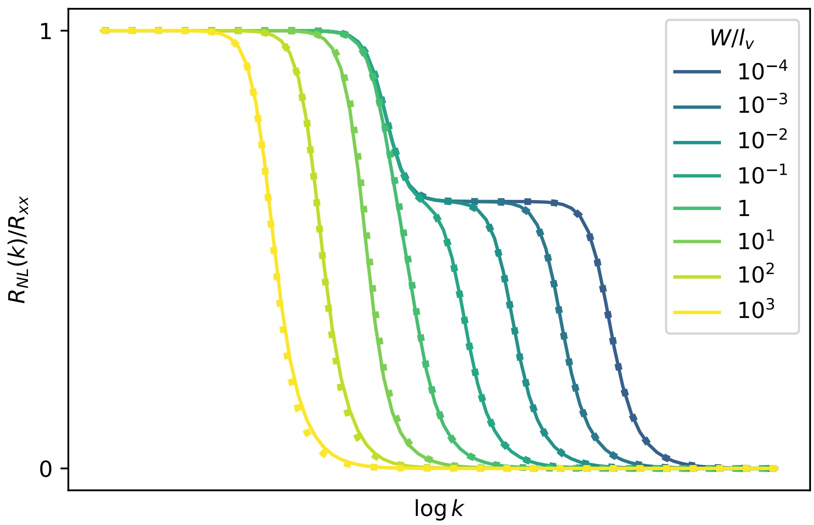

Figure 1.7: Comparison between $R_{NL}(k)$ and $\tilde{R}_{NL}(k)$. The continuous line represents $R_{NL}(k)$, while the dashed line represents $\tilde{R}_{NL}(k)$

The nice thing about this is that if two equations are similar, then their Fourier transform will be too. We can transform $\tilde{R}_{NL}(k)$ with equations 1.55 and 1.57 and we get that

$$\boxed{\tilde{R}_{NL}(x) = \frac{W \rho_{c,xx} e^{-|x|/L_v}}{2L_v[1 + \tan^{-2}(\Theta_{VH})]} - \frac{2\rho_{c,xx}}{\pi[1 + \tan^2(\Theta_{VH})]} \ln \left| \tanh\left(\frac{\pi x}{2W}\right) \right|} \tag{1.61}$$

Infact if we re-create figure 1.6 with the equation above we get figure 1.8

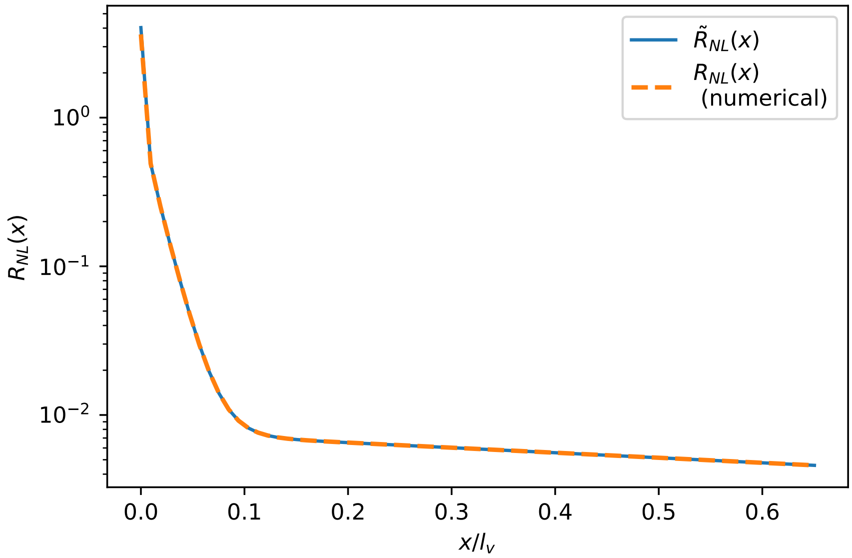

Figure 1.8: As you can see it's impossible to distinguish the difference between the two functions to the naked eye. The parameters are the same as figure 1.8

1.6 $R_{NL}(x)$ as we change ρ_{xx}

Hall effect experiments are generally done in the so-called Hall-bars. There are samples of material with a shape like the one in figure 1.9. This also means that more often than not in experimental setups we cannot change x without changing the geometry of the sample.

