I. BERRY CURVTURE IN THE RASHBA WELL

Let's do a quick example using the Rashba well. The spin portion of the quantum well hamiltonian is:

$$\hat{\mathcal{H}}_R^{spin} = \alpha p \vec{\sigma} \cdot \hat{\phi}_{\vec{p}} - b\sigma^z \tag{1}$$

Now, we would like to calculate the Berry connection for the low-energy band:

$$\vec{\Lambda}_{\vec{p}} = i \langle \vec{p}| \nabla_{\vec{p}} |\vec{p}\rangle \tag{2}$$

The gradient is best expressed in polar coordinates. Since we know that Berry phase for a spin only depends on changes of the Euler angle ϕ of the spin projection on the x-y plane to the x-axis, we can deduce that only the part that depends on $\phi_{\vec{p}}$ will contribute:

$$\vec{\Lambda}_{\vec{p}} = i \langle \vec{p}| \frac{\hat{\phi}_{\vec{p}}}{|p|} \frac{\partial}{\partial \phi_{\vec{p}}} |\vec{p}\rangle = \hat{\phi}_{\vec{p}} \frac{1-\cos\theta_p}{2} \tag{3}$$

where θ_p is the angle of the spin to the z-axis. This is given by:

$$\cos\theta = \frac{b}{\sqrt{\alpha^2 p^2 + b^2}} \tag{4}$$

So:

$$\vec{\Lambda}_{\vec{p}} = \hat{\phi}_{\vec{p}} \frac{1 - \frac{b}{\sqrt{\alpha^2p^2+b^2}}}{2p} \tag{5}$$

A. Shift current

Already here we can see something interesting. Particles at momentum $\vec{p}$ are shifted by a bit in the direction normal to $\vec{p}$ (recall that $\vec{\Lambda}_{\vec{p}}$ is a location shift). If we look at the excited band, then the Berry curvature corresponds to a different θ, with $\cos\theta_p^{exc} = -\cos\theta_p$. When we excite electrons from the bottom band to the top band with a matrix element V_{ge}, the electron's wave function will exhibit a shift in its position, given by:

$$\delta r = \vec{\Lambda}_{\vec{p}}^{exc} - \vec{\Lambda}_{\vec{p}}^{0} - \nabla_{\vec{p}}(arg(V_{ge})) \tag{6}$$

This electronic motion gives rise to the *shift current*

B. Anomalous velocity

What is the Berry curvature? It is:

$$\Omega_{\vec{p}} = \nabla_{\vec{p}} \times \vec{\Lambda}_{\vec{p}} \tag{7}$$

The only terms in the Rashba well that would matter is:

$$\Omega_{\vec{p}} = \left(\hat{p}\frac{\partial}{\partial p} + \hat{\phi}_{\vec{p}} \frac{1}{p}\frac{\partial}{\partial \phi}\right) \times (f(p)\hat{\phi}_{\vec{p}}) \tag{8}$$

Both terms contribute, and we obtain:

$$= \hat{p} \times \hat{\phi}\frac{\partial f}{\partial p} - \hat{\phi} \times \hat{p} f(p)/p \tag{9}$$

where the second term is due to $\frac{\partial \hat{\phi}}{\partial \phi} = -\hat{p}$. This reduces to:

$$= \hat{z}\left(\frac{\partial f(p)}{\partial p} + \frac{f(p)}{p}\right) = \hat{z}\frac{1}{p}\frac{\partial (p f(p))}{\partial p} \tag{10}$$

and finally:

$$\vec{\Omega}_{\vec{p}} = \hat{z}\frac{b\alpha^2}{(b^2+\alpha^2 p^2)^{3/2}} \tag{11}$$

Particularly at $p = 0$ we get a constant result:

$$\Omega_0 = \frac{\alpha^2}{b^2} \tag{12}$$

If we start with an electron at rest at $p = 0$,it will start moving backwards due to the negative band curvature, and sideways:

$$\dot{r} = \frac{\partial \epsilon_{p(t)}}{\partial p} + \dot{\vec{p}} \times (\hat{z}\Omega_p) \tag{13}$$

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II. BERRY CONNECTION AND CURVATURE IN 1D SYSTEMS

Let us next get a feeling for how the Berry phase arises naturally in 1d model and how it is connected to pumping.

