Symmetry Protected Topological Phases and Quantum Geometry

A thesis submitted towards partial fulfilment of
BS-MS Dual Degree Programme

by

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under the guidance of

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Certificate

This is to certify that this thesis entitled "Symmetry Protected Topological Pases and Quantum Geometry" submitted towards the partial fulfilment of the BS-MS dual degree programme at the Indian Institute of Science Education and Research Pune represents original research carried out by " Susmita Singh" at "International Centre for Theoretical Sciences, Bangalore", under the supervision of "Prof Subhro Bhattacharjee" during the academic year 2017-2018.

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I dedicate this thesis to My Family

Declaration

I hereby declare that the matter embodied in the report entitled âĂIJSymmetry Protected Topological Phases and Quantum GeomeryâĂİ are the results of the investigations carried out by me at International Centre for Theoretical Sciences , under the supervision of Prof Subhro Bhattacharjee and the same has not been submitted elsewhere for any other degree.

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Abstract

The observation of Quantum Hall Effect led to the development of interest in topological studies of quantum systems. In the case of Quantum Hall Effect the conductivity of the system acts as the topological invariant which only takes values that are integer multiples of $\frac{e^2}{\hbar}$. In this project we try to understand how the quantum metric behaves when a topological phase transition occurs. Thus, we look for signatures of topological phase transitions in the quantum metric.

We work with different systems. We first analyze the SSH model of Polyacetylene. We see that when the quantum metric, which is defined in terms of the overlap between nearby states diverges at a topological phase transition. This signals that there is no overlap between the states on the two sides of the transition.

We then work with systems in different gauges and see how the metric transforms under the gauge transformation. We have also come up with a rule to tell the transformation of metric in one unit cell to that in another. We then work with the honeycomb lattice and see how the metric behaves when spin inversion symmetry is broken.

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Chapter 1

Geometric Phase of a Quantum System

When a quantum system traverses around a closed adiabatic path, it acquires a phase apart from the dynamical phase. This other phase depends on the geometry of the path it traverse and hence is known as the geometric phase. The geometric phase was first observed by Michael Berry in 1984, and thus it is also known as the Berry's Phase. The geometric phase is a very interesting and consequential feature of quantum systems and has led to the new idea of geometric approach for quantum systems. In this chapter we will briefly describe how the geometric phase appears in quantum systems.

1.1 The Quantum Adiabatic Theorem

Consider a quantum system described by the Hamiltonian $\hat{H}(R_\mu)$,which is dependent on the parameters $\{R_\mu\}$. Then the eigenvalues E and eigenfunctions ψ of the Hamiltonian are also $\{R_\mu\}$ dependent and satisfy the eigenvalue equation:

$$\hat{H}(R_\mu)\psi_n(R_\mu) = E_n(R_\mu)\psi(R_\mu) \tag{1.1}$$

The adiabatic theorem is the statement that if the Hamiltonian is varied 'slowly enough', by varying the parameters $\{R_\mu\}$, then the system remains in the state it started with and only acquires a phase factor. Now the question is how slow is 'slow enough'? The answer to this question is that the frequency of the variation of the Hamiltonian should be much much smaller than the gap between the instantaneous eigenenergies of the system for the quantum adiabatic theorem to hold true.

1.2 Geometric Phase

We will now see how the Berry's phase comes about in the adiabatic evolution of a quantum system.

If the parameter $\{R_\mu\}$ is t, i.e. if we have a time-dependent Hamiltonian, then (1.1) becomes

$$\hat{H}(t)\psi_n(t) = E_n(t)\psi_n(t) \tag{1.2}$$

For the time-dependent Hamiltonian in (1.2), the eigenfunctions and eigenvalues are also time-dependent. But these eiegenfunctions still constitute a complete, orthonormal set at any particular instant of time, such that $\langle\psi_m(t)|\psi_n(t)\rangle = \delta_{mn}$. The general solution to the time-dependent Schrodinger equation can then be given by a linear combination of these eigenfunctions as follows:

$$\psi_n(t) = \sum_n c_n(t)\psi_n(t)e^{\theta_n(t)} \tag{1.3}$$

where $\theta_n(t)$ is the dynamical phase factor given by $\theta_n(t) = -\frac{1}{\hbar}\int_0^t E_n(t')dt'$. On substituting (1.2) in (1.1) we get:

$$i\hbar\sum_n \left(\dot{c_n}\psi_n + c_n\dot{\psi_n} + ic_n\psi_n\dot{\theta_n}\right)e^{i\theta_n} = \sum_n c_n(H\psi_n)e^(i\theta_n) \tag{1.4}$$

The last two terms cancel due to (1.1). Now taking inner product with ψ_m we get:

$$\dot{c_m}(t) = -\sum_n c_n\langle\psi_m|\dot{\psi_n}\rangle e^{i(\theta_n-\theta_m)} \tag{1.5}$$

Taking the time derivative of (1.1) and inner product with ψ_m we get:

$$\langle\psi_m|\dot{H}|\psi_n\rangle + \langle\psi_m|\dot{\psi_n}\rangle = \dot{E}_n\delta_{mn} + E_n\langle\psi_m|\dot{\psi_n}\rangle \tag{1.6}$$

Now, since H is hermitian $\langle\psi_m|H|\dot{\psi_n}\rangle = E_m\langle\psi_m|\dot{\psi_n}\rangle$ Thus, for $m \neq n$ (1.6) becomes:

$$\langle\psi_m|\dot{H}|\psi_n\rangle = (E_n - E_m)\langle\psi_m|\dot{\psi_n}\rangle \tag{1.7}$$

Using this in (1.5) we get:

$$\dot{c}_m(t) = -c_m\langle\psi_m|\dot{\psi_n}\rangle - \sum_n c_n\frac{\langle\psi_m|\dot{H}|\psi_n\rangle}{E_n - E_m}e^{i(\theta_n - theta_m)} \tag{1.8}$$

Now assuming the validity of the adiabatic theorem, i.e. $\dot{H}$ is very small so that we can neglect the last term. We are then left with

$$\dot{c}_m(t) = -c_m\langle\psi_m|\dot{\psi_m}\rangle \tag{1.9}$$

(1.9) has a solution of the form:

$$c_m(t) = c_m(0)e^{i\gamma_m(t)} \tag{1.10}$$

where $\gamma_m(T) = i\int_0^t \langle\psi_m(t')|\dot{\psi}(t')\rangle dt'$.

Now if $\psi_n(t)$ is dependent on some parameter set $\{R_\mu(t)\}$ varying with time, then

$$\partial\psi_n\partial t = (\nabla_R\psi_n)\,.\frac{dR}{dt} \tag{1.11}$$

Then the Berry's phase becomes:

$$\gamma_n(t) = i\int_{R_i}^{R_f} \langle\psi_n|\nabla_R\psi_n\rangle.d\bar{R} \tag{1.12}$$

Now if the system is taken through a closed path in the parameter space, i.e. the parameter values return to the initial set of values at the end of the process, then the geometric phase is given by the line integral around a close loop and is given by the following equation:

$$\gamma_n(T) = i\oint \langle\psi_n|\nabla_R\psi_n\rangle.d\bar{R} \tag{1.13}$$

Thus we see from (1.3) and (1.12) that the state of a quantum system, when taken through an adiabatic closed cycle acquires an additional phase that depends on the geometry of the path traversed in the parameter space, apart from the time dependent dynamical phase factor $\theta_n(t)$.

Chapter 2

Quantum Geometry

The studies of the quantum Hall effect led to the idea of studies of quantum systems in terms topological invariants. Also, the discovery of the geometric phase made possible the studies of the geometry of the space of many electron ground states.

In this chapter we try to build an understanding of the geometry of states of quantum system which are called rays in the Hilbert space. We try to understand quantum geometry in the framework of quantities called Bargmann invariants. We define the Quantum Geometric Tensor in terms of the Bargmann invariants. The Quantum Geometric tensor has a symmetric and antisymmetric part which give the distance metric and the Berry curvature respectively. The topological characterization of quantum systems can be done in terms of the distance metric and the Berry curvature which we try to understand in this project.

2.1 The space of rays

In quantum mechanics the physical state of a system is described by rays in the Hilbert space. By a 'ray' we mean, if there is a state $|\psi\rangle$, which is normalized, i.e. $\langle\psi|\rangle\psi = 1$ and another state $|\psi'\rangle = e^{i\theta}|\psi\rangle$ then the two sates are physically same as they both lead to the same set of observables. This is the state of the quantum system is not physically detectable. Thus, there is a many to one relation from the ray space to the physical state of the system.

To understand this better, we can think of a situation analogous to the 3d real Euclidean space. Then two normalized vectors $\hat{n}$ and $-\hat{n}$ represent the same physical state. Thus, we see that there is no distinction between the forward and backward direction and they both represent the same physical state. We call these objects rays in the Hilbert space.

The quantity that can serve as a one to one correspondence to the physical state of the system is the density matrix or projector defined as:

$$\rho(\psi) = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle} \tag{2.1}$$

We call it a projector because on acting a state $|\chi\rangle$ with $\rho(\psi)$ we get

$$\rho(\psi)|\chi\rangle = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}|\chi\rangle \tag{2.2}$$

$$= \frac{\langle\psi|\chi\rangle}{\langle\psi|\psi\rangle}|\psi\rangle \tag{2.3}$$

This is the projection of $|\chi\rangle$ in state $|\psi\rangle$.

The density matrix/ projector satisfies the following :
•$\rho^2 = \rho$
•$tr(\rho) = 1$.