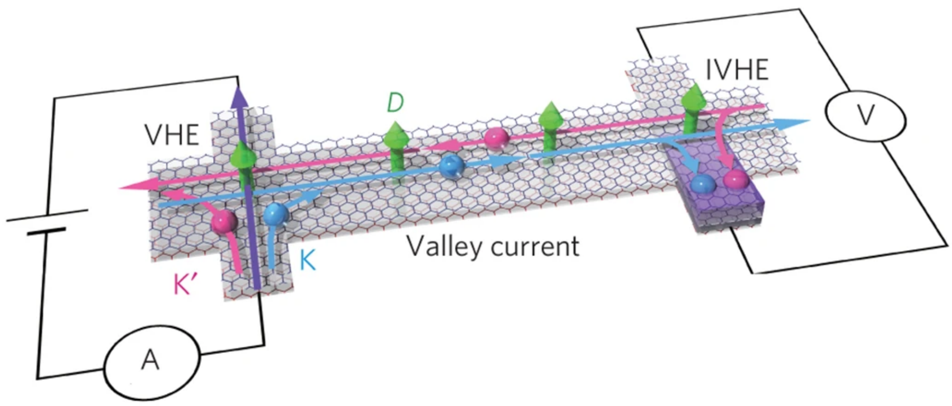

Figure 1.9: Example of the experimental setup

In the previous section we studied how R_{NL} depended on x, and Hall-bars can only measure a single x. One way for having multiple measurements with the same Hall-bar is to change the resistivity of the material by changing the temperature of the setup, and study R_{NL} as we change ρ_{xx}.

For convenience let's re-write equation 1.48

$$R_{NL}(k) = \frac{2\omega(k)}{k\sigma_c}\left\{\frac{\omega(k)}{\tanh(kW/2)} + \frac{k\tan^2(\theta_{VH})}{\tanh[\omega(k)W/2]}\right\}^{-1}$$

For convenience, we are going to change $\tan(\theta_{VH}) = \sigma_v\rho_{xx}$ and do a taylor series expansion of the above equation around $\tan^2(\theta_{VH}) \approx 0$.

$$R_{NL}(k) \approx R_{NL}(k)|_{\tan^2(\theta_{VH})=0} + \frac{\partial}{\partial\tan^2(\theta_{VH})}R_{NL}(k)|_{\tan^2(\theta_{VH})=0}$$

that we are going to re-define as

$$R_{NL}(k) \approx R_{NL}^{(0)}(k) + R_{NL}^{(1)}(k)$$

The zeroth order term gives us this:

$$R_{NL}^{(0)}(k) = \frac{2\rho}{k}\tanh\left(\frac{kW}{2}\right)$$

And if we do a the Fourier transform to get the x dependent form we get the ohmic nonlocal resistivity 1.15

$$R_{NL}^{(0)}(x) = \frac{2\rho}{\pi}\ln\left|\coth\left(\frac{\pi x}{2W}\right)\right| \tag{1.62}$$

Now let's calculate the first order term

$$R_{NL}^{(1)}(k) = -2\rho\frac{\omega(k)}{k}\left[\frac{\omega(k)}{\tanh(Wk/2)}\right]^{-2}k\frac{\tan^2(\theta_{VH})}{\tanh(\omega(k)W/2)} =$$
$$= -2\rho^3\sigma_v^2\tanh^2\left(\frac{kW}{2}\right)\left\{\omega(k)\tanh\left[\frac{\omega(k)W}{2}\right]\right\}^{-1} \equiv \rho^3F(k)$$

where $F(k)$ is defined as follows

$$F(k) \equiv -2\sigma_v^2\tanh^2\left(\frac{kW}{2}\right)\left\{\omega(k)\tanh\left[\frac{\omega(k)W}{2}\right]\right\}^{-1} \tag{1.63}$$

And it doesn't depend on ρ

Putting it all together we get that

$$\lim_{\rho\to 0} R_{NL}(x) = \frac{2\rho}{\pi}\ln\left|\coth\left(\frac{\pi x}{2W}\right)\right| + \rho^3F(x) + o(\rho^5) \tag{1.64}$$

PARLARE DEI REGIMI IN CUI DOMINA ρ^3

Now let's study what happens when $\rho, \tan(\theta_{VH}) \to \infty$. First off let's rewrite equation 1.48 and bring the $\omega(k)$ and k inside the curly braces.

$$R_{NL}(k) = 2\rho \Bigg\{ \underbrace{\frac{k}{\tanh(kW/2)}}_{\substack{\text{cannot be}\\ \text{ignored for } k=0}} + \frac{k^2}{\omega(k)} \frac{\tan^2(\theta_{VH})}{\tanh[\omega(k)W/2]} \Bigg\}^{-1}$$

This limit is a bit tricky to evaluate. First off even thought the right-most term inside the curly braces dominates everywhere except for $k = 0$ this "*small detail*" is crucial. From image 1.10 we can see that the larger ρ gets, the smaller the area around $k = 0$ where the first term dominates.

