I. SPIN ORBIT COUPLING

So far the spin has played a rather secondary role. We would just multiply the number of states by 2. For a long time, however, we knew that spin plays a strong role in the behavior of electronic devices at low temperatures. Now we also know that it plays a very strong role in determining the nature of materials - particularly topological insulators. This story begins with spin orbit coupling.

A. Relativistic effects on electronic motion

Electrons are rather hardy particles. They move in an environemnt with strong fluctuations of an electric field - of the order of volts per angstrom, $E \sim 10^{10} V/m$. And they are moving fast. On top of that, they have a spin. Let's parse all of these facts.

The spin we already discussed. There is a term of the hamiltonian of electrons which is:

$$H = -\gamma \hat{\vec{S}} \cdot \vec{B} \tag{1}$$

with $\gamma = g\frac{e}{2m}$, and g the gyro magnetic ratio.

What happens when something moves quickly through an electric field? It'll see a magnetic field. How much? We can derive it thinking of an electric field produced by a charged plane:

$$E = \frac{\sigma}{\epsilon_0} \tag{2}$$

If the electron moves relative to this plane, from the perspective of the electron, the plane is moving, and has a current:

$$j = \sigma v \tag{3}$$

and therefore the electron sees a magnetic field normal to the motion, and electric field, with magnitude:

$$B = \mu_0 j = \mu_0 v \sigma_v \tag{4}$$

Now, I put σ_v since there is another effect - Lorentz contraction - which changes the effective density of the plane: $\sigma_v = \frac{1}{\sqrt{1-v^2/c^2}}\sigma = \frac{\epsilon_0 E}{\sqrt{1-v^2/c^2}}$. So the electron sees a magnetic field:

$$B = \frac{\mu_0 \epsilon_0 E v}{\sqrt{1-v^2/c^2}} = \frac{\vec{E} \times \vec{v}/c^2}{\sqrt{1-v^2/c^2}} \tag{5}$$

What is the magnitude of this field? Electrons in metals move with speeds of the order $v \sim 10^6 m/s$. The relativistic $1/\sqrt{1-v^2/c^2} \approx 1$. It looks like the resulting field wilil be small , because of the relatively low electronic velocity. But it is enough to produce:

$$B_{SO} \sim 10^{10} V/m \frac{10^6 m/s}{9 \cdot 10^{16} m^2/s^2} \approx 0.1T \tag{6}$$

For electrons with a gyromagnetic factor $g = 2$ this implies an energy of the order of $0.1K$. This is the origin of spin-orbit effects.

B. Dresselhaus interaction

What kind of interaction can we expect for electrons in materials? In bulk materials, the electric field averages to zero, so we don't expect, a priori, a strong effect linear in momentum. But higher orders of electric field in non-inversion-symmetric lattices Also, in the absence of time-reversal symmetry breaking fields, like a magnetic field, the Hamiltonian must be time-reversal symmetric. Since spin and momentum are odd under time-reversal, the total power of momentum and spin must be even. Millie and Gene Dresselhaus suggested that the leading spin-orbit interaction in Zincblende lattices (like GaAs, which is a standard semiconductor for the study of low-diensional electronic phases) consistent with the lattice structure and the origin of the effect is third order in momentum:

$$H_{Dresselhaus} = \beta \left(p_x \sigma^x (p_y^2 - p_z^2) + p_y \sigma^y (p_z^2 - p_x^2) + \beta p_z \sigma^z (p_x^2 - p_y^2) \right) \tag{7}$$

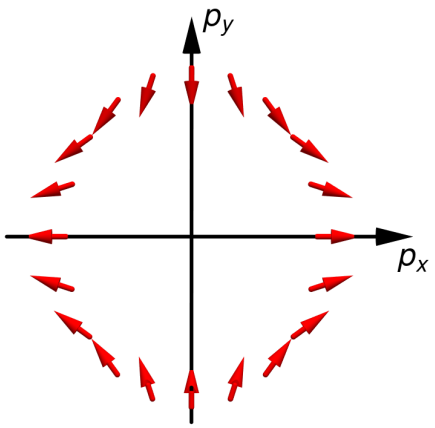

FIG. 1. The spin configuration with Dresselhaus interaction as a function of p_x and p_y for a quantum well or a 3d electron gas for momenta near the 'north-pole' of the Fermi sphere.

The effect on bulk systems is a bit murky due to the large power of momentum. But if we concenterate say on electrons close to the north pole of the fermi sphere, $p_z = p_F$, we see that this interaction reduces to:

$$H_{Dresselahus} = \lambda_D(-p_x\sigma^x + p_y\sigma^y). \tag{8}$$

This makes for a spin pattern that makes an anti-vortex about the fermi sphere north pole.