A. Thouless pump

Consider free particles bound to a wire. It has Hamiltonian:

$$\hat{\mathcal{H}} = \frac{p^2}{2m} \tag{14}$$

Next, subject the poor electrons being subject to a periodic potential $V = 2g\cos(qx+\phi) = ge^{iqx+i\phi} + ge^{-iqx-i\phi}$. This potential clearly scatters momentum p electrons to momentum $p \pm q$. Let's expand the hamiltonian near momentum $q/2$, where we know there will be a gap opened. we write:

$$p = q/2 + \delta p. \tag{15}$$

Then:

$$\hat{\mathcal{H}}_{\delta p}\begin{pmatrix} \psi_{q/2+\delta p} \\ \psi_{-q/2+\delta p} \end{pmatrix} = \begin{pmatrix} \frac{(q/2+\delta p)^2}{2m} & ge^{i\phi} \\ ge^{-i\phi} & \frac{(-q/2+\delta p)^2}{2m} \end{pmatrix}\begin{pmatrix} \psi_{q/2+\delta p} \\ \psi_{-q/2+\delta p} \end{pmatrix} \tag{16}$$

If we expand and remove the trivial offset $q^2/8m$, and also ignore terms that are δp^2 dependent, we end up with the rather appealing. Rename $k = \delta p$, for simplicity, and obtain:

$$\hat{\mathcal{H}}_k = v\sigma^z k + g(\cos\phi\sigma^x + \sin\phi\sigma^y) \tag{17}$$

with $v = q/2m$. Let's start simple. $\phi = 0$. Then the hamiltonian is (really) simply:

$$\hat{\mathcal{H}}_k = v\sigma^z k + g\sigma^x \tag{18}$$

We see a gap open, with energies:

$$E_\pm = \pm\sqrt{v^2k^2+g^2} \tag{19}$$

A filled valence band implies filled momentum states for all momenta $|p| < q/2$. This implies a particular density:

$$n = \int_{-q/2}^{q/2} \frac{dp}{2\pi} = \frac{q}{2\pi} = \frac{1}{a} \tag{20}$$

where a is the periodicity of the periodic potential. Not surprising. One particle per trough! Indeed, if you think of the large potential limit, $g \gg q^2/m$, then that's the only thing one could really have. Particles stuck in the bottom of a periodic potential.

Also, the pseudo spin $\vec{\sigma}$ points in a direction determined by the momentum:

$$\vec{\sigma}_k = -\frac{1}{\sqrt{v^2k^2+g^2}}(g\hat{x}+vk\hat{z}) \tag{21}$$

What is the meaning of the phase ϕ? It is the like a shift in x:

$$\cos(qx+\phi) = \cos(q(x+a\frac{\phi}{2\pi})) \tag{22}$$

This should evoke in your mind the images of a cogwheel turning. So each turn should shift the position by one particle.

As we shift the potential with a nonzero ϕ, so shifts the pseudospin direction of wavefunctions in the bottom band:

$$\vec{\sigma}_k = -\frac{1}{\sqrt{v^2k^2+g^2}}(g\hat{x}\cos\phi + g\hat{y}\sin\phi + vk\hat{z}). \tag{23}$$

How do we see that the particles though are moving from the band structure perspective? Can you guess it? The Berry phase. We would like to trace the shift in location as we change ϕ. Recall that the location operator is given by:

$$x = i\frac{\partial}{\partial k} + i\langle k|\frac{\partial}{\partial k}|k\rangle \tag{24}$$

This is taking into acount the twisting of the wannier wave functions as momentum changes. So we expect that the center of mass of of the particles in the band has a shift given by:

$$\langle x\rangle = \int\limits_{-q/2}^{q/2}\frac{dk}{q}i\langle k|\frac{\partial}{\partial k}|k\rangle = a\int\limits_{-q/2}^{q/2}\frac{dk}{q}i\langle k|\frac{\partial}{\partial k}|k\rangle \tag{25}$$

with $a = 2\pi/q$.

