CUSRA Report: Curvature in SOC Graphene

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1 Preliminaries

1.1 The Derivation of the Berry Phase

Suppose there is a quantum mechanical system with a Hamiltonian H in which the Hamiltonian has a parametric dependence on time t so that we have $H(t)$[1]. We may solve the eigen-pairs of the Hamiltonian: $\psi_n(t), E_n(t)$, such that:

$$H(t)\psi_n(t) = E_n(t)\psi_n(t) \tag{1}$$

Now lets suppose that we have a general solution to the Schrödinger equation $\alpha(t)$ then it follows that:

$$\alpha(t) = \sum_n a_n(t)\psi_n(t) \tag{2}$$

Where $\sum_n |a_n(t)|^2 = 1$. For convenience we will express $a_n(t) = c_n(t)e^{i\theta_n(t)}$, with $\theta_n(t) = -\frac{1}{\hbar}\int_0^t E(t')dt'$. So we have that:

$$\alpha(t) = \sum_n c_n(t)e^{i\theta_n(t)}\psi_n(t) \tag{3}$$

Since α solves the Schrödinger equation we get that

$$\begin{aligned}
\left(i\hbar\frac{\partial}{\partial t} - H\right)\alpha &= 0 \\
\sum_n \left(i\hbar\frac{\partial}{\partial t} - H\right) c_n e^{i\theta_n}\psi_n &= 0 \\
\sum_n i\hbar\frac{\partial}{\partial t} c_n e^{i\theta_n}\psi_n - c_n e^{i\theta_n} H\psi_n &= 0 \\
\sum_n i\hbar\frac{\partial}{\partial t} c_n e^{i\theta_n}\psi_n - c_n e^{i\theta_n} E_n\psi_n &= 0
\end{aligned}$$

If we focus in on the first term

[1] This whole argument is made along the lines of Sakurai &, Napolitano

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}c_n e^{i\theta_n}\psi_n &= i\hbar\left[c_n\psi_n\frac{\partial}{\partial t}e^{i\theta_n} + e^{i\theta_n}\frac{\partial}{\partial t}c_n\psi_n\right] \\
&= i\hbar e^{i\theta_n}\left[ic_n\psi_n\frac{\partial\theta_n}{\partial t} + \frac{\partial c_n}{\partial t}\psi_n + c_n\frac{\partial\psi_n}{\partial t}\right] \\
&= i\hbar e^{i\theta_n}\left[-\frac{i}{\hbar}c_n E_n\psi_n + \frac{\partial c_n}{\partial t}\psi_n + c_n\frac{\partial\psi_n}{\partial t}\right] \\
&= c_n e^{i\theta_n}E_n\psi_n + i\hbar e^{i\theta_n}\left[\frac{\partial c_n}{\partial t}\psi_n + c_n\frac{\partial\psi_n}{\partial t}\right]
\end{aligned}
$$

Notice that the leading term here $c_n e^{i\theta_n}E_n\psi_n$ cancels with the final term in the original sum. Hence we get the equation (by canceling the $i\hbar$ on both sides.

$$
\sum_n e^{i\theta_n}\left[\frac{\partial c_n}{\partial t}\psi_n + c_n\frac{\partial\psi_n}{\partial t}\right] = 0
$$

Using an inner product with ψ_m on both sides we reduct his to

$$
\begin{aligned}
\left\langle\psi_m\middle|\sum_n e^{i\theta_n}\left[\frac{\partial c_n}{\partial t}\psi_n + c_n\frac{\partial\psi_n}{\partial t}\right]\right\rangle &= 0 \\
\sum_n e^{i\theta_n}\frac{\partial c_n}{\partial t}\langle\psi_m|\psi_n\rangle + c_n e^{i\theta_n}\left\langle\psi_m\middle|\frac{\partial\psi_n}{\partial t}\right\rangle &= 0 \\
\sum_n e^{i\theta_n}\frac{\partial c_n}{\partial t}\delta_{mn} + c_n e^{i\theta_n}\left\langle\psi_m\middle|\frac{\partial\psi_n}{\partial t}\right\rangle &= 0 \\
e^{i\theta_m}\frac{\partial c_m}{\partial t} + \sum_n c_n e^{i\theta_n}\left\langle\psi_m\middle|\frac{\partial\psi_n}{\partial t}\right\rangle &= 0 \\
\frac{\partial c_m}{\partial t} &= -\sum_n c_n e^{i(\theta_n-\theta_m)}\left\langle\psi_m\middle|\frac{\partial\psi_n}{\partial t}\right\rangle \\
\frac{\partial c_m}{\partial t} = -c_m\left\langle\psi_m\middle|\frac{\partial\psi_m}{\partial t}\right\rangle &- \sum_{n\neq m} c_n e^{i(\theta_n-\theta_m)}\left\langle\psi_m\middle|\frac{\partial\psi_n}{\partial t}\right\rangle
\end{aligned}
$$

