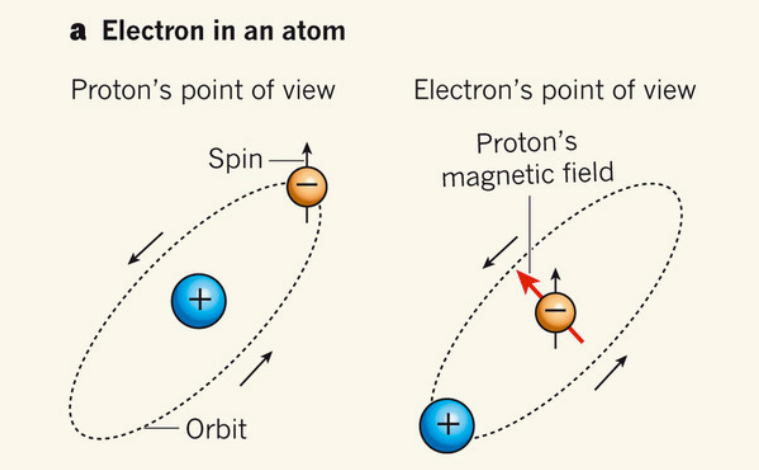
Spin-orbit coupling: a relativistic effect



Binghai Yan

Max Planck Institute for Chemical Physics of Solids, Dresden, Germany
www.cpfs.mpg.de/yan

The Summer School on "Topological Matter States 2016"
Donostia-San Sebastián, Spain, 22-26 Aug 2016

Outline

Spin-orbit coupling in an atom

- Atom SOC
- Contraction of s and p shells

Spin-orbit coupling in solids

- Atomic SOC, such as HgTe
- Rashba effect
- Dresselhaus effect
- SOC in graphene

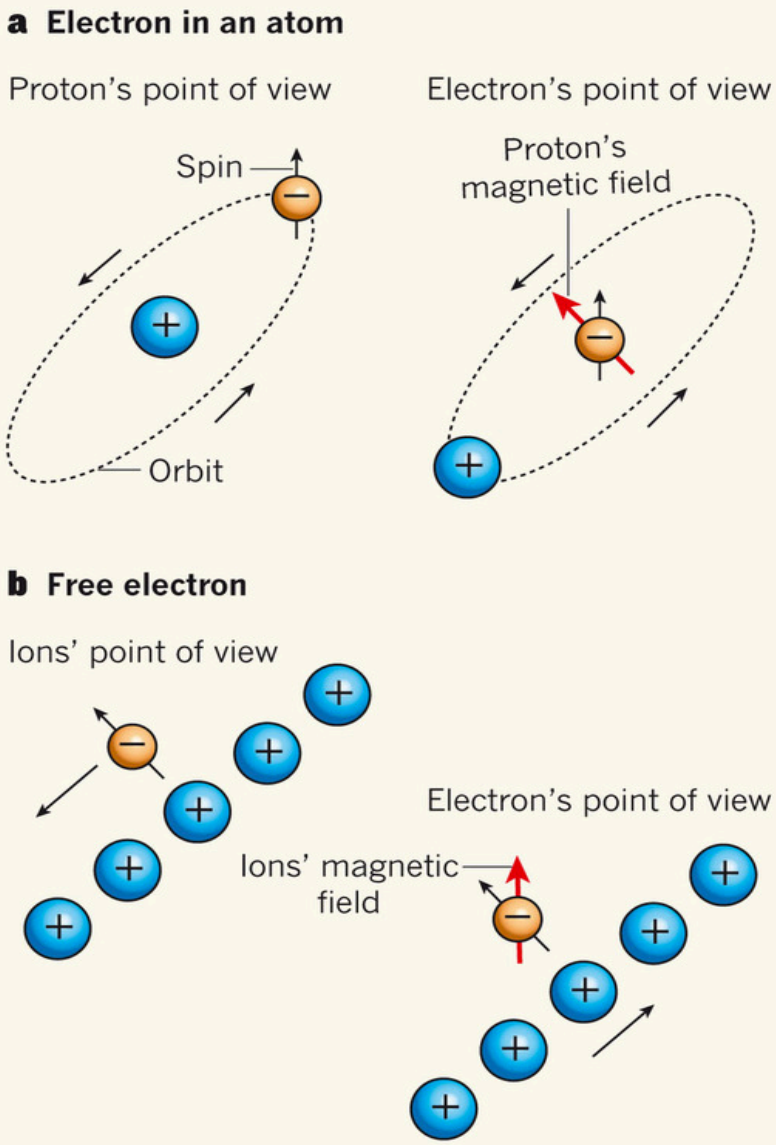
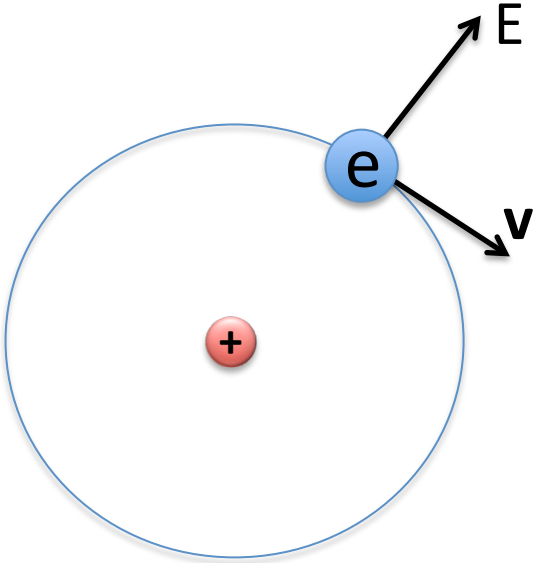


