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 Schrödinger equation for an electron in a solid:

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

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

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

Or since:

\[
\psi_{n,k}(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} u_{n,k}(\vec{r})
\]

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

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

\[
\left( \frac{\hat{\rho} + e\vec{A}(\vec{r}, t)}{2m} \right) \psi(\vec{r}, t) = \frac{\partial \psi(\vec{r}, t)}{\partial t}
\]
The Schrödinger equation is invariant (i.e., does not change) under the following
gauge transformation:

\[
\psi(\vec{r}, t) \rightarrow e^{\frac{i}{\hbar} A(\vec{r}, t) \cdot \vec{E}} \psi(\vec{r}, t)
\]

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

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

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

\[
f(\vec{r}, t) = -\vec{E} \cdot \vec{r} t
\]
Electron Dynamics from Gauge Invariance

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

We are ignoring time derivatives of \(u(\mathbf{r},t)\)

(Adiabaticity assumption)

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

\[
\hbar \mathbf{k}(t) = \hbar \mathbf{k} - e\mathbf{E}t
\]

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

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

So the answer is:

\[
\phi(\mathbf{r},t) = \frac{e^{i\mathbf{k}(t)\cdot\mathbf{r}}}{\sqrt{V}}u_{n,\mathbf{k}(t)}(\mathbf{r})e^{-\frac{i}{\hbar}\int_0^t E_n(\mathbf{k}(t'))dt'}
\]

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

\[
\psi(\mathbf{r},t) = e^{-\frac{i\mathbf{E}\cdot\mathbf{r}}{\hbar}}\phi(\mathbf{r},t) = \frac{e^{i\mathbf{k}(t)\cdot\mathbf{r}}}{\sqrt{V}}u_{n,\mathbf{k}(t)}(\mathbf{r})e^{-\frac{i}{\hbar}\int_0^t E_n(\mathbf{k}(t'))dt'} = \psi_{n,\mathbf{k}(t)}(\mathbf{r})e^{-\frac{i}{\hbar}\int_0^t E_n(\mathbf{k}(t'))dt'}
\]

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Electron Dynamics and Berry’s Phase

Note that the solution:

\[
\phi(\mathbf{r},t) = \frac{e^{i\mathbf{k}(t)\cdot\mathbf{r}}}{\sqrt{V}}u_{n,\mathbf{k}(t)}(\mathbf{r})e^{-\frac{i}{\hbar}\int_0^t E_n(\mathbf{k}(t'))dt'}
\]

is not an exact solution of the equation:

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

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:

\[
\phi(\mathbf{r},t) = \frac{e^{i\mathbf{k}(t)\cdot\mathbf{r}}}{\sqrt{V}}u_{n,\mathbf{k}(t)}(\mathbf{r})e^{-\frac{i}{\hbar}\int_0^t E_n(\mathbf{k}(t'))dt'} + \gamma_{n,\mathbf{k}(t)}
\]

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

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

We get (PTO):
Electron Dynamics and Berry’s Phase

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

\[ \Rightarrow \gamma_{n,k}(t) = i \int_{t=0}^{t} dt' \langle u_{n,k}(t') | \left( \frac{\partial}{\partial t} \right) | u_{n,k}(t') \rangle = i \int_{q=k}^{q=k(t=0)} \langle u_{n,q} | \nabla q | u_{n,q} \rangle dq \]

\[ = \int_{q=k}^{q=k(t=0)} \bar{A}_{n,q} dq \]

The final complete solution is then:

\[ \psi(\vec{r},t) = e^{y} \phi(\vec{r},t) = \frac{e^{i\tilde{k}(t) \cdot \vec{r}}}{\sqrt{V}} u_{n,k}(t) e^{\frac{i}{\hbar} \int_{t_0}^{t} E_n(\tilde{k}(t')) dt'} \]

\[ = \psi_{n,k}(\vec{r}(t)) e^{\frac{i}{\hbar} \int_{t_0}^{t} E_n(\tilde{k}(t')) dt'} \]

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, \( \gamma_{n,k}(t) = \gamma_n(\tilde{k}(t)) \), since it depends on the trajectory of the time-dependent wavevector in reciprocal space

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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:

\[ \theta(\vec{r},t) = \int \frac{d^d k}{(2\pi)^d} f(\vec{k}) e^{-i\vec{k} \cdot \vec{r}_0} \psi_{n,k}(\vec{f}) e^{\frac{i}{\hbar} \int_{t_0}^{t} E_n(\tilde{k}(t')) dt'} \]

\[ = \int \frac{d^d k}{(2\pi)^d} f(\vec{k}) e^{-i\vec{k} \cdot \vec{r}_0} e^{i\tilde{k}(t) \cdot \vec{r}} u_{n,k}(\vec{r}) e^{\frac{i}{\hbar} \int_{t_0}^{t} E_n(\tilde{k}(t')) dt'} \]

Assume that the function \( f(\vec{k}) \) peaks when \( \tilde{k} = \tilde{k}_0 \)

Lets first look at this packet at time \( t = 0 \):

\[ \theta(\vec{r}, t = 0) = \int \frac{d^d k}{(2\pi)^d} f(\vec{k}) e^{-i\vec{k} \cdot \vec{r}_0} e^{i\tilde{k}_0 \cdot \vec{r}} u_{n,k}(\vec{r}) \]

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 \( t = 0 \)?

\[
\theta(\vec{r}, t = 0) = \int \frac{d^d \vec{k}}{(2\pi)^d} f(\vec{k}) e^{-i\vec{k} \cdot \vec{r}_0} e^{i\vec{k} \cdot \vec{r}} \frac{1}{\sqrt{V}} u_{n,\vec{k}}(\vec{r})
\]

One would be inclined to say at \( \vec{r}_0 \)!