At this point we invoke the adiabatic approximation in which the term $\left\langle\psi_m\middle|\frac{\partial\psi_n}{\partial t}\right\rangle \approx 0$. It can be shown that roughly this translates to a slowly varying Hamiltonian. From this then we get a first order separable ODE for c_m:

$$
\frac{\partial c_m}{\partial t} = -\left\langle\psi_m\middle|\frac{\partial\psi_m}{\partial t}\right\rangle c_m
$$

Which if we define the function $\gamma_n(t) = \int_0^t i\left\langle\psi_m\middle|\frac{\partial\psi_m}{\partial t}\right\rangle|_{t=t'}dt'$ then it follows that the solution to the ODE is $c_n(t) = c_n(0)e^{i\gamma_n(t)}$. And so under this adiabatic approximation the general solution is given by

$$
\alpha(t) = \sum_n k_n e^{i[\gamma_n(t)-\theta_n(t)]}\psi_n(t) \tag{4}
$$

1.2 A Digression into Gauge Theory

The function γ_m is called the Berry phase. It has the form

$$\gamma_m(t) = \int_0^t i \left\langle \psi_m \middle| \frac{\partial \psi_m}{\partial t} \right\rangle |_{t=t'} dt' \tag{5}$$

We may assume the the Hamiltonian does not explicitly depend on time but instead depends on a (vector valued) parameter $\vec{r}$ which is itself time dependent. In that context we have that

$$\frac{\partial}{\partial t} = \frac{\partial r^\mu}{\partial t} \frac{\partial}{\partial r^\mu}$$

And so it follows by changing the integration variable we get that another form of γ_m is

$$\begin{gathered} \int_0^t i \left\langle \psi_m \middle| \frac{\partial \psi_m}{\partial t} \right\rangle |_{t=t'} dt' \\ \int_0^t i \left\langle \psi_m \middle| \frac{\partial \psi_m}{\partial r^\mu} \right\rangle |_{\vec{r}(t')} \frac{\partial r^\mu}{\partial t} dt' \\ \int_{\vec{r}(0)}^{\vec{r}(t)} i \left\langle \psi_m \middle| \frac{\partial \psi_m}{\partial r^\mu} \right\rangle dr^\mu \end{gathered}$$

We define the Berry connection one-form A_m as follows:

$$A_m = i \left\langle \psi_m \middle| \frac{\partial \psi_m}{\partial r^\mu} \right\rangle dr^\mu \tag{6}$$

Hence the equation for the Berry phase over a curve $\mathcal{C}$ traced out by $\vec{r}(t)$:

$$\gamma_m(\mathcal{C}) = \int_{\mathcal{C}} A_m \tag{7}$$

In the case where $\vec{r}(0) = \vec{r}(t)$, that is any case where $H(t) = H(0)$ we get that $\mathcal{C}$ is a closed path and so encloses an interior $\mathcal{A}$ (that is $\mathcal{C} = \partial\mathcal{A}$), we can use the generalized Stoke's theorem to write down the following:

$$\gamma_m(\mathcal{C}) = \oint_{\partial\mathcal{A}} A_m = \int_{\mathcal{A}} dA_m = \int_{\mathcal{A}} F_m$$

We call $F_m = dA_m$ the Berry Curvature two-form. These functions A_m and F_m are fields over the parameter space in which the parameter $\vec{r}$ lives, call it $\mathcal{R}$. If we take the name literally then $\mathcal{R}$ is a manifold combined with some Lie group of local transformations G. Moreover, the components of A_m should live in the Lie algebra of this 'gauge' group $\mathfrak{g}$. That being said we don't normally think in this way since given that the components of A_m are real (up to a multiplication of i) it follows that the actual group in question is $\mathrm{U}(1)$ and the mathematics of gauge transformations is therefore not more interesting then in

classical electrodynamics. However, it is still worth thinking in this way as it allows us to understand topological properties of $\mathcal{R}$ formally through the use of the connection A_m.

There is another digression worth noting. There are forms in Chern-Weil theory called Chern classes c_k related to the curvature form F in the following way.

$$\sum_k c_k t^k = \det\left(\frac{F}{2\pi}t + I\right) \tag{8}$$

As such the first Chern class $c_1 = \frac{1}{2\pi}\operatorname{Tr} F^2$. The Chern numbers (of type k) Chern $= \int_{\mathcal{R}} c_k$ are topological invariants of the parameter space $\mathcal{R}$ and say something about the cohomology of the space. I intend in my second report to give a full explanation of this aspect of the research, but as I don't yet understand it I will leave it at this: we will summarize the results in terms of an easily readable Chern number which for us is

$$\text{Chern} = \int_{\mathcal{R}} c_k = \frac{1}{2\pi}\int_{\mathcal{R}} F \tag{9}$$

It is a result in Chern-Weil theory that this number must be an integer. We shall find then that our Chern numbers will be half integral (coming in pairs from K and K' points to cancel each other out) so **technically** the actual Chern number is the sum across both Dirac Points.[3]

1.3 Application of the Previous Section to Our Case (2D Parameter Space)

Now that we have introduced this obscure mathematical objects the A_m one-form and F_m to form, we ought to tie it down to something practicaly. It turns out that in any dimension, a one form can be made into[4] a vector field by simply taking the vector field of its components in the obvious way. Hence we define the Berry connection vector field $\vec{A}_m$ as

$$\vec{A}_m = i\left\langle \psi_m \middle| \vec{\nabla}_{\vec{r}} \psi_m \right\rangle \tag{10}$$