Figure credit: M. Chapman & C. Sá de Melo, Nature 471, 41–42 (2011)

A hydrogen-like atom

$$V(r) = -\frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r}$$ (Z is the atomic number)



$$E_n = -\frac{\mu c^2 Z^2 \alpha^2}{2n^2}$$

$$r_1 \simeq \left(\frac{4\pi\varepsilon_o}{e^2}\right)\frac{\hbar^2}{Zm_e}, \quad \sim Z^{-1}$$

$$v_1 = \frac{Ze^2}{4\pi\epsilon_0\hbar} \sim Z \qquad mv^2 = \frac{Ze^2}{4\pi\epsilon_0 r_n} \sim Z^2$$

$$E = \nabla V(r) = \frac{1}{4\pi}\frac{Ze^2}{r^2}\hat{r} \quad \sim Z^3$$

A hydrogen-like atom

$$E_n = -\frac{\mu c^2 Z^2 \alpha^2}{2n^2} \qquad \sim -13.6\ (Z^2/n^2)\ \text{eV}$$

$$r_1 \simeq \left(\frac{4\pi\varepsilon_o}{e^2}\right)\frac{\hbar^2}{Zm_e}, \qquad \sim a_0 = 0.529\ Z^{-1}\ \text{Å}$$

$$v_1 = \frac{Ze^2}{4\pi\epsilon_0\hbar} \qquad \sim (Z/137)\ c$$

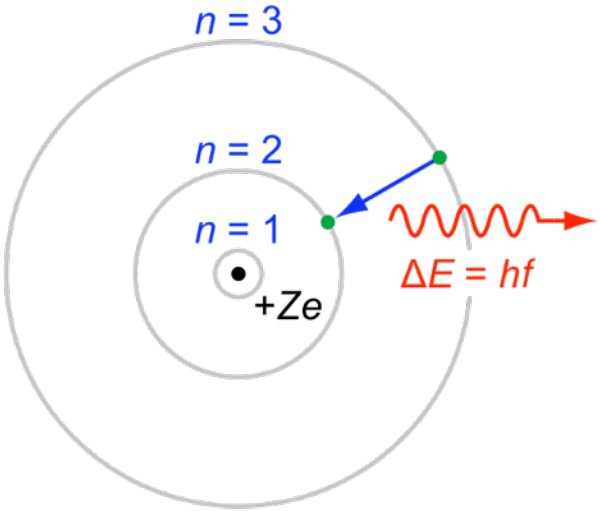
$$\gamma \stackrel{\text{def}}{=} \frac{1}{\sqrt{1 - v^2/c^2}}$$

