Handout 15

Dynamics of Electrons in Energy Bands

In this lecture you will learn:

- The behavior of electrons in energy bands subjected to uniform electric fields
- The dynamical equation for the crystal momentum
- The effective mass tensor and inertia of electrons in energy bands
- Examples
- Magnetic fields
- Appendix: Electron dynamics using gauge invariance arguments, Berry's phase, and Berry's curvature

Electron Dynamics in Energy Bands

1) The quantum states of an electron in a crystal are given by Bloch functions that obey the Schrodinger equation:

$$\hat{H}\,\psi_{n,\vec{k}}(\vec{r}) = E_n(\vec{k})\,\psi_{n,\vec{k}}(\vec{r})$$

where the wavevector $\vec{k}$ is confined to the FBZ and "*n*" is the band index

2) Under a lattice translation, Bloch functions obey the relation:

$$\psi_{n,\vec{k}}(\vec{r}+\vec{R}) = e^{i\,\vec{k}\,.\,\vec{R}}\,\psi_{n,\vec{k}}(\vec{r})$$

Now we ask the following question: if an external potential is added to the crystal Hamiltonian,

$$\hat{H} + \hat{U}(\vec{r},t)$$

then what happens? How do the electrons behave? How do we find the new energies and eigenstates?

The external potential could represent, for example, an applied E-field or an applied B-field, or an electromagnetic wave (like light)

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Periodicity of Energy Bands

Recall from homework that the energy bands are lattice-periodic in the reciprocal space,

$$E_n(\vec{k}+\vec{G}) = E_n(\vec{k})$$

When a function in real space is lattice-periodic, we can expand it in a Fourier series,

$$V(\vec{r}+\vec{R}) = V(\vec{r}) \quad \Rightarrow \quad V(\vec{r}) = \sum_j V(\vec{G}_j)\, e^{i\,\vec{G}_j\,.\,\vec{r}}$$

⇒ When a function is lattice-periodic in reciprocal space, we can also expand it in a Fourier series of the form,

$$E_n(\vec{k}+\vec{G}) = E_n(\vec{k}) \quad \Rightarrow \quad \underbrace{E_n(\vec{k}) = \sum_j E_n(\vec{R}_j)\, e^{i\,\vec{R}_j\,.\,\vec{k}}}_{\text{Fourier representation of energy bands}}$$

A New Operator - I

Consider the following mathematical identity (Taylor expansion):

$$f(x+a) = f(x) + f'(x)\,a + \frac{1}{2} f''(x)\,a^2 + \ldots\ldots\ldots\ldots$$

$$= e^{a\frac{d}{dx}}\, f(x)$$

Generalize to 3 dimensions:

$$f(\vec{r}+\vec{a}) = e^{\vec{a}\,.\,\nabla}\, f(\vec{r})$$

Now go back to the relation:

$$E_n(\vec{k}+\vec{G}) = E_n(\vec{k}) \quad \Rightarrow \quad E_n(\vec{k}) = \sum_j E_n(\vec{R}_j)\, e^{i\,\vec{R}_j\,.\,\vec{k}}$$

and consider the operator:

$$\hat{E}_n(-i\nabla) = \sum_j E_n(\vec{R}_j)\, e^{\vec{R}_j\,.\,\nabla}$$

We apply this operator to a Bloch function from the same band (i.e. the *n*-th band) and see what happens:

$$\hat{E}_n(-i\nabla)\,\psi_{n,\vec{k}}(\vec{r}) = \sum_j E_n(\vec{R}_j)\, e^{\vec{R}_j\,.\,\nabla}\,\psi_{n,\vec{k}}(\vec{r}) = \,?$$

A New Operator - II

$$\hat{E}_n(-i\nabla)\,\psi_{n,\vec{k}}(\vec{r}) = \sum_j E_n(\vec{R}_j)\, e^{\vec{R}_j\cdot\nabla}\, \psi_{n,\vec{k}}(\vec{r})$$
$$= \sum_j E_n(\vec{R}_j)\, \psi_{n,\vec{k}}(\vec{r}+\vec{R}_j)$$
$$= \sum_j E_n(\vec{R}_j)\, e^{i\,\vec{k}\cdot\vec{R}_j}\, \psi_{n,\vec{k}}(\vec{r})$$
$$= E_n(\vec{k})\, \psi_{n,\vec{k}}(\vec{r})$$