In which case we get that $A_m = \vec{A}_m \circ d\vec{r}$ and we understand γ_m as a lign integral of a vector field on a curve in the parameter space. What is more complicated is the understanding of the curvature. In a 2D parametric space the d operator causes the set of all two forms $\Omega^2(\mathcal{R})$ to be 1 dimensional in the

[2] We drop the trace as the group is U(1) so the trace is simply the identity

[3] It must be reiterated that I do not yet understand Chern-Weil theory so this explanation is pieced together from conversations with my Dr. Maiti and my thesis supervisor

[4] by way of isomorphism

following way:

$$F_m = dA_m$$
$$F_m = \frac{\partial \vec{A}_{m,\mu}}{\partial r^\nu} dr^\nu \wedge dr^\mu$$
$$F_m = \frac{\partial \vec{A}_{m,2}}{\partial r^1} dr^1 \wedge dr^2 + \frac{\partial \vec{A}_{m,1}}{\partial r^2} dr^2 \wedge dr^1$$
$$\text{but since} \quad dr^2 \wedge dr^1 = -dr^1 \wedge dr^2$$
$$F_m = \left(\frac{\partial \vec{A}_{m,2}}{\partial r^1} - \frac{\partial \vec{A}_{m,1}}{\partial r^2} \right) dr^1 \wedge dr^2$$
$$F_m = \Omega_m dr^1 \wedge dr^2$$

Hence F_m is a pseudo-scalar because it is like a scalar in that it is one dimensional. Importantly the value Ω_m is called the Berry curvature scalar field (which again only exists in 2D) and has the form.

$$\Omega_m = \frac{\partial \vec{A}_{m,2}}{\partial r^1} - \frac{\partial \vec{A}_{m,1}}{\partial r^2} \tag{11}$$

That said there is a similar line of argumentation in 3D where F_m is a pseudo-vector and we may construct a vector field $\vec{\Omega}_m = \vec{\nabla} \times \vec{A}_m$ sharing the same components. In higher dimensions this analogy fails and we are left thinking of F_m as a 2-form (a rank (0,2) anti-symmetric tensor field) without much recourse for intuition.

1.4 An Example: Spin 1/2 Particles in a Magnetic Field

If we have a spin 1/2 particle in a magnetic field $\vec{B}$ with variable direction then the Hamiltonian of the system is H given by

$$H = \epsilon[\cos\theta \sin\phi \ \sigma_1 + \sin\theta \sin\phi \ \sigma_2 + \cos\phi \ \sigma_3] \tag{12}$$

Where $\vec{B} = B_0 \cos\theta \sin\phi \ \hat{x}_1 + \sin\theta \sin\phi \ \hat{x}_2 + \cos\phi \ \hat{x}_3$ and $\epsilon = CB_0$ and C is a constant allowing for ϵ to have units of energy. By the definition of the Pauli matrices the term M (the inside of the square brackets) takes the form of

$$M = \cos\theta \sin\phi \ \sigma_1 + \sin\theta \sin\phi \ \sigma_2 + \cos\phi \ \sigma_3$$
$$\cos\theta \sin\phi \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + \sin\theta \sin\phi \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} + \cos\phi \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$
$$M = \begin{bmatrix} \cos\phi & \sin\phi(\cos\theta - i\sin\theta) \\ \sin\phi(\cos\theta + i\sin\theta) & -\cos\phi \end{bmatrix}$$
$$M = \begin{bmatrix} \cos\phi & e^{-i\theta}\sin\phi \\ e^{i\theta}\sin\phi & -\cos\phi \end{bmatrix}$$

In this form we can easily find the eigenpairs of the Hamiltonian by finding the eigenpairs of M and multiplying the eigenvalues by H_0. If we do so we get that

$$\begin{aligned} M - \lambda I &= \begin{bmatrix} \cos\phi - \lambda & e^{-i\theta}\sin\phi \\ e^{i\theta}\sin\phi & -(\cos\phi + \lambda) \end{bmatrix} \\ \det(M - \lambda I) &= -(\cos\phi - \lambda)(\cos\phi + \lambda) - \sin^2\phi \\ \lambda^2 - \cos^2\phi - \sin^2\phi &= \lambda^2 - 1 \\ p_M(\lambda) = 0 &\implies \lambda_\pm = \pm 1 \end{aligned}$$

Next we solve the eigenvector for each eigenvalue

$$\begin{aligned} M - \lambda_\pm I &= \begin{bmatrix} \cos\phi \mp 1 & e^{-i\theta}\sin\phi \\ e^{i\theta}\sin\phi & -(\cos\phi \pm 1) \end{bmatrix} \\ &\begin{bmatrix} \mp(1 \mp \cos\phi) & e^{-i\theta}\sin\phi \\ e^{i\theta}\sin\phi & \mp(1 \pm \cos\phi) \end{bmatrix} \end{aligned}$$