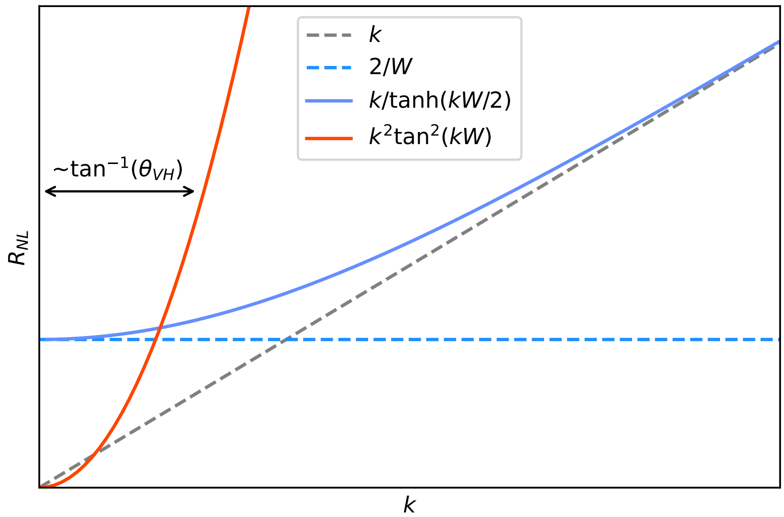

Figure 1.10: The continuous blue line represents the first term, the blue dashed line represents its approximation around $k = 0$ and the gray dashed lines represent its approximation for $k \to \infty$.
The orange parabola represents the right-hand side term $\frac{k^2}{\omega(k)} \frac{\tan^2(\theta_{VH})}{\tanh[\omega(k)W/2]}$

For high values of $\rho, \tan(\theta_{VH})$ the parabola becomes really narrow and it overtakes the first term with $k \approx 0$. This means that we can approximate the first term as being always equal to $2/W$. This means that

$$\lim_{\rho\to\infty} R_{NL}(k) = 2\rho \Bigg\{ \frac{2}{W} + \frac{k^2}{\omega(k)} \frac{\tan^2(\theta_{VH})}{\tanh[\omega(k)W/2]} \Bigg\}^{-1} \tag{1.65}$$

Ok, low let's take a look at this function as we make ρ bigger and bigger

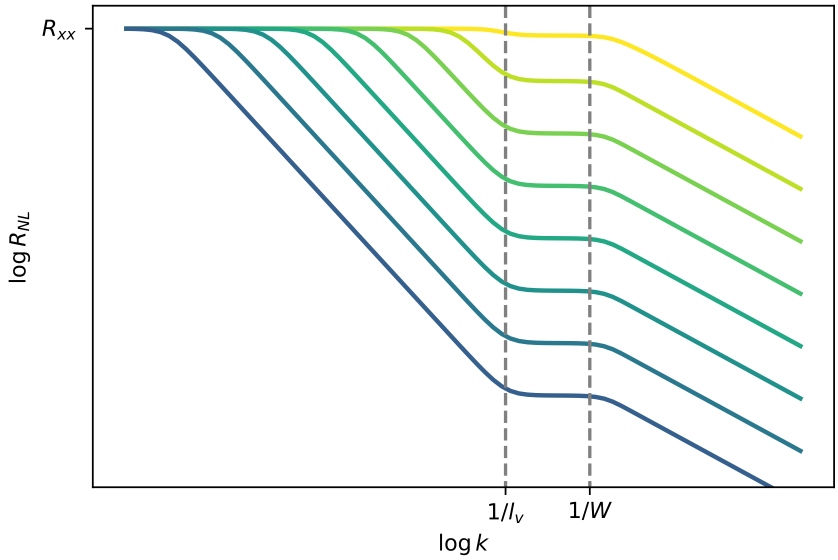

Figure 1.11: In this graph the darker the line color is, the bigger is the value of ρ. Notice how, as we increase ρ the first regime becomes more dominant

As you can see from figure 1.11 are three regimes here. The first one in for $k < l_v^{-1}$, the second one is for $l_v^{-1} < k < W^{-1}$ and the third one is for $W^{-1} < k$

In the first regime ($k < l_v^{-1}$) $R_{NL}(k)$ is similar to a Lorentzian function.

$$\lim_{\rho\to\infty} R_{NL}(k) = 2\rho\left\{\frac{2}{W} + l_v k^2 \frac{\tan^2(\theta_{VH})}{\tanh[W/2l_v]}\right\}^{-1} \tag{1.66}$$

We can re-parametrize it As

$$\lim_{\rho\to\infty} R_{NL}(k) = \frac{R_{xx}}{1+(k/\sigma)^2} \tag{1.67}$$

Where

$$\sigma = \frac{1}{\tan(\theta_{VH})}\sqrt{\frac{2}{l_v W}\tanh\left(\frac{W}{2l_v}\right)}$$

Therefore ρ and the standard deviation of the Lorentzian σ are inversely proportional.

If we do the anti-Fourier transform of this equation to get the position dependent Non-local resistivity we get

$$\mathcal{F}^{-1}\left[\frac{R_{xx}}{1+(k/\sigma)^2}\right] = \frac{1}{2}\rho W\sigma e^{-|x|\sigma} =$$

$$= \frac{\rho W}{\tan(\theta_{VH})}\sqrt{\frac{2}{l_v W}\tanh\left(\frac{W}{2l_v}\right)}\exp\left[\frac{-|x|}{\tan(\theta_{VH})}\sqrt{\frac{2}{l_v W}\tanh\left(\frac{W}{2l_v}\right)}\right] \quad (1.68)$$

Since $\tan(\theta_{VH}) = \rho\sigma_v$, for $\rho \to +\infty$ the equation above converges pointwise to the following saturation constant S

$$\lim_{\rho\to\infty} \mathcal{F}^{-1}\left[\frac{R_{xx}}{1+(k/\sigma)^2}\right] = \frac{1}{\sigma_v}\sqrt{\frac{2W}{l_v}\tanh\left(\frac{W}{2l_v}\right)} \equiv S \quad (1.69)$$

