5. Spin-orbit interaction, top of valence bands

Electron states in atoms are influenced by the inner magnetic field, resulting from the orbital motion. The field tries to orient the spin magnetic moment. This is a relativistic effect, vanishing in the limit of $c \to \infty$.

The spin operator,

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \; \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \; \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{5.1}$$

enters the spin-orbit contribution to the Hamiltonian operator:

$$H_{SO} = \frac{1}{2m^2c^2}(\nabla V \times \vec{p}) \cdot \frac{\hbar \vec{\sigma}}{2} \; . \tag{5.2}$$

An alternate notation use the magnetic moment related to the spin of electron,

$$\vec{\mu} = \frac{-|e|}{mc}\vec{S} = \frac{-|e|}{mc}\frac{\hbar}{2}\frac{\vec{S}}{|\vec{S}|} = \mu_B \frac{\vec{S}}{|\vec{S}|} \; , \tag{5.3}$$

the energy in the magnetic field,

$$H_{SO} = -\vec{\mu} \cdot \vec{H} \ , \tag{5.4}$$

where the intensity H due to the orbital motion is

$$\vec{H} = -\frac{\vec{v}}{c} \times \vec{E} \ . \tag{5.5}$$

Magnetic moment of free electron, μ_B (Bohr magneton) is 9.2740154E-21 erg/gauss, its value in SI is 9.2740154E-24 J/T (1 erg = 1E-7 J, 1 gauss = 1E-4 T); using the appropriate units of energy for the microstructure of matter, it amounts to 58 μeV/T. Magnetic field at the surface of Earth is in the range from 25 to 65 μT; strong permanent neodymium (neodymium-iron-boron) magnets achieve up to 1.3 T.

The spin-orbit part of Hamiltonian in an isolated atom is

$$H_{SO} = \xi(r)(\vec{r} \times \vec{p}) \cdot \vec{S} = \xi(r)\vec{L} \cdot \vec{S} \ , \tag{5.6}$$

where L is orbital angular momentum. Let us consider the atomic p-state (that of l=1). The total angular momentum is represented by the operator

$$\vec{J} = \vec{L} + \vec{S} \ . \tag{5.7}$$

The scalar product (the magnitude squared) involves three terms:

$$\vec{J}\cdot\vec{J}=(\vec{L}+\vec{S})\cdot(\vec{L}+\vec{S})=\vec{L}\cdot\vec{L}+\vec{S}\cdot\vec{S}+(\vec{L}\cdot\vec{S}+\vec{S}\cdot\vec{L})\ , \tag{5.8}$$

where L and S commute (they operate in different vector spaces). However, their projections (m_l and m_s) are not good quantum numbers, since they are coupled by the *SO* interaction; on the other hand, l and s remain good quantum numbers. The appropriate state vectors, allowing us to estimate the product of L and S are therefore

$$\left|\, j,l,s,m_j \right\rangle \ . \tag{5.9}$$

From Eq. (5.8), the diagonal matrix element of the square of total angular momentum is

$$j(j+1)=l(l+1)+s(s+1)+\frac{2}{\hbar^2}\left\langle \vec{L}\cdot\vec{S}\right\rangle\ , \tag{5.10}$$

i.e., the expectation of the product LS is

$$\left\langle \vec{L}\cdot\vec{S}\right\rangle=\frac{\hbar^2}{2}\left[\, j(j+1)-l(l+1)-s(s+1)\right]\ . \tag{5.11}$$