This effect becomes even more pronounced in 2d heterostructures. Such 2d structures could be made by layering semiconductors with different doping such that electons (or holes) are only present in a thin layer between undoped, or oppositely doped semiconductors. The electronic states bound in such heterostructures have a finite z momentum by virtue of being a standing wave between the two boundaries of the layer. Therefore such a layer will have a significant Dresselhaus interaction linear in the in-plane momenta. The strength of this coupling is typically of the order:

$$\beta_{GaAs} \approx 30eV\mathring{A}^3 \tag{9}$$

in GaAs. But in materials with heavy atoms, like InAs, may actually have a much stronger Dresselhaus response of

$$\beta_{InAs} \approx 760eV\mathring{A}^3. \tag{10}$$

Why is it so much stronger? The electric fields that electrons see are stronger. How do we convert this to a planar 2d electron gas residing in a quantum well? Divide by the width of the quantum well:

$$\lambda_D = \frac{\beta}{w^2}. \tag{11}$$

And for $w = 50\mathring{A}$, this is $\lambda_D \sim 10meV\mathring{A}$ for GaAs, or as strong as $\lambda_D \sim 200meV\mathring{A}$ for In As.

C. Rashba SO interaction

But hang on a sec. If we have an electron gas confined to a 2d quantum well, there are also fields associated with the confinement perpendicular to the plane. If the well is uneven, there might be a residual spin orbit interaction arising from this field. This interaction is named after Emmanuel Rashba. It has the form:

$$H_{Rashba} = \alpha\hat{z}\cdot\left(\vec{p}\times\hat{\vec{\sigma}}\right) = \alpha(\sigma^x p_y - \sigma^y p_x). \tag{12}$$

α varies between structures, but has a typical scale of $\alpha = 50 - 100meV\mathring{A}$. Note that the this interaction simply wants the spin locked to the perpendicular to the direction of the momentum.

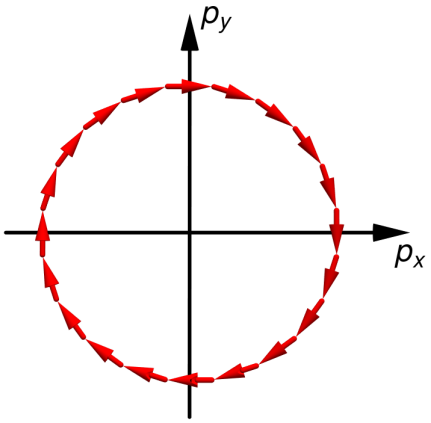

FIG. 2. The spin configuration as a function of p_x and p_y for a quantum well with Rashba interaction.

D. 2DEG with Rashba and magnetic field

For electrons in a quantum well, we expecet a kinetic energy of $H = p^2/2m$. In the presence of Rashba, however, this becomes:

$$H = \frac{p^2}{2m} + \alpha(\sigma^x p_y - \sigma^y p_x) \tag{13}$$

How do we solve this? For every momentum the spin could be pointing clockwise or counterclockwise: $\eta = (\hat{p} \times \vec{\sigma}) \cdot z$ and $\langle \sigma \rangle = \eta \hat{\phi}$, with $\hat{\phi}$ the angular direction in the plane, nad $\eta = \pm 1$ is the helicity of the electrons. Therefore, the electrons split into two branches:

$$H_{\vec{p}} = \frac{\vec{p}^2}{2m} \pm \alpha |\vec{p}| \tag{14}$$

Near zero energ, this is a Dirac cone! $E \approx \pm \alpha p$, with α being a velocity. If we translate the energy to an inverse time ($\hbar = 1$ was used...):

$$v_\alpha = \alpha/\hbar \sim 10^4 m/s. \tag{15}$$

This band structure describes a semi-metal. No gap, but there is a point of vanishing density of states.

The Dirac point is special. It has spin winding about it. Let's add a magnetic field in the z direction. Such a field mixes the two *helicities*. Near the degeneracy point, the electrons obey the hamiltonian:

$$H_{\vec{p}} = \alpha |\vec{p}| \hat{\phi}_{\vec{p}} \cdot \vec{\sigma} - B\gamma\sigma^z. \tag{16}$$

At $p = 0$ the magnetic field will split the degeneracy into a conduction band bottom and valence band top, with energies $\pm\gamma B$, with the spin pointing in the z or $-z$ direction. At larger momenta, the spin tends back to the plane. This is going to be important in the coming discussion. The energy of finite-momentum states is then:

$$E \approx \sqrt{\alpha^2 p^2 + \gamma^2 B^2}. \tag{17}$$

II. BERRY CONNECTION EFFECTS

A. Berry phases

Quantum mechanics has a lot of geometry in it. Using momentum states makes things look so simple, that the geometry is a bit obscured. Let's recover some of the lost complexity.