In the second regime we have already calculated the value the plateau assumes in equation 1.50

$$R_{NL}(k) \approx \frac{\rho W}{1+\tan^2(\theta_{VH})} \quad (1.70)$$

While in the third and last regime

$$R_{NL}(k) \approx \frac{2\rho}{k}\frac{1}{1+\tan^2(\theta_{VH})} \quad (1.71)$$

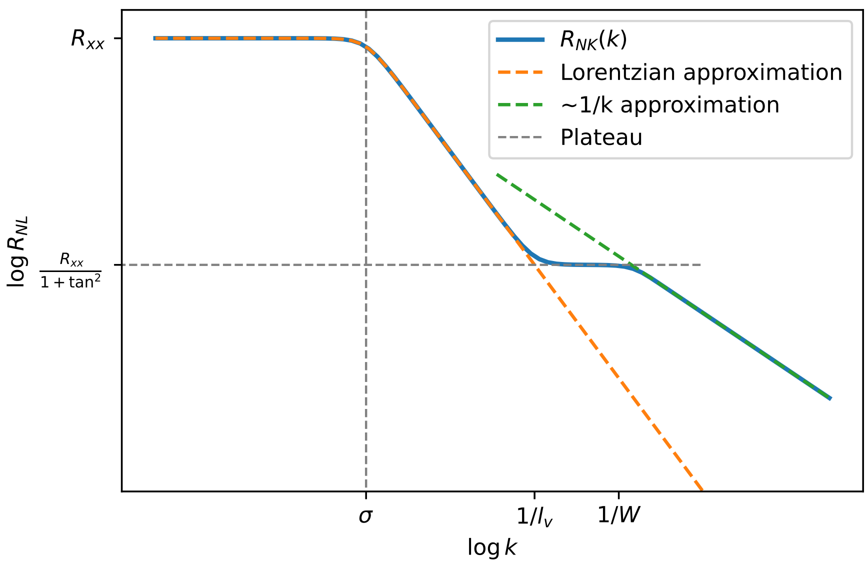

Figure 1.12: The main regimes of this function

Notice how the equations for the second and third regime are both proportional to $\rho/(1+\tan^2(\theta_{VH}))$. This means we can write equation 1.65 as approximately

$$\lim_{\rho\to\infty} R_{NL}(k) = \frac{R_{xx}}{1+(k/\sigma)^2} + \frac{\rho}{1+\tan^2(\theta_{VH})}C(k) \quad (1.72)$$

Where $C(k)$ is a function that doesn't depend on ρ or $\tan(\theta_{VH})$ and it comprehends the second, third regime and eventual corrections in between the approximations[5].
Now let $G(x)$ be it's Fourier anti-transform, then we have that

$$\lim_{\rho\to\infty} R_{NL}(x) = S + \frac{1}{\rho}G(x) \tag{1.73}$$

This means that for $\rho \to +\infty$ the right hand side term vanishes, unless it diverges. And indeed $G(x)$ diverges for $x = 0$. Therefore the limit above has pointwise convergence in $\{x \in \mathbb{R} \,|\, x \neq 0\}$

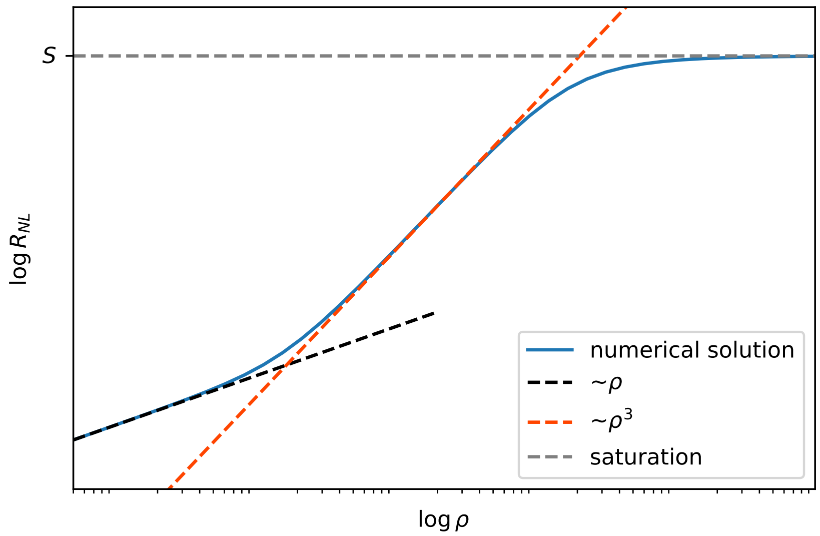

Figure 1.13: The main regimes of this function

[5]Yes, the corrections also are proportional to $\rho/(1 + \tan^2(\theta_{VH}))$ SPIEGA PERCHè

Chapter 2

Berry phase and Berry curvature

2.1 Introduction

Berry phase is the simplest demostration of how geometry and topology can emerge from quantum mechanics and it is in the heart of the quantum Hall effect

Let us consider a physical system described by a Hamiltonian that depends on a set of parameters $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \dots)$. These parameters do not represent the degrees of freedom of the system like position and momentum, rather they describe things such as the mass of a particle, the strenght of a potential and so on.