Next we use the fact that $1 \pm \cos\phi = 2\text{trig}_\pm^2 \frac{\phi}{2}$, and the fact that $\sin\phi = 2\text{trig}_\pm \frac{\phi}{2}\text{trig}_\mp \frac{\phi}{2}$ (where $\text{trig}_+ = \cos, \text{trig}_- = \sin$)

$$\begin{aligned} &\begin{bmatrix} \mp 2\text{trig}_\mp^2 \frac{\phi}{2} & 2e^{-i\theta}\text{trig}_\pm \frac{\phi}{2}\text{trig}_\mp \frac{\phi}{2} \\ 2e^{i\theta}\text{trig}_\pm \frac{\phi}{2}\text{trig}_\mp \frac{\phi}{2} & \mp 2\text{trig}_\pm^2 \frac{\phi}{2} \end{bmatrix} \\ &\cong \begin{bmatrix} 1 & \mp e^{-i\theta}\text{trig}_\pm \frac{\phi}{2}\text{trig}_\mp^{-1} \frac{\phi}{2} \\ 1 & \mp e^{-i\theta}\text{trig}_\pm \frac{\phi}{2}\text{trig}_\mp^{-1} \frac{\phi}{2} \end{bmatrix} \\ &\cong \begin{bmatrix} 1 & \mp e^{-i\theta}\text{trig}_\pm \frac{\phi}{2}\text{trig}_\mp^{-1} \frac{\phi}{2} \\ 0 & 0 \end{bmatrix} = M' \end{aligned}$$

Hence if a vector $M\psi_\pm = \lambda_\pm\psi_\pm \implies (M - \lambda_\pm I)\psi_\pm = 0$ or in otherwords $\psi_\pm \in \text{null}(M - \lambda_\pm I)$ which since the two matrices are similar is equivalent to saying that $\psi_\pm \in \text{null}(M')$. Or in otherwords that $M'\psi_\pm = \vec{0}$. Plugging in the form of M' we derived one can obtain the formula:

$$\psi_\pm^1 = \pm e^{-i\theta}\text{trig}_\pm \frac{\phi}{2}\text{trig}_\mp^{-1} \frac{\phi}{2}\psi_\pm^2$$

We may pick $\psi_\pm^2 = \text{trig}_\mp \frac{\phi}{2}$ without loss of generality to get a normalized vector.

$$\psi_\pm^1 = \pm e^{-i\theta}\text{trig}_\pm \frac{\phi}{2}$$

In summary then, the eigen-pairs of the Hamiltonian are $\psi_\pm, E_\pm$ where

$$E_\pm = \pm\epsilon$$
$$\psi_\pm = \begin{bmatrix} \pm e^{-i\theta}\text{trig}_\pm\frac{\phi}{2} \\ \text{trig}_\mp\frac{\phi}{2} \end{bmatrix}$$

Now that we have solved the eigen-pairs we are prepared to ask the question; what happens if the direction of the magnetic field changes in time[5]. Then we may note that as the magnetic field is a 3D object we need to use the 3D definitions of the Berry connection and curvature. Practically speaking, given the form of the eigenvalues and eigenvectors we are able to use spherical coordinates with $r = \epsilon$

$$\vec{A}_\pm = i\left\langle\psi_\pm\middle|\vec{\nabla}_{\vec{r}}\psi_\pm\right\rangle$$

Now:

$$\vec{\nabla}\psi_\pm = \begin{bmatrix} \frac{\partial\psi_\pm^1}{\partial_\epsilon} & \frac{1}{\epsilon}\frac{\partial\psi_\pm^1}{\partial_\phi} & \frac{1}{\epsilon\sin\phi}\frac{\partial\psi_\pm^1}{\partial_\theta} \\ \frac{\partial\psi_\pm^2}{\partial_\epsilon} & \frac{1}{\epsilon}\frac{\partial\psi_\pm^2}{\partial_\phi} & \frac{1}{\epsilon\sin\phi}\frac{\partial\psi_\pm^2}{\partial_\theta} \end{bmatrix} = \begin{bmatrix} 0 & -\frac{e^{-i\theta}}{\epsilon}\text{trig}_\mp\frac{\phi}{2} & \mp i\frac{e^{-i\theta}}{\epsilon\sin\phi}\text{trig}_\pm\frac{\phi}{2} \\ 0 & \pm\frac{1}{\epsilon}\text{trig}_\pm\frac{\phi}{2} & 0 \end{bmatrix}$$

