Dynamics of Electrons in Energy Bands from Gauge Invariance
Berry's Phase and Berry's Curvature

In this lecture you will learn:

- Electron dynamics using gauge invariance arguments
- Berry's phase and Berry's curvature in solid state physics

Electron Dynamics from Gauge Invariance

Consider the Schrodinger equation for an electron in a solid:

$$\left[\frac{\hat{\vec{P}}^2}{2m}+V\left(\hat{\vec{r}}\right)\right]\psi(\vec{r},t)=i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}$$

We have seen that the stationary solutions are the Bloch states:

$$\left[\frac{\hat{\vec{P}}^2}{2m}+V\left(\hat{\vec{r}}\right)\right]\psi_{n,\vec{k}}(\vec{r})=E_n\left(\vec{k}\right)\psi_{n,\vec{k}}(\vec{r})$$

Or since: $\psi_{n,\vec{k}}(\vec{r})=\dfrac{e^{i\vec{k}.\vec{r}}}{\sqrt{V}}u_{n,\vec{k}}(\vec{r})$

$$\Rightarrow\left[\frac{\left(\hat{\vec{P}}+\hbar\vec{k}\right)^2}{2m}+V\left(\hat{\vec{r}}\right)\right]u_{n,\vec{k}}(\vec{r})=E_n\left(\vec{k}\right)u_{n.\vec{k}}(\vec{r})$$

In the presence of electromagnetic vector and scalar potentials the time-dependent Schrodinger equation becomes:

$$\left[\frac{\left(\hat{\vec{P}}+e\vec{A}\left(\hat{\vec{r}},t\right)\right)^2}{2m}+V\left(\hat{\vec{r}}\right)-e\phi\left(\hat{\vec{r}},t\right)\right]\psi(\vec{r},t)=i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}$$

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$$\left[\frac{\left(\hat{\vec{P}}+e\vec{A}\left(\hat{\vec{r}},t\right)\right)^2}{2m}+V\left(\hat{\vec{r}}\right)-e\phi\left(\hat{\vec{r}},t\right)\right]\psi(\vec{r},t)=i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}$$

The Schrodinger equation is invariant (i.e. does not change) under the following gauge transformation:

$$\vec{A}\left(\hat{\vec{r}},t\right)\to\vec{A}\left(\hat{\vec{r}},t\right)+\nabla f\left(\hat{\vec{r}},t\right)$$

$$\phi\left(\hat{\vec{r}},t\right)\to\phi\left(\hat{\vec{r}},t\right)-\frac{\partial f\left(\hat{\vec{r}},t\right)}{\partial t}$$

$$\psi(\vec{r},t)\to e^{-i\frac{e}{\hbar}f(\vec{r},t)}\psi(\vec{r},t)$$

Now get back to the problem of an electron in an applied electric field. The Schrodinger equation is:

$$\left[\frac{\hat{\vec{P}}^2}{2m}+V\left(\hat{\vec{r}}\right)+e\vec{E}.\hat{\vec{r}}\right]\psi(\vec{r},t)=i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}$$

Perform the following gauge transformation to eliminate the scalar potential in favor of the vector potential:

$$f(\vec{r},t)=-\vec{E}.\vec{r}\,t$$

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We get:

$$\left[\frac{\left(\hat{\vec{P}}-e\vec{E}t\right)^2}{2m}+V\left(\hat{\vec{r}}\right)\right]e^{i\frac{e}{\hbar}\vec{E}.\vec{r}t}\psi(\vec{r},t)=i\hbar\frac{\partial}{\partial t}e^{i\frac{e}{\hbar}\vec{E}.\vec{r}t}\psi(\vec{r},t)$$

Let:

$$\phi(\vec{r},t)=e^{i\frac{e}{\hbar}\vec{E}.\vec{r}t}\psi(\vec{r},t)$$

$$\Rightarrow\left[\frac{\left(\hat{\vec{P}}-e\vec{E}t\right)^2}{2m}+V\left(\hat{\vec{r}}\right)\right]\phi(\vec{r},t)=i\hbar\frac{\partial\phi(\vec{r},t)}{\partial t}$$