For each $H(\boldsymbol{\lambda})$ there exists a set of eigenstates such that

$$H(\boldsymbol{\lambda})\,|n,\boldsymbol{\lambda}\rangle = E_n(\boldsymbol{\lambda})\,|n,\boldsymbol{\lambda}\rangle \tag{2.1}$$

However the equation above does not completely determine the basis function $|n,\boldsymbol{\lambda}\rangle$; We can change arbitrarly the phase $\gamma_n(\boldsymbol{\lambda})$ of any eigenstate which is called *Berry phase*

$$|n,\boldsymbol{\lambda}\rangle \to \underbrace{e^{i\gamma_n(\boldsymbol{\lambda}(t))}}_{\text{Berry phase}}\,|n,\boldsymbol{\lambda}\rangle \tag{2.2}$$

Suppose we start off with a hamiltonian and than we slowly change the parameters for a time T until it reaches a different hamiltonian, this means that $\boldsymbol{\lambda} = \boldsymbol{\lambda}(T)$. For the adiabatic theorem we can say that if we start on an energy eigenstate, and the system changes slowly enough [1], and has no

[1] How slow you have to be in changing the parameters depens on the energy gap from the state you're in to the nearest other state. The smaller the gap, the slower you have to change the parameters. A way of showing this without doing long calculations is the following:
We know from the Heisemberg uncertanty principle that $T\Delta E \geq \hbar/2$. We want the uncertanty in the Energy to be way smaller than the energy gap$E_g \gg \Delta E$, so $E_g \gg \frac{\hbar}{2T}$, so if we make T big enought it can be archieved

degeneracies, then the system will cling on that energy eigenstate.
This means that the equation of motion of a particle that for time $t = 0$ is equal to $|\psi_n(t=0)\rangle = |n, \boldsymbol{\lambda}(0)\rangle$ is

$$|\psi_n(t)\rangle = \underbrace{e^{i\gamma_n(\boldsymbol{\lambda}(t))}}_{\text{Berry phase}} \cdot \underbrace{e^{-\frac{i}{\hbar}\int_0^t E_n(\boldsymbol{\lambda}(t'))dt'}}_{\text{dynamical phase}} |n, \boldsymbol{\lambda}(t)\rangle \tag{2.3}$$

Where the first exponent comes from eq. 2.2. We now insert the equation above into the time-dependent Shrodinger equation

$$i\hbar\partial_t|\psi_n(t)\rangle = H(\boldsymbol{\lambda}(t))|\psi_n(t)\rangle \tag{2.4}$$

By plugging equation 2.3 into the *right* term term of equation 2.4 we get we get that

$$H(\boldsymbol{\lambda}(t))|\psi_n(t)\rangle = E_n(t)\,|\psi_n(t)\rangle \tag{2.5}$$

Andy By plugging equation 2.3 into the *left* term term of equation 2.4 we get we get that

$$i\hbar\partial_t|\psi_n(t)\rangle = -\hbar\dot{\gamma}_n(t)|\psi_n(t)\rangle + E_n(t)|\psi_n(t)\rangle + e^{i\phi_n(t)}\partial_t|n,t\rangle \tag{2.6}$$

where we have defined $e^{i\phi_n(t)} \equiv e^{i\gamma_n(\boldsymbol{\lambda}(t))}e^{-\frac{i}{\hbar}\int_0^t E_n(\boldsymbol{\lambda}(t'))dt'}$

By equating the right terms in equations 2.5 and 2.6 we get that

$$i\hbar e^{i\phi_n t(t)}\partial_t|n,t\rangle = \hbar\dot{\gamma}_n(t)\,|\psi_n(t)\rangle = \hbar\dot{\gamma}_n(t)e^{i\phi_n(t)}\,|n,t\rangle \tag{2.7}$$

now we multiply the term on the left and on the right of equation 2.7 by $\hbar^{-1}e^{-i\phi_n(t)}\,\langle n,t|$

$$\dot{\gamma}_n(t) = i\,\langle n,t|\,\partial_t\,|n,t\rangle \tag{2.8}$$

We can re-express it in terms of $\boldsymbol{\lambda}$

$$\dot{\gamma}_n(t) = \dot{\boldsymbol{\lambda}} \cdot \underbrace{i\,\langle n,t|\,\partial_{\boldsymbol{\lambda}}\,|n,t\rangle}_{\equiv \mathbf{A}_n(\boldsymbol{\lambda})} \tag{2.9}$$