The result above implies that the action of the operator $\hat{E}_n(-i\nabla)$ on a Bloch function belonging to the same band (i.e. *n*-th band) is that of the Hamiltonian!

$$\hat{E}_n(-i\nabla)\,\psi_{n,\vec{k}}(\vec{r}) = \hat{H}\,\psi_{n,\vec{k}}(\vec{r}) = E_n(\vec{k})\,\psi_{n,\vec{k}}(\vec{r})$$

This also implies that if we have a superposition of Bloch functions from a single band then:

$$\hat{H}\sum_{\vec{k}\ \text{in FBZ}} c(\vec{k})\,\psi_{n,\vec{k}}(\vec{r}) = \hat{E}_n(-i\nabla)\sum_{\vec{k}\ \text{in FBZ}} c(\vec{k})\,\psi_{n,\vec{k}}(\vec{r})$$
$$= \sum_{\vec{k}\ \text{in FBZ}} c(\vec{k})\,E_n(\vec{k})\,\psi_{n,\vec{k}}(\vec{r})$$

The Case of Uniform Electric Field

Statement of problem: **Need to solve,**

$$\left[\hat{H} + e\vec{E}\cdot\hat{\vec{r}}\right]\psi(\vec{r},t) = i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}$$

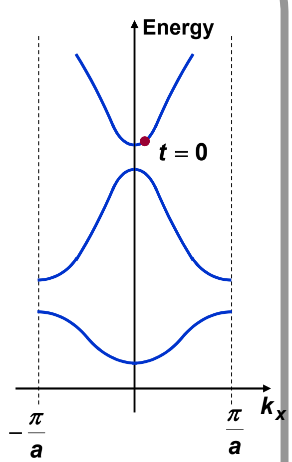
given that at time $t = 0$ the state of the electron is a Bloch function with wavevector $\vec{k}$,

$$\psi(\vec{r},t=0) = \psi_{n,\vec{k}}(\vec{r})$$

Assumption: **Assume that the state at any later time is going to be a Bloch function or a linear combination of Bloch functions belonging to the same band (valid for weak E-fields)**

Then one can replace the Hamiltonian with $\hat{E}_n(-i\nabla)$,

$$\left[\hat{H} + e\vec{E}\cdot\hat{\vec{r}}\right]\psi(\vec{r},t) = i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}$$
$$\Rightarrow \left[E_n(-i\nabla) + e\vec{E}\cdot\hat{\vec{r}}\right]\psi(\vec{r},t) = i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}$$



The Case of Uniform Electric Field

$$\left[\, E_n(-i\nabla) + e\,\vec{E}\,.\,\hat{\vec{r}}\,\right]\psi(\vec{r},t) = i\hbar\,\frac{\partial\psi(\vec{r},t)}{\partial t}$$

Try the following time-dependent solution with a time-dependent energy:

$$\psi(\vec{r},t) = \psi_{n,\vec{k}}(\vec{r})\,\exp\left[-\frac{i}{\hbar}\int_0^t \left(E(t') + e\vec{E}\,.\,\vec{r}\right)dt'\right]$$

First see how the assumed solution behaves under a lattice translation:

$$\psi\left(\vec{r}+\vec{R},t\right) = \psi_{n,\vec{k}}\left(\vec{r}+\vec{R}\right)\exp\left[-\frac{i}{\hbar}\int_0^t \left(E(t') + e\vec{E}\,.\left(\vec{r}+\vec{R}\right)\right)dt'\right]$$

$$= e^{i\left(\vec{k} - \frac{e\,\vec{E}\,t}{\hbar}\right).\vec{R}}\,\psi(\vec{r},t)$$

So the assumed solution looks like a Bloch function with a time dependent k-vector:

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

But we still don't know what is the time-dependent energy *E*(*t*)

The Case of Uniform Electric Field

Take the trial solution and plug it into the equation:

$$\left[\, E_n(-i\nabla) + e\,\vec{E}\,.\,\hat{\vec{r}}\,\right]\psi(\vec{r},t) = i\hbar\,\frac{\partial\psi(\vec{r},t)}{\partial t}$$

