

I. 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:

$$|\psi(0)\rangle = |\psi(1)\rangle. \quad (1)$$

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:

$$H = -\epsilon |\alpha(t)\rangle \langle \alpha(t)| \quad (2)$$

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 $|\psi(\alpha(t))\rangle$ closely. But is the solution for the time dependence:

$$|\psi(t)\rangle = |\alpha(t)\rangle e^{i\epsilon t} \quad (3)$$

Let's substitute into the SE. We expect:

$$i \frac{\partial |\psi\rangle}{\partial t} = -\epsilon |\alpha(t)\rangle \langle \alpha(t)| \cdot |\psi(t)\rangle \quad (4)$$

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

$$RHS = -\epsilon |\alpha(t)\rangle \quad (5)$$

but:

$$LHS = -\epsilon |\alpha(t)\rangle + i \frac{\partial |\alpha(t)\rangle}{\partial t} \quad (6)$$

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:

$$|\psi(t)\rangle = |\alpha(t)\rangle e^{i\epsilon t} \cdot e^{i\lambda(t)}. \quad (7)$$

With this we would have:

$$\langle \alpha(t) | LHS = -\epsilon + i \langle \alpha(t) | \frac{\partial |\alpha(t)\rangle}{\partial t} - \frac{\partial \lambda}{\partial t} = \langle \alpha(t) | LHS = -\epsilon \quad (8)$$

and ultimately:

$$\frac{\partial \lambda}{\partial t} = i \langle \alpha(t) | \frac{\partial |\alpha(t)\rangle}{\partial t} \quad (9)$$

$\lambda(t)$ 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 consider an electron in the 2d quantum well with Rashba interaction (Eq. ??) 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 $T^{-1} \gg \alpha p_0$.

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:

$$|\theta, \phi\rangle = \begin{pmatrix} \cos \frac{\theta}{2} \\ e^{-i\phi} \sin \frac{\theta}{2} \end{pmatrix} \quad (10)$$

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:

$$\frac{\partial \lambda}{\partial t} = i \langle \theta(t), \phi(t) | \frac{\partial |\theta(t), \phi(t)\rangle}{\partial t}. \quad (11)$$

Clearly we need to calculate the time derivative:

$$\frac{\partial |\theta(t), \phi(t)\rangle}{\partial t} = \frac{\dot{\theta}}{2} \begin{pmatrix} \sin \frac{\theta}{2} \\ e^{-i\phi} \cos \frac{\theta}{2} \end{pmatrix} - i\dot{\phi} \begin{pmatrix} 0 \\ e^{-i\phi} \sin \frac{\theta}{2} \end{pmatrix} \quad (12)$$

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

$$\langle \theta, \phi | \frac{\partial |\theta(t), \phi(t)\rangle}{\partial t} = -\dot{\phi} e^{-i\phi} \sin^2 \frac{\theta}{2} = -i\dot{\phi} \frac{1 - \cos \theta(t)}{2}. \quad (13)$$

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:

$$\frac{\partial \lambda}{\partial t} = \frac{1}{2} \dot{\phi} (1 - \cos(\pi/2)) = \frac{1}{2} \dot{\phi} \quad (14)$$

Actually, here is a better interpretation:

$$\frac{\partial \lambda}{\partial t} = \dot{\phi} \int_0^{\pi/2} d\theta \sin \theta \rightarrow \lambda = \int_0^{\pi/2} d\phi \int_0^{\pi/2} \sin \theta d\theta. \quad (15)$$

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:

$$\lambda = \frac{\pi/2}{2} = \pi/4. \quad (16)$$

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

Now we can do the Berry phase for the circling 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:

$$\lambda = \frac{\Delta\phi}{2} = \pi \quad (17)$$

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 forced through a funny motion. But in fact, we were looking at a more general problem. We had a wave function for a momentum state:

$$|\psi(t)\rangle = \psi(t) |p(t)\rangle \quad (18)$$

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:

$$i \langle p(t) | \frac{\partial}{\partial t} | \psi(t) \rangle = i \frac{\partial \psi(t)}{\partial t} + \psi(t) i \langle p(t) | \frac{\partial}{\partial t} | p(t) \rangle = \epsilon_p \psi(t) \quad (19)$$

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

$$i \langle p(t) | \frac{\partial}{\partial t} | p(t) \rangle = \dot{\vec{p}}^i \langle p(t) | \frac{\partial}{\partial \vec{p}^i} | p(t) \rangle \quad (20)$$

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

$$\psi(p, t) \rightarrow \psi(p, t) e^{-i \int^{\vec{p}} d\vec{p} \cdot \vec{\Lambda}_{\vec{p}}} \quad (21)$$

with

$$\vec{\Lambda}_{\vec{p}} = -i \langle p | \nabla_p | p \rangle \quad (22)$$

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:

$$\psi(r, t) \rightarrow \psi(r, t) e^{ie \int^{\vec{r}} d\vec{r} \cdot \vec{A}}. \quad (23)$$

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

$$\dot{p} = -\nabla_{\vec{r}} V(\vec{r}), \quad \dot{r} = \nabla_{\vec{p}} \epsilon_{\vec{p}} \quad (24)$$

With the vector potential we would have:

$$\dot{p} = -\nabla_{\vec{r}} V(\vec{r}) + e\dot{r} \times \nabla_{\vec{r}} \vec{A} - e\dot{\vec{A}}, \quad \dot{r} = \nabla_{\vec{p}} \epsilon_{\vec{p}} \quad (25)$$

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 \vec{r} side of the equation. This would give:

$$\dot{p} = -\nabla_{\vec{r}} V(\vec{r}) + e\dot{r} \times \nabla_{\vec{r}} \vec{A} - e\dot{\vec{A}}, \quad \dot{r} = \nabla_{\vec{p}} \epsilon_{\vec{p}} - \dot{p} \times \nabla_{\vec{p}} \vec{\Lambda}_{\vec{p}} + \dot{\vec{\Lambda}}_{\vec{p}} \quad (26)$$

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

$$\dot{r} = \nabla_{\vec{p}} \epsilon_{\vec{p}} - \vec{F} \times \nabla_{\vec{p}} \vec{\Lambda}_{\vec{p}} + \dot{\vec{\Lambda}}_{\vec{p}} \quad (27)$$

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:

$$-\vec{F} \times \nabla_{\vec{p}} \vec{\Lambda}_{\vec{p}} = -\vec{F} \times \vec{\Omega}_{\vec{p}} \quad (28)$$

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:

$$\dot{\vec{\Lambda}}_{\vec{p}}, \quad (29)$$

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:

$$\Delta \vec{r} = \vec{\Lambda}_{\vec{p}} \quad (30)$$