Consider a quantum system, with a state continuously parametrized by a parameter $0 \leq \alpha \leq 1$, $|\psi(\alpha)\rangle$ with:

$$|\psi(0)\rangle = |\psi(1)\rangle\,. \tag{18}$$

So that the state returns to the original one after a full cycle. While α parametrizes the continuous state family $|\psi(L)\rangle$, it does not yet describe the time evolution of the system. Let's assume a hamiltonian:

$$H = -\epsilon \left|\alpha(t)\right\rangle \left\langle\alpha(t)\right| \tag{19}$$

and that at $t = 0$, $\alpha = 0$ and $|\psi\rangle = |\psi(\alpha = 0)\rangle$. As time progresses, α changes. Let us assume that α changes very slowly in time. This assumption of adiabaticity allows us to expect that the wavefunction will follow the states $|\psi(\alpha(t))\rangle$ closley. But is the solution for the time depndence:

$$|\psi(t)\rangle = |\alpha(t)\rangle\, e^{i\epsilon t}? \tag{20}$$

Let's substitute into the SE. We expect:

$$i\frac{\partial \left|\psi\right\rangle}{\partial t} = -\epsilon \left|\alpha(t)\right\rangle \left\langle\alpha(t)\right| \cdot \left|\psi(t)\right\rangle \tag{21}$$

and the two sides of the equation become (canceling the exponent between the sides):

$$RHS = -\epsilon \left|\alpha(t)\right\rangle \tag{22}$$

but:

$$LHS = -\epsilon \left|\alpha(t)\right\rangle + i\frac{\partial \left|\alpha(t)\right\rangle}{\partial t} \tag{23}$$

That last term shouldn't be there! Let's see. We are neglecting the possibility of exciting the state to something that is orthogonal to $\alpha(t)$. This is the assumption of adiabaticity. But there might be a component of the time derivative $\frac{\partial|\alpha(t)\rangle}{\partial t}$ along the direction of $|\alpha(t)\rangle$. How would we handle that?

Looks like we need to modify our assumption to something like:

$$|\psi(t)\rangle = |\alpha(t)\rangle\, e^{i\epsilon t} \cdot e^{-i\lambda(t)}. \tag{24}$$

With this we would have:

$$\left\langle\alpha(t)\right| LHS = -\epsilon + i \left\langle\alpha(t)\right| \frac{\partial \left|\alpha(t)\right\rangle}{\partial t} + \frac{\partial \lambda}{\partial t} = \left\langle\alpha(t)\right| RHS = -\epsilon \tag{25}$$

and ultimately:

$$\frac{\partial \lambda}{\partial t} = -i \left\langle\alpha(t)\right| \frac{\partial \left|\alpha(t)\right\rangle}{\partial t} \tag{26}$$

$\lambda(t)$ is the Berry phase.

B. Spin berry phase

The best place to explore the effects of this Berry phase is with spin. For instance, we could conisder an electron in the 2d quantum well with Rashba interaction (Eq. 13) that starts in the low energy state at momentum $\vec{p} = p_0(\hat{x}\cos(\beta) + \hat{y}\sin(\beta))$, and let $\beta(t) = 2\pi t/T$ for $0 < t < T$. with $T^{-1} \ll \alpha p_0$.

A spin that points in the Euler angles θ to the z-axis, and when projected to the x-y plane forms an angle ϕ to the x axis has the spinor:

$$|\theta, \phi\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix} \tag{27}$$

Let's not have any prejudices regarding the directions of the spin as a function of time, and just assume a trajectory $\theta(t), \phi(t)$. Then the Berry phase for the evolution is:

$$\frac{\partial \lambda}{\partial t} = -i \left\langle\theta(t), \phi(t)\right| \frac{\partial \left|\theta(t), \phi(t)\right\rangle}{\partial t}. \tag{28}$$

Clearlt we need to calculate the time derivative:

$$\frac{\partial \left|\theta(t),\phi(t)\right\rangle}{\partial t} = \frac{\dot{\theta}}{2}\begin{pmatrix} \sin\frac{\theta}{2} \\ e^{i\phi}\cos\frac{\theta}{2}\end{pmatrix} + i\dot{\phi}\begin{pmatrix} 0 \\ e^{i\phi}\sin\frac{\theta}{2}\end{pmatrix} \tag{29}$$

Contracting this result with the bra $\langle\theta,\phi|$ then gives:

$$\langle\theta,\phi|\frac{\partial \left|\theta(t),\phi(t)\right\rangle}{\partial t} = \dot{\phi}e^{i\phi}\sin^2\frac{\theta}{2} = i\dot{\phi}\frac{1-\cos\theta(t)}{2}. \tag{30}$$