Lorentz factor

Relativistic effect

$$m = \gamma m_0 = m_0/\sqrt{1-(v/c)^2}.$$

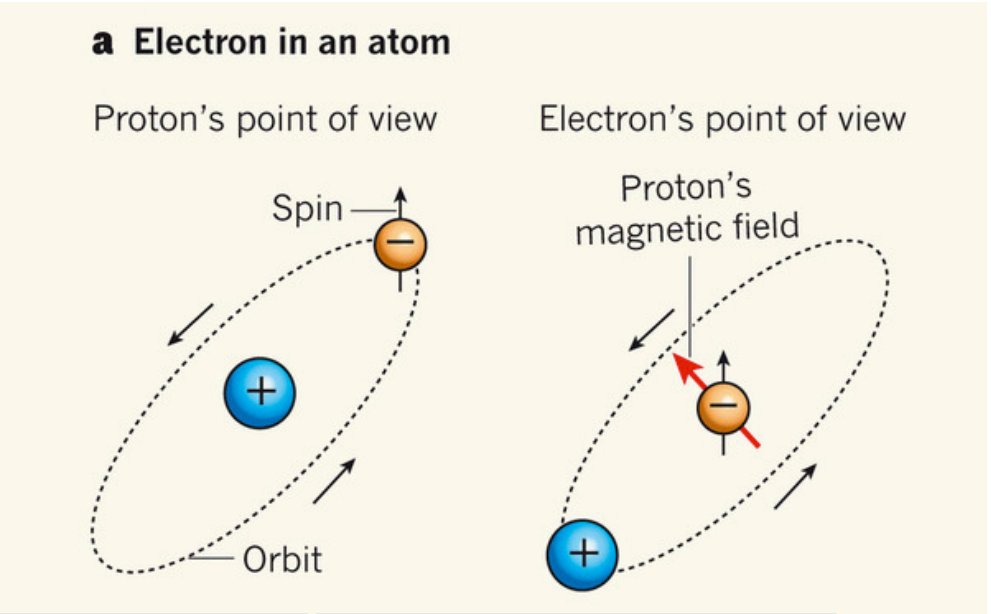
$$a_0 = \hbar^2/me^2.$$



A hydrogen-like atom

Lorentz transformation

$$\mathbf{E}_{\parallel}{}' = \mathbf{E}_{\parallel}$$
$$\mathbf{B}_{\parallel}{}' = \mathbf{B}_{\parallel}$$
$$\mathbf{E}_{\perp}{}' = \gamma(\mathbf{E}_{\perp} + \mathbf{v} \times \mathbf{B})$$
$$\mathbf{B}_{\perp}{}' = \gamma\left(\mathbf{B}_{\perp} - \frac{1}{c^2}\mathbf{v} \times \mathbf{E}\right)$$



$$\mathbf{B} = \frac{1}{c^2}\mathbf{E} \times \mathbf{v}. \quad \sim Z^4$$

$$\mathbf{E} = -\frac{\mathbf{r}}{r}\phi' \qquad \mathbf{B} = -\frac{1}{rc^2}\phi'\mathbf{r} \times \mathbf{v}$$

As $\mathbf{l} = \mathbf{r} \times \mathbf{p}$, and hence $\mathbf{r} \times \mathbf{v} = \frac{1}{m_e}\mathbf{l}$, we get the Hamiltonian