Now we have to solve a time-dependent equation BUT the Hamiltonian is now lattice periodic! Assume, in the spirit of Bloch's analysis, solution of the form:

$$\varphi(\vec{r},t)=\frac{e^{i\vec{k}.\vec{r}}}{\sqrt{V}}u(\vec{r},t)e^{-\frac{i}{\hbar}\int_0^t E(t')dt'}$$

And plug the assumed form in the above equation to get:

Electron Dynamics from Gauge Invariance

$$\left[\frac{\left(\hat{\vec{P}}+\hbar\vec{k}-e\vec{E}t\right)^2}{2m}+V\left(\hat{\vec{r}}\right)\right]u\left(\vec{r},t\right)=E\left(t\right)u\left(\vec{r},t\right)$$

We are ignoring time derivatives of $u\left(\vec{r},t\right)$

(Adiabaticity assumption)

If one now defines a time-dependent wavevector as follows:

$$\hbar\vec{k}(t)=\hbar\vec{k}-e\vec{E}t$$

Then the above equation is just the familiar equation for the periodic part of a Bloch function whose wavevector is time dependent:

$$\left[\frac{\left(\hat{\vec{P}}+\hbar\vec{k}(t)\right)^2}{2m}+V\left(\hat{\vec{r}}\right)\right]u_{n,\vec{k}(t)}(\vec{r})=E_n\left(\vec{k}(t)\right)u_{n,\vec{k}(t)}(\vec{r})$$

So the answer is:

$$\phi(\vec{r},t)=\frac{e^{i\vec{k}.\vec{r}}}{\sqrt{V}}u_{n,\vec{k}(t)}(\vec{r})e^{-\frac{i}{\hbar}\int_0^t E_n\left(\vec{k}(t')\right)dt'}$$

And finally the solution of the original problem is (as expected):

$$\psi(\vec{r},t)=e^{-i\frac{e}{\hbar}\vec{E}.\vec{r}t}\phi(\vec{r},t)=\frac{e^{i\vec{k}(t).\vec{r}}}{\sqrt{V}}u_{n,\vec{k}(t)}(\vec{r})e^{-\frac{i}{\hbar}\int_0^t E_n\left(\vec{k}(t')\right)dt'}=\psi_{n,\vec{k}(t)}(\vec{r})e^{-\frac{i}{\hbar}\int_0^t E_n\left(\vec{k}(t')\right)dt'}$$

Electron Dynamics and Berry's Phase

Note that the solution:

$$\phi(\vec{r},t)=\frac{e^{i\vec{k}.\vec{r}}}{\sqrt{V}}u_{n,\vec{k}(t)}(\vec{r})e^{-\frac{i}{\hbar}\int_0^t E_n\left(\vec{k}(t')\right)dt'}$$

$$\hbar\vec{k}(t)=\hbar\vec{k}-e\vec{E}t$$

is not an exact solution of the equation:

$$\left[\frac{\left(\hat{\vec{P}}-e\vec{E}t\right)^2}{2m}+V\left(\hat{\vec{r}}\right)\right]\phi(\vec{r},t)=i\hbar\frac{\partial\phi(\vec{r},t)}{\partial t}$$

It misses a very important phase factor even if the time dependence is not fast enough to cause transitions between states (adiabaticity). To capture this we try:

$$\phi(\vec{r},t)=\frac{e^{i\vec{k}.\vec{r}}}{\sqrt{V}}u_{n,\vec{k}(t)}(\vec{r})e^{-\frac{i}{\hbar}\int_0^t E_n\left(\vec{k}(t')\right)dt'+i\underbrace{\gamma_{n,\vec{k}}(t)}_{\text{Added phase}}}$$