LHS (first term):

$$E_n(-i\nabla)\,\psi(\vec{r},t) = \sum_j E_n\left(\vec{R}_j\right)e^{\vec{R}_j\,.\,\nabla}\psi(\vec{r},t)$$

$$= \sum_j E_n\left(\vec{R}_j\right)\psi\left(\vec{r}+\vec{R}_j,t\right)$$

$$= \sum_j E_n\left(\vec{R}_j\right)e^{i\left(\vec{k} - \frac{e\,\vec{E}}{\hbar}t\right).\vec{R}_j}\psi(\vec{r},t)$$

$$= E_n\left(\vec{k} - \frac{e\,\vec{E}}{\hbar}t\right)\psi(\vec{r},t)$$

RHS:

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

The Case of Uniform Electric Field

Putting it together:

$$\left[E_n(-i\nabla) + e\vec{E}\,.\,\hat{\vec{r}} \right]\psi(\vec{r},t) = i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t}$$

$$\Rightarrow \left[E_n\left(\vec{k} - \frac{e\vec{E}\,t}{\hbar}\right) + e\vec{E}\,.\,\hat{\vec{r}} \right]\psi(\vec{r},t) = \left[E(t) + e\vec{E}\,.\,\hat{\vec{r}} \right]\psi(\vec{r},t)$$

$$\Rightarrow E(t) = E_n\left(\vec{k} - \frac{e\vec{E}\,t}{\hbar}\right)$$

The time-dependent energy is consistent with our solution being a Bloch function with a time-dependent k-vector,

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

So the solution for the initial condition:

$$\psi(\vec{r},t=0) = \psi_{n,\vec{k}}(\vec{r})$$

is approximately a Bloch function with a time-dependent k-vector:

$$\psi(\vec{r},t) = \psi_{n,\vec{k}(t)}(\vec{r})\,\exp\left[-\frac{i}{\hbar}\int_0^t E_n(k(t'))\,dt'\right]$$

The Case of Uniform Electric Field

Final result: In the presence of a uniform electric field the electrons in energy bands have a time-dependent crystal momentum that satisfies the dynamical equation:

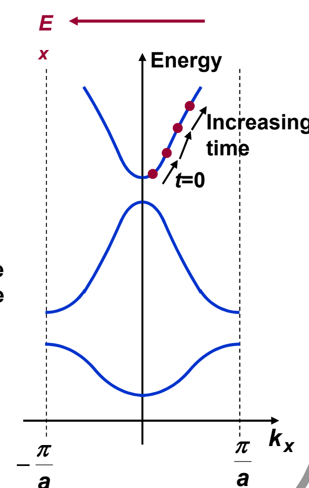
$$\frac{d\,\hbar\vec{k}(t)}{dt} = -e\,\vec{E}$$

$\Rightarrow$ The rate of change of the crystal momentum is equal to the force on the electron

Note that (perhaps) the more intuitive result that the rate of change of the average electron momentum equals the applied force DOES NOT hold,

$$\frac{d\,\langle\psi(\vec{r},t)|\hat{P}|\psi(\vec{r},t)\rangle}{dt} \neq -e\,\vec{E}$$

The dynamical equation is instead given in terms of the crystal momentum



What Happened to Ehrenfest's Theorem of QM?

In quantum mechanics, Ehrenfest's theorem is the closest to Newton's second law.

Ehrenfest's theorem: For a time dependent quantum state, the rate of change of the average momentum equals the average force:

$$\frac{d\,\langle\psi(\vec{r},t)|\hat{P}|\psi(\vec{r},t)\rangle}{dt} = \langle\psi(\vec{r},t)|\hat{F}(\vec{r})|\psi(\vec{r},t)\rangle$$

We saw that for electrons in solids, in the presence of a uniform applied E-field, the following equation does not hold:

$$\frac{d\,\langle\psi(\vec{r},t)|\hat{P}|\psi(\vec{r},t)\rangle}{dt} \neq \langle\psi(\vec{r},t)|-e\,\vec{E}|\psi(\vec{r},t)\rangle = -e\,\vec{E}$$

