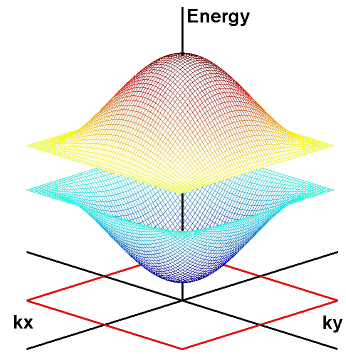
Handout on

Crystal Symmetries and Energy Bands

In this lecture you will learn:

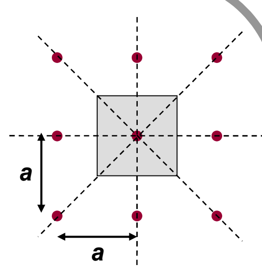
- The relationship between symmetries and energy bands in the absence of spin-orbit coupling
- The relationship between symmetries and energy bands in the presence of spin-orbit coupling



Symmetry and Energy Bands

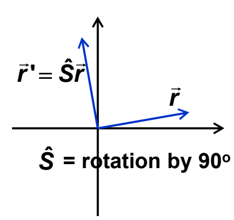
The crystal potential $V(\vec{r})$ generally has certain other symmetries in addition to the lattice translation symmetry:

$$V(\vec{r}+\vec{R}) = V(\vec{r})$$



For example, the 2D potential of a square atomic lattice, as shown, has the following symmetries:

a) Symmetry under rotations by 90, 180, and 270 degrees
b) Symmetry under reflections w.r.t. x-axis and y-axis
c) Symmetry under reflections w.r.t. the two diagonals

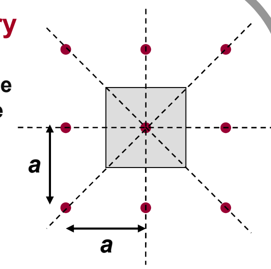


Let $\hat{S}$ be the operator (in matrix representation) for any one of these symmetry operations then:

$$\vec{r}' = \hat{S}\vec{r}$$

$$\Rightarrow V(\hat{S}\vec{r}) = V(\vec{r})$$

Crystal Point-Group Symmetry

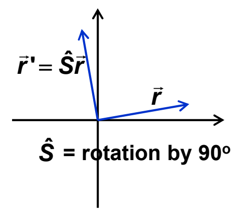


Point-Group Symmetry

The point group symmetry operation of a lattice are all those operations that leave the lattice unchanged and at least one point of the lattice remains unmoved under the operation

Point group symmetry operations can include:

i) Rotations (w.r.t. to axes of rotation)
ii) Reflections (across lines or planes)
iii) Inversions (w.r.t. to a point)



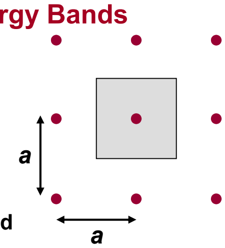
Let $\hat{S}$ be the operator for a point-group symmetry operation, such that:

$$V\left(\hat{S}\vec{r}\right) = V(\vec{r})$$

The operator $\hat{S}$ is unitary:

$$\hat{S}^T = \vec{S}^{-1} \Rightarrow \text{unitary}$$

Crystal Point-Group Symmetry and Energy Bands



Let $\hat{S}$ be the operator for a point-group symmetry operation, such that:

$$\vec{r}' = \hat{S}\vec{r} \qquad \left\{\hat{S}^T = \vec{S}^{-1} \Rightarrow \text{unitary}\right.$$

$$\Rightarrow V\left(\hat{S}\vec{r}\right) = V(\vec{r})$$

Suppose one has solved the Shrodinger equation and obtained the energy and wavefunction of a Bloch State $\psi_{n,\vec{k}}(\vec{r})$

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

Now replace $\vec{r}$ by $\hat{S}\vec{r}$ everywhere in the Schrodinger equation:

$$\left[-\frac{\hbar^2\nabla^2_{\hat{S}\vec{r}}}{2m} + V\left(\hat{S}\vec{r}\right)\right]\psi_{n,\vec{k}}\left(\hat{S}\vec{r}\right) = E_n\left(\vec{k}\right)\psi_{n,\vec{k}}\left(\hat{S}\vec{r}\right) \longrightarrow \left\{\begin{array}{l}\nabla^2_{\hat{S}\vec{r}} = \nabla^2_{\vec{r}} \\ \text{Laplacian is} \\ \text{invariant}\end{array}\right.$$

$$\Rightarrow \left[-\frac{\hbar^2\nabla^2_{\vec{r}}}{2m} + V(\vec{r})\right]\psi_{n,\vec{k}}\left(\hat{S}\vec{r}\right) = E_n\left(\vec{k}\right)\psi_{n,\vec{k}}\left(\hat{S}\vec{r}\right)$$

Crystal Point-Group Symmetry and Energy Bands

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

The above equation says that the function $\psi_{n,\vec{k}}(\hat{S}\vec{r})$ is also a Bloch state with the same energy as $\psi_{n,\vec{k}}(\vec{r})$ (we have found a new eigenfunction!)

The question is if we really have found a new eigenfunction or not, and if so what is the wavevector of this new eigenfunction

We know that Bloch functions have the property that: $\psi_{n,\vec{k}}(\vec{r}+\vec{R})=e^{i\,\vec{k}\,.\,\vec{R}}\,\psi_{n,\vec{k}}(\vec{r})$

So we try this on $\psi_{n,\vec{k}}(\hat{S}\vec{r})$:

$$\psi_{n,\vec{k}}(\hat{S}(\vec{r}+\vec{R}))=\psi_{n,\vec{k}}(\hat{S}\vec{r}+\hat{S}\vec{R}) \longrightarrow \left\{\ \hat{S}\vec{R}\ \text{is also a lattice vector}\right.$$

$$=e^{i\,\vec{k}\,.\,\hat{S}\vec{R}}\,\psi_{n,\vec{k}}(\hat{S}\vec{r})=e^{i\left[\hat{S}^{-1}\vec{k}\right].\,\vec{R}}\,\psi_{n,\vec{k}}(\hat{S}\vec{r}) \longrightarrow \left\{\ \vec{k}.(\hat{S}\vec{R})=(\hat{S}^{-1}\vec{k}).\vec{R}\right.$$

$\Rightarrow$ $\psi_{n,\vec{k}}(\hat{S}\vec{r})$ **is a Bloch function with wavevector** $\hat{S}^{-1}\vec{k}$ **and energy** $E_n(\vec{k})$

$$\Rightarrow \psi_{n,\vec{k}}(\hat{S}\vec{r})=\psi_{n,\hat{S}^{-1}\vec{k}}(\vec{r})$$

Crystal Point-Group Symmetry and Energy Bands

So we finally have for the symmetry operation $\hat{S}$:

$$\Rightarrow \psi_{n,\vec{k}}(\hat{S}\vec{r})=\psi_{n,\hat{S}^{-1}\vec{k}}(\vec{r})$$

We also know that the eigenenergy of $\psi_{n,\hat{S}^{-1}\vec{k}}(\vec{r})$ is $E_n(\vec{k})$
Therefore:

$$E_n(\hat{S}^{-1}\vec{k})=E_n(\vec{k})$$

Or, equivalently:

$$E_n(\hat{S}\vec{k})=E_n(\vec{k})$$

Important Lessons:

1) If $\hat{S}$ is a symmetry of the potential such that in real-space we have:

$$V(\hat{S}\vec{r})=V(\vec{r})$$

then the energy bands also enjoy the symmetry of the potential such that in k-space:

$$E_n(\hat{S}\vec{k})=E_n(\vec{k})$$

2) Degeneracies in the energy bands can therefore arise from crystal point-group symmetries!

