I. BERRY CONNECTION EFFECTS

A. Berry connection, semiclassical equations of motion, and curvature

The result above for the spin should be taken really seriously. Indeed we calculated the Berry phase for a spin forcced through a funny motion. But in fact, we were looking at a more general problem. We had a wave function for a momentum state:

$$|\psi(t)\rangle = \psi(t)\,|p(t)\rangle \tag{1}$$

It is really tempting to try to write down a Schroedinger equation simply for $\psi(t)$. If we did, and projected it on $\langle p(t)|$ then we would have:

$$i\,\langle p(t)|\,\frac{\partial}{\partial t}\,|\psi(t)\rangle = i\frac{\partial\psi(t)}{\partial t} + \psi(t) i\,\langle p(t)|\,\frac{\partial}{\partial t}\,|p(t)\rangle = \epsilon_p\psi(t) \tag{2}$$

But we recognize here the Berry phase! We can process it a bit to be:

$$i\,\langle p(t)|\,\frac{\partial}{\partial t}\,|p(t)\rangle = \dot{\vec{p}} i\,\langle p(t)|\,\frac{\partial}{\partial\vec{p}}\,|p(t)\rangle \tag{3}$$

We could absorb this term in the wave function, though,by saying:

$$\psi(p,t) \to \psi(p,t)e^{i\int^{\vec{p}} d\vec{p}\cdot\Lambda_{\vec{p}}} \tag{4}$$

with

$$\vec{\Lambda}_{\vec{p}} = i\,\langle p|\,\nabla_p\,|p\rangle \tag{5}$$

is called the Berry connection.

Wait! This is really familiar! This is like doing a gauge transformation to absorb a vector potential in the wave function, to get rid of the minimum coupling prescription: $p - eA = \frac{1}{i}\frac{\partial}{\partial\vec{r}} - e\vec{A}$ leads to:

$$\psi(r,t) \to \psi(r,t)e^{ie\int^{\vec{r}} d\vec{r}\cdot\vec{A}}. \tag{6}$$

Now, for this case we know what the equations of motion are. First, without a vector potential, we would have:

$$\dot{p} = -\nabla_{\vec{r}}V(\vec{r}),\ \dot{r} = \nabla_{\vec{p}}\epsilon_{\vec{p}} \tag{7}$$

With the vector potential we would have:

$$\dot{p} = -\nabla_{\vec{r}}V(\vec{r}) + e\dot{r}\times\nabla_{\vec{r}}\vec{A} - e\dot{\vec{A}},\ \dot{r} = \nabla_{\vec{p}}\epsilon_{\vec{p}} \tag{8}$$

By analogy, and since p and r are conjugate to each other, then, when we have $\vec{\Lambda}_{\vec{p}}$, we must also add similar terms to the $\dot{\vec{r}}$ side of the equation. This would give:

$$\dot{p} = -\nabla_{\vec{r}}V(\vec{r}) + e\dot{r}\times\nabla_{\vec{r}}\vec{A} - e\dot{\vec{A}},\ \dot{r} = \nabla_{\vec{p}}\epsilon_{\vec{p}} - \dot{p}\times\nabla_{\vec{p}}\vec{\Lambda}_{\vec{p}} + \dot{\vec{\Lambda}}_{\vec{p}} \tag{9}$$

And concentrating on the second part, and writing $\dot{\vec{p}} = \vec{F}$ we have:

$$\dot{r} = \nabla_{\vec{p}}\epsilon_{\vec{p}} + \vec{F}\times\nabla_{\vec{p}}\vec{\Lambda}_{\vec{p}} - \dot{\vec{\Lambda}}_{\vec{p}} \tag{10}$$

The first piece is the group velocity. But we see that when there is a nonzero Berry connection, there is an *anomalous velocity* normal to the force applied:

$$\vec{F}\times\nabla_{\vec{p}}\vec{\Lambda}_{\vec{p}} = \vec{F}\times\vec{\Omega}_{\vec{p}} \tag{11}$$

The newly defined $\vec{\Omega}_{\vec{p}}$ is called the Berry curvature. It is the dual, or analog, of the magnetic field.