A quick word on how the Berry phase emerged here. In practice, we were treating the electrons in this band as if they were spin-1/2's. But they are not! They are spinless in this example. Furthermore, we would like to be thinking of the states as simple momentum states, with $|k\rangle \sim e^{ikx}$, and ignore the spinor structure. This is possible, if we take into account the Berry connection that emerges from the pseudospin. You can see that if we had applied $\hat{x} = i\frac{\partial}{\partial k}$ on the spinor wave function $|k\rangle = e^{ikx}\begin{pmatrix} u_k \\ v_k \end{pmatrix}$, we would have gotten the Berry connection above.

Now, we would like to trace this change as a function of ϕ:

$$\Delta x = \int\limits_0^{2\pi} d\phi\frac{\partial}{\partial\phi}\frac{1}{q}\int\limits_{-q/2}^{q/2} dki\langle k|\frac{\partial}{\partial k}|k\rangle \tag{26}$$

For the example we have, for a given ϕ the product $i\langle k|\frac{\partial}{\partial k}|k\rangle = 0$ since k only changes that lattitude of the spin, while the Berry connection depends on the longtitude (which incidentally is ϕ). So looks like we don't have any shift... Is there no effect?

We must have forgotten something. As we change ϕ, what happens to the wave functions? They acquire a Berry phase due to ϕ. Where is it in our calculation? That's right. Missing. Each state $|k\rangle$ should get slapped with a Berry phase due to the shift of ϕ:

$$|k\rangle \to |k\rangle e^{i\lambda_\phi}, \; \frac{\partial\lambda_\phi}{\partial\phi} = i\langle k|\frac{\partial}{\partial\phi}|k\rangle \tag{27}$$

So Eq. (26) should be changed to accomodate the different $|k\rangle$ states:

$$\Delta x = \int\limits_0^{2\pi} d\phi\frac{\partial}{\partial\phi}\frac{1}{q}\int\limits_{-q/2}^{q/2} dki\left(e^{-i\lambda_\phi}\langle k|\frac{\partial}{\partial k}\left(|k\rangle e^{i\lambda_\phi}\right)\right) \tag{28}$$

Just doing the algebra yields:

$$= \frac{1}{q}\int d\phi \int dk \left(\frac{\partial \Lambda_k}{\partial \phi} - \frac{\partial^2}{\partial k \partial \phi}\lambda_\phi\right) \tag{29}$$

but we recognize:

$$\frac{\partial \lambda_\phi}{\partial \phi} = i \langle k| \frac{\partial}{\partial \phi}|k\rangle = \Lambda_\phi \tag{30}$$

The Berry connection as if ϕ were a momentum. So this is:

$$= \frac{2\pi}{q}\int \frac{d\phi}{2\pi} \int dk \left(\frac{\partial \Lambda_k}{\partial \phi} - \frac{\partial}{\partial k}\Lambda_\phi\right) = a\int \frac{d\phi}{2\pi}\int dk \hat{z}\cdot \nabla_{k,\phi}\times \vec{\Lambda} \tag{31}$$

So the curl of a Berry connection $\vec{\Lambda} = \hat{\phi}\Lambda_\phi + \hat{k}\Lambda_k$. But this curl is just the Berry curvature:

$$\Omega = \hat{z}\cdot \nabla_{k,\phi}\times \vec{\Lambda} \tag{32}$$

assuming that $\hat{\phi}\times \hat{k} = \hat{z}$.

But what is finally the result?

$$\Lambda_k = 0,\ \Lambda_\phi = \frac{1}{2}(1-\cos\theta) = \frac{1}{2}(1 - \langle \sigma^z \rangle) \tag{33}$$

And the final displacement upona shift by 2π is:

$$a\frac{d\phi}{2\pi}\int dk(-\frac{\partial}{\partial k})\Lambda_\phi(k) = a\cdot (\Lambda_{-k_{max}} - \Lambda_{k_{max}}) = a \tag{34}$$

Why is it quantized? Since the spin covered the full bloch sphere. As a result, the integrated Berry curvature was $4\pi/2$, which gives the desired result.

This is the description of the quantum Thouless pump. It shows how the quantized value of the current produced - one particle per cycle, and exactly one particle per cycle, arises due to the topological nature of the pseudospin of the electrons in the filled band.

