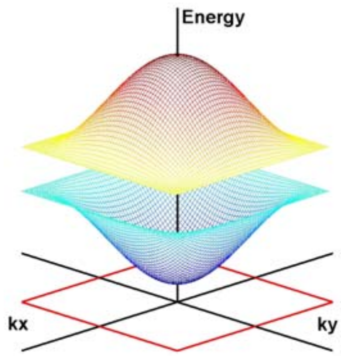
Handout on

Crystal Symmetries and Energy Bands

In this lecture you will learn:

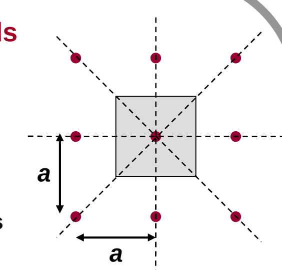
- **The relationship between symmetries and energy bands in the absence of spin-orbit coupling**
- **The relationship between symmetries and energy bands in the presence of spin-orbit coupling**



Symmetry and Energy Bands

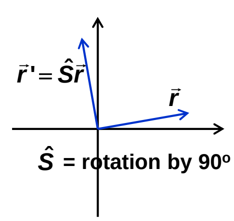
The crystal potential $V(\vec{r})$ generally has certain other symmetries in addition to the lattice translation symmetry:

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



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**

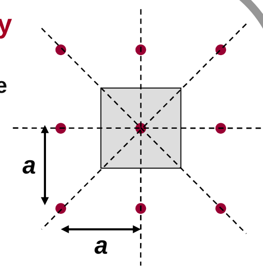


Let $\hat{S}$ be the operator (in matrix representation) for any one of these symmetry operations then:

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

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

Crystal Point-Group Symmetry

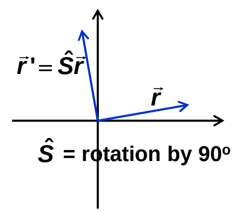


Point-Group Symmetry

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)



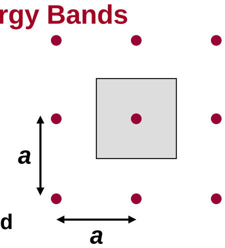
Let $\hat{S}$ be the operator for a point-group symmetry operation, such that:

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

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

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

Crystal Point-Group Symmetry and Energy Bands



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

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

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

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

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

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

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

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

$\nabla^2_{\hat{S}\vec{r}} = \nabla^2_{\vec{r}}$

Laplacian is invariant

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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 $\psi_{n,\vec{k}}(\hat{S}\vec{r})$:

$$\psi_{n,\vec{k}}(\hat{S}(\vec{r}+\vec{R}))=\psi_{n,\vec{k}}(\hat{S}\vec{r}+\hat{S}\vec{R})$$ → $\hat{S}\vec{R}$ **is also a lattice vector**

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

$\Rightarrow$ $\psi_{n,\vec{k}}(\hat{S}\vec{r})$ **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:

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

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

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

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

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:

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

χ **=Quantum number for the two spin degrees of freedom**

Spin-Orbit Interaction and Bloch Functions

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

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

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

We label them with an additional subscript χ **that can take two different values:**

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

Spin-Orbit Interaction and Bloch Functions

In the presence of spin-orbit coupling, spin is not a good quantum number!

$$\left[\hat{H},\hat{\vec{\sigma}}\right]\neq 0$$

$\Rightarrow$ Eigenstates cannot be labeled by the spin quantum number
So what do we do?!

Near the atoms, where the potential is approximately radial, one can write:

$$H_{so}=-i\frac{\hbar^2}{4m^2c^2}\hat{\vec{\sigma}}\cdot\left[\nabla_{\vec{r}}V\left(\hat{\vec{r}}\right)\times\vec{\nabla}_{\vec{r}}\right]\approx\frac{\hbar}{4m^2c^2}\frac{1}{r}\frac{dV(r)}{dr}\hat{\vec{\sigma}}\cdot\left[\hat{\vec{r}}\times\hat{\vec{P}}\right]=\frac{\hbar}{4m^2c^2}\frac{1}{r}\frac{dV(r)}{dr}\hat{\vec{\sigma}}\cdot\hat{\vec{L}}$$