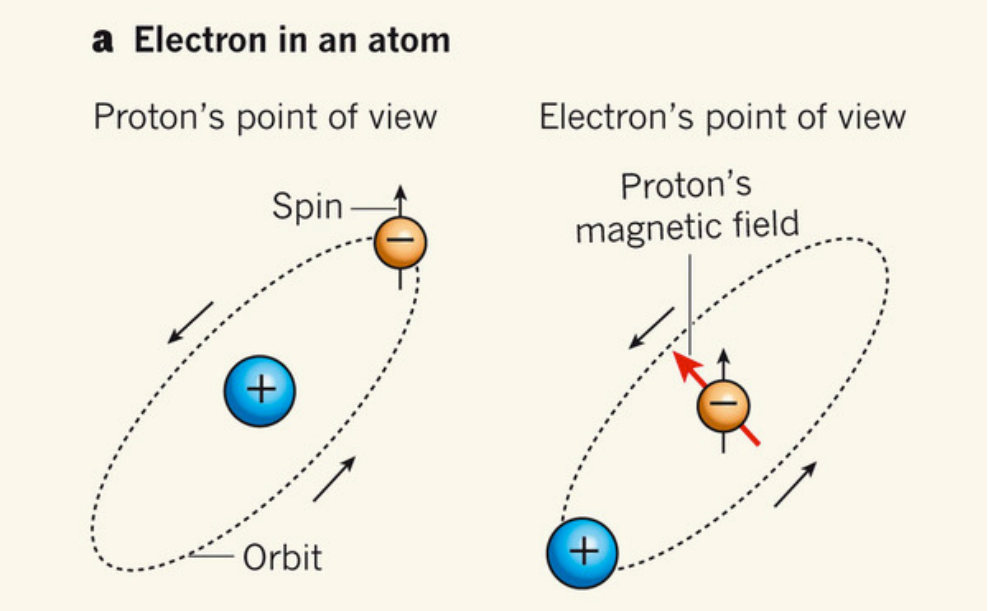
$$h_{\mathrm{SO}} = -\mu_{\mathbf{e}} \cdot \mathbf{B} = \frac{1}{m_e r c^2}\phi' \mu \cdot \mathbf{l} = \frac{e}{m_e^2 r c^2}\phi' \mathbf{s} \cdot \mathbf{l},$$

1/2
Thomas factor

Relativistic effects

Relativity:
Switch the coordinate frame
Moving E → $\mathbf{B} = \frac{1}{c^2}\mathbf{E} \times \mathbf{v}.$

Quantum spin:
Electron has a spin ***s*** → ***h* = -μ_s•*B***



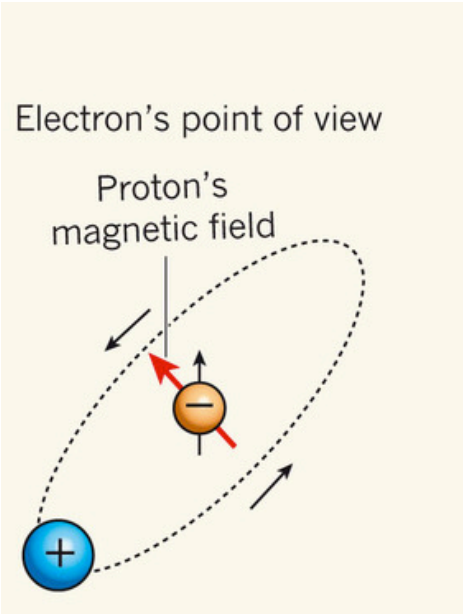
The Relativistic Hamiltonian

$$\left[\frac{1}{2m_e}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 - \frac{e\hbar}{2m_e c}\underset{\sim}{\sigma}\cdot\vec{\nabla}\times\vec{A} - \frac{\vec{p}^4}{8m_e^3c^3} + \frac{e\hbar^2}{8m_e^2c^2}\vec{\nabla}\cdot\vec{\nabla}\phi - \frac{e\hbar}{4m_e^2c^2}\underset{\sim}{\sigma}\cdot\vec{\nabla}\phi\times\vec{p}\right]\psi = (E^{nr} - e\phi)\,\psi.$$

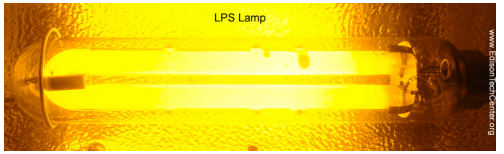
The Fully Relativistic Hamiltonian

Tab. 1.1 Summary of relativistic and spin-dependent interaction terms.