2.2 Bargmann Invariants

We know any measurable quantity of a state $|\psi\rangle$ can be written in terms of the projectors $\rho(\psi)$ defined in (2.1). Noting this, we define a sequence of quantities called Bargmann invariants by the following equation:

$$B^N(\psi_1, \psi_2, ..., \psi_N) = tr\left(\prod_{n=1}^{N} \rho(\psi_n)\right) \tag{2.4}$$

To see how these invaariants are relevant, let us consider the inner product $\langle\psi|\chi\rangle$. This is the probability amplitude for a system in state $|\chi\rangle$ to be found in state $|\psi\rangle$. The measurable quantity here is the square of the probability amplitude, that is:

$$|\langle\psi|\chi\rangle|^2 = tr(\rho(\psi)\rho(\chi)) \tag{2.5}$$

We see that the RHS is the second Bargmann invariant. The third and higher Bargmann invariants have a phase Ω^N associated with them which satisfies:

$$B^N(\psi_1, \psi_2, ..., \psi_N) = e^{i\Omega^N(\psi_1,\psi_2,...,\psi_N)}|B^N(\psi_1, \psi_2, ..., \psi_N)|$$

Here $\Omega^N(\psi_1, \psi_2, ..., \psi_N)$ is the phase of the N vertex Bargmann invariant with vertices at $\psi_1, \psi_2, ..., \psi_N$. We will later relate the phase of the Bargamnn invariants to th egeometric phase.

2.3 Distance and the Quantum metric

We work in a subspace of the states of a quantum system. The states are parameterized by a local N coordinate system. We denote the local coordinates by η_a, where a=1,2,...,N. We define the distance between two nearby points using the second Bargmann invariant as follows:

$$d(\psi_1, \psi_2) = \sqrt{1 - B^2(\psi_1, \psi_2)^{\lambda/2}} \tag{2.6}$$

where λ is a real number ≥ 1. Notice that the distance is maximum, i.e. 1 between two orthogonal states and is zero between a state and itself. On Taylor expansion we see that

$$d^2(\eta + d\eta, \eta) = \frac{\lambda}{4} tr(\partial_a \rho(\eta) \partial_b \rho(\eta)) d\eta^a d\eta^b \tag{2.7}$$

where $\{\eta_\mu\}$ is the set of parameters on which ψ depends and ∂_a means $\frac{\partial}{\partial_{\eta_\mu}}$. On comparing (2.7) with

$$d(\eta + d\eta, \eta)^2 = \sum_{a,b} g_{a,b}(\eta) d\eta^a d\eta^b \tag{2.8}$$

we get

$$g_{ab}(\eta) = \frac{\lambda}{4} tr(\partial_a \rho(\eta) \partial_b \rho(\eta)) \tag{2.9}$$

Thus the space of rays has a geometry in which the notion of distance can be described in terms of the metric in (2.9).

2.4 Phase of Bargmann Invariants

Let's look at the phase of a three vertex Bargmann invariant. When the the three vertices of the Bargmann invariant are very close to each other, the phase will be given by

$$\Omega^3(\eta, \eta + d\eta_1, \eta + d\eta_2) = Im(ln(tr(\rho(\eta)\rho(\eta + d\eta_1)\rho(\eta + d\eta_2)))) \tag{2.10}$$

Again, using Taylor expansion and making use of the properties $tr(\rho)^2 = tr(\rho) = 1$ and thus $tr(\partial_a \rho \partial_b \rho) = -tr(\rho \partial_a \partial_b \rho)$ we get

$$\Omega(\eta, \eta + d\eta_1, \eta + d\eta_2) = \frac{1}{2i} tr(\rho(\eta)[\partial_a \rho(\eta), \partial_b \rho(\eta)]) d\eta_1^a d\eta_2^b \tag{2.11}$$

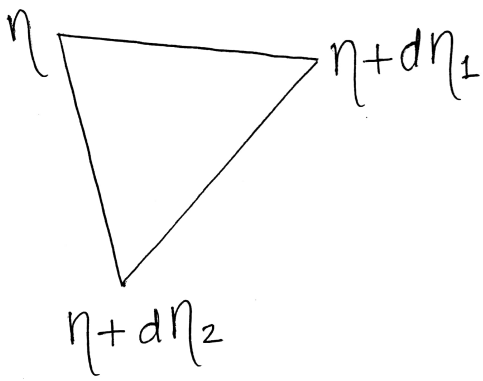

Figure 2.1: Three states close to each other as discussed in (2.10)

We define an antisymmetric tensor

$$F_{ab}(\eta) = \frac{1}{2i} tr(\rho(\eta)[\partial_a \rho(\eta), \partial_b \rho(\eta)]) \tag{2.12}$$

Now for any N vertex Bargmann invariant can be divided into triangles and the phase associated with the N vertex Bargmann invariant can be written as a sum of the phase of the 3 vertex Bargmann invariants as follows:

$$\Omega(\partial\Sigma) = \int_\Sigma F_{ab}(\eta) d\eta^a \wedge \eta^b \tag{2.13}$$

Where $\partial\Sigma$ denotes the closed Bargmann curve, Σ is the surface whose boundary is $\partial\Sigma$ and $d\eta^a \wedge \eta^b$ is a wedge product. Although there can be many surfaces with $\partial\Sigma$ as their boundary, we know that the phase of the Bargmann invariant is independent of the triangulation i.e. chice of the surface. Therefore $F_{ab}(\eta)$ must be a closed two-form.

$$\partial_a F_{bc} + \partial_b F_{ca} + \partial_c F_{ab} = 0 \tag{2.14}$$

Also, since F is a closed form it can locally be written as dA where A is a one-form. If we choose

$$A_a = \frac{1}{i} \langle \eta | \partial_a | \eta \rangle \tag{2.15}$$

we get back F as defined in (2.12). The phase of the Bargmann invariant can now be written as a line integral along $\partial\Sigma$ as

$$\Omega(\partial\Sigma) = \oint_{\partial\Sigma} A_a d\eta^a \tag{2.16}$$

We note that this A defined in (2.15) is the Berry connection differing only by a factor of 2. (2.16) is then the statement that the berry phase is given by the line integral of the Berry connection.

2.5 The Quantum Geometric Tensor

The quantum geometric tensor is defined as the sum of the symmetric tensor g_{ab} and the antisymmetric tensor F_{ab}.

$$Q_{ab} = g_{ab} + F_{ab} \tag{2.17}$$

This can be compared to the quantum geometric tensor obtained from the covariant derivative of $|\psi\rangle$ as follows.

Consider the covariant derivative of $|\psi'\rangle = e^{i\theta}|\psi\rangle$

$$D_a|\psi'\rangle = |\partial_a\psi\rangle - i\partial_a\theta|\psi\rangle$$

Construct an object

$$q_{ab} = \langle D_a\psi|D_b\psi\rangle$$

and

$$g'_{ab} = \frac{q_{ab} + q_{ba}}{2}$$
$$F'_{ab} = \frac{q_{ab} - q_{ba}}{2i}$$

On using the definition of covariant derivative as given above we get

$$g'ab = \frac{\langle\partial_a\psi|\partial_b\psi\rangle + \langle\partial_b\psi|\partial_a\psi\rangle}{2} + \partial_a\theta\partial_b\theta$$
$$F'_{ab} = \frac{\langle\partial_a\psi|\partial_b\psi\rangle - \langle\partial_b\psi|\partial_a\psi\rangle}{2i}$$

and

$$q_{ab} = g'_{ab} + iF'_{ab}$$

On comparing g_{ab}, F_{ab} from (16) with the above mentioned g'_{ab} and F'_{ab} using the definition of $\rho(\psi)$ we see that

$$g_{ab} = 2g'_{ab}$$
$$F_{ab} = 2F'_{ab}$$

Thus we see a correspondence between the quantum geometric tensors defined in two different ways.
We now proceed to discuss several examples of tight binding models that exhibit topological phases in trying to understand their signature in both g and F.

Chapter 3

Quantum metric in 1d: The Polyacetylene system

In this chapter we work with a simple 1d quantum system, namely the Su-Schrieffer Heeger model of Polyacetylene. We analyze the properties of the quantum metric, which in this case is a scalar, both qualitatively and quantitatively.

3.1 Polyacetylene (The SSH model)

Polyacetylene is a special case of the Su-Schrieffer-Heeger model in which the hopping probabilities between two sites are different. It is carbon compound with alternate double and single bonds between carbon atoms. Thus we have electrons hopping on a 1d chain with staggered hopping probabilities.

We choose a two site unit cell with sublattice labels a and b as shown in fig.(3.1).

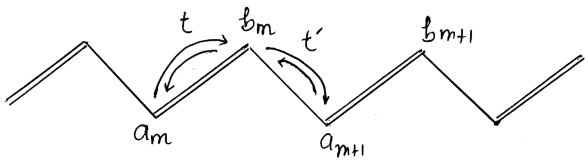

Figure 3.1: Polyacetylene chain with the two-site unit cell having sublattice labels a and b

The hamiltonian of the system is given by

$$H = -\sum_m \left(t(a_m^\dagger b_m + h.c) + t'(b_m^\dagger a_{m+1} + h.c)\right) \tag{3.1}$$

Taking the Fourier transform of (**??**) using

$$a_m = \sqrt{\tfrac{a}{2\pi}} \sum_{k=-\pi/a}^{\pi/a} e^{ikma} a_k$$
$$b_m = \sqrt{\tfrac{a}{2\pi}} \sum_{k=-\pi/a}^{\pi/a} e^{ikma} b_k$$

we get, on setting 'a'=1 for simplicity,

$$H_k = -\sum_k \begin{bmatrix} a_k^\dagger & b_k^\dagger \end{bmatrix} \begin{bmatrix} 0 & t + t'e^{-ik} \\ t + t'e^{ik} & 0 \end{bmatrix} \begin{bmatrix} a_k \\ b_k \end{bmatrix} \tag{3.2}$$

On solving this Hamiltonian we get 2 bands.

$$\epsilon_k = \pm\sqrt{t^2 + t'^2 + 2tt'\cos(k)} \tag{3.3}$$

We set $t = 1$ and plot the dispersion relation with varying t' which is equivalent to varying t'/t ratio.

