Notes:

- **Exam this week!** Settled on Friday afternoon 2-4. [I will get room.]

- Covers: Through ch. 10 (tight binding material, today). Format, open book (Ashcroft & Mermin) – you should have a paper copy!

Symmetry & electrons in crystals

(& see ch. 8 of A&M)

$$T_{\vec{R}} f(\vec{r}) = f(\vec{r} + \vec{R})$$

$$\left[H, T_{\vec{R}}\right] = 0$$

Crystal translation operator, commutes with Hamiltonian

$$\Longrightarrow \quad T_{\vec{R}} \psi = c_{\vec{R}} \psi$$

Energy eigenstates = translation eigenstates

Periodic boundary conditions:

$$\left(T_{\vec{a}_i}\right)^{N_i} \psi = \left(c_{\vec{a}_i}\right)^{N_i} \psi \equiv \psi$$

Thus:

$$c_{\vec{a}_i} = e^{i\vec{k}\cdot\vec{a}_i}$$

Bloch theorem!

Symmetry & electrons in crystals

$$T_{\vec{R}} f(\vec{r}) = f(\vec{r} + \vec{R}) \qquad \left[H, T_{\vec{R}}\right] = 0$$

Crystal translation symmetry

$$\Longrightarrow \quad T_{\vec{R}}\psi = c_{\vec{R}}\psi$$

Energy eigenstates also translation eigenstates

$$\left[H, T_{\vec{r}}\right] = 0 \quad \Longleftrightarrow \quad \vec{p}_{\vec{r}} = \text{constant of motion}$$

$$\left[H, T_{\vec{R}}\right] = 0 \quad \Longleftrightarrow$$

Crystal momentum constant of motion:

$\vec{k}$ *within one Brillouin zone*

$$\vec{k}' = \vec{k} \pm \vec{K}$$

Symmetry & electrons in crystals

$$T_{\vec{R}} f(\vec{r}) = f(\vec{r} + \vec{R})$$ Crystal translation symmetry

$$[H, T_{\vec{R}}] = 0$$ ⟺ Crystal momentum constant of motion:

$\vec{k}$ *within one Brillouin zone*

Time reversal invariance: $\vec{k} \Rightarrow -\vec{k}$ (complex conjugation reverses sign of *t*-dependent Schrödinger equation.)

Thus Band-structure mirror symmetric in *k*

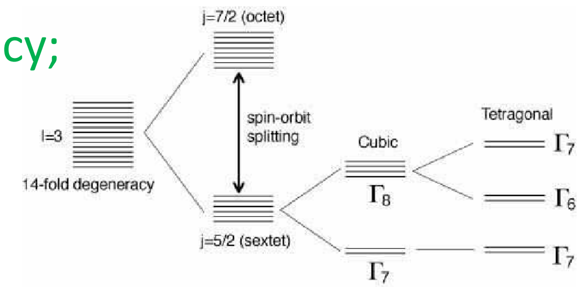
- even if crystal basis has *no* inversion symmetry
- but only for nonmagnetic cases

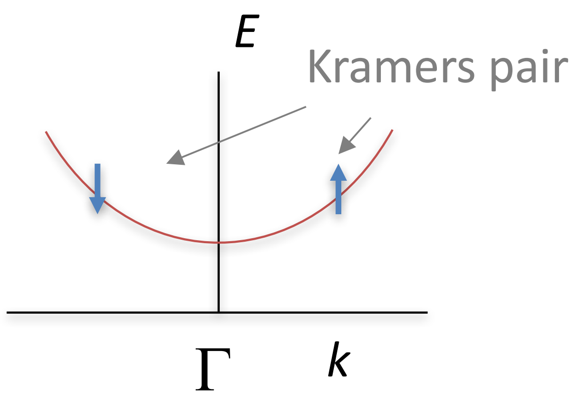
Symmetry & electrons in crystals

Time reversal: $\vec{k} \Rightarrow -\vec{k}$ Also spin: $s \Rightarrow -s$

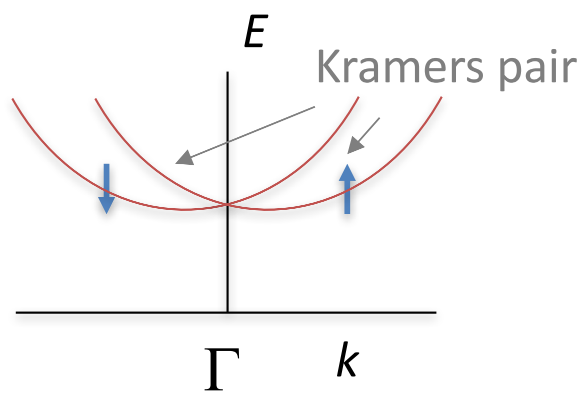
$$\psi(\vec{k}, s) = \psi(-\vec{k}, -s)$$