Time Reversal Symmetry and Energy Bands

Suppose we have solved the time dependent Schrodinger and obtained the Bloch state $\psi_{n,\vec{k}}(\vec{r})$ with energy $E_n(\vec{k})$:

$$\left[-\frac{\hbar^2\nabla^2}{2m}+V(\vec{r})\right]\psi_{n,\vec{k}}(\vec{r},t)=i\hbar\frac{\partial\psi_{n,\vec{k}}(\vec{r},t)}{\partial t} \longrightarrow \psi_{n,\vec{k}}(\vec{r},t)=\psi_{n,\vec{k}}(\vec{r})\,e^{-i\frac{E_n(\vec{k})}{\hbar}t}$$

After plugging the solution in the time-dependent equation, we get:

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

If we take the complex conjugate of the above equation, we get:

$$\left[-\frac{\hbar^2\nabla^2}{2m}+V(\vec{r})\right]\psi^*_{n,\vec{k}}(\vec{r})=E_n(\vec{k})\psi^*_{n,\vec{k}}(\vec{r})$$

We have found another Bloch function, i.e. $\psi^*_{n,\vec{k}}(\vec{r})$, with the same energy as $\psi_{n,\vec{k}}(\vec{r})$

Question: What is the physical significance of the state $\psi^*_{n,\vec{k}}(\vec{r})$?

Time Reversal Symmetry and Energy Bands

Suppose we have solved the time dependent Schrodinger and obtained the Bloch state $\psi_{n,\vec{k}}(\vec{r})$ with energy $E_n(\vec{k})$:

$$\left[-\frac{\hbar^2\nabla^2}{2m}+V(\vec{r})\right]\psi_{n,\vec{k}}(\vec{r},t)=i\hbar\frac{\partial\psi_{n,\vec{k}}(\vec{r},t)}{\partial t} \longrightarrow \psi_{n,\vec{k}}(\vec{r},t)=\psi_{n,\vec{k}}(\vec{r})\,e^{-i\frac{E_n(\vec{k})}{\hbar}t}$$

Lets see if we can find a solution under time-reversal (i.e. when t is replaced by $-t$):

$$\Rightarrow\left[-\frac{\hbar^2\nabla^2}{2m}+V(\vec{r})\right]\psi_{n,\vec{k}}(\vec{r},-t)=-i\hbar\frac{\partial\psi_{n,\vec{k}}(\vec{r},-t)}{\partial t}$$

The above does not look like a Schrodinger equation so we complex conjugate it:

$$\Rightarrow\left[-\frac{\hbar^2\nabla^2}{2m}+V(\vec{r})\right]\psi^*_{n,\vec{k}}(\vec{r},-t)=i\hbar\frac{\partial\psi^*_{n,\vec{k}}(\vec{r},-t)}{\partial t}$$

This means that $\psi^*_{n,\vec{k}}(\vec{r},-t)$ is the time-reversed state corresponding to the state $\psi_{n,\vec{k}}(\vec{r},t)$

$$\psi^*_{n,\vec{k}}(\vec{r},-t)=\psi^*_{n,\vec{k}}(\vec{r})\,e^{-i\frac{E_n(\vec{k})}{\hbar}t} \longrightarrow \left[-\frac{\hbar^2\nabla^2}{2m}+V(\vec{r})\right]\psi^*_{n,\vec{k}}(\vec{r})=E_n(\vec{k})\psi^*_{n,\vec{k}}(\vec{r})$$

The function $\psi^*_{n,\vec{k}}(\vec{r})$ is the time-reversed Bloch state corresponding to $\psi_{n,\vec{k}}(\vec{r})$

Time Reversal Symmetry and Energy Bands

$$\left[-\frac{\hbar^2\nabla^2}{2m}+V(\vec{r})\right]\psi^*_{n,\vec{k}}(\vec{r})=E_n(\vec{k})\psi^*_{n,\vec{k}}(\vec{r})$$

We have found another Bloch function, i.e. $\psi^*_{n,\vec{k}}(\vec{r})$, with the same energy as $\psi_{n,\vec{k}}(\vec{r})$

The question is if we really have found a new eigenfunction or not, and if so what is the wavevector of this new eigenfunction

We know that Bloch functions have the property that: $\psi_{n,\vec{k}}(\vec{r}+\vec{R})=e^{i\,\vec{k}\,.\,\vec{R}}\,\psi_{n,\vec{k}}(\vec{r})$

So we try this on $\psi^*_{n,\vec{k}}(\vec{r})$:

$$\psi^*_{n,\vec{k}}(\vec{r}+\vec{R})=\left[\psi_{n,\vec{k}}(\vec{r}+\vec{R})\right]^*=\left[e^{i\,\vec{k}\,.\,\vec{R}}\,\psi_{n,\vec{k}}(\vec{r})\right]^*=e^{i\,[-\vec{k}]\,.\,\vec{R}}\,\psi^*_{n,\vec{k}}(\vec{r})$$

$\Rightarrow$ $\psi^*_{n,\vec{k}}(\vec{r})$ is a Bloch function with wavevector $-\vec{k}$ and energy $E_n(\vec{k})$

$\Rightarrow$ $\psi_{n,-\vec{k}}(\vec{r})=\psi^*_{n,\vec{k}}(\vec{r})$ and $E_n(-\vec{k})=E_n(\vec{k})$

Important Lesson:
Time reversal symmetry implies that $E_n(-\vec{k})=E_n(\vec{k})$ even if the crystal lacks spatial inversion symmetry (e.g. GaAs, InP, etc)

Spin-Orbit Interaction in Solids

An electron moving in an electric field sees an effective magnetic field given by:

$$\vec{B}_{eff}=\frac{\vec{E}\times\vec{P}}{2mc^2}\longrightarrow$$

The additional factor of 2 is coming from Thomas precession

The electron has a magnetic moment $\vec{\mu}$ related to its spin angular momentum $\vec{S}$ by:

$$\vec{\mu}=-g\frac{\mu_B}{\hbar}\vec{S}\longrightarrow\hat{\vec{S}}=\frac{\hbar}{2}\hat{\vec{\sigma}}\qquad\mu_B=\frac{e\hbar}{2m}\qquad g\approx 2\longrightarrow\hat{\vec{\mu}}=-\mu_B\hat{\vec{\sigma}}$$

$$\hat{\vec{\sigma}}=\hat{\sigma}_x\hat{x}+\hat{\sigma}_y\hat{y}+\hat{\sigma}_z\hat{z}\quad\left\{\ \hat{\sigma}_x=\begin{bmatrix}0&1\\1&0\end{bmatrix}\qquad\hat{\sigma}_y=\begin{bmatrix}0&-i\\i&0\end{bmatrix}\qquad\hat{\sigma}_z=\begin{bmatrix}1&0\\0&-1\end{bmatrix}\right.$$