The reason is that in solids, in the presence of an applied E-field, the electrons not only feel the force from the applied E-field but they also feel the force from the periodic atomic potential. If all forces are correctly taken into account then, of course, Ehrenfest's theorem would hold. But it is more useful and simpler to use the dynamical equation involving the crystal momentum:

$$\frac{d\,\hbar\vec{k}(t)}{dt} = -e\,\vec{E}$$

Another Look at the Dynamical Equation: Energy Conservation

One can also derive the dynamical equation: $\frac{d\,\hbar\vec{k}(t)}{dt} = -e\,\vec{E}$

from arguments involving energy conservation

Consider an electron with an initial Bloch state with wavevector $\vec{k}$. Suppose in the presence of an E-field the wavevector is time-dependent - but we don't know what is the time dependence:

$$\frac{d\,\vec{k}(t)}{dt} = ?$$

In time δt the electron energy will increase by:

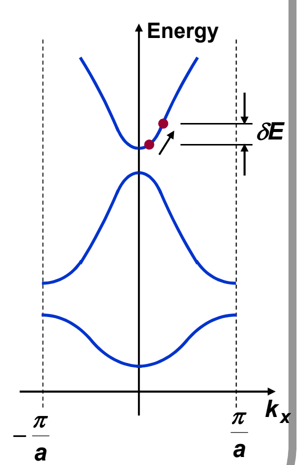
$$\delta E = \nabla E_n(\vec{k}) . \frac{d\,\vec{k}(t)}{dt}\,\delta t \qquad (1)$$

The increase in electron energy also equals the work done by the E-field on the electron in time δt:

$$\delta E = \vec{v}_n(\vec{k}) . (-e\vec{E})\;\delta t \qquad (2)$$

Equating (1) and (2) gives:

$$\frac{d\,\hbar\vec{k}(t)}{dt} = -e\,\vec{E}$$



Effective Mass Tensor and Acceleration

Consider a solid in which the energy dispersion near a band extremum is given by:

$$E_n(\vec{k}) = E_n(\vec{k}_o) + \frac{\hbar^2}{2}(\vec{k}-\vec{k}_o)^T \, . \, M^{-1} \, . \, (\vec{k}-\vec{k}_o)$$

The average velocity is:

$$\vec{v}_n(\vec{k}) = M^{-1} \, . \, \hbar \, (\vec{k}-\vec{k}_o)$$

Consequently, the rate of change of the velocity satisfies:

$$\frac{d\,\vec{v}_n(\vec{k}(t))}{dt} = M^{-1} \, . \, \frac{d\,\hbar\,\vec{k}(t)}{dt}$$

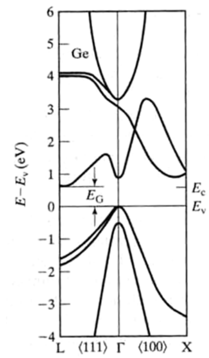
In the presence of an E-field the crystal momentum changes as:

$$\frac{d\,\hbar\vec{k}(t)}{dt} = -e\,\vec{E}$$

Therefore:

$$\frac{d\,\vec{v}_n(\vec{k}(t))}{dt} = M^{-1} \, . \, \frac{d\,\hbar\,\vec{k}(t)}{dt} = M^{-1} \, . \, -e\vec{E}$$

$$\Rightarrow \frac{d\,\vec{v}_n(t)}{dt} = -e\,M^{-1} \, . \, \vec{E}$$



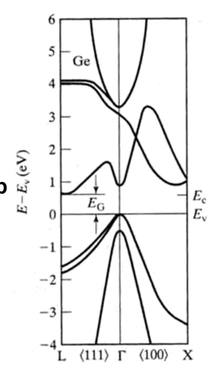
Effective Mass Tensor and Acceleration

$$\frac{d\,\vec{v}_n(t)}{dt} = -e\,M^{-1} \, . \, \vec{E} \qquad \text{Or :} \qquad M \, . \, \frac{d\,\vec{v}_n(t)}{dt} = -e\,\vec{E}$$

The acceleration of electrons in energy bands in response to an applied force is governed by the effective mass tensor.

The above relation shows that the effective mass tensor, which up to this point just represented coefficients for Taylor expansion of the energy dispersion relation, is also a measure of the inertia of electrons in energy bands just like ordinary mass is a measure of the inertia of free electrons.