We can do several things with this example. We could pretend that ϕ is really a momentum in another direction, and then get a $2d$ phase with something quantized. We will do this next time. But before, let's do more 1d stuff. In particular, localized instanton modes, and a proper topological 1d phase.

B. Relation of the Berry curvature to spin winding

Several of you have wondered about the explicit relatioship, which I advertized but never proven or even shown really, beteween the berry phase flux and the winding of the spin. Here is then the proof.

Let's assume that we have two parameters. k_x and k_y, that parametrize the spn of a spin-1/2 state in a closed manifold. I'm not quite sure why these parameters were exactly chosen. They just came to me somehow from midair. I really don't know... The Berry curvature flux is:

$$\int dk_y \int dk_x \Omega_{\vec{k}} = i\int dk_y \int dk_x \sum_{i,j=x,y} \epsilon^{ij}\frac{\partial}{\partial k_i}\Lambda_j \tag{35}$$

with $\Lambda_j = i\left\langle \vec{k}\right| \frac{\partial}{\partial k_j}\left|\vec{k}\right\rangle$, and $\epsilon^{xx} = \epsilon^{yy} = 0$, $\epsilon^{xy} = -\epsilon^{yx} = 1$. Clearly, the first derivative must fall on the $\left\langle \vec{k}\right|$, otherwise, the antisymmetric tensor will kill the double derivative:

$$\sum_{i,j=x,y} \epsilon^{ij}\left\langle \vec{k}\right| \frac{\partial^2}{\partial k_i \partial k_j}\left|\vec{k}\right\rangle = 0. \tag{36}$$

Therefore:

$$\int dk_y \int dk_x \Omega_{\vec{k}} = i\int dk_y \int dk_x \sum_{i,j=x,y} \epsilon^{ij}\frac{\partial}{\partial k_i}\left\langle \vec{k}\right| \frac{\partial}{\partial k_j}\left|\vec{k}\right\rangle \tag{37}$$

Now we need a leap of faith. Let's prove that we can upgrade the expression above to:

$$\int dk_y \int dk_x \Omega_{\vec{k}} = i \int dk_y \int dk_x \sum_{i,j=x,y} \epsilon^{ij} \mathrm{Tr}\left(\frac{\partial}{\partial k_i} \left(\left|\vec{k}\right\rangle \left\langle \vec{k}\right| \right) \frac{\partial}{\partial k_j} \left(\left|\vec{k}\right\rangle \left\langle \vec{k}\right| \right) \left|\vec{k}\right\rangle \left\langle \vec{k}\right| \right) \tag{38}$$

It is easy to prove this using the antisymmetric matrix. Any term that has a product of $\Lambda_i \Lambda_j$ dies upon summation. To see this explicitly, we can do the following:

$$\begin{aligned} \int dk_y \int dk_x \sum_{i,j=x,y} \epsilon^{ij} \tfrac{\partial}{\partial k_i} \left\langle \vec{k}\right| \tfrac{\partial}{\partial k_j} \left|\vec{k}\right\rangle &= \int dk_y \int dk_x \sum_{i,j=x,y} \epsilon^{ij} \left\langle \vec{k}\right| \left[\tfrac{\partial}{\partial k_i} \left(\left|\vec{k}\right\rangle \left\langle \vec{k}\right| \right) - \tfrac{\partial}{\partial k_i} \left|\vec{k}\right\rangle \right] \left\langle \vec{k}\right| \tfrac{\partial}{\partial k_j} \left|\vec{k}\right\rangle \\ &= \int dk_y \int dk_x \sum_{i,j=x,y} \epsilon^{ij} \left\langle \vec{k}\right| \tfrac{\partial}{\partial k_i} \left(\left|\vec{k}\right\rangle \left\langle \vec{k}\right| \right) \tfrac{\partial}{\partial k_j} \left|\vec{k}\right\rangle \end{aligned} \tag{39}$$

The last equality follows since:

$$\sum_{i,j=x,y} \epsilon^{ij} \left\langle \vec{k}\right| \frac{\partial}{\partial k_i} \left|\vec{k}\right\rangle \left\langle \vec{k}\right| \frac{\partial}{\partial k_j} \left|\vec{k}\right\rangle = 0 \tag{40}$$