Perturbation	Description	Magnitude
$\frac{1}{2m_e}\left(\vec{p}-\frac{e}{c}\vec{A}\right)^2$	The nonrelativistic motion, $p^2/2m_e$, and the interaction terms $\frac{e}{2m_ec}\vec{A}\cdot\vec{\nabla}+\frac{e^2}{2m_ec^2}\vec{A}\cdot\vec{A}$. The latter terms are responsible for absorption and emission; they can be written as $-e\vec{r}\cdot\vec{E}$ (see Section 4.1.1).	$\gtrsim 10^5$ cm^{-1}
$\frac{e\hbar}{2m_ec}\boldsymbol{\sigma}\cdot\vec{\nabla}\times\vec{A}$	The spin-1/2 ($\vec{s}=\boldsymbol{\sigma}/2$) interaction with a magnetic field ($\vec{B}\equiv\vec{\nabla}\times\vec{A}$). This term gives the correct g-factor, $g=2$, and magnetic moment of the electron, $\mu=\frac{e\hbar}{2m_ec}g\vec{s}$.	≈ 1 cm^{-1}
$\frac{\vec{p}^4}{8m_e^3c^3}$	Relativistic mass correction term.	≈ 0.1 cm^{-1}
$\frac{e\hbar^2}{8m_e^2c^2}\vec{\nabla}\cdot\vec{\nabla}\phi$	The "Darwin" term responsible for s-state shifts. It represents the relativistic nonlocalizability of the electron and is related to both the negative-energy sea and its rapid motion.	< 0.1 cm^{-1}
$\frac{e\hbar}{4m_e^2c^2}\boldsymbol{\sigma}\cdot\vec{\nabla}\phi\times\vec{p}$	Spin–orbit interaction. As shown in Problem 1.4, this term can be written as $\frac{e\hbar^2}{2m_e^2c^2}\frac{1}{r}\frac{d\phi}{dr}\left(\vec{l}\cdot\vec{s}\right)$, where $\vec{l}$ is the orbital angular momentum. In contrast to the previous term, this does not affect s states.	10–10^3 cm^{-1}



Experimental consequence: fine structure



Na

Total angular momentum,

$$\vec{j} = \vec{l} + \vec{s},$$

with eigenvalues (of $\vec{j}^2$) $j(j+1)$.
values that $\vec{j}$ can assume are

$$j = \begin{cases} l \pm \frac{1}{2}, & l \neq 0, \\ \frac{1}{2}, & l = 0. \end{cases} \qquad \Delta E_{nlj} = \Delta E_R + \Delta E_{so} = \alpha^2 \mathcal{R}_M \left(\frac{3}{4n} - \frac{1}{j+\frac{1}{2}} \right) \frac{Z^4}{n^3}.$$

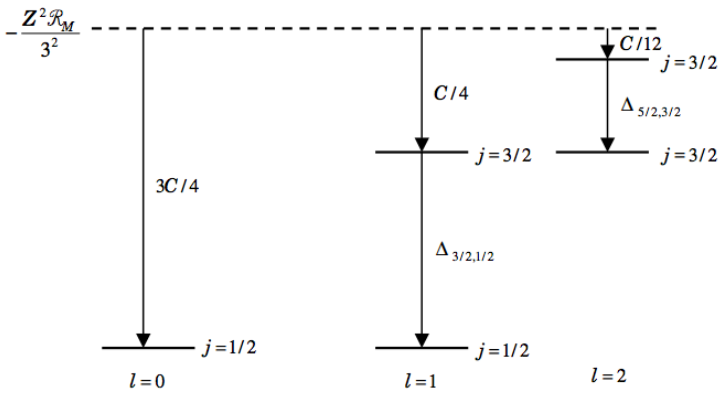
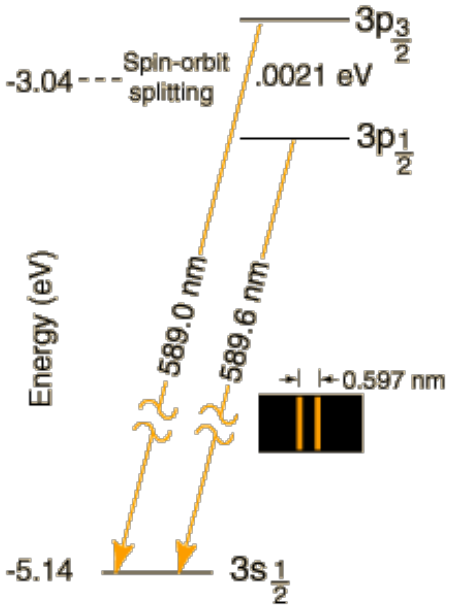


Fig. 1.7 Fine structure of hydrogen-like ions in wavenumbers for $n = 3$ where $C = \alpha^2 Z^4 \mathcal{R}_M / n^3$ and $\Delta_{j+1,j} = \Delta E_{nlj+1} - \Delta E_{nlj} = C/l\,(l+1)$. The levels are all shifted below $-Z^2\mathcal{R}_M/n^2$, the nonrelativistic energy.