Written out in component form we have:



$$\frac{d}{dt}\begin{bmatrix} v_{x,n}(t) \\ v_{y,n}(t) \\ v_{z,n}(t) \end{bmatrix} = -e \begin{bmatrix} 1/m_{xx} & 1/m_{xy} & 1/m_{xz} \\ 1/m_{yx} & 1/m_{yy} & 1/m_{yz} \\ 1/m_{zx} & 1/m_{zy} & 1/m_{zz} \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}$$

In general, the electrons are accelerated in a direction different from the direction of the force due to the applied E-field !

Example: Conduction and Heavy-Hole Valence Bands of GaAs

Consider the conduction band of GaAs near the band bottom at the Γ-point:

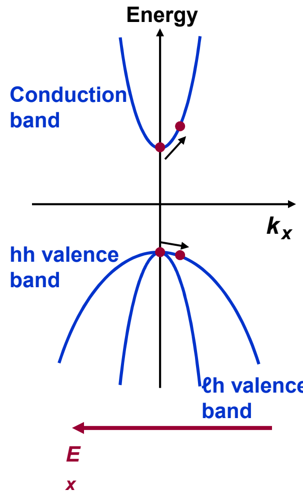
$$M^{-1} = \begin{bmatrix} 1/m_e & 0 & 0 \\ 0 & 1/m_e & 0 \\ 0 & 0 & 1/m_e \end{bmatrix}$$

$$\frac{d\,\vec{v}_c(t)}{dt} = -e\,M^{-1}\,.\,\vec{E} = -\frac{e}{m_e}\,\vec{E}$$

Now consider the heavy-hole valence band of GaAs near the band maximum at the Γ-point:

$$M^{-1} = \begin{bmatrix} -1/m_{hh} & 0 & 0 \\ 0 & -1/m_{hh} & 0 \\ 0 & 0 & -1/m_{hh} \end{bmatrix}$$

$$\frac{d\,\vec{v}_{hh}(t)}{dt} = -e\,M^{-1}\,.\,\vec{E} = \frac{e}{m_{hh}}\,\vec{E}$$



Electrons in the valence band are accelerated in the direction opposite to the force acting upon them due to the applied E-field

Example: Conduction Band of Silicon

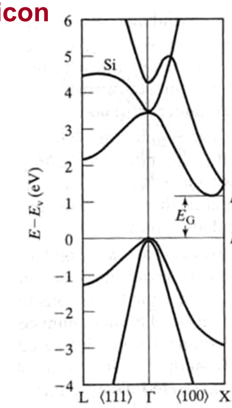
In Silicon there are six conduction band minima (valleys) that occur along the six Γ-X directions. For the one that occurs along the Γ-X(2π/a,0,0) direction:

$$\vec{k}_o = 0.85\left(\frac{2\pi}{a},0,0\right)$$

$$M^{-1} = \begin{bmatrix} 1/m_\ell & 0 & 0 \\ 0 & 1/m_t & 0 \\ 0 & 0 & 1/m_t \end{bmatrix}$$

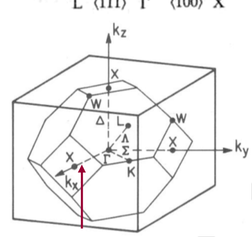
Not isotropic!

$m_\ell = 0.92\,m$
$m_t = 0.19\,m$



This implies:

$$\frac{d}{dt}\begin{bmatrix} v_{x,c}(t) \\ v_{y,c}(t) \\ v_{z,c}(t) \end{bmatrix} = -e\begin{bmatrix} 1/m_\ell & 0 & 0 \\ 0 & 1/m_t & 0 \\ 0 & 0 & 1/m_t \end{bmatrix}\begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}$$



Electrons in this valley have larger inertia (i.e. larger mass) for E-field applied in the x-direction (i.e. the longitudinal direction) and smaller inertia (i.e. smaller mass) for E-field applied in the y- or z-directions (i.e. the transverse directions)

Generalization to Include Applied Magnetic Fields

We had for only electric fields:

$$\frac{d\,\hbar\vec{k}(t)}{dt} = -e\,\vec{E} \quad \xrightarrow{\text{(assuming parabolic energy band dispersion)}} \quad M\,.\frac{d\,\vec{v}_n\left(\vec{k}(t)\right)}{dt} = -e\,\vec{E}$$