In general, the Bloch wavefunction is a superposition of atomic orbitals:

$$\psi_{n,\vec{k},\chi}(\vec{r})=e^{i\vec{k}.\vec{r}}\sum_j\frac{e^{i\vec{k}.\left(\vec{R}_j-\vec{r}\right)}}{\sqrt{N}}\sum_n e^{i\vec{k}.\vec{d}_n}\left\{c_{n,\uparrow}\left(\vec{k}\right)e\begin{bmatrix}\alpha_n\left(\vec{r}-\vec{R}_j-\vec{d}_n\right)\\0\end{bmatrix}+c_{n,\downarrow}\left(\vec{k}\right)\begin{bmatrix}0\\\beta_n\left(\vec{r}-\vec{R}_j-\vec{d}_n\right)\end{bmatrix}\right\}$$

At the zone center (Γ point), the Bloch wavefunction is:

$$\psi_{n,\vec{k},\chi}(\vec{r})=\sum_j\frac{1}{\sqrt{N}}\sum_n\left\{c_{n,\uparrow}\left(\vec{k}\right)\begin{bmatrix}\alpha_n\left(\vec{r}-\vec{R}_j-\vec{d}_n\right)\\0\end{bmatrix}+c_{n,\downarrow}\left(\vec{k}\right)\begin{bmatrix}0\\\beta_n\left(\vec{r}-\vec{R}_j-\vec{d}_n\right)\end{bmatrix}\right\}$$

The only spatial dependence at the zone center comes from the atomic orbitals

Spin-Orbit Interaction and Bloch Functions

So at the zone center the atomic orbitals can be chosen to be eigenstates of the total angular momentum in order to diagonalize the spin-orbit Hamiltonian

$$\hat{\vec{J}}=\hat{\vec{L}}+\hat{\vec{S}}=\hat{\vec{L}}+\frac{\hbar}{2}\hat{\vec{\sigma}}\qquad\qquad \hat{J}^2=\hat{L}^2+\hat{S}^2+\hat{\vec{L}}.\hat{\vec{S}}$$

If the Bloch functions at the zone center can be chosen to be eigenvalues of $\hat{J}^2$ and $\hat{J}_z$ then, H_{so}, proportional to:

$$\hat{\vec{L}}.\hat{\vec{S}}=\hat{J}^2-\hat{L}^2-\hat{S}^2$$

will be diagnonalized!

The two Bloch solutions for a band at the zone center can be chosen to correspond to two different eigenvalues of $\hat{J}_z$ and the same value of $\hat{J}^2$:

$$\hat{J}_z\,\psi_{n,\vec{k}=0,\chi}(\vec{r})=\chi\,\psi_{n,\vec{k}=0,\chi}(\vec{r})\qquad\left\{\chi=j_1\quad or\quad \chi=j_2\right.$$

If the crystal has time reversal symmetry then at the zone center one can always choose:

$$j_2=-j_1$$

Spin-Orbit Interaction and Bloch Functions

Example – Six Valence Bands of Si, GaAs, and InP (…..Contd):

HH Band:

$$\hat{J}^2\,\psi_{HH,\vec{k}=0,\pm 3/2}(\vec{r}) = \frac{3}{2}\left(\frac{3}{2}+1\right)\hbar^2\;\psi_{HH,\vec{k}=0,\pm 3/2}(\vec{r})$$

$$\hat{J}_z\,\psi_{HH,\vec{k}=0,3/2}(\vec{r}) = +\frac{3}{2}\hbar\;\psi_{HH,\vec{k}=0,3/2}(\vec{r})$$

$$\hat{J}_z\,\psi_{HH,\vec{k}=0,-3/2}(\vec{r}) = -\frac{3}{2}\hbar\;\psi_{HH,\vec{k}=0,-3/2}(\vec{r})$$

LH Band:

$$\hat{J}^2\,\psi_{LH,\vec{k}=0,\pm 1/2}(\vec{r}) = \frac{3}{2}\left(\frac{3}{2}+1\right)\hbar^2\;\psi_{LH,\vec{k}=0,\pm 1/2}(\vec{r})$$

$$\hat{J}_z\,\psi_{LH,\vec{k}=0,1/2}(\vec{r}) = +\frac{1}{2}\hbar\;\psi_{LH,\vec{k}=0,1/2}(\vec{r})$$

$$\hat{J}_z\,\psi_{LH,\vec{k}=0,-1/2}(\vec{r}) = -\frac{1}{2}\hbar\;\psi_{LH,\vec{k}=0,-1/2}(\vec{r})$$