The interaction between the electron spin and the effective magnetic field adds a new term to the Hamiltonian:

$$\hat{H}_{so}=-\hat{\vec{\mu}}.\vec{B}_{eff}=\mu_B\hat{\vec{\sigma}}.\vec{B}_{eff}=\mu_B\hat{\vec{\sigma}}\,.\,\frac{1}{2mc^2}\left[\frac{\nabla V(\hat{\vec{r}})}{e}\times\hat{\vec{P}}\right]=\frac{\hbar}{4m^2c^2}\hat{\vec{\sigma}}\,.\left[\nabla V(\hat{\vec{r}})\times\hat{\vec{P}}\right]$$

Spin-Orbit Interaction and Bloch Functions

In the absence of spin-orbit interaction we had:

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

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

Electron states with spin-up and spin-down were degenerate $\left\{ E_{n,\uparrow}(\vec{k}) = E_{n,\downarrow}(\vec{k}) \right.$

In the presence of spin-orbit coupling the Hamiltonian becomes:

$$\hat{H} = \hat{H}_o + \hat{H}_{so}$$

$$\hat{H}_{so} = \frac{\hbar}{4m^2c^2} \hat{\vec{\sigma}} \cdot \left[\nabla_{\vec{r}} V(\hat{\vec{r}}) \times \hat{\vec{P}}\right] = -i \frac{\hbar^2}{4m^2c^2} \hat{\vec{\sigma}} \cdot \left[\nabla_{\vec{r}} V(\hat{\vec{r}}) \times \vec{\nabla}_{\vec{r}}\right]$$

Since the Hamiltonian is now spin-dependent, pure spin-up or pure spin-down states are no longer the eigenstates of the Hamiltonian

The eigenstates can be written most generally as a superposition of up and down spin states, or:

$$\psi_{n,\vec{k},\chi}(\vec{r}) = \begin{bmatrix} \alpha_{n,\vec{k}}(\vec{r}) \\ \beta_{n,\vec{k}}(\vec{r}) \end{bmatrix} = \alpha_{n,\vec{k}}(\vec{r}) |\uparrow\rangle + \beta_{n,\vec{k}}(\vec{r}) |\downarrow\rangle$$

χ =Quantum number for the two spin degrees of freedom, usually taken to be +1 or -1

Spin-Orbit Interaction and Bloch Functions

$$\hat{H} \begin{bmatrix} \alpha_{n,\vec{k}}(\vec{r}) \\ \beta_{n,\vec{k}}(\vec{r}) \end{bmatrix} = E_{n,\chi}(\vec{k}) \begin{bmatrix} \alpha_{n,\vec{k}}(\vec{r}) \\ \beta_{n,\vec{k}}(\vec{r}) \end{bmatrix}$$

$$\left\{-\frac{\hbar^2 \nabla_{\vec{r}}^2}{2m} + V(\vec{r}) - i \frac{\hbar^2}{4m^2c^2} \hat{\vec{\sigma}} \cdot \left[\nabla_{\vec{r}} V(\hat{\vec{r}}) \times \vec{\nabla}_{\vec{r}}\right]\right\} \begin{bmatrix} \alpha_{n,\vec{k}}(\vec{r}) \\ \beta_{n,\vec{k}}(\vec{r}) \end{bmatrix} = E_{n,\chi}(\vec{k}) \begin{bmatrix} \alpha_{n,\vec{k}}(\vec{r}) \\ \beta_{n,\vec{k}}(\vec{r}) \end{bmatrix}$$

For each wavevector in the FBZ, and for each band index, one will obtain two solutions of the above equation

We label one as χ = +1 and the other with χ = -1 and in general $E_{n,-\chi}(\vec{k}) \neq E_{n,\chi}(\vec{k})$

These two solutions will correspond to spins pointing in two different directions (usually collinear and opposite directions). Let these directions be specified by $\hat{n}$ at the location $\vec{r}$:

$$\hat{\vec{\sigma}}.\hat{n}\, \psi_{n,\vec{k},\chi}(\vec{r}) = +1\, \psi_{n,\vec{k},\chi}(\vec{r})$$

$$\hat{\vec{\sigma}}.\hat{n}\, \psi_{n,\vec{k},-\chi}(\vec{r}) = -1\, \psi_{n,\vec{k},-\chi}(\vec{r})$$

Spin-Orbit Interaction and Lattice Symmetries

In the presence of spin-orbit interaction we have the Schrodinger equation:

$$\left\{-\frac{\hbar^2\nabla_{\vec r}^2}{2m}+V(\vec r)-i\frac{\hbar^2}{4m^2c^2}\,\hat{\vec\sigma}\,.\left[\nabla_{\vec r}V(\hat{\vec r})\times\vec\nabla_{\vec r}\right]\right\}\begin{bmatrix}\alpha_{n,\vec k}(\vec r)\\ \beta_{n,\vec k}(\vec r)\end{bmatrix}=E_{n,\chi}(\vec k)\begin{bmatrix}\alpha_{n,\vec k}(\vec r)\\ \beta_{n,\vec k}(\vec r)\end{bmatrix}$$

Lattice Translation Symmetry:

$$\psi_{n,\vec k,\chi}(\vec r+\vec R)=\begin{bmatrix}\alpha_{n,\vec k}(\vec r+\vec R)\\ \beta_{n,\vec k}(\vec r+\vec R)\end{bmatrix}=\begin{bmatrix}e^{i\vec k.\vec R}\alpha_{n,\vec k}(\vec r)\\ e^{i\vec k.\vec R}\beta_{n,\vec k}(\vec r)\end{bmatrix}=e^{i\vec k.\vec R}\psi_{n,\vec k,\chi}(\vec r)$$

Rotation Symmetry:

Let $\hat S$ be an operator belonging to the rotation subgroup of the crystal point-group, such that:

$$V(\hat S\vec r)=V(\vec r) \qquad \left\{\hat S^T=\hat S^{-1}\Rightarrow \text{unitary}\right.$$

(The case of inversion symmetry will be treated separately)

Spin-Orbit Interaction and Rotation Symmetry

Suppose we have found the solution to the Schrodinger equation:

$$\left\{-\frac{\hbar^2\nabla_{\vec r}^2}{2m}+V(\vec r)-i\frac{\hbar^2}{4m^2c^2}\,\hat{\vec\sigma}\,.\left[\nabla_{\vec r}V(\hat{\vec r})\times\vec\nabla_{\vec r}\right]\right\}\begin{bmatrix}\alpha_{n,\vec k}(\vec r)\\ \beta_{n,\vec k}(\vec r)\end{bmatrix}=E_{n,\chi}(\vec k)\begin{bmatrix}\alpha_{n,\vec k}(\vec r)\\ \beta_{n,\vec k}(\vec r)\end{bmatrix}$$