Where $\mathbf{A}_n(\boldsymbol{\lambda})$ called the **Berry connection** This means that we can calculate the total change in $\gamma_n(t)$ can be obtained by doing a line integral in the space of parameters $\boldsymbol{\lambda}$ over the path $\mathcal{P}$ of values that $\boldsymbol{\lambda}$ assumes during the time evolution

$$\gamma_n = \int_{\mathcal{P}} \mathbf{A}_n(\boldsymbol{\lambda}) \cdot d\boldsymbol{\lambda} \tag{2.10}$$

$$|n, \boldsymbol{\lambda}\rangle \to e^{if_n(\boldsymbol{\lambda})}\,|n, \boldsymbol{\lambda}\rangle \tag{2.11}$$

Keep in mind however that the eigenstates are defined up to a phase, meaning that we can re-define the base vectors like so (equation 2.11). If we apply this substitution into the formula of $\mathbf{A}_n$ we have that

$$\mathbf{A}_n(\boldsymbol{\lambda}) = i \langle n,t| \partial_{\boldsymbol{\lambda}} |n,t\rangle \rightarrow i \langle n,t| \partial_{\boldsymbol{\lambda}} |n,t\rangle - \partial_{\boldsymbol{\lambda}} f_n(\boldsymbol{\lambda})$$

$$\mathbf{A}_n \rightarrow \mathbf{A}_n - \partial_{\boldsymbol{\lambda}} f_n \tag{2.12}$$

So the system is invariant under the gauge transformation in equation 2.12. If we do this transformation to equation 2.10 we have that

$$\gamma_n = \int_{\mathcal{P}} \mathbf{A}_n(\boldsymbol{\lambda}) \cdot d\boldsymbol{\lambda} - \int_{\mathcal{P}} \partial_{\boldsymbol{\lambda}} f_n(\boldsymbol{\lambda}) \cdot d\boldsymbol{\lambda} = \int_{\mathcal{P}} \mathbf{A}_n(\boldsymbol{\lambda}) \cdot d\boldsymbol{\lambda} + f(\boldsymbol{\lambda}(0)) - f(\boldsymbol{\lambda}(T))$$

This means that if the path $\mathcal{P}$ is open we can always choose a function f_n such that $f(\boldsymbol{\lambda}(0)) - f(\boldsymbol{\lambda}(T)) = \int_{\mathcal{P}} \mathbf{A}_n(\boldsymbol{\lambda}) \cdot d\boldsymbol{\lambda}$, thus we can conclude that one can always choose a suitable $f(\boldsymbol{\lambda})$ such that γ_n accumulated along the path $\mathcal{P}$ is calceled out leaving equation 2.3 with only the dynamical phase. However if the path is closed $\boldsymbol{\lambda}(0) = \boldsymbol{\lambda}(T)$, in order to make the phase change in equation 2.11 single value we must have that

$$e^{f(\boldsymbol{\lambda}(0)) - f(\boldsymbol{\lambda}(T))} = 1$$

so

$$f(\boldsymbol{\lambda}(0)) - f(\boldsymbol{\lambda}(T)) = 2n\pi \quad n \in \mathbb{R}$$

This leads us to the important result that

$$\gamma_n = \oint_{\mathcal{P}} \mathbf{A}_n(\boldsymbol{\lambda}) \cdot d\boldsymbol{\lambda} + 2n\pi \tag{2.13}$$

This time, if the line integral is not a multiple of 2π (and there is no reason why it should) there is no way of choosing a suitable f_n to cancel it out and the Berry phase in equation 2.3 is there to stay

2.2 Berry curvature

In EM the field thensor $F_{\mu\nu}$ is defined as in equation 2.14. Since Berry conenction has the same Gauge invariance as the one of the EM vector potential it is useful to define, a gauge field tensor derived from the Berry connection:

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu \tag{2.14}$$

$$\Omega^n_{\mu\nu} = \partial_\mu A^n_\nu(\boldsymbol{\lambda}) - \partial_\nu A^n_\mu(\boldsymbol{\lambda}) \tag{2.15}$$

This new field tensor is defined as **Berry curvature** and it is gauge independent just like $F_{\mu\nu}$![2]

[2] The notation has changed a bit, now $A^n_\mu \equiv (\mathbf{A}_n)_\mu$

2.2.1 Other formulas for $\Omega_{\mu\nu}$

With a few mathematical steps it is possible to re cast the Berry curvature into a different form that might be useful later

$$\partial_\mu A^n_\mu = i\partial_\mu \langle n, \boldsymbol{\lambda}| \partial_\nu n, \boldsymbol{\lambda}\rangle = i \langle \partial_\mu n, \boldsymbol{\lambda}| \partial_\nu n, \boldsymbol{\lambda}\rangle + i \langle n, \boldsymbol{\lambda}| \partial_\mu \partial_\nu n, \boldsymbol{\lambda}\rangle$$

$$\boxed{\Omega^n_{\mu\nu} = i \langle \partial_\mu n| \partial_\nu n\rangle - i \langle \partial_\nu n| \partial_\mu n\rangle} \tag{2.16}$$