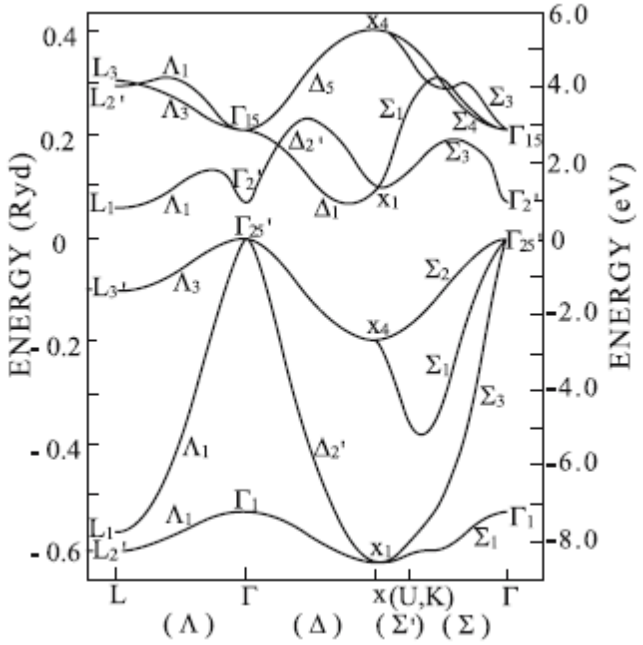
For atomic p-states (l=1, s=1/2), possible values of j are 3/2 or ½; consequently

$$\left\langle \vec{L}\cdot\vec{S}\right\rangle = \frac{\hbar^2}{2} \text{ pro } j = 3/2 \,, \left\langle \vec{L}\cdot\vec{S}\right\rangle = -\hbar^2 \text{ pro } j = 1/2 \,. \tag{5.12}$$

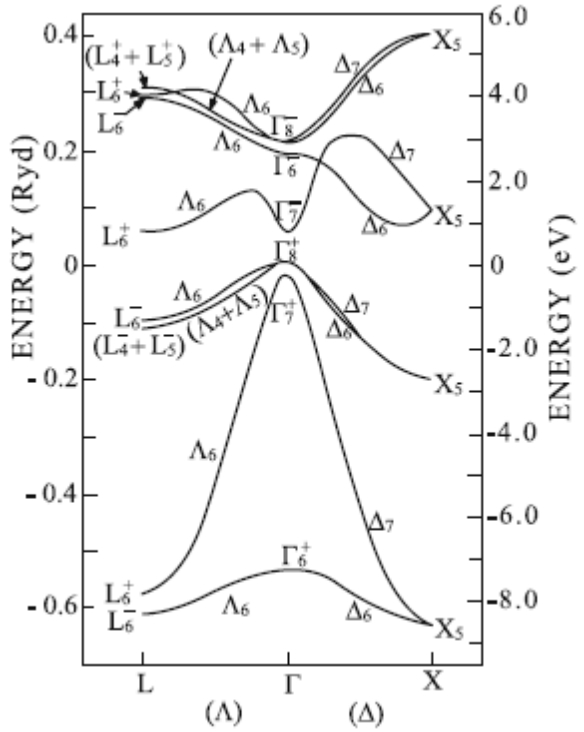
Spin-orbit interaction leads to the energy splitting of the states with the total angular momentum of 3/2 a 1/2. Atomic s-state is not influenced by the *SO* interaction, the spin degeneracy is retained. Further, atomic *d*-state splits into 6-fold degenerate state $D_{5/2}$ and 4-fold degenerate $D_{3/2}$.

diamond	$Z = 6$	$\triangle E = 0.006$ eV
silicon	$Z = 14$	$\triangle E = 0.044$ eV
germanium	$Z = 32$	$\triangle E = 0.29$ eV
InSb { In	$Z = 49$	$\triangle E = 0.9$ eV
InSb { Sb	$Z = 51$	

Atomic numbers and SO splitting of the top of valence bands.



Bandstructure of Ge without the *SO* interaction (Dresselhaus). Note the erroneous dispersion of the lowest valence band.



Bandstructure of Ge with the *SO* interaction included (Dresselhaus). Note the erroneous dispersion of the lowest valence band.

Double groups – include symmetry operations of the spin variable (rotations by o 2π change the sign of the state vector).