Because if one looks at the gradient of the phase w.r.t. \( \vec{k} \), evaluates it at \( \vec{k}_0 \), and sets it equal to zero, one obtains: \( \vec{r} = \vec{r}_0 \)

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:

\[
\phi_{n,\vec{k}} = \int \vec{A}_{n,q} \, d\vec{q}
\]

\[
\theta(\vec{r}, t = 0) = \int \frac{d^d \vec{k}}{(2\pi)^d} f(\vec{k}) e^{-i\vec{k} \cdot \vec{r}_0} e^{i\vec{k} \cdot \vec{r}} \frac{1}{\sqrt{V}} u_{n,\vec{k}}(\vec{r}) e^{i\phi_{n,\vec{k}}(\vec{r})}
\]

Finally, at time \( t = 0 \), the packet is sitting at \( \vec{r}_0 \) ! We will work with this packet now.

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Bloch Velocity and Berry’s Phase

Now at time \( t \):

\[
\theta(\vec{r}, t) = \int \frac{d^d \vec{k}}{(2\pi)^d} f(\vec{k}) e^{-i\vec{k} \cdot \vec{r}_0} e^{i\vec{k} \cdot \vec{r}(\vec{k}(t))} \frac{1}{\sqrt{V}} u_{n,\vec{k}(t)}(\vec{r}) e^{i\phi_{n,\vec{k}(t)}(\vec{r})} e^{i\int \frac{1}{\hbar} E_n(\vec{k}(t)) dt + i\gamma_n(\vec{k}(t))}
\]

We again write it as:

\[
\theta(\vec{r}, t) = \int \frac{d^d \vec{k}}{(2\pi)^d} f(\vec{k}) e^{-i\vec{k} \cdot \vec{r}_0} e^{i\vec{k} \cdot \vec{r}(\vec{k}(t))} \frac{1}{\sqrt{V}} u_{n,\vec{k}(t)}(\vec{r}) e^{i\phi_{n,\vec{k}(t)}(\vec{r})} e^{i\int \frac{1}{\hbar} E_n(\vec{k}(t)) dt + i\gamma_n(\vec{k}(t))}
\]

Now:

\[
\phi_{n,\vec{k}}(t) = \phi_{n,\vec{k}(t)}(t) + \gamma_n(\vec{k}(t)) = \int \vec{A}_{n,q} \, d\vec{q} + \int q = \vec{k} \vec{A}_{n,q} \, d\vec{q} - \int q = \vec{k} \vec{A}_{n,q} \, d\vec{q}
\]

\[
\Rightarrow \nabla_{\vec{k}} \left[ \phi_{n,\vec{k}}(t) - \phi_{n,\vec{k}(t)}(t) + \gamma_n(\vec{k}(t)) \right]_{\vec{k} = \vec{k}_0} = -\frac{\hbar}{E_t} \nabla_{\vec{q}} \times \vec{A}_{n,q} \bigg|_{\vec{q} = \vec{k}_0}
\]

Also:

\[
-\frac{1}{\hbar} \nabla_{\vec{k}} \left[ \int \frac{1}{\hbar} E_n(\vec{k}(t)) dt \right]_{\vec{k} = \vec{k}_0} = -\frac{\hbar}{E_t} \left( \gamma_n(\vec{k}_0) + \frac{1}{\hbar} \nabla_{\vec{k}} E_n(\vec{k}(t)) \bigg|_{\vec{k} = \vec{k}_0} \right)
\]
Bloch Velocity and Berry’s Phase

The wavepacket at time $t$ is:

$$\rho(r,t) = \int \frac{d^d k}{(2\pi)^d} f(k) e^{-ik \cdot r} \left( e^{i\phi_{n,k,t}(r)} \right) \frac{\partial^{(t)} E}{\partial V} u_{n,k}(r) e^{i\phi_{n,k}(r)} \frac{d}{dt} - i\frac{d}{dt} E_n(k(t)) dt + i\Omega_n(k(t))$$

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

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

The packet group velocity is then:

$$\vec{v}_g(k_o) = \frac{1}{\hbar} \nabla_k E_n(k)_{\hat{k}_o} + \frac{e}{\hbar} \vec{E} \times \left( \nabla_q \times \vec{A}_{n,q} \right) \bigg|_{\vec{q} = \hat{k}_o}$$

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):

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

The quantity:

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

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):

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

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

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

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

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