And the solution is:

$$\psi_{n,\vec k,\chi}(\vec r)=\begin{bmatrix}\alpha_{n,\vec k}(\vec r)\\ \beta_{n,\vec k}(\vec r)\end{bmatrix} \qquad \Leftrightarrow \qquad E_{n,\chi}(\vec k)$$

We replace $\vec r$ by $\hat S\vec r$ everywhere in the Schrodinger equation:

$$\left\{-\frac{\hbar^2\nabla_{\hat S\vec r}^2}{2m}+V(\hat S\vec r)-i\frac{\hbar^2}{4m^2c^2}\,\hat{\vec\sigma}\,.\left[\nabla_{\hat S\vec r}V(\hat S\hat{\vec r})\times\vec\nabla_{\hat S\vec r}\right]\right\}\begin{bmatrix}\alpha_{n,\vec k}(\hat S\vec r)\\ \beta_{n,\vec k}(\hat S\vec r)\end{bmatrix}=E_{n,\chi}(\vec k)\begin{bmatrix}\alpha_{n,\vec k}(\hat S\vec r)\\ \beta_{n,\vec k}(\hat S\vec r)\end{bmatrix}$$

$$\Rightarrow\left\{-\frac{\hbar^2\nabla_{\vec r}^2}{2m}+V(\vec r)-i\frac{\hbar^2}{4m^2c^2}\,\hat{\vec\sigma}\,.\,\hat S\left[\nabla_{\vec r}V(\hat{\vec r})\times\vec\nabla_{\vec r}\right]\right\}\begin{bmatrix}\alpha_{n,\vec k}(\hat S\vec r)\\ \beta_{n,\vec k}(\hat S\vec r)\end{bmatrix}=E_{n,\chi}(\vec k)\begin{bmatrix}\alpha_{n,\vec k}(\hat S\vec r)\\ \beta_{n,\vec k}(\hat S\vec r)\end{bmatrix}$$

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Spin-Orbit Interaction and Rotation Symmetry

$$\left\{-\frac{\hbar^2\nabla_{\vec{r}}^2}{2m}+V(\vec{r})-i\frac{\hbar^2}{4m^2c^2}\hat{\vec{\sigma}}\,.\,\hat{S}\left[\nabla_{\vec{r}}V\left(\hat{\vec{r}}\right)\times\vec{\nabla}_{\vec{r}}\right]\right\}\begin{bmatrix}\alpha_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\\ \beta_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\end{bmatrix}=E_{n,\chi}\left(\vec{k}\right)\begin{bmatrix}\alpha_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\\ \beta_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\end{bmatrix}$$

The above equation does not look like the Schrodinger equation!

We define a unitary spin rotation operator $\hat{R}_{\hat{S}}$ that operates in the Hilbert space of spins and rotates spin states in the sense of the operator $\hat{S}$

Consider a spin vector pointing in the $\hat{n}$ direction:

$$\hat{\vec{\sigma}}.\hat{n}\begin{bmatrix}a\\ b\end{bmatrix}=+1\begin{bmatrix}a\\ b\end{bmatrix}$$

$$\Rightarrow \hat{\vec{\sigma}}.\hat{n}\hat{R}_{\hat{S}}^{-1}\hat{R}_{\hat{S}}\begin{bmatrix}a\\ b\end{bmatrix}=+1\begin{bmatrix}a\\ b\end{bmatrix}$$

$$\Rightarrow \hat{R}_{\hat{S}}\hat{\vec{\sigma}}.\hat{n}\hat{R}_{\hat{S}}^{-1}\hat{R}_{\hat{S}}\begin{bmatrix}a\\ b\end{bmatrix}=+1\,\hat{R}_{\hat{S}}\begin{bmatrix}a\\ b\end{bmatrix}$$

$$\Rightarrow \left(\hat{\vec{\sigma}}.\hat{S}\hat{n}\right)\hat{R}_{\hat{S}}\begin{bmatrix}a\\ b\end{bmatrix}=+1\,\hat{R}_{\hat{S}}\begin{bmatrix}a\\ b\end{bmatrix}$$

The spin rotation operators have the property: $\hat{R}_{\hat{S}}\left(\hat{\vec{\sigma}}.\hat{n}\right)\hat{R}_{\hat{S}}^{-1}=\hat{\vec{\sigma}}.\hat{S}\hat{n}$

Spin-Orbit Interaction and Point-Group Symmetry

Start from:

$$\left\{-\frac{\hbar^2\nabla_{\vec{r}}^2}{2m}+V(\vec{r})-i\frac{\hbar^2}{4m^2c^2}\hat{\vec{\sigma}}\,.\,\hat{S}\left[\nabla_{\vec{r}}V\left(\hat{\vec{r}}\right)\times\vec{\nabla}_{\vec{r}}\right]\right\}\begin{bmatrix}\alpha_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\\ \beta_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\end{bmatrix}=E_{n,\chi}\left(\vec{k}\right)\begin{bmatrix}\alpha_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\\ \beta_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\end{bmatrix}$$

Introduce spin rotation operator $\hat{R}_{\hat{S}}$ corresponding to the rotation generated by the matrix $\hat{S}$:

$$\hat{R}_{\hat{S}}^{-1}\left\{-\frac{\hbar^2\nabla_{\vec{r}}^2}{2m}+V(\vec{r})-i\frac{\hbar^2}{4m^2c^2}\hat{\vec{\sigma}}\,.\,\hat{S}\left[\nabla_{\vec{r}}V\left(\hat{\vec{r}}\right)\times\vec{\nabla}_{\vec{r}}\right]\right\}\hat{R}_{\hat{S}}\hat{R}_{\hat{S}}^{-1}\begin{bmatrix}\alpha_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\\ \beta_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\end{bmatrix}=E_{n,\chi}\left(\vec{k}\right)\hat{R}_{\hat{S}}^{-1}\begin{bmatrix}\alpha_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\\ \beta_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\end{bmatrix}$$

$$\left\{-\frac{\hbar^2\nabla_{\vec{r}}^2}{2m}+V(\vec{r})-i\frac{\hbar^2}{4m^2c^2}\hat{\vec{\sigma}}\,.\left[\nabla_{\vec{r}}V\left(\hat{\vec{r}}\right)\times\vec{\nabla}_{\vec{r}}\right]\right\}\hat{R}_{\hat{S}}^{-1}\begin{bmatrix}\alpha_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\\ \beta_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\end{bmatrix}=E_{n,\chi}\left(\vec{k}\right)\hat{R}_{\hat{S}}^{-1}\begin{bmatrix}\alpha_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\\ \beta_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\end{bmatrix}$$