Magnetic fields can also be included as follows:

$$\frac{d\,\hbar\vec{k}(t)}{dt} = -e\,\vec{E} - e\,\vec{v}_n\left(\vec{k}(t)\right)\times\vec{B}$$

(assuming parabolic energy band dispersion)

$$M\,.\frac{d\,\vec{v}_n\left(\vec{k}(t)\right)}{dt} = -e\,\vec{E} - e\,\vec{v}_n\left(\vec{k}(t)\right)\times\vec{B}$$

Note: If the energy band dispersion is not parabolic (as in graphene) then the equations on the right hand side have no meaning

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

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

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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Appendix: Electron Dynamics from Gauge Invariance

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

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

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

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

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

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:

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

Appendix: Electron Dynamics from Gauge Invariance

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:

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

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

Appendix: Electron Dynamics from Gauge Invariance

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

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):

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

Appendix: 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. To capture this we try:

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

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):

Appendix: Electron Dynamics and Berry's Phase

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

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

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

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

Appendix: 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:

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

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

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

In the absence of Berry's phase the group velocity of the packet can be found from the usual stationary phase argument:

$$v_g(\vec{k}_o)(\vec{k}-\vec{k}_o) = \frac{1}{\hbar}\frac{d}{dt}\int_{t'=0}^{t'=t}dt'\left(E_n(\vec{k}-e\vec{E}t/\hbar) - -E_n(\vec{k}_o - e\vec{E}t/\hbar)\right)$$

$$\Rightarrow v_g(\vec{k}_o) = \frac{1}{\hbar}\nabla_{\vec{k}}E_n(\vec{k})\Big|_{\vec{k}_o}$$

Appendix: Bloch Velocity and Berry's Phase

In the presence of Berry's phase the group velocity of the packet from the stationary phase argument gives an extra term:

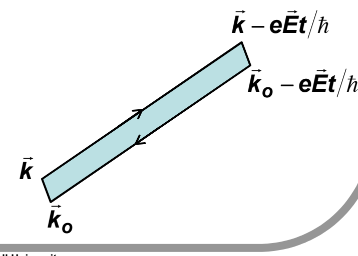
$$v_g(\vec{k}_o).(\vec{k}-\vec{k}_o)=\frac{1}{\hbar}\nabla_{\vec{k}}E_n(\vec{k})\Big|_{\vec{k}_o}.(\vec{k}-\vec{k}_o)-\frac{d}{dt}\left[\gamma_n(\vec{k}-e\vec{E}t/\hbar)-\gamma_n(\vec{k}_o-e\vec{E}t/\hbar)\right]$$

$$v_g(\vec{k}_o).(\vec{k}-\vec{k}_o)=\frac{1}{\hbar}\nabla_{\vec{k}}E_n(\vec{k})\Big|_{\vec{k}_o}.(\vec{k}-\vec{k}_o)-\frac{d}{dt}\left[\int_{\vec{q}=\vec{k}}^{\vec{q}=\vec{k}-e\vec{E}t/\hbar}\vec{A}_{n,q}.d\vec{q}-\int_{\vec{q}=\vec{k}_o}^{\vec{q}=\vec{k}_o-e\vec{E}t/\hbar}\vec{A}_{n,q}.d\vec{q}\right]$$

The second term in brackets represents the rate of change of the (oriented) area of the figure below and equals:

$$-\frac{d}{dt}\left[\int_{\vec{q}=\vec{k}}^{\vec{q}=\vec{k}-e\vec{E}t/\hbar}\vec{A}_{n,q}.d\vec{q}-\int_{\vec{q}=\vec{k}_o}^{\vec{q}=\vec{k}_o-e\vec{E}t/\hbar}\vec{A}_{n,q}.d\vec{q}\right]=-\nabla_{\vec{q}}\times\vec{A}_{n,\vec{q}}\Big|_{\vec{q}=\vec{k}_o}.\left[\frac{e}{\hbar}\vec{E}\times(\vec{k}-\vec{k}_o)\right]$$

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



The packet group velocity is then:

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

Appendix: 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)

If a solid possesses time reversal symmetry (all materials in the absence of an external magnetic field):

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

If a solid possesses inversion symmetry (like 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 (like Si, Ge):

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