SO Band:

$$\hat{J}^2\,\psi_{SO,\vec{k}=0,\pm 1/2}(\vec{r}) = \frac{1}{2}\left(\frac{1}{2}+1\right)\hbar^2\;\psi_{SO,\vec{k}=0,\pm 1/2}(\vec{r})$$

$$\hat{J}_z\,\psi_{SO,\vec{k}=0,1/2}(\vec{r}) = +\frac{1}{2}\hbar\;\psi_{SO,\vec{k}=0,1/2}(\vec{r})$$

$$\hat{J}_z\,\psi_{SO,\vec{k}=0,-1/2}(\vec{r}) = -\frac{1}{2}\hbar\;\psi_{SO,\vec{k}=0,-1/2}(\vec{r})$$

Slightly away from zone center, one can use k.p perturbation theory with the spin-orbit coupling term included in the perturbing Hamiltonian:

$$\hat{H}_{k.p} = \frac{\hbar^2 k^2}{2m} + \hbar\vec{k}.\left(\frac{\vec{P}}{m} + \frac{\hbar}{4m^2c^2}\left[\hat{\vec{\sigma}} \times \nabla_{\vec{r}} V(\hat{\vec{r}})\right]\right)$$

Thus, it is safe to assume that the Bloch eigenstates chosen as above will remain reasonably good eigenstates of $\hat{J}_z$ even slightly away from the zone center

Spin-Orbit Interaction and Lattice Symmetries

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

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

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:

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

(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:

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

And the solution is:

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

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

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

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

Spin-Orbit Interaction and Rotation Symmetry

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

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

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:

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

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:

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

And the solution is:

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

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

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

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

Spin-Orbit Interaction and Inversion Symmetry

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

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:

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

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

Also, since the total angular momentum operators are invariant under spatial inversion:

$$\hat{J}_z\,\psi_{n,\vec{k},\chi}(\vec{r}) = \chi\,\psi_{n,\vec{k},\chi}(\vec{r})$$

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

Spin-Orbit Interaction and Inversion Symmetry

So the new eigenstate found has the same angular momentum as the original state!

Therefore, we can write:

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

Summary:

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

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

have the same energy:

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

Spin-Orbit Interaction and Time Reversal Symmetry

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

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

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 $-t$):

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

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

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

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:

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

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

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

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

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

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:

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

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

Q: What are the quantum numbers of the time-reversed state $\begin{bmatrix}-\beta^*_{n,\vec{k}}(\vec{r})\\ \alpha^*_{n,\vec{k}}(\vec{r})\end{bmatrix}$?

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:

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

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:

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

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:

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

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

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

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

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

Note: the new solution is the time-reversed solution found previously!

Spin-Orbit Interaction and Time Reversal Symmetry

Under lattice translation we get for the new solution:

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

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, this means that the above state has spin opposite to the state:

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

But what about:

$$\hat{J}_z\begin{bmatrix}-\beta^*_{n,\vec{k}}(\vec{r})\\ \alpha^*_{n,\vec{k}}(\vec{r})\end{bmatrix} = \hat{J}_z\left[-i\hat{\sigma}_y\,\psi^*_{n,\vec{k},\chi}(\vec{r})\right] = ?$$

Spin-Orbit Interaction and Time Reversal Symmetry

$$\hat{J}_z \begin{bmatrix} -\beta^*_{n,\vec{k}}(\vec{r}) \\ \alpha^*_{n,\vec{k}}(\vec{r}) \end{bmatrix} = \hat{J}_z \left[-i\hat{\sigma}_y \, \psi^*_{n,\vec{k},\chi}(\vec{r}) \right] = ?$$