The above equation shows that the new state:

$$\hat{R}_{\hat{S}}^{-1}\begin{bmatrix}\alpha_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\\ \beta_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\end{bmatrix}$$

satisfies the Schrodinger equation and has the same energy as the state: $\begin{bmatrix}\alpha_{n,\vec{k}}\left(\vec{r}\right)\\ \beta_{n,\vec{k}}\left(\vec{r}\right)\end{bmatrix}$

Spin-Orbit Interaction and Point-Group Symmetry

Since:

$$\hat{R}_{\hat{S}}^{-1}\begin{bmatrix}\alpha_{n,\vec{k}}\left(\hat{S}\left(\vec{r}+\vec{R}\right)\right)\\ \beta_{n,\vec{k}}\left(\hat{S}\left(\vec{r}+\vec{R}\right)\right)\end{bmatrix}=e^{i\vec{k}.\hat{S}\vec{R}}\ \hat{R}_{\hat{S}}^{-1}\begin{bmatrix}\alpha_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\\ \beta_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\end{bmatrix}=e^{i\hat{S}^{-1}\vec{k}.\vec{R}}\ \hat{R}_{\hat{S}}^{-1}\begin{bmatrix}\alpha_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\\ \beta_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\end{bmatrix}$$

The new state is a Bloch state with wavevector $\hat{S}^{-1}\vec{k}$

Summary:

If $\hat{S}$ is an operator for a point-group symmetry operation then the two states given by:

$$\psi_{n,\vec{k},\chi}(\vec{r})=\begin{bmatrix}\alpha_{n,\vec{k}}(\vec{r})\\ \beta_{n,\vec{k}}(\vec{r})\end{bmatrix}$$

$$\psi_{n,\hat{S}^{-1}\vec{k},\chi'}(\vec{r})=\hat{R}_{\hat{S}}^{-1}\begin{bmatrix}\alpha_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\\ \beta_{n,\vec{k}}\left(\hat{S}\vec{r}\right)\end{bmatrix}$$

This represents a rotated (in space) version of the original Bloch state. Even the spin is rotated appropriately by the spin rotation operator.

have the same energy:

$$E_{n,\chi'}\left(\hat{S}^{-1}\vec{k}\right)=E_{n,\chi}\left(\vec{k}\right)$$

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Spin-Orbit Interaction and Inversion Symmetry

Suppose the crystal potential has inversion symmetry:

$$V(-\vec{r})=V(\vec{r})$$

Suppose we have found the solution to the Schrodinger equation:

$$\left\{-\frac{\hbar^2\nabla_{\vec{r}}^2}{2m}+V(\vec{r})-i\frac{\hbar^2}{4m^2c^2}\hat{\vec{\sigma}}\,.\left[\nabla_{\vec{r}}V\left(\hat{\vec{r}}\right)\times\nabla_{\vec{r}}\right]\right\}\begin{bmatrix}\alpha_{n,\vec{k}}(\vec{r})\\ \beta_{n,\vec{k}}(\vec{r})\end{bmatrix}=E_{n,\chi}\left(\vec{k}\right)\begin{bmatrix}\alpha_{n,\vec{k}}(\vec{r})\\ \beta_{n,\vec{k}}(\vec{r})\end{bmatrix}$$

And the solution is:

$$\psi_{n,\vec{k},\chi}(\vec{r})=\begin{bmatrix}\alpha_{n,\vec{k}}(\vec{r})\\ \beta_{n,\vec{k}}(\vec{r})\end{bmatrix}\qquad\Leftrightarrow\qquad E_{n,\chi}\left(\vec{k}\right)$$

We replace $\vec{r}$ by $-\vec{r}$ everywhere in the Schrodinger equation:

$$\left\{-\frac{\hbar^2\nabla_{-\vec{r}}^2}{2m}+V(-\vec{r})-i\frac{\hbar^2}{4m^2c^2}\hat{\vec{\sigma}}\,.\left[\nabla_{-\vec{r}}V\left(-\hat{\vec{r}}\right)\times\nabla_{-\vec{r}}\right]\right\}\begin{bmatrix}\alpha_{n,\vec{k}}(-\vec{r})\\ \beta_{n,\vec{k}}(-\vec{r})\end{bmatrix}=E_{n,\chi}\left(\vec{k}\right)\begin{bmatrix}\alpha_{n,\vec{k}}(-\vec{r})\\ \beta_{n,\vec{k}}(-\vec{r})\end{bmatrix}$$

$$\Rightarrow\left\{-\frac{\hbar^2\nabla_{\vec{r}}^2}{2m}+V(\vec{r})-i\frac{\hbar^2}{4m^2c^2}\hat{\vec{\sigma}}\,.\left[\nabla_{\vec{r}}V\left(\hat{\vec{r}}\right)\times\nabla_{\vec{r}}\right]\right\}\begin{bmatrix}\alpha_{n,\vec{k}}(-\vec{r})\\ \beta_{n,\vec{k}}(-\vec{r})\end{bmatrix}=E_{n,\chi}\left(\vec{k}\right)\begin{bmatrix}\alpha_{n,\vec{k}}(-\vec{r})\\ \beta_{n,\vec{k}}(-\vec{r})\end{bmatrix}$$

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Spin-Orbit Interaction and Inversion Symmetry

$$\left\{-\frac{\hbar^2\nabla^2_{\vec r}}{2m}+V(\vec r)-i\frac{\hbar^2}{4m^2c^2}\hat{\vec\sigma}\,.\left[\nabla_{\vec r}V(\hat{\vec r})\times\vec\nabla_{\vec r}\right]\right\}\begin{bmatrix}\alpha_{n,\vec k}(-\vec r)\\ \beta_{n,\vec k}(-\vec r)\end{bmatrix}=E_{n,\chi}(\vec k)\begin{bmatrix}\alpha_{n,\vec k}(-\vec r)\\ \beta_{n,\vec k}(-\vec r)\end{bmatrix}$$

The above equation shows that the new state: $\begin{bmatrix}\alpha_{n,\vec k}(-\vec r)\\ \beta_{n,\vec k}(-\vec r)\end{bmatrix}$

satisfies the Schrodinger equation and has the same energy as the state: $\begin{bmatrix}\alpha_{n,\vec k}(\vec r)\\ \beta_{n,\vec k}(\vec r)\end{bmatrix}$

Since:

$$\begin{bmatrix}\alpha_{n,\vec k}\left(-\left(\vec r+\vec R\right)\right)\\ \beta_{n,\vec k}\left(-\left(\vec r+\vec R\right)\right)\end{bmatrix}=e^{i(-\vec k).\vec R}\begin{bmatrix}\alpha_{n,\vec k}(-\vec r)\\ \beta_{n,\vec k}(-\vec r)\end{bmatrix}$$

the new state is a Bloch state with wavevector $-\vec k$

In most cases, the new state: $\begin{bmatrix}\alpha_{n,\vec k}(-\vec r)\\ \beta_{n,\vec k}(-\vec r)\end{bmatrix}$

has the same spin direction as the state: $\begin{bmatrix}\alpha_{n,\vec k}(\vec r)\\ \beta_{n,\vec k}(\vec r)\end{bmatrix}$