As we can see from Fig (3.2) the dispersion has a gap when the ration $\frac{t'}{t}$is small and large.At $t = t'$ we have a gapless spectrum. The points ($k = \pm\pi$) where the two bands meet are called the Dirac points and the dispersion around these points is linear in the momentum. We expand the Hamiltonian (3.2) around the Dirac points using:

$$a_m = e^{i\pi m} \sum_q e^{iqm} a_{1q} + e^{-i\pi m} \sum_{q'} e^{-iq'm} a_{2q'} \tag{3.4}$$
$$b_m = e^{i\pi m} \sum_q e^{iqm} b_{1q} + e^{-i\pi m} \sum_{q'} e^{-iq'm} b_{2q'} \tag{3.5}$$

we get

$$\hat{H}_{1q} = \sum_q \begin{bmatrix} a_{1q}^\dagger & b_{1q}^\dagger \end{bmatrix} \begin{bmatrix} 0 & t - t' + iqt' \\ t - t' - iqt' & 0 \end{bmatrix} \begin{bmatrix} a_{1q} \\ b_{1q} \end{bmatrix} \tag{3.6}$$

and

$$\hat{H}_{2q} = \sum_q \begin{bmatrix} a_{2q}^\dagger & b_{2q}^\dagger \end{bmatrix} \begin{bmatrix} 0 & t - t' - iqt' \\ t - t' + iqt' & 0 \end{bmatrix} \begin{bmatrix} a_{2q} \\ b_{2q} \end{bmatrix} \tag{3.7}$$

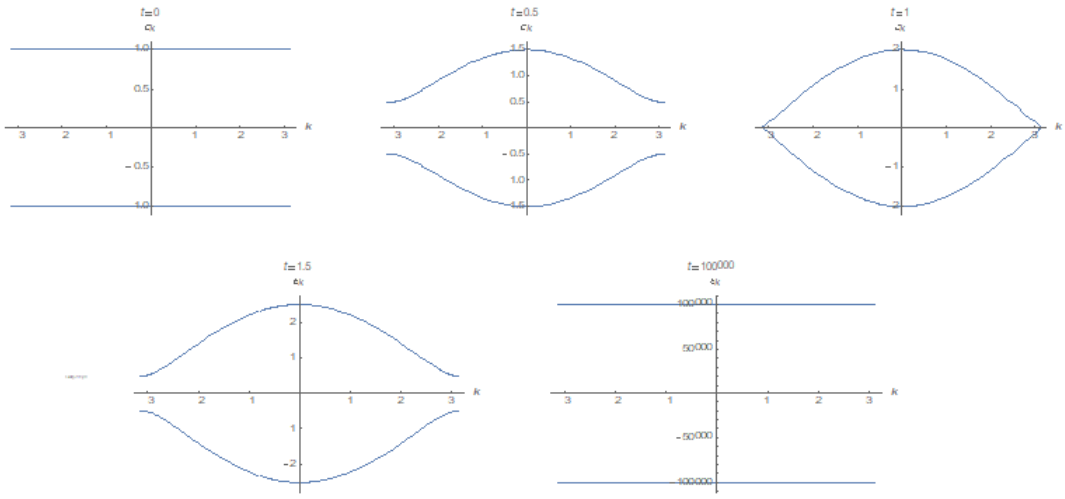

Figure 3.2: Dispersion realtion for the system with different t':t. The gap closes as t' increases(t is set to 1). And it opens again as t' exceeds 1.

Here H_{1q} is the hamiltonian expanded around $k = \pi$ nd H_{2q} is what we get on expanding around $k = -\pi$.

(3.6) and (3.7) can be written as:

$$H_{1q} = \psi_{1q}^{\dagger} \left(m_{-} \sigma^{x} + i t' \sigma^{y} \partial_{q} \right) \psi_{1q} \tag{3.8}$$

$$H_{2q} = \psi_{2q}^{\dagger} \left(m_{-} \sigma^{x} - i t' \sigma^{y} \partial_{q} \right) \psi_{2q} \tag{3.9}$$

Here σ represents the sublattice index and $\psi_{iq} = \begin{bmatrix} a_{iq} & b_{iq} \end{bmatrix}^{T}$ and $m_{-} = t - t'$ (3.8) and (3.9) can be combined as follows:

$$H_{q} = \psi_{q}^{\dagger} \left(m_{-} \sigma^{x} - i t \sigma^{z} \tau^{z} \partial_{q} \right) \psi_{q} \tag{3.10}$$

Here τ represents the valley index and $\psi_{q} = \begin{bmatrix} a_{1q} & b_{1q} & a_{2q} & b_{2q} \end{bmatrix}^{T}$ We see from (3.10) that the Hamiltonian looks like a Dirac equation, where $m_{-} = t - t'$ acts like the mass which opens up a gap in the spectrum as we can see from fig. (3.2).

3.2 Zero modes

To solve for the zero modes we consider the following equation:

$$H_{1q} \psi_{10} = 0 \tag{3.11}$$

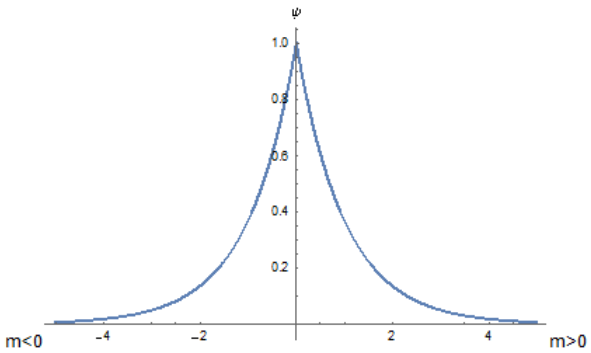

Figure 3.3: The zero modes for $m < 0$ and $m > 0$ concatenated ($m = \frac{m_-}{t'}$)

$$\begin{bmatrix} 0 & m_- + t'\partial_q \\ m_- - t'\partial_q & 0 \end{bmatrix} \begin{bmatrix} u_1 \\ v_1 \end{bmatrix} = 0 \begin{bmatrix} u_1 \\ v_1 \end{bmatrix}$$

On solving the above system of linear equations we get two possible linearly independent solutions:

$$\psi_{10} = e^{-\int \frac{m_-}{t'} dx} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \text{ and } \psi_{10} = e^{\int \frac{m_-}{t'} dx} \begin{bmatrix} 1 \\ 0 \end{bmatrix}.$$

The two solutions are depicted graphically in Fig.(3.3).

3.3 Quantum metric

The quantum metric gives the distance between two nearby states in the space of rays as given by (2.9)

Now we calculate the quantum metric for the polyacetylene system. We solve for the eigenvalues and eigenstates of H_k in (3.2), taking a=1 for simplicity.
We get the eigenvalues

$$\epsilon_\pm(k) = \sqrt{t^2 + t'^2 + 2tt'\cos(k)} \tag{3.12}$$

and eigenstates

$$\psi_\pm(k) = \begin{bmatrix} t + t'e^{-ik} \\ \pm\epsilon(k) \end{bmatrix} \tag{3.13}$$

Next we calculate the density matrices using:

$$\rho_\pm = \frac{|\psi_\pm\rangle\langle\psi_\pm|}{\langle\psi_\pm|\psi_\pm\rangle} \tag{3.14}$$

This gives

$$\rho_{\pm} = \frac{1}{2}\begin{bmatrix} 1 & \frac{\pm\epsilon(k)}{t+t'e^(ik)} \\ \frac{\pm\epsilon(k)}{t+t'e^(-ik)} & 1 \end{bmatrix} \tag{3.15}$$

Now using (2.9) we get

$$g_{kk}(\psi_+) = \frac{1}{2}\frac{t'^2(t' + t\cos(k))}{(t + t'e^{-ik})^2(t + t'e^{ik})^2} \tag{3.16}$$

Similarly we get

$$g_{kk}(\psi_-) = g_{kk}(\psi_+) \tag{3.17}$$

We now wish to calculate the quantum metric w.r.t to the hamiltonian expanded around the dirac points i.e the quantity $g_{qq}(\rho\pm)$. We have the following hamiltonian:

$$H_{1q} = \begin{bmatrix} 0 & m_- + iqt' \\ m_- - iqt' & 0 \end{bmatrix} \tag{3.18}$$

Solving for the eigenvalues and eigenstates we get

$$\epsilon_{\pm}(q) = \pm\sqrt{m_-^2 + q^2t'^2} \tag{3.19}$$

$$\psi_{\pm}(q) = \begin{bmatrix} m - - + iqt' \\ \epsilon_{\pm}(q) \end{bmatrix} \tag{3.20}$$

Proceeding as before we get

$$g_{qq}(\rho_+) = g_{qq}(\rho_-) = g_{qq} = \frac{t'^2}{\epsilon(q)^2} - \frac{t'^4q^2}{\epsilon(q)^4} \tag{3.21}$$

Using (3.19), (3.21) becomes

$$g_{qq} = \frac{t'^2\Delta^2}{(\Delta^2 + t'^2q^2)^2} \tag{3.22}$$

Where $\Delta = m_-$ is a measure of the gap in the band structure. Let us define another variable η as

$$\eta = \frac{t'q}{\Delta} \tag{3.23}$$

Then we have the following forms of g_{qq} in the two limits:

$$g_{qq} = \frac{t'^2}{\Delta^2(1+\eta^2)} \sim \frac{t'^2}{\Delta^2}; \quad \text{when} \quad \eta << 1(q \to 0) \tag{3.24}$$

$$g_{qq} = \frac{\eta^2}{q^2(1+\eta^2)^2} \sim \frac{1}{q^2\eta^4}; \quad \text{when} \quad \eta >> 1(\Delta \to 0) \tag{3.25}$$

We see that g_{qq} dependence on q and Δ is inverse square in both the limits as listed in (3.24) and (3.25).