And hence since $\left\langle\psi_\pm\middle|\vec{\nabla}_{\vec{r}}\psi_\pm\right\rangle = \psi_\pm^\dagger\vec{\nabla}\psi_\pm$ we get that

$$\begin{aligned}\left\langle\psi_\pm\middle|\vec{\nabla}_{\vec{r}}\psi_\pm\right\rangle &= \begin{bmatrix}\pm e^{i\theta}\text{trig}_\pm\frac{\phi}{2} & \text{trig}_\mp\frac{\phi}{2}\end{bmatrix}\begin{bmatrix} 0 & -\frac{e^{-i\theta}}{\epsilon}\text{trig}_\mp\frac{\phi}{2} & \mp i\frac{e^{-i\theta}}{\epsilon\sin\phi}\text{trig}_\pm\frac{\phi}{2} \\ 0 & \pm\frac{1}{\epsilon}\text{trig}_\pm\frac{\phi}{2} & 0 \end{bmatrix} \\ &= \begin{bmatrix} 0 & \frac{1}{\epsilon}\left(\mp\text{trig}_\mp\frac{\phi}{2}\text{trig}_\pm\frac{\phi}{2} \pm \text{trig}_\mp\frac{\phi}{2}\text{trig}_\pm\frac{\phi}{2}\right) & \frac{1}{\epsilon\sin\phi}\left(0 - i\text{trig}_\pm^2\frac{\phi}{2}\right)\end{bmatrix} \\ &= \begin{bmatrix} 0 & 0 & \frac{-i\text{trig}_\pm^2\frac{\phi}{2}}{\epsilon\sin\phi}\end{bmatrix}\end{aligned}$$

And so since we know that $\vec{A}_\pm = i\left\langle\psi_\pm\middle|\vec{\nabla}_{\vec{r}}\psi_\pm\right\rangle$ it follows that all we get is the simple statement that

$$\vec{A}_\pm = \frac{\text{trig}_\pm^2\frac{\phi}{2}}{\epsilon\sin\phi}\hat{\theta}$$

Moreover we can extract the Berry curvature vector (again by definition)[6]

$$\begin{aligned}\vec{\Omega}_\pm = \vec{\nabla}\times\vec{A}_\pm = \frac{1}{\epsilon\sin\phi}\left[\frac{\partial\sin\phi A_\pm^\theta}{\partial\phi} - \frac{\partial A_\pm^\phi}{\partial\theta}\right]\hat{\epsilon} &= \frac{1}{\epsilon^2\sin\phi}\frac{\partial\text{trig}_\pm^2\frac{\phi}{2}}{\partial\phi}\hat{\epsilon} \\ \mp\frac{\text{trig}_\pm\frac{\phi}{2}\text{trig}_\mp\frac{\phi}{2}}{\epsilon^2\sin\phi}\hat{\epsilon} = \mp\frac{\sin\phi}{2\epsilon^2\sin\phi}\hat{\epsilon} &= \mp\frac{1}{2\epsilon^2}\hat{\epsilon}\end{aligned}$$

[5] In such a way that the adiabatic approximation holds

[6] ignoring the $\hat{\theta}$ and $\hat{\phi}$ terms in the curl which go to 0 by inspection

We have worked through this very difficult result if for no other reason than to demonstrate what I have done in the much more complicated case to follow where writing the equations explicitly would not have been possible. Now that I have brought it up, its time to introduce the quantum system this research is all about.

1.5 Our Example: SOC in Graphene about Dirac Points

Now the example I just worked out in[7] detail throughout the last section is a particularly simple example of finding a Berry curvature. This report deals with a system that is mathematically not too dissimilar, although intuitively very different.

To be more clear, the system I am concerned with is that of a graphene lattice: a hexagonal network of bonded carbon atoms which looks like a honeycomb. There is an electron somewhere in this lattice, and it has a certain probability of moving from one carbon atom to a different one. Of course I am speaking loosely to say this, what I mean is that there is a wave-function describing an electron that is delocalized over the lattice and the interaction controlling transitions of the electrons "location" between atoms is given by the Hamiltonian.

More precisely, we are working in the regime of the nearest neighboor tight binding approximation in a system large enough for Bloch's theorem to be used (again in approximation). This means that the graphene lattice is large relative to the size of the individual bond lengths, and that "the electron will only jump from one atom to the nearest adjacent atom (or neighbour)".

In addition this report does not care about the global behaviour of the Hamiltonian but only at the behaviour around any of the Dirac points (places in the parameter space where the Hamiltonian looks linear) of which there are two types; K and K'. Expanded locally [8] the Hamiltonian takes the form of h.

$$h = \tau x\sigma_1 + y\sigma_2 \tag{13}$$

Where $\tau = \pm 1$ for K and K' points respectively and x, y are variables that we will change adiabatically like ϵ, θ, ϕ in the previous example.

Lastly the Hamiltonian this report focuses on is not this specific Hamiltonian but in principle the most general Hamiltonian that can be constructed out of h while factoring in spin in such a way as to preserve the rotational symmetry of the lattice. That is it is the Hamiltonian of spin orbit coupling (SOC) in graphene near Dirac points. I will leave my description of this system here for now but will go into more detail in a later section.

[7] extreme

[8] By this I mean if we do a first order Taylor expansion of the Hamiltonian as functions in the parameter space about the Dirac points

2 Motivation

In short this section has the goal of answering a question left in the air after the first section in which I derived in detail the derivation of the Berry curvature, and calculated it in a toy problem. Why should we care about the curvature? Put in a little more detail: the Berry phase can only be related to the Berry curvature if there is a closed path $\partial\mathcal{A}$ in the parameter space over which the system evolves. If no such path exists then the only relevant entity we can speak of in the wave function is the Berry connection.