So we can write: $\psi_{n,-\vec k,\chi}(\vec r)=\begin{bmatrix}\alpha_{n,\vec k}(-\vec r)\\ \beta_{n,\vec k}(-\vec r)\end{bmatrix}$

Spin-Orbit Interaction and Inversion Symmetry

Summary:

If the crystal potential has inversion symmetry then the two states given by:

$$\psi_{n,\vec k,\chi}(\vec r)=\begin{bmatrix}\alpha_{n,\vec k}(\vec r)\\ \beta_{n,\vec k}(\vec r)\end{bmatrix}\qquad \psi_{n,-\vec k,\chi}(\vec r)=\begin{bmatrix}\alpha_{n,\vec k}(-\vec r)\\ \beta_{n,\vec k}(-\vec r)\end{bmatrix}$$

have the same energy:

$$E_{n,\chi}(-\vec k)=E_{n,\chi}(\vec k)$$

Spin-Orbit Interaction and Time Reversal Symmetry

Consider the Bloch function:

$$\psi_{n,\vec{k},\chi}(\vec{r}) = \begin{bmatrix} \alpha_{n,\vec{k}}(\vec{r}) \\ \beta_{n,\vec{k}}(\vec{r}) \end{bmatrix} = \alpha_{n,\vec{k}}(\vec{r})|\uparrow\rangle + \beta_{n,\vec{k}}(\vec{r})|\downarrow\rangle$$

Suppose the Bloch function corresponds to the spin pointing in the direction of the unit vector $\hat{n}$ at the location $\vec{r}$:

$$\hat{\vec{\sigma}}.\hat{n}\,\psi_{n,\vec{k},\chi}(\vec{r}) = \hat{\vec{\sigma}}.\hat{n}\begin{bmatrix} \alpha_{n,\vec{k}}(\vec{r}) \\ \beta_{n,\vec{k}}(\vec{r}) \end{bmatrix} = +1\begin{bmatrix} \alpha_{n,\vec{k}}(\vec{r}) \\ \beta_{n,\vec{k}}(\vec{r}) \end{bmatrix} = +1\,\psi_{n,\vec{k},\chi}(\vec{r})$$

What if we want the state with the opposite spin at the same location?

The answer is:

$$-i\hat{\sigma}_y\,\psi^*_{n,\vec{k},\chi}(\vec{r}) = \begin{bmatrix} -\beta^*_{n,\vec{k}}(\vec{r}) \\ \alpha^*_{n,\vec{k}}(\vec{r}) \end{bmatrix}$$

Proof:

$$\begin{aligned}\hat{\vec{\sigma}}.\hat{n}\left[-i\hat{\sigma}_y\,\psi^*_{n,\vec{k},\chi}(\vec{r})\right] &= -i\left[-\hat{\vec{\sigma}}^*.\hat{n}\,\hat{\sigma}_y\,\psi_{n,\vec{k},\chi}(\vec{r})\right]^* \\ &= -i\left[-\hat{\sigma}_y\hat{\sigma}_y\hat{\vec{\sigma}}^*.\hat{n}\,\hat{\sigma}_y\hat{\sigma}_y\hat{\sigma}_y\,\psi_{n,\vec{k},\chi}(\vec{r})\right]^* = -i\left[\hat{\sigma}_y\hat{\vec{\sigma}}.\hat{n}\,\psi_{n,\vec{k},\chi}(\vec{r})\right]^* \\ &= -i\left[\hat{\sigma}_y\,\psi_{n,\vec{k},\chi}(\vec{r})\right]^* = -1\left[-i\hat{\sigma}_y\,\psi^*_{n,\vec{k},\chi}(\vec{r})\right]\end{aligned}$$

$$\left\{\hat{\vec{\sigma}} = \hat{\sigma}_x\hat{x} + \hat{\sigma}_y\hat{y} + \hat{\sigma}_z\hat{z} \quad \Rightarrow \quad \hat{\vec{\sigma}}^* = \hat{\sigma}_x\hat{x} - \hat{\sigma}_y\hat{y} + \hat{\sigma}_z\hat{z} \neq \hat{\vec{\sigma}}\right\}$$

Spin-Orbit Interaction and Time Reversal Symmetry

In the presence of spin-orbit interaction we have the Schrodinger equation:

$$\left\{-\frac{\hbar^2\nabla^2_{\vec{r}}}{2m} + V(\vec{r}) - i\frac{\hbar^2}{4m^2c^2}\,\hat{\vec{\sigma}}\,.\left[\nabla V(\hat{\vec{r}})\times\vec{\nabla}\right]\right\}\begin{bmatrix} \alpha_{n,\vec{k}}(\vec{r}) \\ \beta_{n,\vec{k}}(\vec{r}) \end{bmatrix} = E_{n,\chi}(\vec{k})\begin{bmatrix} \alpha_{n,\vec{k}}(\vec{r}) \\ \beta_{n,\vec{k}}(\vec{r}) \end{bmatrix}$$

Suppose we have solved it and found the solution: $\psi_{n,\vec{k},\chi}(\vec{r}) = \begin{bmatrix} \alpha_{n,\vec{k}}(\vec{r}) \\ \beta_{n,\vec{k}}(\vec{r}) \end{bmatrix} \Leftrightarrow E_{n,\chi}(\vec{k})$

We complex conjugate it:

$$\left\{-\frac{\hbar^2\nabla^2_{\vec{r}}}{2m} + V(\vec{r}) + i\frac{\hbar^2}{4m^2c^2}\,\hat{\vec{\sigma}}^*\,.\left[\nabla V(\hat{\vec{r}})\times\vec{\nabla}\right]\right\}\begin{bmatrix} \alpha^*_{n,\vec{k}}(\vec{r}) \\ \beta^*_{n,\vec{k}}(\vec{r}) \end{bmatrix} = E_{n,\chi}(\vec{k})\begin{bmatrix} \alpha^*_{n,\vec{k}}(\vec{r}) \\ \beta^*_{n,\vec{k}}(\vec{r}) \end{bmatrix}$$

It does not look like the original Schrodinger equation!