It is also possible to express Ω in terms of the eigenstates of the Hamiltonian with some mathematical manipulation

$$\langle n'| H |n\rangle = \delta_{n'n} \to \partial_\mu \langle n'| H |n\rangle = 0$$

$$\begin{aligned}
\partial_\mu \langle n'| H |n\rangle &= \langle \partial_\mu n'| H |n\rangle + \langle n'| H |\partial_\mu n\rangle + \langle n'| \partial_\mu H |n\rangle \\
E_n \langle \partial_\mu n'| n\rangle + E_{n'} \langle n'| \partial_\mu n\rangle &= \langle n'| \partial_\mu H |n\rangle \\
(E_{n'} - E_n) \langle n'| \partial_\mu n\rangle &= \langle n'| \partial_\mu H |n\rangle \\
\langle n'| \partial_\mu n\rangle &= \frac{\langle n'| \partial_\mu H |n\rangle}{E_{n'} - E_n}
\end{aligned} \tag{2.17}$$

Now we write equation 2.16 like so

$$\Omega^n_{\mu\nu} = i \langle \partial_\mu n| \partial_\nu n\rangle - (\mu \leftrightarrow \nu) = i \sum_{n' \neq n} \langle \partial_\mu n| n'\rangle \langle n'| \partial_\nu n\rangle - (\mu \leftrightarrow \nu)$$

By plugging in above equation 2.17 we get

$$\boxed{\Omega^n_{\mu\nu} = i \sum_{n' \neq n} \frac{\langle n| \partial_\mu H |n'\rangle \langle n'| \partial_\nu H |n\rangle}{(E_{n'} - E_n)^2} - (\mu \leftrightarrow \nu)} \tag{2.18}$$

This last form of the Berry curvature has the advantage that no differentiation of the wavefunction is needed. This equation also tells us that

$$\sum_n \Omega^n_{\mu\nu}(\boldsymbol{\lambda}) = 0$$

2.3 Stokes' Theorem

From the Stokes theorem we have that

$$\gamma_n = \oint_{\mathcal{P}} A^n_\mu \, d\lambda^\mu = \frac{1}{2} \int_\Sigma \Omega^n_{\mu\nu} \, d\lambda^\mu \wedge d\lambda^\nu \tag{2.19}$$

where we have used the Einstein convention of summation and the $\wedge$ operator represents the exterior product

There is a subtelty in this last equation, as we know the Berry curvature

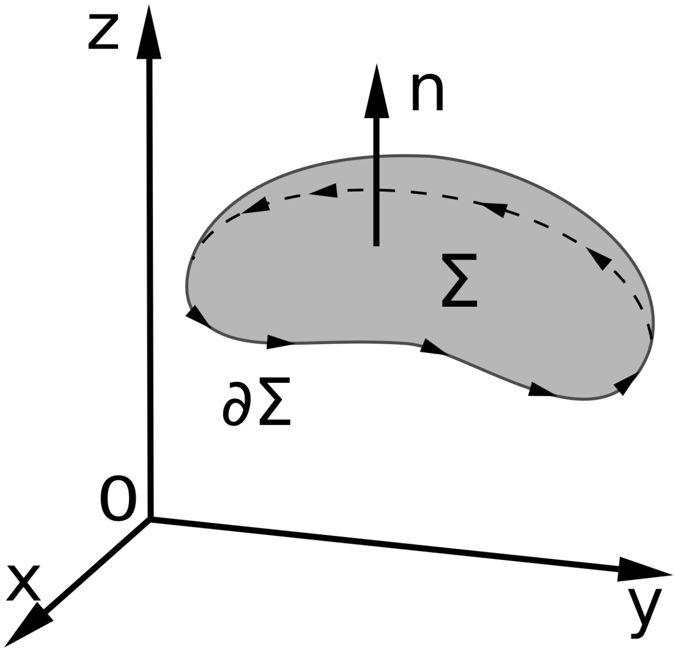

Figure 2.1: Here we divide the surface of the sphere in two different surfaces $\mathcal{A}$ and $\mathcal{B}$ that share the edge $\mathcal{P}$

tensor in Gauge-invariant, so the integral over the surface is too, but the integral over the closed path of the Berry connection is defined up to a factor $2n\pi$ that is gauge dependant. So is there a modulo 2π ambiguity or not?
The answer is that if γ_n is to be determined using the knowledge of $|n, \boldsymbol{\lambda}\rangle$ only on the curve $\mathcal{P}$ then it is really well defined modulo 2π. In this case we can re-write equation 2.19 as

$$\frac{1}{2}\int_{\Sigma} \Omega^n_{\mu\nu}\, d\lambda^\mu \wedge d\lambda^\nu := \oint_{\mathcal{P}} A^n_\mu \, d\lambda^\mu$$

Meaning that the integral over the surface $\pm$ is equal to *one of the values of* the integrals along the closed path $\mathcal{P}$

But what kind of Gauge gives the "correct" answer? If we choose a gauge that is continuous and smooth everywhere along the surface Σ including on its boundary $\mathcal{P}$ then equation 2.19 becomes unambiguous.
While it is possible to make a radical gauge transformation that shifts γ_n by 2π when regarding $|n, \boldsymbol{\lambda}\rangle$ as a function defined only in the neighborhood of $\mathcal{P}$, such a gauge change cannot be smoothly continued into the interior $\mathcal{S}$ without creating a vortex-like singularity of $\gamma_n(\boldsymbol{\lambda})$.