Plugging it in, multiplying both sides by $u^*_{n,\vec{k}(t)}(\vec{r})$, integrating, and using the fact that:

$$\left[\frac{\left(\hat{\vec{P}}+\hbar\vec{k}(t)\right)^2}{2m}+V\left(\hat{\vec{r}}\right)\right]u_{n,\vec{k}(t)}(\vec{r})=E_n\left(\vec{k}(t)\right)u_{n,\vec{k}(t)}(\vec{r})$$

We get (PTO):

Electron Dynamics and Berry's Phase

$$\frac{\partial \gamma_{n,\vec{k}}(t)}{\partial t} = i\int d^d\vec{r}\, u^*_{n,\vec{k}(t)}(\vec{r})\frac{\partial}{\partial t}u_{n,\vec{k}(t)}(\vec{r}) = i\left\langle u_{n,\vec{k}(t)}\left|\frac{\partial}{\partial t}\right|u_{n,\vec{k}(t)}\right\rangle$$

$$\Rightarrow \gamma_{n,\vec{k}}(t) = i\int_{t=0}^{t} dt' \left\langle u_{n,\vec{k}(t')}\left|\frac{\partial}{\partial t'}\right|u_{n,\vec{k}(t')}\right\rangle = i\int_{\vec{q}=\vec{k}(t=0)}^{\vec{q}=\vec{k}(t)} \left\langle u_{n,\vec{q}}\left|\nabla_{\vec{q}}\right|u_{n,\vec{q}}\right\rangle . d\vec{q}$$

$$= \int_{\vec{q}=\vec{k}(t=0)}^{\vec{q}=\vec{k}(t)} \vec{A}_{n,q}. d\vec{q} \qquad \left\{ \vec{A}_{\vec{q}} = i\left\langle u_{n,\vec{q}}\left|\nabla_{\vec{q}}\right|u_{n,\vec{q}}\right\rangle \right.$$

The final complete solution is then:

$$\psi(\vec{r},t) = e^{-i\frac{e}{\hbar}\vec{E}.\vec{r}t}\phi(\vec{r},t) = \frac{e^{i\vec{k}(t).\vec{r}}}{\sqrt{V}}u_{n,\vec{k}(t)}(\vec{r})e^{-\frac{i}{\hbar}\int_0^t E_n(\vec{k}(t'))dt' + i\gamma_{n,\vec{k}}(t)}$$

$$= \psi_{n,\vec{k}(t)}(\vec{r})e^{-\frac{i}{\hbar}\int_0^t E_n(\vec{k}(t'))dt'} \underbrace{e^{i\gamma_{n,\vec{k}}(t)}}_{\text{Berry's phase}}$$

The extra phase factor is called the Berry's phase and appears in many places in physics (and in optics)

It is appropriate to write the Berry's phase as, $\gamma_{n,\vec{k}}(t) = \gamma_n(\vec{k}(t))$**, since it depends on the trajectory of the time-dependent wavevector in reciprocal space**

Bloch Velocity and Berry's Phase

The velocity of an electron packet in the presence of an E-field is not the same as in the absence of it

Consider an electron packet made up of the time-dependent Bloch functions:

$$\theta(\vec{r},t) = \int \frac{d^d\vec{k}}{(2\pi)^2} f(\vec{k})e^{-i\vec{k}.\vec{r}_o}\psi_{n,\vec{k}(t)}(\vec{r})e^{-\frac{i}{\hbar}\int_0^t E_n(\vec{k}(t'))dt' + i\gamma_n(\vec{k}(t))}$$

$$= \int \frac{d^d\vec{k}}{(2\pi)^2} f(\vec{k})e^{-i\vec{k}.\vec{r}_o}\frac{e^{i\vec{k}(t).\vec{r}}}{\sqrt{V}}u_{n,\vec{k}(t)}(\vec{r})e^{-\frac{i}{\hbar}\int_0^t E_n(\vec{k}(t'))dt' + i\gamma_n(\vec{k}(t))}$$