When the system is also time dependent (fluctuating lattice, or something like that) we have another piece to the anomalous velocity:

$$\dot{\vec{\Lambda}}_{\vec{p}}, \tag{12}$$

which is the analog to the EMF due to a change in flux. This implies that the Berry connection is really a shift in the wave packet location:

$$\Delta\vec{r} = \vec{\Lambda}_{\vec{p}} \tag{13}$$

II. 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:

$$\hat{\mathcal{H}}_R^{spin} = \alpha p \vec{\sigma} \cdot \hat{\phi}_{\vec{p}} - B\sigma^z \tag{14}$$

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

$$\vec{\Lambda}_{\vec{p}} = i \langle \vec{p} | \nabla_{\vec{p}} | \vec{p} \rangle \tag{15}$$

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:

$$\vec{\Lambda}_{\vec{p}} = i \langle \vec{p} | \frac{\hat{\phi}_{\vec{p}}}{|p|} \frac{\partial}{\partial \phi_{\vec{p}}} | \vec{p} \rangle = \hat{\phi}_{\vec{p}} \frac{1 - \cos\theta_p}{2} \tag{16}$$

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

$$\cos\theta = \frac{b}{\sqrt{\alpha^2 p^2 + b^2}} \tag{17}$$

So:

$$\vec{\Lambda}_{\vec{p}} = \hat{\phi}_{\vec{p}} \frac{1 - \frac{b}{\sqrt{\alpha^2 p^2 + b^2}}}{2p} \tag{18}$$

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:

$$\delta r = \vec{\Lambda}_{\vec{p}}^{exc} - \vec{\Lambda}_{\vec{p}}^{0} - \nabla_{\vec{p}}(arg(V_{ge})) \tag{19}$$

This electronic motion gives rise to the *shift current*

B. Anomalous velocity

What is the Berry curvature? It is:

$$\Omega_{\vec{p}} = \nabla_{\vec{p}} \times \vec{\Lambda}_{\vec{p}} \tag{20}$$

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

$$\Omega_{\vec{p}} = \left(\hat{p} \frac{\partial}{\partial p} + \hat{\phi}_{\vec{p}} \frac{1}{p} \frac{\partial}{\partial \phi} \right) \times (f(p) \hat{\phi}_{\vec{p}} \tag{21}$$

Both terms contribute, and we obtain:

$$= \hat{p} \times \hat{\phi} \frac{\partial f}{\partial p} - \hat{\phi} \times \hat{p} f(p) \tag{22}$$

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

$$= \hat{z} \left(\frac{\partial f(p)}{\partial p} + \frac{f(p)}{p} \right) = \hat{z} \frac{1}{p} \frac{\partial (p f(p))}{\partial p} \tag{23}$$

and finally:

$$\vec{\Omega}_{\vec{p}} = \hat{z}\frac{b\alpha^2}{(b^2+\alpha^2p^2)^{3/2}} \tag{24}$$

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

$$\Omega_0 = \frac{\alpha^2}{b^2} \tag{25}$$

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

$$\dot{r} = \frac{\partial \epsilon_{p(t)}}{\partial p} + \dot{\vec{p}} \times (\hat{z}\Omega_p) \tag{26}$$

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III. 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:

$$\hat{\mathcal{H}} = \frac{p^2}{2m} \tag{27}$$

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:

$$p = q/2 + \delta p. \tag{28}$$

Then:

$$\hat{\mathcal{H}}_{\delta p}\begin{pmatrix} \psi_{q/2+\delta p} \\ \psi_{-q/2+\delta p}\end{pmatrix} = \begin{pmatrix} \frac{(q/2+\delta p)^2}{2m} & ge^{i\phi} \\ ge^{-i\phi} & \frac{(-q/2+\delta p)^2}{2m}\end{pmatrix}\begin{pmatrix} \psi_{q/2+\delta p} \\ \psi_{-q/2+\delta p}\end{pmatrix} \tag{29}$$