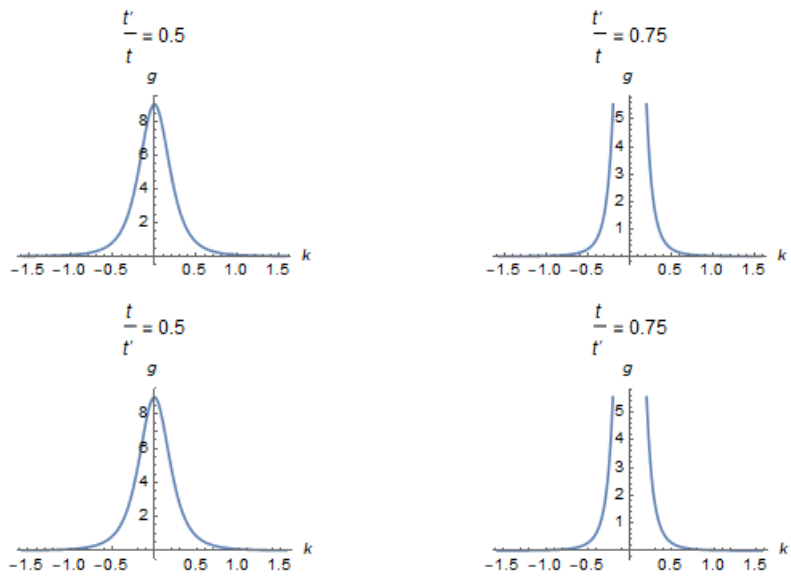

Figure 3.4: Variation of g as t'/t varies. Note that the metric diverges as it reaches near the critical point t'/t=1. This can also be seen from (3.11) when $\Delta \to 0$.

Chapter 4

Quantum metric under gauge transformation

In this chapter we will try to understand how the quantum metric transforms under gauge transformations. For this, we will work with a special class of systems in 2d called π flux systems.

4.1 Pi-flux systems

For any system with a certain vector potential A-distribution the flux through a placket is given by:

$$\phi = \oint A.dl \tag{4.1}$$

Any system that has $\phi = \pi$ will be called a pi-flux system.

4.2 Pi-flux system in two different gauges

We look at systems as shown in the figure (4.1). In the above diagrams the wavy lines have vector potential $A = \pi$ on moving along positive x and $A = -\pi$ on moving in the opposite direction and the straight lines have $A = 0$. We see that the distribution of A in the two systems is different but the flux through each square placket in both the cases is

$$\phi = \sum_{\square} A.dl = \pm\pi \tag{4.2}$$

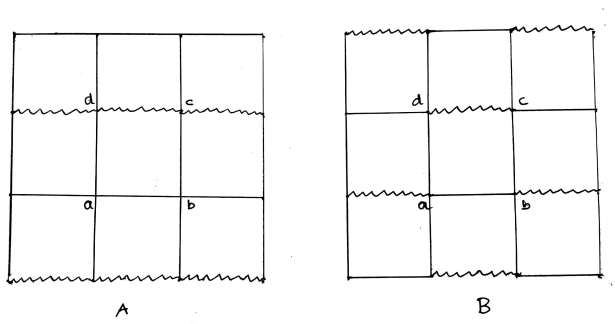

Figure 4.1: Two different gauges

These are thus two different gauges of the same system.
The Hamiltonian for both the gauges is given by

$$H = \sum_{<ij>} c_i^\dagger e^{iA_{ij}} c_j \tag{4.3}$$

We can see from (4.3) that the directionality of A does not matter as

$$e^{i\pi} = e^{-i\pi}$$

Statement: Given a system whose Hamiltonian is dependent on the set of parameters $\{k_\mu\}$ in two different gauges, call them A and B, then one can find a transformation between k_{μ_A} and k_{μ_B} such that for each k_{μ_A} in the first gauge there is a corresponding k_{μ_B} in the second gauge that gives the same eigenvalue as that given in the first gauge. We will find such a transformation between the above two gauges.

Let's first find the Hamiltonians for the two gauges.
Gauge A: We choose a four-sight unit cell with basis $\begin{bmatrix} a & b & c & d \end{bmatrix}$. Now, from (4.3) and using Fourier transform

$$a_j = \sum_k e^{ik.r_j} a_k \tag{4.4}$$

and similarly for b,c and d. We get

$$H_{k_A} = \begin{bmatrix} 0 & 2Cos(k_y) & 0 & -2Cos(k_x) \\ 2Cos(k_y) & 0 & 2Cos(k_x) & 0 \\ 0 & 2Cos(k_x) & 0 & 2Cos(k_y) \\ -2Cos(k_x) & 0 & 2Cos(k_y) & 0 \end{bmatrix} \tag{4.5}$$

Gauge B: Following the same procedure for the second gauge we get

$$H_{k_B} = \begin{bmatrix} 0 & 2Cos(k_y) & 0 & 2iSin(k_x) \\ 2Cos(k_y) & 0 & -2iSin(k_x) & 0 \\ 0 & 2iSin(k_x) & 0 & 2Cos(k_y) \\ -2iSin(k_x) & 0 & 2Cos(k_y) & 0 \end{bmatrix} \tag{4.6}$$

H_{k_A} has eigenvalues $\pm\sqrt{2}\sqrt{2 + Cos(2k_x) + Cos(2k_y)}$ each with a double degeneracy. H_{k_B} has eigenvalues $\pm\sqrt{2}\sqrt{2 - Cos(2k_x) + Cos(2k_y)}$ again with double degeneracy. And the transformation between k_A and k_B such that we get the same eigenvalues for both the Hamiltonians is

$$k_{x_B} = k_{x_A} - \frac{\pi}{2} \tag{4.7}$$

$$k_{y_B} = k_{y_A} \tag{4.8}$$

4.3 Quantum metric calculations

We will now look at how the quantum metric looks in the two gauges. Using (2.9) for the two gauges we get

$$g_{k_x k_{y_A}} = \frac{1}{(2 + \cos(2k_x) + \cos(2k_y))^2} \begin{bmatrix} 4\cos(k_y)^2 \sin(k_x)^2 & -\sin(2k_x)\sin(2k_y) \\ -\sin(2k_x)\sin(2k_y) & 4\cos(k_x)^2 \sin(k_y)^2 \end{bmatrix} \tag{4.9}$$

$$g_{k_x k_{y_B}} = \frac{1}{(2 - \cos(2k_x) + \cos(2k_y))^2} \begin{bmatrix} 4\cos(k_y)^2 \cos(k_x)^2 & \sin(2k_x)\sin(2k_y) \\ \sin(2k_x)\sin(2k_y) & 4\sin(k_y)^2 \sin(k_x)^2 \end{bmatrix} \tag{4.10}$$

Notice that the quantum metrics in (4.9) and (4.10) also follow the transformation law (4.7) and (4.8). i.e.

$$g_{k_x k_{y_B}} = g_{k_x - \frac{\pi}{2} k_{y_A}} \tag{4.11}$$

We can check the validity of (4.11) by comparing the values of components of g in the two gauges. For eg,

$$g_{k_x k_{x_A}}(0,0) = g_{k_x k_{x_B}}(\pi/2, 0) = 0 \tag{4.12}$$

$$g_{k_x k_{y_A}}(\pi,\pi) = g_{k_x k_{y_B}}(3\pi/2, \pi) = 0 \tag{4.13}$$

$$g_{k_y k_{y_A}}(0,\pi/2) = g_{k_y k_{y_B}}(\pi/2, \pi/2) = 1 \tag{4.14}$$

$$\tag{4.15}$$

The plots of different components of g along specific path are given in figure (4.2). We can note from the plots of g in the two gauges that they

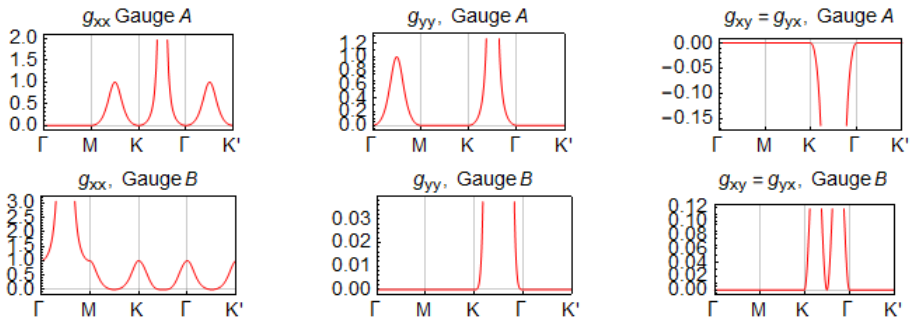

Figure 4.2: Quantum metric plots in two gauges

diverge near the critical points in both the gauges, a feature also noted in the case of polyacetylene. We have also established that the quantum metric transforms as the reciprocal lattice vectors under a gauge transformation.

Chapter 5

Quantum metric with different unit cells

In this chapter we will work with π flux systems with diagonal hopping, which, as we will see, opens up a gap in the spectrum. We will calculate the quantum metric with different unit cells and try to understand whether there is a rule by which the quantum metric in one unit cell can be converted into the quantum metric in another unit cell.

5.1 Gauge 1

Consider a π-flux system which has a potential distribution such that the hopping probabilities are given by (5.1)-(5.4).

$$t_{i,i+\hat{x}} = it_1 \tag{5.1}$$
$$t_{i,i+\hat{y}} = it_1(-1)^{ix} \tag{5.2}$$
$$t_{i,i+\hat{x}+\hat{y}} = it_2(-1)^{ix+1} \tag{5.3}$$
$$t_{i,i+\hat{x}-\hat{y}} = it_2(-1)^{ix} \tag{5.4}$$

Where i denotes the position $(i\hat{x} + i\hat{y})$. With this distribution the system looks like as shown in figure (5.1). Going along the arrows adds a flux of $\frac{\pi}{2}$ and going against the direction of the arrows adds a flux of $-\frac{\pi}{2}$.