Next, we need to defining the projector $P_{\vec{k}} = \left|\vec{k}\right\rangle \left\langle \vec{k}\right| = \frac{1}{2} + \frac{1}{2} \hat{n}_{\vec{k}} \cdot \vec{\sigma}$ which projects on the state $\left|\vec{k}\right\rangle$, using:

$$\hat{n}_{\vec{k}} \cdot \vec{\sigma} \left|\vec{k}\right\rangle = \left|\vec{k}\right\rangle . \tag{41}$$

Using this simplifies the expression a bit, and we proceed to modify the second derivative in the expression:

$$\begin{aligned} & i \int dk_y \int dk_x \sum_{i,j=x,y} \epsilon^{ij} \left\langle \vec{k}\right| \tfrac{\partial P_{\vec{k}}}{\partial k_i} \tfrac{\partial}{\partial k_j} \left|\vec{k}\right\rangle \\ &= i \int dk_y \int dk_x \sum_{i,j=x,y} \epsilon^{ij} \left\langle \vec{k}\right| \tfrac{\partial P_{\vec{k}}}{\partial k_i} \left[\tfrac{\partial}{\partial k_j} \left(\left|\vec{k}\right\rangle \left\langle \vec{k}\right| \right) - \left|\vec{k}\right\rangle \tfrac{\partial}{\partial k_j} \left\langle \vec{k}\right| \right] \left|\vec{k}\right\rangle \end{aligned} \tag{42}$$

Now:

$$\begin{aligned} & \sum_{i,j=x,y} \epsilon^{ij} \left\langle \vec{k}\right| \tfrac{\partial P_{\vec{k}}}{\partial k_i} \left|\vec{k}\right\rangle \left(\tfrac{\partial}{\partial k_j} \left\langle \vec{k}\right| \right) \left|\vec{k}\right\rangle \\ &= \sum_{i,j=x,y} \epsilon^{ij} \left[\tfrac{\partial \left\langle \vec{k}\right|}{\partial k_i} \left|\vec{k}\right\rangle \tfrac{\partial \left\langle \vec{k}\right|}{\partial k_j} \left|\vec{k}\right\rangle - \left\langle \vec{k}\right| \tfrac{\partial \left|\vec{k}\right\rangle}{\partial k_i} \left\langle \vec{k}\right| \tfrac{\partial \left|\vec{k}\right\rangle}{\partial k_j} \right] = 0 \end{aligned} \tag{43}$$

So the correction term in Eq. (42) can be ignored. It vanishes. Then picking up from Eq. (42), we find:

$$\int dk_y \int dk_x \Omega_{\vec{k}} = i \int dk_y \int dk_x \sum_{i,j=x,y} \epsilon^{ij} \mathrm{Tr}\left[\frac{\partial P_{\vec{k}}}{\partial k_i} \frac{\partial P_{\vec{k}}}{\partial k_j} \left|\vec{k}\right\rangle \left\langle \vec{k}\right| \right] = i \int dk_y \int dk_x \sum_{i,j=x,y} \mathrm{Tr} P_{\vec{k}} [\frac{\partial}{\partial k_x} P_{\vec{k}}, \frac{\partial}{\partial k_y} P_{\vec{k}}] \tag{44}$$

The only contributing terms in the commutator are the ones with the unit vector. These yield a pali matrix. Unless they find another pauli matrix, the trace would kill them. So this reduces further to:

$$\int dk_y \int dk_x \Omega_{\vec{k}} = \frac{i}{8} \int dk_y \int dk_x \sum_{i,j=x,y} \mathrm{Tr}\left(\hat{n}_{\vec{k}} \cdot \vec{\sigma} \left[\frac{\partial \hat{n}_{\vec{k}}}{\partial k_x} \cdot \vec{\sigma}, \frac{\partial \hat{n}_{\vec{k}}}{\partial k_y} \cdot \vec{\sigma} \right] \right). \tag{45}$$

And the only waythat this is nonzero, is if the pauli matrices form a triple product:

$$\mathrm{Tr}(\sigma^x [\sigma^y, \sigma^z]) = 4i. \tag{46}$$

This reduces the integral to a simple vector identity:

$$\int dk_y \int dk_x \Omega_{\vec{k}} = -\frac{1}{2} \int dk_y \int dk_x \sum_{i,j=x,y} \hat{n}_{\vec{k}} \cdot \left(\frac{\partial \hat{n}_{\vec{k}}}{\partial k_x} \times \frac{\partial \hat{n}_{\vec{k}}}{\partial k_y} \right) \tag{47}$$

This is nothing but half the Poyntriagin integral which tells you how much of the unit sphere is explored by the unit vector $\hat{n}_{\vec{k}}$.