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:

$$\hat{\mathcal{H}}_k = v\sigma^z k + g(\cos\phi\sigma^x + \sin\phi\sigma^y) \tag{30}$$

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

$$\hat{\mathcal{H}}_k = v\sigma^z k + g\sigma^x \tag{31}$$

We see a gap open, with energies:

$$E_\pm = \pm\sqrt{v^2k^2+g^2} \tag{32}$$

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

$$n = \int_{-q/2}^{q/2} \frac{dp}{2\pi} = \frac{q}{2\pi} = \frac{1}{a} \tag{33}$$

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:

$$\vec{\sigma}_k = -\frac{1}{\sqrt{v^2k^2+g^2}}(g\hat{x}+vk\hat{z}) \tag{34}$$

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

$$\cos(qx+\phi) = \cos(q(x+a\frac{\phi}{2\pi})) \tag{35}$$

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:

$$\vec{\sigma}_k = -\frac{1}{\sqrt{v^2k^2+g^2}}(g\hat{x}\cos\phi + g\hat{y}\sin\phi + vk\hat{z}). \tag{36}$$

How do we see this from the band structure? You guessed it. Berry phase. We would like to trace the shift in location as we change ϕ. Recall that the location operator is given by:

$$x = i\frac{\partial}{\partial k} + i\langle k|\frac{\partial}{\partial k}|k\rangle \tag{37}$$

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:

$$\langle x\rangle = \frac{1}{q}\int\limits_{-q/2}^{q/2}\frac{dk}{2\pi}i\langle k|\frac{\partial}{\partial k}|k\rangle \tag{38}$$

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

$$\Delta x = \int\limits_0^{2\pi} d\phi\frac{\partial}{\partial\phi}\frac{1}{q}\int\limits_{-q/2}^{q/2}\frac{dk}{2\pi}i\langle k|\frac{\partial}{\partial k}|k\rangle \tag{39}$$

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:

$$|k\rangle \to |k\rangle e^{i\lambda_\phi},\ \frac{\partial\lambda_\phi}{\partial\phi} = i\langle k|\frac{\partial}{\partial\phi}|k\rangle \tag{40}$$

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

$$\Delta x = \int\limits_0^{2\pi} d\phi\frac{\partial}{\partial\phi}\frac{1}{q}\int\limits_{-q/2}^{q/2} dki\left(e^{-i\lambda_\phi}\langle k|\frac{\partial}{\partial k}\left(|k\rangle e^{i\lambda_\phi}\right)\right) \tag{41}$$

Just doing the algebra yields:

$$= \frac{1}{2\pi q}\int d\phi\int dk\left(\frac{\partial\Lambda_k}{\partial\phi} - \frac{\partial^2}{\partial k\partial\phi}\lambda_\phi\right) \tag{42}$$

but we recognize:

$$\frac{\partial \lambda_\phi}{\partial \phi} = i \langle k| \frac{\partial}{\partial \phi} |k\rangle = \Lambda_\phi \tag{43}$$

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

$$= \frac{2\pi}{q} \int \frac{d\phi}{2\pi} \int dk \left(\frac{\partial \Lambda_k}{\partial \phi} - \frac{\partial}{\partial k} \Lambda_\phi \right) = a \int \frac{d\phi}{2\pi} \int dk \hat{z} \cdot \nabla_{k,\phi} \times \vec{\Lambda} \tag{44}$$

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:

$$\Omega = \hat{z} \cdot \nabla_{k,\phi} \times \vec{\Lambda} \tag{45}$$

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

But what is finally the result?

$$\Lambda_k = 0,\, \Lambda_\phi = \frac{1}{2}(1 - \cos\theta) = \frac{1}{2}(1 - \langle \sigma^z \rangle) \tag{46}$$

And the final displacement upona shift by 2π is:

$$a \frac{d\phi}{2\pi} \int dk (-\frac{\partial}{\partial k}) \Lambda_\phi(k) = a \cdot (\Lambda_{-k_{max}} - \Lambda_{k_{max}}) = a \tag{47}$$

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.