Start from:

$$\hat{J}_z \, \psi_{n,\vec{k},\chi}(\vec{r}) = \chi \psi_{n,\vec{k},\chi}(\vec{r})$$
$$\Rightarrow \left(\hat{L}_z + \hat{S}_z\right) \psi_{n,\vec{k},\chi}(\vec{r}) = \chi \psi_{n,\vec{k},\chi}(\vec{r})$$
$$\Rightarrow \left(\hat{L}_z + \hat{S}_z\right)^* \psi^*_{n,\vec{k},\chi}(\vec{r}) = \chi \psi^*_{n,\vec{k},\chi}(\vec{r})$$
$$\Rightarrow \left(-\hat{L}_z + \hat{S}_z\right) \psi^*_{n,\vec{k},\chi}(\vec{r}) = \chi \psi^*_{n,\vec{k},\chi}(\vec{r})$$
$$\Rightarrow \left(-\hat{L}_z + \hat{S}_z\right)\left(i\hat{\sigma}_y\right)\left(-i\hat{\sigma}_y\right) \psi^*_{n,\vec{k},\chi}(\vec{r}) = \chi \psi^*_{n,\vec{k},\chi}(\vec{r}) \qquad \left\{ \hat{\sigma}_y \hat{\sigma}_y = \hat{1} \right.$$
$$\Rightarrow \left(-i\hat{\sigma}_y\right)\left(-\hat{L}_z + \hat{S}_z\right)\left(i\hat{\sigma}_y\right)\left(-i\hat{\sigma}_y\right) \psi_{n,\vec{k},\chi}(\vec{r}) = \chi \left(-i\hat{\sigma}_y\right) \psi^*_{n,\vec{k},\chi}(\vec{r})$$
$$\Rightarrow \left(-\hat{L}_z - \hat{S}_z\right)\left(-i\hat{\sigma}_y\right) \psi^*_{n,\vec{k},\chi}(\vec{r}) = \chi \left(-i\hat{\sigma}_y\right) \psi^*_{n,\vec{k},\chi}(\vec{r})$$
$$\Rightarrow \left(\hat{L}_z + \hat{S}_z\right)\left(-i\hat{\sigma}_y\right) \psi^*_{n,\vec{k},\chi}(\vec{r}) = -\chi \left(-i\hat{\sigma}_y\right) \psi^*_{n,\vec{k},\chi}(\vec{r})$$
$$\Rightarrow \hat{J}_z \left(-i\hat{\sigma}_y\right) \psi^*_{n,\vec{k},\chi}(\vec{r}) = -\chi \left(-i\hat{\sigma}_y\right) \psi^*_{n,\vec{k},\chi}(\vec{r})$$

Spin-Orbit Interaction and Time Reversal Symmetry

Therefore, the new solution is also an eigenfunction of $\hat{J}_z$ with an eigenvalue $-\chi$:

$$\hat{J}_z \left(-i\hat{\sigma}_y\right) \psi^*_{n,\vec{k},\chi}(\vec{r}) = -\chi \left(-i\hat{\sigma}_y\right) \psi^*_{n,\vec{k},\chi}(\vec{r})$$

Therefore, the new solution is the 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 $\psi_{n,\vec{k},\chi}(\vec{r})$:

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

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:

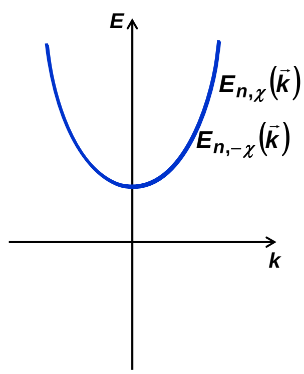
$$E_{n,-\chi}(\vec{k}) = E_{n,\chi}(\vec{k}) \longrightarrow$$

There is spin (or rather total angular momentum) degeneracy!

Crystals which do not have inversion symmetry, spin degeneracy of the bands is not guaranteed

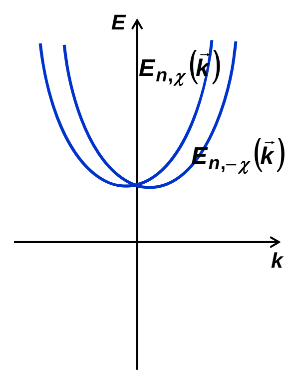
Crystal Inversion Symmetry and Time Reversal Symmetry

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

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

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