Moreover, even if we have such a path, the curvature only appears as a part of the phase of the wave-function α and therefore has no ability to influence the probability density function $|\alpha|^2$. Even further none of the usual observables we compute in quantum mechanics (position, momentum, etc.) would be able to detect it either as it has no positional dependence. So therefore the question remains; why should one care about the Berry curvature?

The answer is that while at this level there seems to be no use, in other levels of analysis (transport theory and wave-packet Lagrangian mechanics as well as others) there is a clear use for it. For example, consider the off diagonal conductivity of a topological insulator σ_{xy}[9], one can show[10] these terms satisfy

$$\sigma_{xy} \propto \int_{\mathcal{R}} \Omega \tag{14}$$

Additionally there is an argument to be made[11] that the curvature scalar appears in a Lagrangian formulation of wave-packet semi-classical mechanics in the following sense. Suppose we have a lattice (as we do in this case) then we may break the lattice up into smaller subsystems. Within each of these subsystems there will be a time-dependent parameters and hence each of these will give rise to curvatures. From the eigenvectors in each local subsystem one may construct a wave-packet Ψ in a particular way. Additionally one may construct variables which behave like classical position $\vec{q}$ and momentum $\vec{p}$ for this wave-packet. Then if one uses the Lagrangian formulation of quantum mechanics with Lagrangian L

$$L = \langle\Psi| i\hbar\frac{\partial}{\partial t} - H |\Psi\rangle \tag{15}$$

and the principle of stationary action, one can arrive at a set of equations of motion for these new positions and momenta that take the form

$$\frac{dq^\mu}{dt} = \frac{\partial E}{\partial p^\mu} + f(\Omega), \;\; \frac{dp^\mu}{dt} = \frac{\partial E}{\partial q^\mu} \tag{16}$$

Where f is a function of the curvature. This will be the next step in my research in which I try and apply the computed curvatures in this semi classical

[9] Here σ has nothing to do with Pauli matrices, this is just a coincidence

[10] B. Bernevig, *Topological Insulators and Topological Superconductors,* Princeton University Press, 2013. (pg .14)

[11] and one which I do not yet completely understand

theory, but I do not yet understand it well enough to elaborate any further than that.

3 Our Hamiltonian

3.1 The Spin Blind Terms

Firstly, we again begin with the Hamiltonian discussed in the first introduction to the system of SOC graphene h. If we wish to add spin to this Hamiltonian, the simplest possible way to do that is to make this system "spin-blind" that is let this system act on spin states by non-action (identity). Hence we define the graphene spin-blind Hamiltonian term G as

$$G = h \otimes s_0 \tag{17}$$

Additionally we can add a third dimensional term which was missing from h in such a way that the system is still spin-blind. We call this term A and we introduce a parameter (although not one which changes in time) a to control it. In the literature this is often called the Delta term, and $a = \Delta$

$$A = a\sigma_3 \otimes s_0 \tag{18}$$

3.2 The Lattice Blind Term

Now in another sense we should define terms which act on spin states non-trivially but act on lattice states by identity. The term which does this while still preserving the planar symmetry of the lattice is called C and is controlled by c. In the literature it is called the Valley-Zeeman term and $c = \lambda_{\mathrm{VZ}}$. For reasons concerning time-reversal symmetry[12] the C term and all the terms to follow include the τ parameter.

$$C = c\tau\sigma_0 \otimes s_3 \tag{19}$$

3.3 The Mixed Terms

Lastly, there are two additional terms which mix up lattice states and spin states. The first, B (controlled by b) does not directly interfere with the lattice states anymore than the A term as it does not influence σ_1, or σ_2. In the literature this is called the Kane-Mele term and $b = \lambda_{\mathrm{KM}}$.

$$B = b\tau\sigma_3 \otimes s_3 \tag{20}$$

Finally, and most purnishously, the D term mixes up spin and lattice states in a more aggressive way than the B term as it directly mixes up σ_1 with σ_2

[12] which will be a central aspect of the second phase of my research

with s_1 and s_2.In the litterature this is the Rashba term and its controlling parameter $d = \lambda_{\mathrm{R}}$.

$$D = d(\tau\sigma_1 \otimes s_2 - \sigma_2 \otimes s_1) \tag{21}$$

3.4 The Full Hamiltonian

In total the full Hamiltonian for this report is H

$$H = G + A + B + C + D \tag{22}$$

Any of these terms can be set to 0 by setting the controlling parameter to 0. It must be reiterated that the parameters $a, ...d$ are not time dependent and play no direct role in finding the curvature. The eigen-problem for the full Hamiltonian what we call the ABCD case, is not tractable. We need to selectively set some terms to 0 to get tractable cases. These turned out to be:

- the ABC case
- the AD case

the BD case was deemed not important as in physical systems the D term dominates. The ACD, and CD cases were also not tractable (in a sense that will be made clear in a subsequent section). So the Hamiltonians' this report is about are:

- $G + A + B + C$
- $G + A + D$

4 The Method

We can note that H is a 4D matrix similar to the toy problem from the introduction and so the solution for the curvatures will be identical. To reiterate what was done for the toy problem:

1. Find the eigen-pairs E_m, ψ_m of the Hamiltonian
2. Normalize the eigenvectors so that they represent realise-able wave functions[13]
3. Compute the Berry connection vectors from the eigenvectors using

$$\vec{A}_m = i \left\langle \psi_m \middle| \vec{\nabla}_{\vec{r}} \psi_m \right\rangle \tag{23}$$

[13] In the toy problem I was able to solve the wave-functions already normalized. These ones are too complicated for that and so require an extra step.