5.1.1 Hamiltonian

We now calculate the Hamiltonian for this system. Let's choose a four-site unit-cell with basis $\begin{bmatrix} a & b & c & d \end{bmatrix}$. Take $t_1 = 1$ and $t_2 = t$. We will have terms like

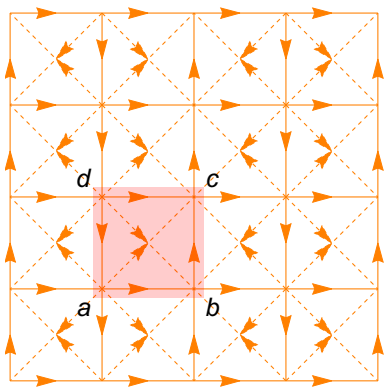

Figure 5.1: Pi-flux distribution

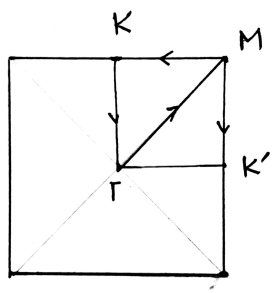

Figure 5.2: Brilluin zone for the system

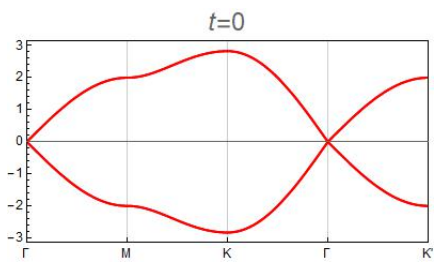

Figure 5.3: Dispersion along the path $\Gamma \to M \to K \to \Gamma \to M \to K'$ *when* $t = 0$

$$H_{ab} = i(1 - \exp(-ik_x)) \tag{5.5}$$
$$H_{ac} = it(1 + \exp(-ik_x) + \exp(-i(k_x + k_y)) + \exp(-ik_y)) \tag{5.6}$$
$$H_{ad} = i(-1 + \exp(-ik_y)) \tag{5.7}$$
$$H_{bc} = i(1 - exp(-ik_y)) \tag{5.8}$$
$$H_{bd} = it(-1 - \exp(-ik_y) - \exp(i(k_x - k_y)) - \exp(ik_x)) \tag{5.9}$$
$$H_{cd} = i(-1 + \exp(ik_x))m \tag{5.10}$$

Thus the Hamiltonian looks like

$$H = \sum_k \begin{bmatrix} a_k^\dagger & b_k^\dagger & c_k^\dagger & d_k^\dagger \end{bmatrix} \begin{bmatrix} 0 & H_{ab} & H_{ac} & H_{ad} \\ H_{ab}^\dagger & 0 & H_{bc} & H_{bd} \\ H_{ac}^\dagger & H_{bc}^\dagger & 0 & H_{cd} \\ H_{ad}^\dagger & H_{bd}^\dagger & H_{cd}^\dagger & 0 \end{bmatrix} \begin{bmatrix} a_k \\ b_k \\ c_k \\ d_k \end{bmatrix} \tag{5.11}$$

5.1.2 Dirac points and Dirac cones

The Brilluin zone for our system is a square as shown in figure (5.2). If we plot the dispersion along the path $\Gamma \to M \to K \to \Gamma \to M \to K'$, we get two Dirac points, both at Γ.

5.1.3 Quantum metric

Quantum metric with 4-site unit cell

Let's look at gauge 1, as described in fig (5.1) first. To calculate the quantum metric in gauge 1 with 4-site unit cell, we expand the Hamiltonian in (5.11) around the Dirac point (0,0). This gives (neglecting terms of the order $\mathcal{O}(tq), \mathcal{O}(q^2)$ and higher):

$$h_{ab} = -q_x \tag{5.12}$$
$$h_{ac} = 4it \tag{5.13}$$
$$h_{ad} = q_y \tag{5.14}$$
$$h_{bc} = -q_y \tag{5.15}$$
$$h_{bd} = -4it \tag{5.16}$$
$$h_{cd} = -q_x \tag{5.17}$$

Where (q_x, q_y) are momentum values near the Dirac point (0,0). Now the soft mode hamiltonian h is given by :

$$h = \sum_q \begin{bmatrix} \tilde{a}_q^\dagger & \tilde{b}_q^\dagger & \tilde{c}_q^\dagger & \tilde{d}_q^\dagger \end{bmatrix} \begin{bmatrix} 0 & -q_x & 4it & q_y \\ -q_x & 0 & -q_y & -4it \\ -4it & -q_y & 0 & -q_x \\ q_y & 4it & -q_x & 0 \end{bmatrix} \begin{bmatrix} \tilde{a}_q & \tilde{b}_q & \tilde{c}_q & \tilde{d}_q \end{bmatrix} \quad (5.18)$$

where $\tilde{a}_q, \tilde{b}_q$ etc are wavefunctions around the Dirac point (0,0). In this case we get two pairs of degenerate bands, out of which two are ground states. The quantum metric g in this case will be a tensor of rank (2,2) with components of the form $g^{ij}_{\mu\nu}$, where $\mu, \nu = q_x, q_y$ and $i, j = 1, 2$ (band index). On using (2.9) we get the following:

$$g^{(4)}_{q_x q_x} = \begin{bmatrix} \frac{16t^2+q_y^2}{(16t^2+q_x^2+q_y^2)^2} & \frac{(16t^2+q_y^2)^2}{(16t^2+q_x^2+q_y^2)^3} \\ \frac{(16t^2+q_y^2)^2}{(16t^2+q_x^2+q_y^2)^3} & \frac{16t^2+q_y^2}{(16t^2+q_x^2+q_y^2)^2} \end{bmatrix} \quad (5.19)$$

$$g^{(4)}_{q_x q_y} = \begin{bmatrix} \frac{-q_x q_y}{(16t^2+q_x^2+q_y^2)^2} & \frac{-q_x q_y (16t^2+q_y^2}{2(16t^2+q_x^2+q_y)^2)^3} \\ \frac{-q_x q_y (16t^2+q_y^2}{2(16t^2+q_x^2+q_y)^2)^3} & \frac{-q_x q_y}{(16t^2+q_x^2+q_y^2)^2} \end{bmatrix} \quad (5.20)$$

$$g^{(4)}_{q_y q_y} = \begin{bmatrix} \frac{16t^2+q_x^2}{(16t^2+q_x^2+q_y^2)^2} & \frac{-256t^4+q_x^2 q_y^2-16t^2(q_x^2+q_y^2)}{2(16t^2+q_x^2+q_y^2)^3} \\ \frac{-256t^4+q_x^2 q_y^2-16t^2(q_x^2+q_y^2)}{2(16t^2+q_x^2+q_y^2)^3} & \frac{16t^2+q_x^2}{(16t^2+q_x^2+q_y^2)^2} \end{bmatrix} \quad (5.21)$$

Quantum metric with 2-site unit cell

For the calculation with 2-site unit cell, we select the unit cell as shown in fig 7 with sublattice indices a and b. The Hamiltonian is given as follows:

$$\begin{aligned} H = i \sum_R [&(a^\dagger(R)b(R) + b^\dagger a(R+\hat{x} - h.c.) \\ &+ (a^\dagger(R+\hat{y})a(R) - h.c.) + (b^\dagger(R)b(R+\hat{y}) - h.c.) \\ &+ t((a^\dagger(R)b(R+\hat{y}) + a^\dagger(R)b(R-\hat{x}+\hat{y}) - h.c.) \\ &+ (a^\dagger(R+\hat{y})b(R) + a^\dagger(R+\hat{x}+\hat{y})b(R) - h.c.))] \end{aligned} \quad (5.22)$$

For the soft mode expansion of the Hamiltonian in eq (65) we expand $a(R)$ and $b(R)$ around the Dirac points $k_1 = (0, 0)$ and $k_2 = (0, \pi)$ in terms of wavefunctions a_{iq} b_{iq}, where i =1,2 is the valley index.

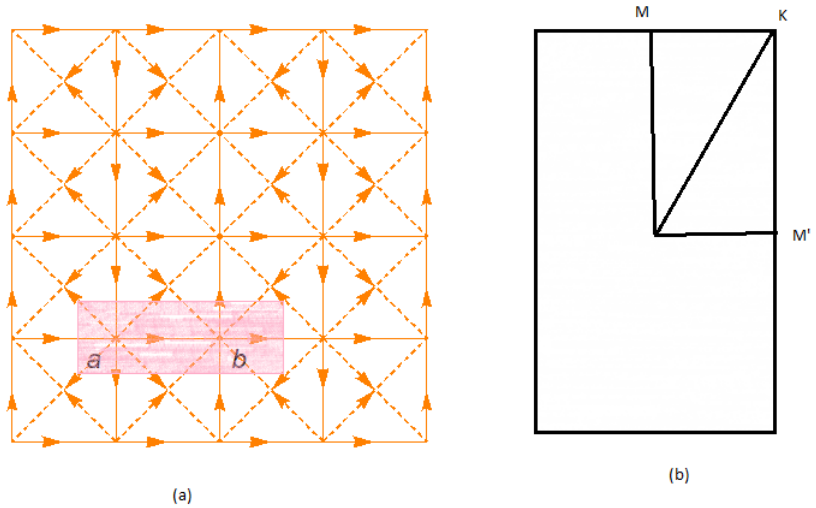

Figure 5.4: (a) The 2-site unit cell and (b) the Brillouin zone for the 2-site unit cell in gauge 1

$$a(R) = \exp(ik1.R)\sum_{q}\exp(iq.R)a_{1q} + \exp(ik_2.R)\sum_{q'}\exp(iq'.R)a_{2q'} \quad (5.23)$$

$$b(R) = \exp(ik1.R)\sum_{q}\exp(iq.R)b_{1q} + \exp(ik_2.R)\sum_{q'}\exp(iq'.R)b_{2q'} \quad (5.24)$$