Assume that the function $f(\vec{k})$ **peaks when** $\vec{k} = \vec{k}_o$

Lets first look at this packet at time t **= 0:**

$$\theta(\vec{r},t=0) = \int \frac{d^d\vec{k}}{(2\pi)^2} f(\vec{k})e^{-i\vec{k}.\vec{r}_o}\frac{e^{i\vec{k}.\vec{r}}}{\sqrt{V}}u_{n,\vec{k}}(\vec{r})$$

Where is the packet sitting in space at time t **= 0?**

Bloch Velocity and Berry's Phase

Where is the packet sitting in space at time $t = 0$?

$$\theta\left(\vec{r},t=0\right)=\int\frac{d^d\vec{k}}{(2\pi)^2}f\left(\vec{k}\right)e^{-i\vec{k}.\vec{r}_o}\,\frac{e^{i\vec{k}.\vec{r}}}{\sqrt{V}}\,u_{n,\vec{k}}\left(\vec{r}\right)$$

One would be inclined to say at $\vec{r}_o$!

Because if one looks at the gradient of the phase w.r.t. $\vec{k}$, evaluates it at $\vec{k}_o$, and sets it equal to zero, one obtains: $\vec{r}=\vec{r}_o$

However, this argument would work if the Bloch function did not carry a phase factor ……but it does!

This Bloch function phase can be cancelled if the following phase is added to our packet:

$$\phi_{n,\vec{k}}=\int^{\vec{k}}\vec{A}_{n,q}.d\vec{q}$$

$$\theta\left(\vec{r},t=0\right)=\int\frac{d^d\vec{k}}{(2\pi)^2}f\left(\vec{k}\right)e^{-i\vec{k}.\vec{r}_o}e^{i\phi_{n,\vec{k}}}\,\frac{e^{i\vec{k}.\vec{r}}}{\sqrt{V}}\,u_{n,\vec{k}}\left(\vec{r}\right)$$

Finally, at time t=0, the packet is sitting at $\vec{r}_o$! We will work with this packet now.

Bloch Velocity and Berry's Phase

Now at time t:

$$\theta\left(\vec{r},t\right)=\int\frac{d^d\vec{k}}{(2\pi)^2}f\left(\vec{k}\right)e^{-i\vec{k}.\vec{r}_o}e^{i\phi_{n,\vec{k}}}\,\frac{e^{i\vec{k}(t).\vec{r}}}{\sqrt{V}}\,u_{n,\vec{k}(t)}\left(\vec{r}\right)e^{-\frac{i}{\hbar}\int_0^t E_n\left(\vec{k}(t')\right)dt'+i\gamma_n\left(\vec{k}(t)\right)}$$

We again write it as:

$$\theta\left(\vec{r},t\right)=\int\frac{d^d\vec{k}}{(2\pi)^2}f\left(\vec{k}\right)e^{-i\vec{k}.\vec{r}_o}e^{i\left(\phi_{n,\vec{k}}-\phi_{n,\vec{k}(t)}\right)}\,\frac{e^{i\vec{k}(t).\vec{r}}}{\sqrt{V}}\,\underbrace{u_{n,\vec{k}(t)}\left(\vec{r}\right)e^{i\phi_{n,\vec{k}(t)}}}_{\text{Phase of the Bloch function has been cancelled}}e^{-\frac{i}{\hbar}\int_0^t E_n\left(\vec{k}(t')\right)dt'+i\gamma_n\left(\vec{k}(t)\right)}$$