Note that:

$$\hat{\vec{\sigma}} = \hat{\sigma}_x\hat{x} + \hat{\sigma}_y\hat{y} + \hat{\sigma}_z\hat{z}$$

$$\Rightarrow \hat{\vec{\sigma}}^* = \hat{\sigma}_x\hat{x} - \hat{\sigma}_y\hat{y} + \hat{\sigma}_z\hat{z} \neq \hat{\vec{\sigma}}$$

Spin-Orbit Interaction and Time Reversal Symmetry

Given an eigenvalue matrix equation:

$$Av = \lambda v$$

One can always perform a unitary transformation with matrix T and obtain:

$$TAT^{-1}Tv = \lambda Tv \qquad \begin{cases} B = TAT^{-1} \\ u = Tv \end{cases}$$

$$\Rightarrow Bu = \lambda u$$

So try a transformation with the unitary matrix $-i\hat{\sigma}_y$ with the equation:

$$\left(-i\hat{\sigma}_y\right)\left\{-\frac{\hbar^2\nabla_{\vec{r}}^2}{2m} + V(\vec{r}) + i\frac{\hbar^2}{4m^2c^2}\hat{\vec{\sigma}}^* \cdot \left[\nabla V\left(\hat{\vec{r}}\right)\times\vec{\nabla}\right]\right\}\left(+i\hat{\sigma}_y\right)\left(-i\hat{\sigma}_y\right)\begin{bmatrix}\alpha^*_{n,\vec{k}}(\vec{r})\\ \beta^*_{n,\vec{k}}(\vec{r})\end{bmatrix} = E_{n,\chi}\left(\vec{k}\right)\left(-i\hat{\sigma}_y\right)\begin{bmatrix}\alpha^*_{n,\vec{k}}(\vec{r})\\ \beta^*_{n,\vec{k}}(\vec{r})\end{bmatrix}$$

$$\Rightarrow \left\{-\frac{\hbar^2\nabla_{\vec{r}}^2}{2m} + V(\vec{r}) - i\frac{\hbar^2}{4m^2c^2}\hat{\vec{\sigma}} \cdot \left[\nabla V\left(\hat{\vec{r}}\right)\times\vec{\nabla}\right]\right\}\begin{bmatrix}-\beta^*_{n,\vec{k}}(\vec{r})\\ \alpha^*_{n,\vec{k}}(\vec{r})\end{bmatrix} = E_{n,\chi}\left(\vec{k}\right)\begin{bmatrix}-\beta^*_{n,\vec{k}}(\vec{r})\\ \alpha^*_{n,\vec{k}}(\vec{r})\end{bmatrix}$$

We have found a new solution: $\begin{bmatrix}-\beta^*_{n,\vec{k}}(\vec{r})\\ \alpha^*_{n,\vec{k}}(\vec{r})\end{bmatrix}$

with the same energy $E_{n,\chi}\left(\vec{k}\right)$ as the original solution: $\psi_{n,\vec{k},\chi}(\vec{r}) = \begin{bmatrix}\alpha_{n,\vec{k}}(\vec{r})\\ \beta_{n,\vec{k}}(\vec{r})\end{bmatrix}$

Question: What is the physical significance of the new solution?

Spin-Orbit Interaction and Time Reversal Symmetry

Under lattice translation we get for the new solution:

$$\begin{bmatrix}-\beta^*_{n,\vec{k}}\left(\vec{r}+\vec{R}\right)\\ \alpha^*_{n,\vec{k}}\left(\vec{r}+\vec{R}\right)\end{bmatrix} = e^{-i\vec{k}.\vec{R}}\begin{bmatrix}-\beta^*_{n,\vec{k}}(\vec{r})\\ \alpha^*_{n,\vec{k}}(\vec{r})\end{bmatrix}$$

So the new solution is a Bloch state with wavevector $-\vec{k}$

$$\psi_{n,-\vec{k},?}(\vec{r}) = \begin{bmatrix}-\beta^*_{n,\vec{k}}(\vec{r})\\ \alpha^*_{n,\vec{k}}(\vec{r})\end{bmatrix}$$

Note that the new solution found can also be written as:

$$-i\hat{\sigma}_y\,\psi^*_{n,\vec{k},\chi}(\vec{r}) = \begin{bmatrix}-\beta^*_{n,\vec{k}}(\vec{r})\\ \alpha^*_{n,\vec{k}}(\vec{r})\end{bmatrix}$$

But as shown earlier, the above state has spin opposite to the state $\psi_{n,\vec{k},\chi}(\vec{r}) = \begin{bmatrix}\alpha_{n,\vec{k}}(\vec{r})\\ \beta_{n,\vec{k}}(\vec{r})\end{bmatrix}$

Therefore, the new solution is a Bloch state $\psi_{n,-\vec{k},-\chi}(\vec{r})$, i.e.:

$$\psi_{n,-\vec{k},-\chi}(\vec{r}) = -i\hat{\sigma}_y\,\psi^*_{n,\vec{k},\chi}(\vec{r}) = \begin{bmatrix}-\beta^*_{n,\vec{k}}(\vec{r})\\ \alpha^*_{n,\vec{k}}(\vec{r})\end{bmatrix}$$

And we have also found that its energy is the same as that of the state $\psi_{n,\vec{k},\chi}(\vec{r})$:

$$E_{n,-\chi}\left(-\vec{k}\right) = E_{n,\chi}\left(\vec{k}\right)$$

Spin-Orbit Interaction and Time Reversal Symmetry

In the presence of spin-orbit interaction we have the time-dependent Schrodinger equation:

$$\left\{-\frac{\hbar^2\nabla_{\vec r}^2}{2m}+V(\vec r)-i\frac{\hbar^2}{4m^2c^2}\hat{\vec\sigma}\cdot\left[\nabla V(\hat{\vec r})\times\hat{\vec\nabla}\right]\right\}\begin{bmatrix}\alpha_{n,\vec k}(\vec r,t)\\ \beta_{n,\vec k}(\vec r,t)\end{bmatrix}=i\hbar\frac{\partial}{\partial t}\begin{bmatrix}\alpha_{n,\vec k}(\vec r,t)\\ \beta_{n,\vec k}(\vec r,t)\end{bmatrix}$$

Solution is:

$$\psi_{n,\vec k,\chi}(\vec r,t)=\begin{bmatrix}\alpha_{n,\vec k}(\vec r,t)\\ \beta_{n,\vec k}(\vec r,t)\end{bmatrix}=\begin{bmatrix}\alpha_{n,\vec k}(\vec r)e^{-iE_{n,\chi}(\vec k)t}\\ \beta_{n,\vec k}(\vec r)e^{-iE_{n,\chi}(\vec k)t}\end{bmatrix}=\psi_{n,\vec k,\chi}(\vec r)e^{-iE_{n,\chi}(\vec k)t}$$

Lets see if we can find a solution under time-reversal (i.e. when *t* is replaced by *–t*):

$$\left\{-\frac{\hbar^2\nabla_{\vec r}^2}{2m}+V(\vec r)-i\frac{\hbar^2}{4m^2c^2}\hat{\vec\sigma}\cdot\left[\nabla V(\hat{\vec r})\times\hat{\vec\nabla}\right]\right\}\begin{bmatrix}\alpha_{n,\vec k}(\vec r,-t)\\ \beta_{n,\vec k}(\vec r,-t)\end{bmatrix}=-i\hbar\frac{\partial}{\partial t}\begin{bmatrix}\alpha_{n,\vec k}(\vec r,-t)\\ \beta_{n,\vec k}(\vec r,-t)\end{bmatrix}$$

The above does not look like a Schrodinger equation so we complex conjugate it:

$$\left\{-\frac{\hbar^2\nabla_{\vec r}^2}{2m}+V(\vec r)+i\frac{\hbar^2}{4m^2c^2}\hat{\vec\sigma}^*\cdot\left[\nabla V(\hat{\vec r})\times\hat{\vec\nabla}\right]\right\}\begin{bmatrix}\alpha^*_{n,\vec k}(\vec r,-t)\\ \beta^*_{n,\vec k}(\vec r,-t)\end{bmatrix}=i\hbar\frac{\partial}{\partial t}\begin{bmatrix}\alpha^*_{n,\vec k}(\vec r,-t)\\ \beta^*_{n,\vec k}(\vec r,-t)\end{bmatrix}$$

And it still does not look like the original Schrodinger equation!