Now the full soft-mode Hamiltonian is given as follows:

$$H_q = H_{1q} + H_{2q} \quad (5.25)$$

where,

$$H_{1q} = \begin{bmatrix} a_{1q}^{\dagger} & b_{1q}^{\dagger} \end{bmatrix} \begin{bmatrix} 2q_y & -q_x + 4it \\ -q_x - 4it & -2q_y \end{bmatrix} \begin{bmatrix} a_{1q} & b_{1q} \end{bmatrix} \quad (5.26)$$

$$H_{2q} = \begin{bmatrix} a_{2q}^{\dagger} & b_{2q}^{\dagger} \end{bmatrix} \begin{bmatrix} -2q_y & -q_x - 4it \\ -q_x + 4it & 2q_y \end{bmatrix} \begin{bmatrix} a_{2q} & b_{2q} \end{bmatrix} \quad (5.27)$$

From eq (69) and (70), H_q can be written as:

$$H = \tau_z(2q_y\sigma_z - 4t\sigma_y) - iq_x\sigma_x) \quad (5.28)$$

Here τ is the valley index. Now we will do the $g_{\mu\nu}$ calculations for the Hamitonian in eq (68) using (2.9)

$$g^{(2)}_{q_x q_x} = \frac{2(4t^2 + q_y^2}{(16t^2 + q_x^2 + 4q_y^2)^2} \quad (5.29)$$

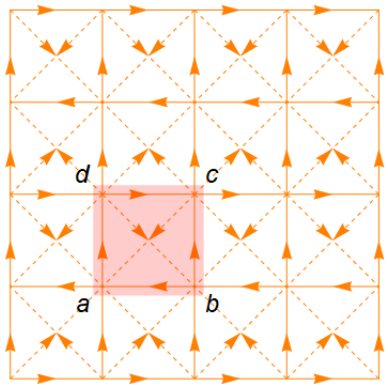

Figure 5.5: π flux distribution in second gauge

$$g^{(2)}_{q_x q_y} = \frac{-2q_x q_y}{(16t^2 + q_x^2 + 4q_y^2)^2} \tag{5.30}$$

$$g^{(2)}_{q_y q_y} = \frac{2(16t^2 + q_x^2)}{(16t^2 + q_x^2 + 4q_y^2)^2} \tag{5.31}$$

5.2 Gauge 2

We now work with a π flux system in a different gauge as shown in fig

5.2.1 Hamiltonian

Following the convention, that the flux added when traveling along the arrow is $\frac{\pi}{2}$ and when traveling opposite to the the direction of the arrow, is $-\frac{\pi}{2}$ we get the Hamiltonian with 4-site unit cell for the system.

$$H_{ab} = i(1 - \exp(-ik_x)) \tag{5.32}$$

$$H_{bc} = it(1 + \exp(-ik_x) + \exp(-i(k_x + k_y)) + \exp(-ik_y)) \tag{5.33}$$

$$H_{ad} = i(1 - \exp(-ik_y)) \tag{5.34}$$

$$H_{bc} = i(1 - \exp(-ik_y)) \tag{5.35}$$

$$H_{bd} = it(1 + \exp(ik_x) + \exp(-ik_y) + \exp(i(k_x - k_y)) \tag{5.36}$$

$$H_{cd} = i(1 - \exp(ik_x)) \tag{5.37}$$

With the basis $\begin{bmatrix} a & b & c & d \end{bmatrix}^T$ we get the following Hamiltonian for the system:

$$H = \sum_k \begin{bmatrix} a_k^\dagger & b_k^\dagger & c_k^\dagger & d_k^\dagger \end{bmatrix} \begin{bmatrix} 0 & H_{ab} & H_{ac} & H_{ad} \\ H_{ab}^\dagger & 0 & H_{bc} & H_{bd} \\ H_{ac}^\dagger & H_{bc}^\dagger & 0 & H_{cd} \\ H_{ad}^\dagger & H_{bd}^\dagger & H_{cd}^\dagger & 0 \end{bmatrix} \begin{bmatrix} a_k \\ b_k \\ c_k \\ d_k \end{bmatrix} \tag{5.38}$$

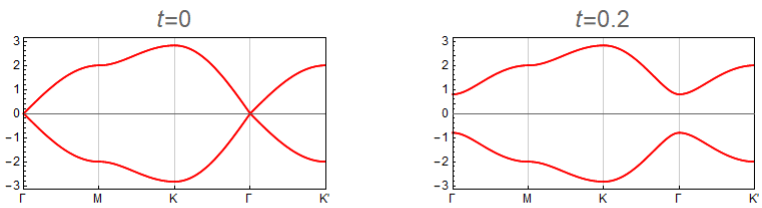

Figure 5.6: Band structure for the system without and with the diagonal hopping term

5.2.2 Dirac points

We plot the band structure for the system with $t = 0$ and nonzero t. We see that there are two Dirac points in the $t = 0$ case at Γ. The gap opens up at nonzero t.

5.2.3 Quantum metric

Quantum metric with 4-site unit cell

We calculate the quantum metric with the 4-site unit cell for Hamiltonian as defined by (5.32)-(5.37) and (5.38) by expanding the Hamiltonian around the Dirac point(Γ) (0,0) and get:

$$H_q = \sum_q \begin{bmatrix} a_q^\dagger & b_q^\dagger & c_q^\dagger & d_q^\dagger \end{bmatrix} \begin{bmatrix} 0 & -q_x & 4it & -q_y \\ -q_x & 0 & -q_y & 4it \\ -4it & -q_y & 0 & q_x \\ -q_y & -4it & q_x & 0 \end{bmatrix} \begin{bmatrix} a_q \\ b_q \\ c_q \\ d_q \end{bmatrix} \tag{5.39}$$

We calculate the quantum metric using (2.9) and get:

$$g^{(4)}_{q_x q_x} = \begin{bmatrix} \frac{16t^2+q_y^2}{(16t^2+q_x^2+q_y^2)^2} & \frac{(16t^2+q_y^2)^2}{(16t^2+q_x^2+q_y^2)^3} \\ \frac{(16t^2+q_y^2)^2}{(16t^2+q_x^2+q_y^2)^3} & \frac{16t^2+q_y^2}{(16t^2+q_x^2+q_y^2)^2} \end{bmatrix} \tag{5.40}$$

$$g^{(4)}_{q_x q_y} = \begin{bmatrix} \frac{-q_x q_y}{(16t^2+q_x^2+q_y^2)^2} & \frac{-q_x q_y (16t^2+q_y)^2}{2(16t^2+q_x^2+q_y^2)^3} \\ \frac{-q_x q_y (16t^2+q_y)^2}{2(16t^2+q_x^2+q_y^2)^3} & \frac{-q_x q_y}{(16t^2+q_x^2+q_y^2)^2} \end{bmatrix} \tag{5.41}$$

$$g^{(4)}_{q_y q_y} = \begin{bmatrix} \frac{16t^2+q_x^2}{(16t^2+q_x^2+q_y^2)^2} & \frac{-256t^4+q_x^2q_y^2-16t^2(q_x^2+q_y^2)}{2(16t^2+q_x^2+q_y^2)^3} \\ \frac{-256t^4+q_x^2q_y^2-16t^2(q_x^2+q_y^2)}{2(16t^2+q_x^2+q_y^2)^3} & \frac{16t^2+q_x^2}{(16t^2+q_x^2+q_y^2)^2} \end{bmatrix} \tag{5.42}$$

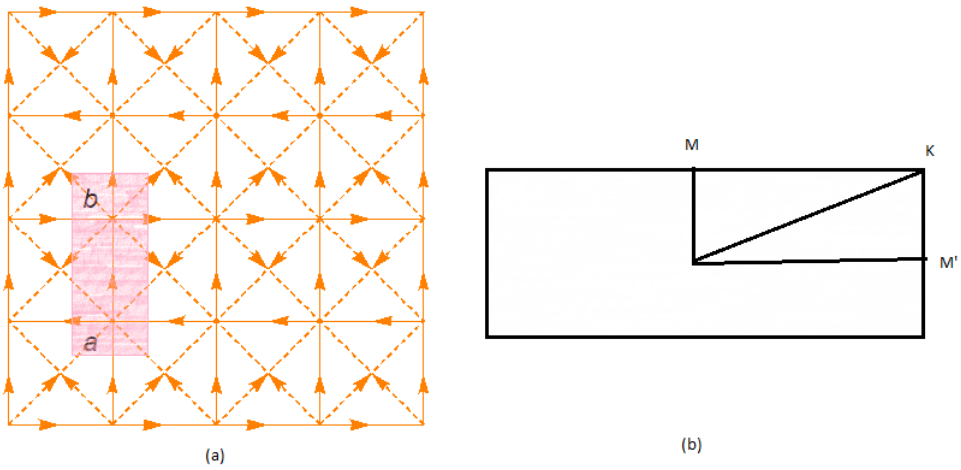

Figure 5.7: (a) The 2-site unit cell and (b) the Brillouin zone for the 2-site unit cell in gauge 2

Quantum metric with 2-site unit cell

To calculate the quantum metric with 2 site unit cell as shown in fig. we expand the 2-site Hamiltonian in (5.43) around the Dirac points (0,0) and $(\pi, 0)$ and get the soft mode Hamiltonian in (5.45)-(5.47).

$$\begin{aligned} H = i\sum_R [&(a^\dagger(R)b(R) - h.c) + (a^\dagger(R)a(R+\hat{x}) - h.c) \\ &+ t\{(a^\dagger(R)b(R+\hat{x}) - h.c) + (a^\dagger(R)b(R+\hat{x}-\hat{y}) - h.c)\} \\ &+ (b^\dagger(R)a(R+\hat{y}) - h.c) + (b^\dagger(R+\hat{x})b(R) - h.c) \\ &- t\{(b^\dagger(R)a(R+\hat{x}) - h.c) + (b^\dagger(R)a(R-\hat{x}+\hat{y}) - h.c)\}] \end{aligned} \tag{5.43}$$