Kramers degeneracy;
lifted by B field





Basis with inversion symmetry
(in <u>direct-space</u>)



No inversion symmetry in direct space.
Splitting may be due to *spin-orbit coupling*

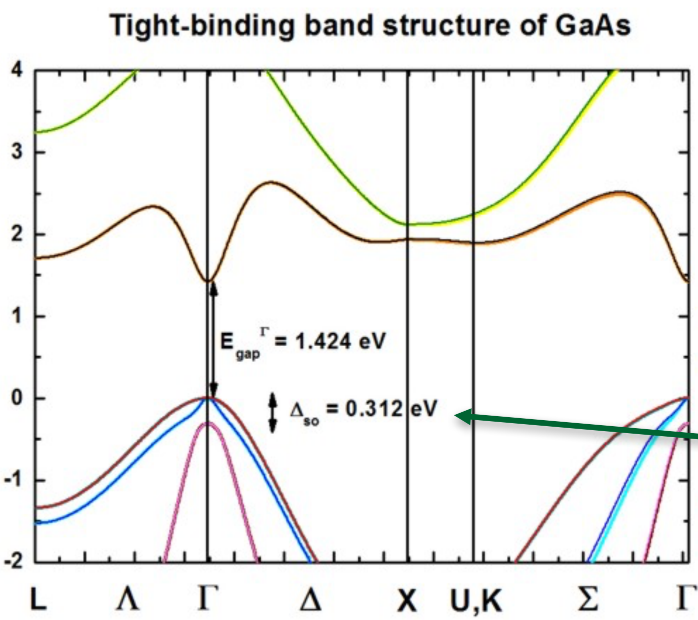
Spin-orbit coupling:

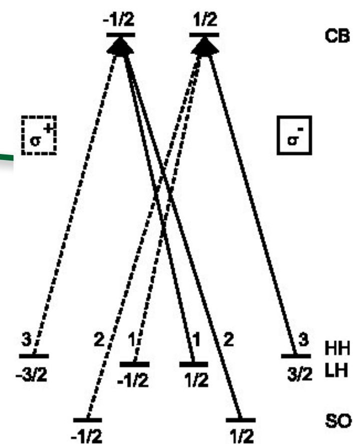
$$H \propto \frac{1}{r}\frac{dU}{dr}\vec{S}\cdot\vec{L}$$

Have assumed spin + orbit states independent up to now.

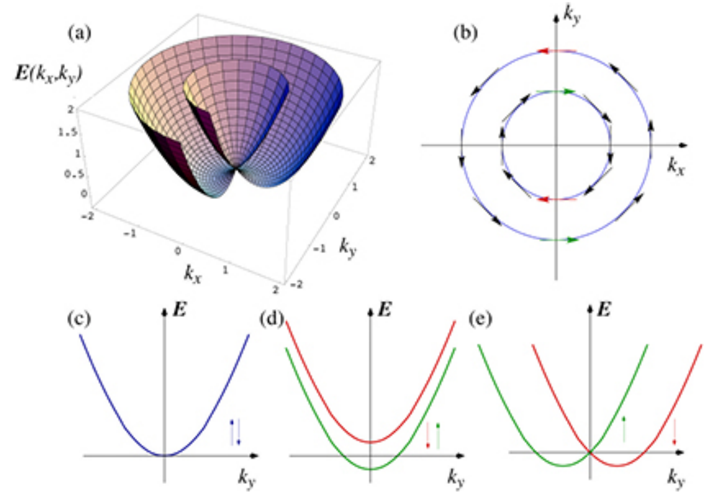
Spin-orbit small splittings; largest for heavy atoms, noticed particularly at band edges.

Issues of much current interest: spintronics; topological insulators.





Split-off holes; optical polarization in GaAs



Rashba effect; spins coupled to carrier transport (2D layers)