4. Compute the Berry curvature scalars from the connection

$$\Omega_m = \frac{\partial \vec{A}_{m,2}}{\partial r^1} - \frac{\partial \vec{A}_{m,1}}{\partial r^2} \tag{24}$$

5. Compute (if possible) the Chern number using $\text{Chern}_m = \frac{1}{2\pi} \int_{\mathbb{R}^2} \Omega_m dr_1 dr_2$

6. Show the graph of each eigenvalue and its corresponding curvature or Chern number to learn something interesting about the topology of the system.[14]

To preform these steps, I have written a program in *Mathematica* that makes use of a rotational symmetry in the problem to do everything in polar coordinates. That said the computation is purely symbolic. There are no numerical approximations here, all subsequent results are analytically true given the approximations needed to arrive at the Hamiltonian.

I should give a note on what is meant by intractability. I say that a case is intractable if the program fails at a particular step, and there is no alternative exploit for which I can solve the problem by hand. The ABCD case fails at step 1. The ACD , the CD, and AD cases all fail at step 2. The only reason we have a solution for the AD case was because there are a set of substitutions that can be made and exploited to easily normalize much faster than the program (in that it terminates) and then continue by hand. If such an exploit can be found for the ACD case, we would have a much more general curvature like with the ABC case.

Lastly before I show the result I should explain what I mean when I say that the Chern numbers and curvatures tell us something interesting about the topology of the parameter space. If the Chern numbers are 0 then the system is topologically trivial, that is we should expect no holes in parameter space. Else the Chern number **should** be 1/2 (as the total Chern number is 0 and there are 2 Dirac points). Which would imply that while globally the space is trivial, locally about each Dirac point this system is nontrivial in opposite ways. This would have physical implications as it would influence the behaviour of the wave-function via the Berry phase.

5 Results

5.1 the ABC case

Firstly, here are the eigenvalues and the respective curvatures and Chern numbers

$$E_{nm} = n\left[c - m\sqrt{(a+nb)^2 + r^2}\right] \tag{25}$$

[14] This last point connects very closely to the talk of Chern numbers mentioned in the digression into gauge theory

$$\Omega_{nm} = m\frac{a+nb}{2\left[(a+nb)^2+r^2\right]^{3/2}} \tag{26}$$

+

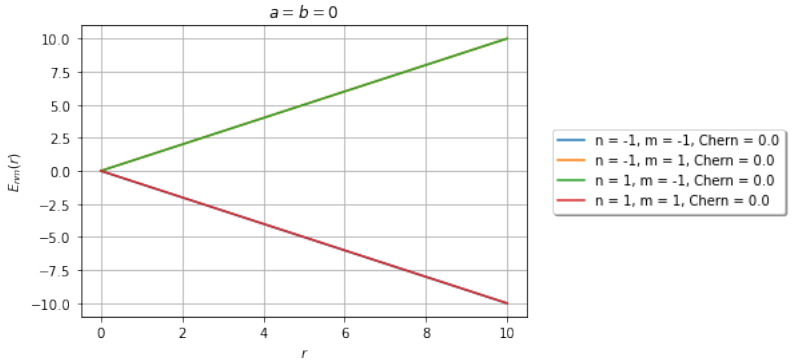
$$\text{Chern}_{nm} = m\ \text{sgn}(a+nb)\frac{1}{2} \tag{27}$$

Where $n, m = \pm 1$.

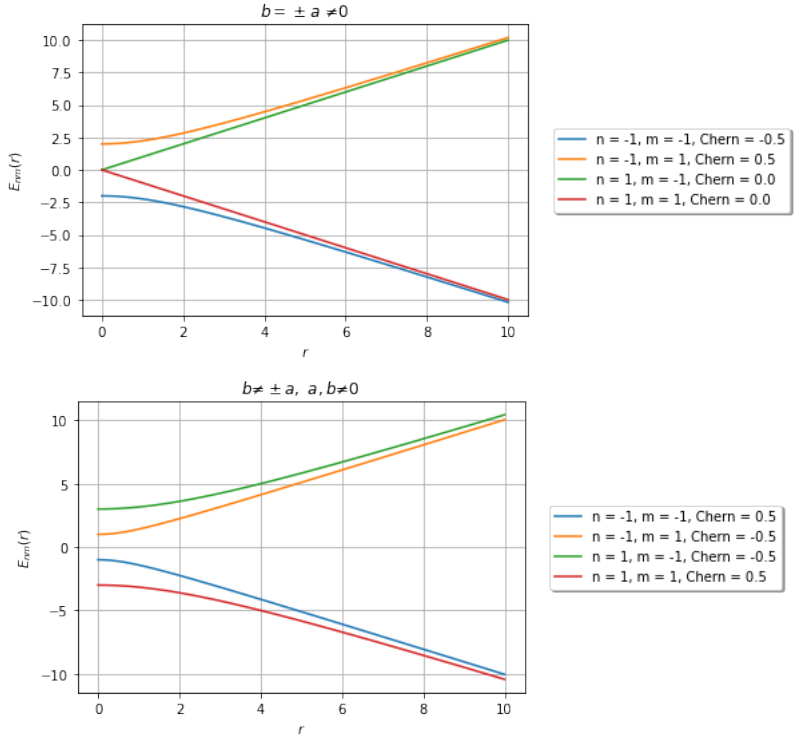
We can confirm that the curvature found here in the limit of $c = 0$ should match the AB case Hamiltonian looked at in the literature[15], and we find them to be exactly equal. Just looking at the results is a little opaque, so lets see identify three different cases of interest.