This is a neat little result. You can get a sense for it if you think of a spin that starts off at the $\hat{z}$ direction ($\theta=\phi=0$) and, say, goes down to the $\hat{x}$ ($\theta=\pi/2,\phi=0$) direction, then to the $\hat{y}$ ($\theta=\pi/2,\phi=\pi/2$)direction, and back to $\hat{z}$ ($\theta=0,\phi=\pi/2$), and then don't forget to bring ϕ back! Go to $\theta=\phi=0$. What do we get? For the first part and last two parts - nothing. $\dot{\phi}=0$ in the first and third segments. On the last segment $1-\cos\theta=0$. In the second one, though, we have:

$$\frac{\partial\lambda}{\partial t} = \frac{1}{2}\dot{\phi}(1-\cos(\pi/2) = \frac{1}{2}\dot{\phi} \tag{31}$$

Actually, here is a better interpretation:

$$\frac{\partial\lambda}{\partial t} = \dot{\phi}\int_0^{\pi/2} d\theta\sin\theta \rightarrow \lambda = \int_0^{\pi/2} d\phi\int_0^{\pi/2}\sin\theta d\theta. \tag{32}$$

Why is that better? Clearly this is the solid angle of the spin's motion! Well, divided by 2. Spin-1/2 after all... For the octant marked, we get:

$$\lambda = \frac{\pi/2}{2} = \pi/4. \tag{33}$$

If we were to cover the whole sphere, we would get $4\pi/2$.

Now we can do the Berry phase for the circlig electron in the Rashba quantum well. $\theta=\pi/2$, and $\Delta\phi=2\pi$. We get the solid angle of half a sphere, divided by 2:

$$\lambda = \frac{\Delta\phi}{2} = \pi \tag{34}$$

Neat. The spin wave function changes sign after this turn. Again, should be familiar - spin-1/2!

C. 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:

$$\left|\psi(t)\right\rangle = \psi(t)\left|p(t)\right\rangle \tag{35}$$

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:

$$i\left\langle p(t)\right|\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = i\frac{\partial\psi(t)}{\partial t} + \psi(t)i\left\langle p(t)\right|\frac{\partial}{\partial t}\left|p(t)\right\rangle = \epsilon_p\psi(t) \tag{36}$$

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

$$i\left\langle p(t)\right|\frac{\partial}{\partial t}\left|p(t)\right\rangle = \dot{\vec{p}}i\left\langle p(t)\right|\frac{\partial}{\partial\vec{p}}\left|p(t)\right\rangle \tag{37}$$

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

$$\psi(p,t)\rightarrow\psi(p,t)e^{i\int^{\vec{p}}d\vec{p}\cdot\Lambda_{\vec{p}}} \tag{38}$$

with

$$\vec{\Lambda}_{\vec{p}} = i \langle p | \nabla_p | p \rangle \tag{39}$$

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:

$$\psi(r,t) \to \psi(r,t) e^{ie \int^{\vec{r}} d\vec{r} \cdot \vec{A}}. \tag{40}$$

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

$$\dot{p} = -\nabla_{\vec{r}} V(\vec{r}),\ \dot{r} = \nabla_{\vec{p}} \epsilon_{\vec{p}} \tag{41}$$

With the vector potential we would have:

$$\dot{p} = -\nabla_{\vec{r}} V(\vec{r}) + e\dot{r} \times \left(\nabla_{\vec{r}} \times \vec{A} \right) - e\dot{\vec{A}},\ \dot{r} = \nabla_{\vec{p}} \epsilon_{\vec{p}} \tag{42}$$

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:

$$\dot{p} = -\nabla_{\vec{r}} V(\vec{r}) + e\dot{r} \times \left(\nabla_{\vec{r}} \times \vec{A} \right) - e\dot{\vec{A}},\ \dot{r} = \nabla_{\vec{p}} \epsilon_{\vec{p}} - \dot{p} \times \left(\nabla_{\vec{p}} \times \vec{\Lambda}_{\vec{p}} \right) + \dot{\vec{\Lambda}}_{\vec{p}} \tag{43}$$

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

$$\dot{r} = \nabla_{\vec{p}} \epsilon_{\vec{p}} + \vec{F} \times \left(\nabla_{\vec{p}} \times \vec{\Lambda}_{\vec{p}} \right) - \dot{\vec{\Lambda}}_{\vec{p}} \tag{44}$$

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:

$$\vec{F} \times \left(\nabla_{\vec{p}} \times \vec{\Lambda}_{\vec{p}} \right) = \vec{F} \times \vec{\Omega}_{\vec{p}} \tag{45}$$

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:

$$\dot{\vec{\Lambda}}_{\vec{p}}, \tag{46}$$

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:

$$\Delta \vec{r} = \vec{\Lambda}_{\vec{p}} \tag{47}$$