Next we use the expansion of the wavefunction near the two Dirac points $(0,0)$ and $(\pi, 0)$ as follows:

$$a(R) = \sum_q e^{iq.R} a_{1q} + e^{i\pi R_x} \sum_{q'} e^{iq'.R} a_{2q'} \tag{5.44}$$

$$b(R) = \sum_q e^{iq.R} b_{1q} + e^{i\pi R_x} \sum_{q'} e^{iq'.R} b_{2q'} \tag{5.45}$$

and get

$$H_{1q} = \sum_q \begin{bmatrix} a_{1q}^\dagger & b_{1q}^\dagger \end{bmatrix} \begin{bmatrix} -2q_x & -q_y + 4it \\ -q_y - 4it & 2q_x \end{bmatrix} \begin{bmatrix} a_{1q} \\ b_{1q} \end{bmatrix} \tag{5.46}$$

$$H_{2q} = \sum_q \begin{bmatrix} a_{2q}^\dagger & b_{2q}^\dagger \end{bmatrix} \begin{bmatrix} 2q_x & -q_y - 4it \\ -q_y - 4it & -2q_x \end{bmatrix} \begin{bmatrix} a_{2q} \\ b_{2q} \end{bmatrix} \tag{5.47}$$

Here H_{1q} and H_{2q} are the soft mode expansions of the Hamiltonian around the Dirac points $(0,0)$ and $(\pi,0)$ respectively. (5.46) and (5.47) can be combined as follows:

$$H = \tau^z(-2q_x\sigma^z - 4t\sigma_y) - q_y\sigma^x \tag{5.48}$$

where τ is the valley index. The quantum metric in the 2-site unit cell case will be a scalar since there is only one occupied band. We use (2.9) to get the following:

$$g^{(2)}_{q_xq_x} = \frac{2(16t^2 + q_y^2}{(16t^2 + 4q_x^2 + q_y^2)^2} \tag{5.49}$$

$$g^{(2)}_{q_xq_y} = \frac{-2q_xq_y}{(16t^2 + 4q_x^2 + q_y^2)^2} \tag{5.50}$$

$$g^{(2)}_{q_yq_y} = \frac{2(4t^2 + q_x^2)}{(16t^2 + 4q_x^2 + q_y^2)^2} \tag{5.51}$$

5.3 Analysis

In this section we will see how the metric changes in different unit cells and reestablish the relation we obtained for quantum metric under gauge transformation.

5.3.1 Comparison of quantum metric with 4-site and 2-site unit cell

In Gauge 1

If we compare the Quantum metric with 4-site unit cell and 2-site unit cell in gauge 1 as in (5.19)-(5.21) and (5.29)-(5.31), we get the following relations:

$$g^{(2)}_{q_xq_x}(q_y \to \frac{q_y}{2}) = \frac{1}{4}Tr[g^{(4)}_{q_xq_x}] \tag{5.52}$$

$$g^{(2)}_{q_xq_y}(q_y \to \frac{q_y}{2}) = \frac{1}{2}Tr[g^{(4)}_{q_xq_y}] \tag{5.53}$$

$$g^{(2)}_{q_yq_y}(q_y \to \frac{q_y}{2}) = Tr[g^{(4)}_{q_xq_y}] \tag{5.54}$$

From (5.52) (5.54) we see that the metric in 2-site unit cell which is a scalar is the trace of the metric obtained by using the 4-site unit cell times a prefactor, i.e.

$$g^{(2)}_{q_\mu q_\nu} = f(\mu\nu) Tr[g^{(4)}_{q_\mu q_\nu}] \tag{5.55}$$

where the prefactor $f(\mu\nu)$ is given as follows.

$$f(\mu\nu) = \frac{1}{4}\left(\frac{1}{\lambda_\mu \lambda_\nu}\right) \tag{5.56}$$

where $\mu, \nu = x, y$ and λ_μ is the scaling factor for the μ component between the two unit cells. In this case $\lambda_x = 1$ and $\lambda_y = \frac{1}{2}$.

In Gauge 2

We do similar comparisons for metric in gauge 2 and find:

$$g^{(2)}_{q_x q_x}(q_x \to \frac{q_x}{2}) = Tr[g^{(4)}_{q_x q_x}] \tag{5.57}$$

$$g^{(2)}_{q_x q_y}(q_x \to \frac{q_x}{2}) = \frac{1}{2} Tr[g^{(4)}_{q_x q_y}] \tag{5.58}$$

$$g^{(2)}_{q_y q_y}(q_x \to \frac{q_x}{2}) = \frac{1}{4} Tr[g^{(4)}_{q_x q_y}] \tag{5.59}$$

We can see that (5.57)-(5.59) satisfy (5.56) with $\lambda_x = \frac{1}{2}$ and $\lambda_y = 1$.

5.3.2 Check for metric under gauge transformation rule

Now to check the validity of our metric under the gauge transformation rule we compare the metric with 2-site unit cell in both the gauges. We know that the gauge transformation here is:

$$q_x \to q_y \tag{5.60}$$

$$q_y \to q_x \tag{5.61}$$

Now due to the above gauge transformation we need to compare the $g^{(2)}_{q_x q_x}$ in one gauge with $g^{(2)}_{q_y q_y}$ in the other. On doing so we find that $g^{(2)}_{q_x q_x}(q_x, q_y)$ in gauge is equal to $g^{(2)}_{q_y q_y}(q_y, q_x)$ in gauge 2. This holds for other components of the quantum metric as well. Same analysis can be done with the metric for 4-site unit cell also. It turns out that the rule is valid in that case also. Thus, we see that our rule for the metric under gauge transformation holds well in all the cases we have considered. Also, we have found out a rule for the transformation of metric with different sizes of the unit cell.

Chapter 6

Quantum Metric in Honeycomb Lattice

In this chapter we calculate the quantum metric for the honeycomb lattice. We first calculate it for a Hamiltonian that has the usual nearest neighbor hopping and next nearest neighbor spin dependent hopping terms. We then calculate the metric for a Hamiltonian with a third term, that is the Rashba spin-orbit coupling term. The Rashba term breaks the spin s_z inversion symmetry. Our aim in this chapter is to understand how the violation of the spin inversion symmetry shows up in the quantum metric.

6.1 The Honeycomb lattice

The honeycomb lattice looks as shown in figure, with a two sublattice (a and b) unit cell. The nearest neighbor distances are:

$$\hat{r}_1 = -\hat{y} \tag{6.1}$$

$$\hat{r}_2 = \frac{\sqrt{3}}{2}\hat{x} + \frac{\hat{y}}{2} \tag{6.2}$$

$$\hat{r}_3 = -\frac{\sqrt{3}}{2}\hat{x} + \frac{\hat{y}}{2} \tag{6.3}$$

6.2 Hamiltonian without the Rashba term

The Hamiltonian without the Rashba term is given as follows:

$$H = \sum_{<ij>\alpha} t c^\dagger_{i\alpha} c_{j\alpha} + \sum_{<<ij>>\alpha\beta} i t_2 v_{ij} s^z_{\alpha\beta} c^\dagger_{i\alpha} c_{j\beta} \tag{6.4}$$

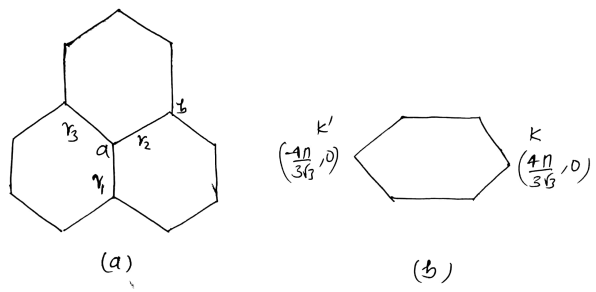

Figure 6.1: (a) The honeycomb lattice(b) The two Dirac points K and K'

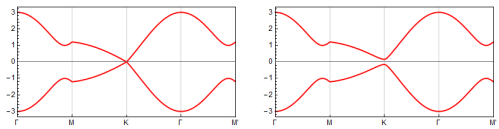

Figure 6.2: The spectrum for the Hamiltonian with two terms. The next nearest neighbor term opens up the gap in the spectrum as seen in the second picture

The first term in the Hamiltonian is the nearest neighbor hopping. Let's call it H_1. The second term is the spin dependent next nearest neighbor hopping term. α, β are the spin indices. The spin dependent amplitude $v_{ij} = (2/\sqrt{3})(\hat{d}_1 X \hat{d}_2)_z = \pm 1$. Here $\hat{d}_1$ and $\hat{d}_2$ are unit vectors along the two bonds joining site i and j.

To diagonalize the Hamiltonian we take the Fourier transform. We do it term y term as follows:

$$H_1(k) = t \sum_k [a_k^\dagger b_k (e^{i(\frac{\sqrt{3}}{2}k_x + \frac{k_y}{2})} + e^{-ik_y} + e^{i(-\frac{\sqrt{3}}{2}k_x + \frac{k_y}{2})}) + h.c] \tag{6.5}$$

We have suppressed the spin indices in the above equation as H_1 is the same for both the spin components.
Next we calculate the second term in the Hamiltonian.

$$\begin{aligned} H_2(k) = 2t_2 \sum_k \sum_{\alpha\beta} s^z_{\alpha\beta} [a^\dagger_{k\alpha} a_{k\beta} (\sin(\sqrt{3}k_x) - 2(\sin(\frac{\sqrt{3}}{2}k_x)\cos(\frac{3}{2}k_y)) \\ - b^\dagger_{k\alpha} b_{k\beta} (\sin(\sqrt{3}k_x) - 2(\sin(\frac{\sqrt{3}}{2}k_x)\cos(\frac{3}{2}k_y))] \end{aligned} \tag{6.6}$$

We plot the spectrum for this Hamiltonian and see that there are two Dirac points in the spectrum at $K = (4\pi/3\sqrt{3}, 0)$ and $K' = (-4\pi/3\sqrt{3}, 0)$. The next nearest neighbor term results in the gap opening, as we can see from the plots.