Now:

$$\phi_{n,\vec{k}}-\phi_{n,\vec{k}(t)}+\gamma_n\left(\vec{k}(t)\right)=\int^{\vec{q}=\vec{k}}\vec{A}_{n,q}.d\vec{q}+\int_{\vec{q}=\vec{k}}^{\vec{q}=\vec{k}-e\vec{E}t/\hbar}\vec{A}_{n,q}.d\vec{q}-\int^{\vec{q}=\vec{k}-e\vec{E}t/\hbar}\vec{A}_{n,q}.d\vec{q}$$

$$\Rightarrow\nabla_{\vec{k}}\left[\phi_{n,\vec{k}}-\phi_{n,\vec{k}(t)}+\gamma_n\left(\vec{k}(t)\right)\right]_{\vec{k}=\vec{k}_o}=-\frac{e}{\hbar}\vec{E}t\times\left(\nabla_{\vec{q}}\times\vec{A}_{n,\vec{q}}\right)\Big|_{\vec{q}=\vec{k}_o}$$

Also:

$$-\frac{1}{\hbar}\nabla_{\vec{k}}\left[\int_0^t E_n\left(\vec{k}(t')\right)dt'\right]_{\vec{k}=\vec{k}_o}=-\vec{v}_g\left(\vec{k}_o\right)t$$

$$\left\{\;v_g\left(\vec{k}_o\right)=\frac{1}{\hbar}\nabla_{\vec{k}}E_n\left(\vec{k}\right)\Big|_{\vec{k}_o}\right.$$

Bloch Velocity and Berry's Phase

The wavepacket at time *t* is:

$$\theta(\vec{r},t) = \int \frac{d^d\vec{k}}{(2\pi)^2} f(\vec{k})\, e^{-i\vec{k}.\vec{r}_o} e^{i\left(\phi_{n,\vec{k}} - \phi_{n,\vec{k}(t)}\right)} \frac{e^{i\vec{k}(t).\vec{r}}}{\sqrt{V}} u_{n,\vec{k}(t)}(\vec{r})\, e^{i\phi_{n,\vec{k}(t)}} e^{-\frac{i}{\hbar}\int_0^t E_n\left(\vec{k}(t')\right)dt' + i\gamma_n\left(\vec{k}(t)\right)}$$

Now if one takes the gradient of the phase w.r.t. $\vec{k}$, evaluates it at $\vec{k}_o$, and sets it equal to zero, one obtains:

$$\vec{r} = \vec{r}_o + \vec{v}_g(\vec{k}_o)\, t + \frac{e}{\hbar}\vec{E}t \times \left(\nabla_{\vec{q}} \times \vec{A}_{n,\vec{q}}\right)\Big|_{\vec{q}=\vec{k}_o}$$

The packet group velocity is then:

$$v_g(\vec{k}_o) = \frac{1}{\hbar}\nabla_{\vec{k}} E_n(\vec{k})\Big|_{\vec{k}_o} + \frac{e}{\hbar}\vec{E} \times \left(\nabla_{\vec{q}} \times \vec{A}_{n,\vec{q}}\Big|_{\vec{q}=\vec{k}_o}\right)$$

Berry's Phase and Berry's Curvature

So, more generally, one can write the velocity of Bloch electrons (in the presence of a field as):

$$\vec{v}_n(\vec{k}) = \frac{1}{\hbar}\nabla_{\vec{k}} E_n(\vec{k}) - \frac{d\vec{k}}{dt} \times \left(\nabla_{\vec{k}} \times \vec{A}_{n,\vec{k}}\right)$$

The quantity:

$$\vec{\Omega}_n(\vec{k}) = \nabla_{\vec{k}} \times \vec{A}_{n,\vec{k}}$$

is called Berry's curvature and plays an important role in many different places in solid state physics (spin Hall effect for example). It acts like a magnetic field in k-space.

If a solid possesses time reversal symmetry (e.g. all materials in the absence of magnetic fields):

$$\vec{\Omega}_n(-\vec{k}) = -\vec{\Omega}_n(\vec{k})$$

If a solid possesses inversion symmetry (e.g. Si, Ge):

$$\vec{\Omega}_n(-\vec{k}) = \vec{\Omega}_n(\vec{k})$$

It follows that if a solid possesses both time reversal symmetry and inversion symmetry (e.g. Si, Ge):

$$\vec{\Omega}_n(\vec{k}) = 0$$