C. Jackiw-Rebbi mode

The Thouless pump is like a prototype of a topological phase. We'll learn quickly that topological phases are often synonymous with having an edge state protected by symmetry. This edge state is already obvious from the Thouless example.

What happens if the phase of the potential changes from being $\phi = 0$, $x < 0$ to $\phi = \pi$, $x > 0$. This implies a change of sign of g:

$$\hat{\mathcal{H}}_k = vk\sigma^z + |g| sign(x)\sigma^x \tag{48}$$

If we draw this potential, it'll like a missing step. For this potential this will imply a zero mode. Let's derive it. First, write the hamiltonian fully in real space:

$$\hat{\mathcal{H}} = v\frac{1}{i}\frac{\partial}{\partial x}\sigma^z + |g| sign(x)\sigma^x \tag{49}$$

First, how can I be so confident that it is a zero mode? Symmetries. This particular model has a particle-hole symmetry which maps the Hamiltonian to minus itself. Particle-hole transformations must be antiunitary:

$$\mathcal{C} = \sigma^z \hat{K} \tag{50}$$

with $\hat{K} i \hat{K} = -i$. We have:

$$\mathcal{C}\hat{\mathcal{H}}\mathcal{C} = -\hat{\mathcal{H}} \tag{51}$$

So if we are expecting one state $|\psi\rangle$ with energy ϵ, we would also have another state:

$$|\psi'\rangle = \mathcal{C}\,|\psi\rangle\,,\, with\, \epsilon' = -\epsilon \tag{52}$$

But if there is only one state, then we must have $\epsilon = \epsilon' = 0$.

Armed with this we can look for the state:

$$E\,|\psi(x)\rangle = 0 = v\frac{1}{i}\sigma^z\frac{\partial\,|\psi(x)\rangle}{\partial x} + |g| sign(x)\sigma^x\,|\psi(x)\rangle \tag{53}$$

Let's guess:

$$|\psi(x)\rangle = \begin{pmatrix} u \\ v \end{pmatrix} e^{-\gamma|x|} \tag{54}$$

Why the u, v independent of the sign of x? Because the wave function must be cntinuous at $x = 0$. Plugging in we get:

$$(iv\gamma sign(x)\sigma^z + |g| sign(x)\sigma^x)\begin{pmatrix} u \\ v \end{pmatrix} = 0 \tag{55}$$

Multiplying from the left by the bracketed operator, we get:

$$(-\gamma^2 v^2 + g^2)\begin{pmatrix} u \\ v \end{pmatrix} = 0 \tag{56}$$

so $\gamma = g/v$ is obligatory. Putting this insight back in Eq. (55) we get:

$$|g| sign(x)\,(i\sigma^z + \sigma^x)\begin{pmatrix} u \\ v \end{pmatrix} = 0 \tag{57}$$

does this have a solution? Yes!

$$\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} i \\ 1 \end{pmatrix} \tag{58}$$

So the mode is:

$$|\psi(x)\rangle = \frac{g/2v}{\sqrt{2}}\begin{pmatrix} i \\ 1 \end{pmatrix} e^{-|gx|/v} \tag{59}$$

with normalization even!

Is it symmetry under $\mathcal{C}$? Sure is! This is the Jackiw Rebbi protected mode. You can see that if you have a juncion with a $\Delta\phi \neq \pi$ the state loses its protection, and the hamiltonian loses the particle-hole symmetry. This shifts gradually the state from $\epsilon = 0$ towards the valence or conduction band, until when $\phi = 0$ it gets absorbed. This, along with time-reversal and chiral symmetries will be explored in the problem set.