6.2.1 Quantum metric calculations

We now calculate the quantum metric for the Hamiltonian with the two terms H_1 and H_2. To do so we first calculate the soft mode Hamiltonian around the two Dirac points using:

$$a(R) = e^{iK.R} \sum_q e^{iq.R} a_{1q} + e^{ik'.R} \sum_{q'} e^{-iq'.R} a_{2q} \tag{6.7}$$

$$b(R) = e^{iK.R} \sum_q e^{iq.R} b_{1q} + e^{ik'.R} \sum_{q'} e^{-iq'.R} b_{2q} \tag{6.8}$$

This gives us the soft mode Hamiltonian that looks like:

$$H(q) = \tau^z(-3\sqrt{3}s^z t_2 \sigma^z + \frac{3}{2} t q_y \sigma^y) - \frac{3}{2} q_x \sigma^x \tag{6.9}$$

Here τ represents the valley index (K,K'), s represents the spin index and σ represents the subllatice freedom (a or b). The soft mode Hamiltonian near the two Dirac points thus looks like:

$$H(q) = \sum_q \begin{bmatrix} a_{1\uparrow}^\dagger & b_{1\uparrow}^\dagger & a_{1\downarrow}\dagger & b_{1\downarrow}\dagger \end{bmatrix} \begin{bmatrix} -3\sqrt{3}t_2 & -\frac{3}{2}(q_x + iq_y) & 0 & 0 \\ -\frac{3}{2}(q_x - iq_y) & 3\sqrt{3}t_2 & 0 & 0 \\ 0 & 0 & 3\sqrt{3}t_2 & -\frac{3}{2}(q_x + iq_y) \\ 0 & 0 & -\frac{3}{2}(q_x - iq_y) & -3\sqrt{3}t_2 \end{bmatrix} \begin{bmatrix} a_{1\uparrow} \\ b_{1\uparrow} \\ a_{1\downarrow} \\ b_{1\downarrow} \end{bmatrix} \tag{6.10}$$

near K and

$$H(q) = \sum_q \begin{bmatrix} a_{2\uparrow}^\dagger & b_{2\uparrow}^\dagger & a_{2\downarrow}\dagger & b_{2\downarrow}\dagger \end{bmatrix} \begin{bmatrix} 3\sqrt{3}t_2 & -\frac{3}{2}(q_x - iq_y) & 0 & 0 \\ -\frac{3}{2}(q_x + iq_y) & -3\sqrt{3}t_2 & 0 & 0 \\ 0 & 0 & -3\sqrt{3}t_2 & -\frac{3}{2}(q_x - iq_y) \\ 0 & 0 & -\frac{3}{2}(q_x + iq_y) & 3\sqrt{3}t_2 \end{bmatrix} \begin{bmatrix} a_{2\uparrow} \\ b_{2\uparrow} \\ a_{2\downarrow} \\ b_{2\downarrow} \end{bmatrix} \tag{6.11}$$

near K'. Using these soft mode Hamiltonians we calculate the quantum metric for the system and get:

$$g_{q_x q_x} = \begin{bmatrix} \frac{12m^2+q_y^2}{2(12m^2+q_x^2+q_y^2)^2} & 0 \\ 0 & \frac{12m^2+q_y^2}{2(12m^2+q_x^2+q_y^2)^2} \end{bmatrix} \tag{6.12}$$

$$g_{q_xq_y} = \begin{bmatrix} \frac{-q_xq_y}{2(12m^2+q_x^2+q_y^2)^2} & 0 \\ 0 & \frac{-q_xq_y}{2(12m^2+q_x^2+q_y^2)^2} \end{bmatrix} \tag{6.13}$$

$$g_{q_yq_y} = \begin{bmatrix} \frac{12m^2+q_x^2}{2(12m^2+q_x^2+q_y^2)^2} & 0 \\ 0 & \frac{12m^2+q_x^2}{2(12m^2+q_x^2+q_y^2)^2} \end{bmatrix} \tag{6.14}$$

Near both the Dirac points.

6.3 Calculations with Rashba term

The Rashba term is given by:

$$H_R = it_3\hat{z}.(s_{\alpha\beta} \times d)c_{i\alpha}^{\dagger}c_{j\beta} \tag{6.15}$$

On addin the Rashba term (6.15) to the Hamiltonian (6.4) we get the soft mode Hamiltonian near the two Dirac points K and K', respectively:

$$H_{1q} = \sum_q \psi_{1q}^{\dagger} \begin{bmatrix} -3\sqrt{3}t_2 & -\frac{3}{2}t(q_x+iq_y) & 0 & -3it_3 \\ -\frac{3}{2}t(q_x-iq_y) & 3\sqrt{3}t_2 & 0 & 0 \\ 0 & 0 & 3\sqrt{3}t_2 & -\frac{3}{2}t(q_x+iq_y) \\ 3it_3 & 0 & -\frac{3}{2}t(q_x-iq_y) & -3\sqrt{3}t_2 \end{bmatrix} \psi_{1q} \tag{6.16}$$

$$H_{2q} = \sum_q \psi_{2q}^{\dagger} \begin{bmatrix} 3\sqrt{3}t_2 & -\frac{3}{2}t(q_x-iq_y) & 0 & 0 \\ -\frac{3}{2}t(q_x+iq_y) & -3\sqrt{3}t_2 & 3it_3 & 0 \\ 0 & -3it_3 & -3\sqrt{3}t_2 & -\frac{3}{2}t(q_x-iq_y) \\ 0 & 0 & -\frac{3}{2}t(q_x+iq_y) & 3\sqrt{3}t_2 \end{bmatrix} \psi_{2q} \tag{6.17}$$

Where $\psi_{iq} = \begin{bmatrix} a_{iq\uparrow} & b_{iq\uparrow} & a_{iq\downarrow} & b_{iq\downarrow} \end{bmatrix}$, i=1,2.

6.3.1 Quantum metric calculations

Next, we do the calculation for the quantum metric using the soft-mode Hamiltonians in (6.16) and (6.17). Now since there are two occupied bands the quantum metric is a (2,2) tensor. It can be written in terms of the 2×2 Identity matrix and the Pauli matrices as follows:

$$g_{\mu\nu} = \frac{g_{\mu\nu}^{11} + g_{\mu\nu}^{22}}{2} I_2 + \frac{g_{\mu\nu}^{11} - g_{\mu\nu}^{22}}{2}\sigma_z + \frac{g_{\mu\nu}^{12} + g_{\mu\nu}^{21}}{2}\sigma_x + i\frac{g_{\mu\nu}^{12} + g_{\mu\nu}^{21}}{2}\sigma_y \tag{6.18}$$

Let's call

$$\frac{g^{11}_{\mu\nu} + g^{22}_{\mu\nu}}{2} = A \tag{6.19}$$

$$\frac{g^{12}_{\mu\nu} + g^{21}_{\mu\nu}}{2} = B \tag{6.20}$$

$$i\frac{g^{12}_{\mu\nu} + g^{21}_{\mu\nu}}{2} = C \tag{6.21}$$

$$\frac{g^{11}_{\mu\nu} - g^{22}_{\mu\nu}}{2} = D \tag{6.22}$$

It turns out that when we write the metric in the form (6.18), we get the coefficients A, B, C, D to be the same for the metric near both the Dirac points.

The spin-orbit coupling terms in the Hamiltonian for the honeycomb lattice make it a Symmetry Protected Topological phase which shows Spin Quantum Hall Effect. And as we can see from the metric equations without the Rashba term, the metric diverges near the transition as $1/q^2$. Similar behavior occurs with the Rashba term also.

6.4 Summary and Conclusions

From the calculations of the quantum metric that we have studied in this project, we see that the metric diverges near a topological phase transition. We see this from the plots for the metric in the 1d Polyacetylene case and in the 2d π flux systems. We have also found the analytical forms of the metric in different systems. From our studies we conclude that the quantum metric diversges, near a transition, wherein a mass-less Dirac fermion becomes massive.

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Appendix A

Calculation of quantum metric

We have from (2.6)

$$d(\psi_1, \psi_2) = \sqrt{1 - B^2(\psi_1, \psi_2)^{\lambda/2}}$$

Now if we consider the distance between two neighboring points η and $\eta + d\eta$ we have the square of the distance between these points using (5) and the definition of the Bargmann invariants:

$$d^2(\eta, \eta + d\eta) = 1 - tr((\rho(\eta)\rho(\eta + d\eta)))^{\frac{\lambda}{2}} \tag{A.1}$$

We next use the properties of the projector $\rho^2 = \rho$ and thus $tr(\rho^2) = tr(\rho) = 1$. On differenciating this we get

$$tr(\rho\partial_a\rho) = 0 \rightarrow tr(\partial_a\rho\partial_b\rho) = -tr(\rho\partial_a\partial_b\rho) \tag{A.2}$$

Now on doing Taylor expansion for $\rho(\eta + d\eta)$ in RHS of (51) we get

$$d^2(\eta, \eta + d\eta) = 1 - (tr(\rho(\eta) + \partial_a\rho d\eta^a + \frac{1}{2}\partial_a\partial_b\rho d\eta^a d\eta^b)\rho(\eta))^{\frac{\lambda}{2}} \tag{A.3}$$

Using (52) we will have no contribution from terms with linear differentials and $tr(\rho^2) = 1$ will cancel the 1 in RHS and we are left with $\frac{\lambda}{4}tr(\partial_a\rho\partial_b\rho)d\eta^a d\eta^b$. This gives

$$d^2(\eta, \eta + d\eta) = \frac{\lambda}{4}tr(\partial_a\rho\partial_b\rho)d\eta^a d\eta^b \tag{A.4}$$