- $a = b = 0 \implies \text{Chern}_{mn} = 0$
- $b = \pm a \neq 0 \implies \text{Chern}_{m+} = 0,\ |\text{Chern}_{m-}| = \frac{1}{2}$ in canceling pairs
- $b \neq \pm a, a$ or $b \neq 0 \implies \text{Chern}_{m+} = 0,\ |\text{Chern}_{mn}| = \frac{1}{2}$ in canceling pairs. In this final case we choose to make both $a, b \neq 0$ as this lifts the degeneracy and makes the picture easier to understand.

We can plot each of these cases to gain some intuition on the topology of the parameter space.



[15] Zhou, B., Katsuhisa, T., Kawaguchi, T., Tanaka, Y. Law K., *Spin-orbit coupling induced valley Hall effects in transition-metal dichalcogenides*, Communications Physics, 2019. This Hamiltonian appears in two completely different contexts in this paper where the parameters x, y, a, b have nothing to do with SOC in graphene. But since the Hamiltonians are mathematically identical the curvatures should be (and are) as well.



We note the following trend: Chern numbers become nonzero exactly when gaps open up between pairs of lines in the spectrum.

5.2 The AD case

As mentioned prior, the AD case is intractable with the algorithm. However, introducing the following substitutions makes the problem analytically solveable. These substitutions are:

$$\epsilon_m = \sqrt{r^2 + d^2} + md, \cos\phi_m = \frac{a}{\sqrt{a^2 + \epsilon_m^2}}, \cos\gamma = \frac{d}{\sqrt{r^2 + d^2}}$$

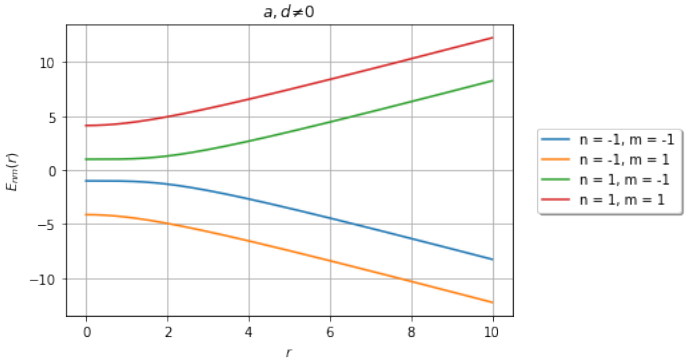
we get the following results [16]

$$E_{nm} = n\sqrt{a^2 + \epsilon_m^2} \tag{28}$$

$$\Omega_{nm} = -\frac{n}{2r}\cos\phi_m \sin^2\gamma \left[\sin^2\phi\left(\frac{1 - m\cos\gamma}{1 + m\cos\gamma}\right) - m\cos\gamma\right] \tag{29}$$

To visualize this, here is a generic example of the spectrum

[16] One would expect the Chern numbers to again be 0 or ±1/2 but the integration is nontrivial and I have not yet done it



6 Where to go from here

At this point there are a couple things left to do, and I can split the list up into the theoretical goals, computational goals, and application goals.

6.1 Theoretical Goals

First it would be nice to understand exactly what the Chern numbers and classes measure. For this reason will seek to get a better handle on Chern-Weil theory.

Additionally as the global Chern numbers must be integral it follows that there should be some reason for this present in the algebra that generates this Hamiltonian $\mathfrak{su}(4)$. The question is why should the flip $\tau \to -\tau$ cause $\Omega \to -\Omega$.[17]

6.2 Computational Goals

I still need to compute (analytically or numerically) the Chern number in the AD case and verify the prediction of $\pm 1/2$. Additionally I could potentially look for another trick to exploit in the ACD case as was done in AD[18]

6.3 Application Goals

Lastly I need to use the curvatures found in both cases to derive observable properties. Either transport properties like the conductivity or else using the wave-packet equations of motion [19]

[17] Dr. Maiti has hinted that this might be related to time reversal
[18] this seems unlikely
[19] which Dr. Maiti and I are both still learning