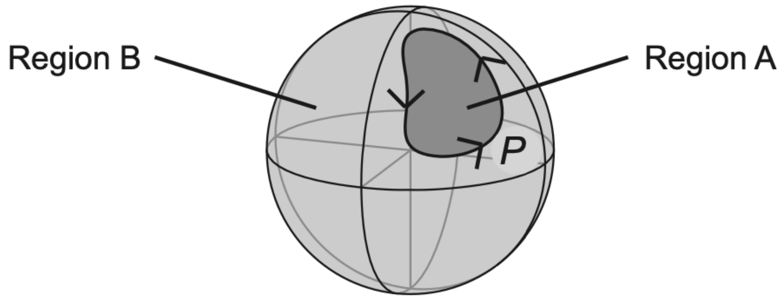

Figure 2.2: Here we divide the surface of the sphere in two different surfaces $\mathcal{A}$ and $\mathcal{B}$ that share the edge $\mathcal{P}$

2.4 Chern Theorem

Let's take as an example Gauss's theorem. It tells us that the flux of the field through a closed surface is equal to the charges inside.
Now let's calculate the flux of the Berry curvature thorugh a closed surface. We can divide the closed surface as two different open surfaces that share the same edge $\mathcal{P}$.
Thanks to stokes theorem the flux throught the surface $\mathcal{A}$ is $\oint_{\mathcal{P}} \mathbf{A} \cdot d\boldsymbol{\lambda}$, but the flux throught the surface $\mathcal{B}$ is $-\oint_{\mathcal{P}} \mathbf{A} \cdot d\boldsymbol{\lambda}$.
Theese two integrals must be equal modulo 2π, so

$$\oint_{\mathcal{S}} \Omega^n_{\mu\nu} d\lambda^\mu \wedge d\lambda^\nu = 2\pi C \qquad C \in \mathbb{Z} \tag{2.20}$$

This means that the flux thought a closed surface of the Berry curvature is quantized

The constant C in known as the Chern number. Note that when the Chern index is nonzero, it is impossible to construct a smooth and continuous gauge over the entire surface $\mathcal{S}$. If such a gauge did exist, then we could apply Stokes' theorem directly to the entire surface and conclude that the Chern number vanishes, in contradiction with the assumpti
But what are theese "pseudo-charges" inside the closed surface that generate the flux?
In E.M. a simple way to spot charges (or monopoles) is to look at the field tensor and see if as some point it diverges as $1/(\mathbf{r} - \mathbf{r_0})^2$. Let's take a look

at $\Omega_{\mu\nu}$ (eq. 2.18) and see if we can spot anything similar [3]

$$\Omega^n_{\mu\nu} = i \sum_{n' \neq n} \frac{\langle n| \partial_\mu H |n'\rangle \wedge \langle n'| \partial_\nu H |n\rangle}{\underbrace{[E_{n'}(\boldsymbol{\lambda}) - E_n(\boldsymbol{\lambda})]^2}_{\substack{\text{what happens if for some } \boldsymbol{\lambda}=\boldsymbol{\lambda}_d \\ \text{the two energies are the same?}}}} \tag{2.21}$$

So, suppose that for some $\boldsymbol{\lambda} = \boldsymbol{\lambda}_d$ we have that $E_n(\boldsymbol{\lambda}_d) = E_m(\boldsymbol{\lambda}_d)$, now we expand the energies near $\boldsymbol{\lambda}_d$ at first order

$$\begin{cases} E_n(\boldsymbol{\lambda}) \approx E_n(\boldsymbol{\lambda}_d) + \partial_{\boldsymbol{\lambda}} E_n|_{\boldsymbol{\lambda}=\boldsymbol{\lambda}_d} \cdot (\boldsymbol{\lambda} - \boldsymbol{\lambda}_d) \\ E_m(\boldsymbol{\lambda}) \approx E_n(\boldsymbol{\lambda}_d) + \partial_{\boldsymbol{\lambda}} E_m|_{\boldsymbol{\lambda}=\boldsymbol{\lambda}_d} \cdot (\boldsymbol{\lambda} - \boldsymbol{\lambda}_d) \end{cases}$$

This means that

$$E_n(\boldsymbol{\lambda}) - E_m(\boldsymbol{\lambda}) \approx \partial_{\boldsymbol{\lambda}}(E_n - E_m)|_{\boldsymbol{\lambda}=\boldsymbol{\lambda}_d} \cdot (\boldsymbol{\lambda} - \boldsymbol{\lambda}_d)$$

so the denominator of the berry curvature near $\boldsymbol{\lambda}_d$ goes like $1/(\boldsymbol{\lambda} - \boldsymbol{\lambda}_d)^2$. This means that there are "charges" or "monopoles" that induce the flux throught the closed surface, and they are localized where 2 (or more) energy levels cross

[3] In the equation below I expressed explicitely the $\boldsymbol{\lambda}$ dependence in the denomiator and condensed the fomula using the wedge product $\wedge$

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