Spin-Orbit Interaction and Time Reversal Symmetry

Given an eigenvalue matrix equation:

$$Av=\lambda v$$

One can always perform a unitary transformation with matrix *T* and obtain:

$$\begin{aligned}&TAT^{-1}Tv=\lambda Tv\\ &\Rightarrow Bu=\lambda u\end{aligned}\qquad\left\{\begin{aligned}&B=TAT^{-1}\\ &u=Tv\end{aligned}\right.$$

So try a transformation with the unitary matrix $-i\hat\sigma_y$ with the equation:

$$\left\{-\frac{\hbar^2\nabla_{\vec r}^2}{2m}+V(\vec r)+i\frac{\hbar^2}{4m^2c^2}\hat{\vec\sigma}^*\cdot\left[\nabla V(\hat{\vec r})\times\hat{\vec\nabla}\right]\right\}\begin{bmatrix}\alpha^*_{n,\vec k}(\vec r,-t)\\ \beta^*_{n,\vec k}(\vec r,-t)\end{bmatrix}=i\hbar\frac{\partial}{\partial t}\begin{bmatrix}\alpha^*_{n,\vec k}(\vec r,-t)\\ \beta^*_{n,\vec k}(\vec r,-t)\end{bmatrix}$$

$$\left(-i\hat\sigma_y\right)\left\{-\frac{\hbar^2\nabla_{\vec r}^2}{2m}+V(\vec r)+i\frac{\hbar^2}{4m^2c^2}\hat{\vec\sigma}^*\cdot\left[\nabla V(\hat{\vec r})\times\hat{\vec\nabla}\right]\right\}\left(+i\hat\sigma_y\right)\left(-i\hat\sigma_y\right)\begin{bmatrix}\alpha^*_{n,\vec k}(\vec r,-t)\\ \beta^*_{n,\vec k}(\vec r,-t)\end{bmatrix}=i\hbar\frac{\partial}{\partial t}\left(-i\hat\sigma_y\right)\begin{bmatrix}\alpha^*_{n,\vec k}(\vec r,-t)\\ \beta^*_{n,\vec k}(\vec r,-t)\end{bmatrix}$$

$$\Rightarrow\left\{-\frac{\hbar^2\nabla_{\vec r}^2}{2m}+V(\vec r)-i\frac{\hbar^2}{4m^2c^2}\hat{\vec\sigma}\cdot\left[\nabla V(\hat{\vec r})\times\hat{\vec\nabla}\right]\right\}\begin{bmatrix}-\beta^*_{n,\vec k}(\vec r,-t)\\ \alpha^*_{n,\vec k}(\vec r,-t)\end{bmatrix}=i\hbar\frac{\partial}{\partial t}\begin{bmatrix}-\beta^*_{n,\vec k}(\vec r,-t)\\ \alpha^*_{n,\vec k}(\vec r,-t)\end{bmatrix}$$

The above equation now looks like the time-dependent Schrodinger equation

Spin-Orbit Interaction and Time Reversal Symmetry

Summary:

Corresponding to the Bloch state:

$$\psi_{n,\vec{k},\chi}(\vec{r},t)=\begin{bmatrix}\alpha_{n,\vec{k}}(\vec{r},t)\\ \beta_{n,\vec{k}}(\vec{r},t)\end{bmatrix}=\begin{bmatrix}\alpha_{n,\vec{k}}(\vec{r})e^{-iE_{n,\chi}(\vec{k})t}\\ \beta_{n,\vec{k}}(\vec{r})e^{-iE_{n,\chi}(\vec{k})t}\end{bmatrix}=\psi_{n,\vec{k},\chi}(\vec{r})e^{-iE_{n,\chi}(\vec{k})t}$$

with energy:

$$E_{n,\chi}(\vec{k})$$

the time-reversed Bloch state is:

$$\begin{bmatrix}-\beta^*_{n,\vec{k}}(\vec{r},-t)\\ \alpha^*_{n,\vec{k}}(\vec{r},-t)\end{bmatrix}=\begin{bmatrix}-\beta^*_{n,\vec{k}}(\vec{r})e^{-iE_{n,\chi}(\vec{k})t}\\ \alpha^*_{n,\vec{k}}(\vec{r})e^{-iE_{n,\chi}(\vec{k})t}\end{bmatrix}=\psi_{n,-\vec{k},-\chi}(\vec{r})e^{-iE_{n,\chi}(\vec{k})t}$$

and the time-reversed state has the same energy as the original state:

$$E_{n,-\chi}(-\vec{k})=E_{n,\chi}(\vec{k})$$

Crystal Inversion Symmetry and Time Reversal Symmetry

Time reversal symmetry implies:

$$E_{n,-\chi}(-\vec{k})=E_{n,\chi}(\vec{k})$$

Inversion symmetry implies:

$$E_{n,\chi}(-\vec{k})=E_{n,\chi}(\vec{k})$$

In crystals which have inversion and time reversal symmetries the above two imply:

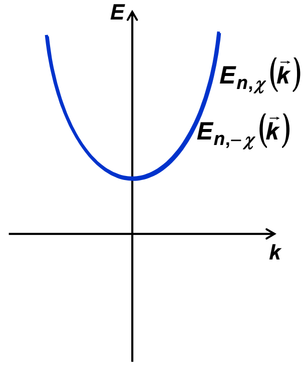
$$E_{n,-\chi}(\vec{k})=E_{n,\chi}(\vec{k}) \longrightarrow$$ **There is spin degeneracy!**

In crystals which do not have inversion symmetry the above two do not guarantee spin degeneracy. In general:

$$E_{n,-\chi}(\vec{k})\neq E_{n,\chi}(\vec{k}) \longrightarrow$$ **Bands with different spins can have different energy dispersion relations**

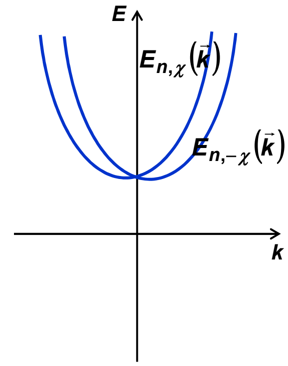
Crystal Inversion Symmetry and Time Reversal Symmetry

Cartoon (and much exaggerated) sketches of the conduction bands of Ge and GaAs are shown below:



Ge

$$E_{n,-\chi}(\vec{k}) = E_{n,\chi}(\vec{k})$$



GaAs

$$E_{n,-\chi}(\vec{k}) \neq E_{n,\chi}(\vec{k})$$