	$\{E\}$	$\{3C_2/3\hat{E}C_2\}$	$\{6S_4\}$	$\{6\sigma/6\hat{E}\sigma\}$	$\{8C_3\}$	$\{\hat{E}\}$	$\{6\hat{E}S_4\}$	$\{8\hat{E}C_3\}$
Γ_1	1	1	1	1	1	1	1	1
Γ_2	1	1	−1	−1	1	1	−1	1
Γ_3	2	2	0	0	−1	2	0	−1
Γ_4	3	−1	−1	1	0	3	−1	0
Γ_5	3	−1	1	−1	0	3	1	0
Γ_6	2	0	$\sqrt{2}$	0	1	−2	$-\sqrt{2}$	−1
Γ_7	2	0	$-\sqrt{2}$	0	1	−2	$\sqrt{2}$	−1
Γ_8	4	0	0	0	−1	−4	0	1

Characters of irreducible representation of the double group of the zincblene structure at the center of the Brillouin zone, Γ.

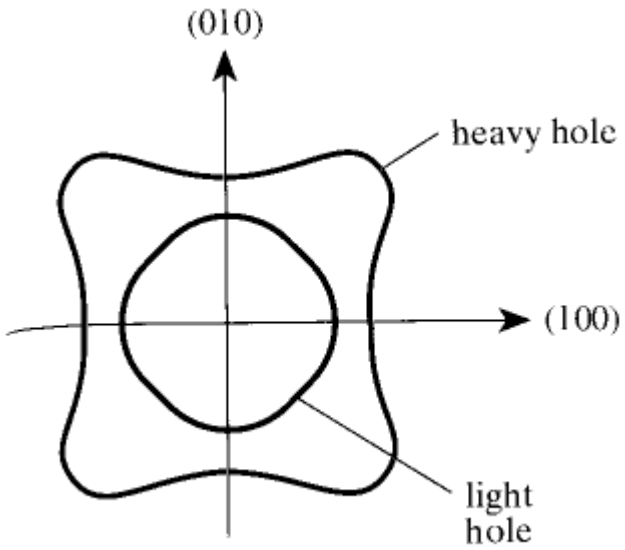
Dispersion of the topmost valence states close to Γ(„warping“):

$$E_{\pm}(k) = Ak^2 \pm \sqrt{B^2k^4 + C^2(k_x^2k_y^2 + k_z^2k_y^2 + k_x^2k_z^2)}\ . \qquad (5.13)$$

Table 2.24. Valence band parameters A and B in units of $(\hbar^2/2m)$ and $|C|^2$ in units of $(\hbar^2/2m)^2$. The spin–orbit splitting of the valence bands Δ_0 is given in units of eV. The averaged experimental (exp) and theoretical [th, obtained from A, B, C^2 with (2.67, 69)] values of the effective masses of the heavy hole (hh), light hole (lh) and spin–orbit split-off hole (so) valence bands are in units of the free electron mass. (2.11, 12)

	A	B	$\|C\|^2$	Δ_0	m_{hh}/m_0		m_{lh}/m_0		m_{so}/m_0	
				[eV]	exp	th	exp	th	exp	th
Si	−4.25	−0.63	24	0.044	0.54	0.45	0.15	0.14	0.23	0.24
Ge	−13.4	−8.5	173	0.295	0.34	0.43	0.043	0.041	0.095	0.1
GaAs	−7.0	−4.5	38	0.341	0.53	0.78	0.08	0.08	0.15	0.17
InP	−5.04	−3.1	41	0.11	0.58	0.53	0.12	0.12	0.12	0.2
InAs	−20.4	−16.6	167	0.38	0.4	0.4	0.026	0.026	0.14	0.10
GaSb	−13.3	−8.8	230	0.75	0.8	0.9	0.05	0.04	—	0.15
InSb	−40.1	−36.2	492	0.81	0.42	0.48	0.016	0.013	—	0.12
GaP	−4.05	−0.98	16	0.08	0.57	0.5	0.18	0.17	—	0.25

Parameters of the topmost valence states close to Γ.



Contours of constant energy around the Brillouin zone center Γ.

Heavy- and light-hole bands, effective masses averaged over directions:

$$\frac{1}{m^*_{hh}} = \frac{1}{\hbar^2}\left[-2A + 2B\left(1 + \frac{2|C|^2}{15B^2}\right)\right], \tag{5.14}$$

$$\frac{1}{m^*_{lh}} = \frac{1}{\hbar^2}\left[-2A - 2B\left(1 + \frac{2|C|^2}{15B^2}\right)\right]. \tag{5.15}$$