μ_s g B = (5.79 x 10^{-5} eV/T)2B = 0.0021 eV

B = 18 Tesla

A huge field

Experimental consequence: *sp* contraction

$$\langle v_r \rangle_{1s} = Z$$

$$= 80 \text{ for Hg}$$

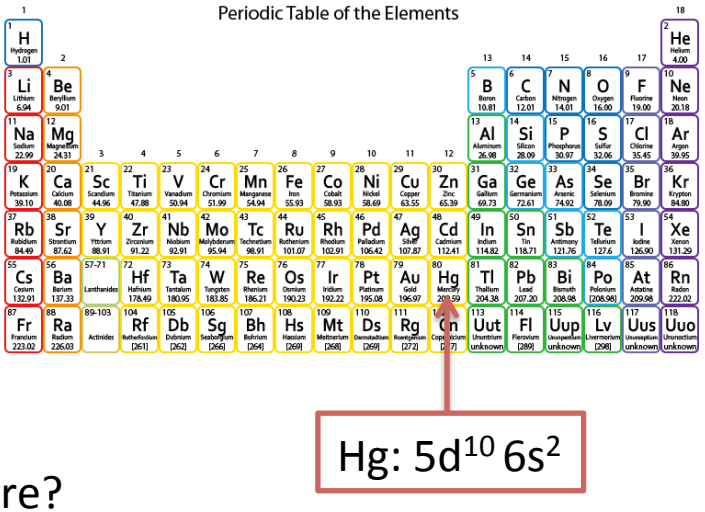
$$c, \text{ is } = 137.035999679$$

$$\gamma \overset{\text{def}}{=} \frac{1}{\sqrt{1 - v^2/c^2}} = 123\ \%$$

$$m = \gamma m_0$$

$$a_{rel} = \frac{\hbar^2}{me^2} = a_0/\gamma = a_0 81\%$$

$$\Delta E_{nlj} = \Delta E_R + \Delta E_{so} = \alpha^2 \mathcal{R}_M \left(\frac{3}{4n} - \frac{1}{j+\frac{1}{2}} \right) \frac{Z^4}{n^3}.$$



- Contraction of s and p shells, decrease in E_n
- Expansion of d and f shells, increase in E_n

Example 1: Hg

- Why Hg is in a liquid metal at room temperature?

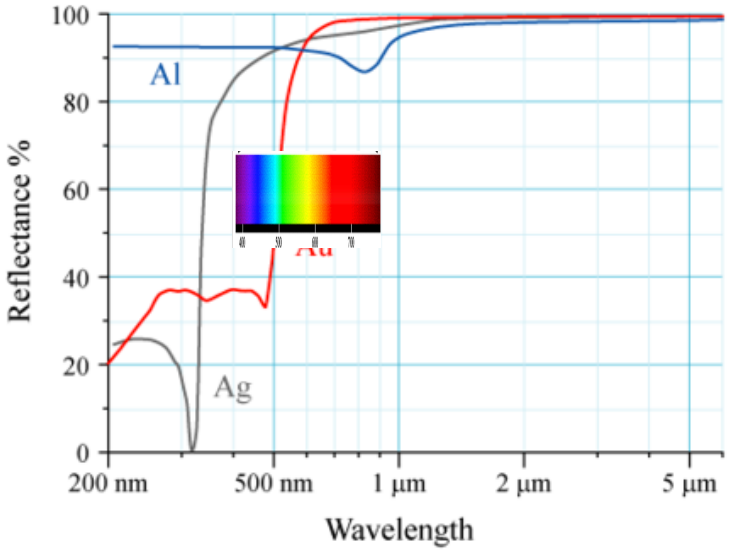
The $6s^2$ orbital is contracted so much that they only weakly contribute to any bonding, which is weak vdW type.

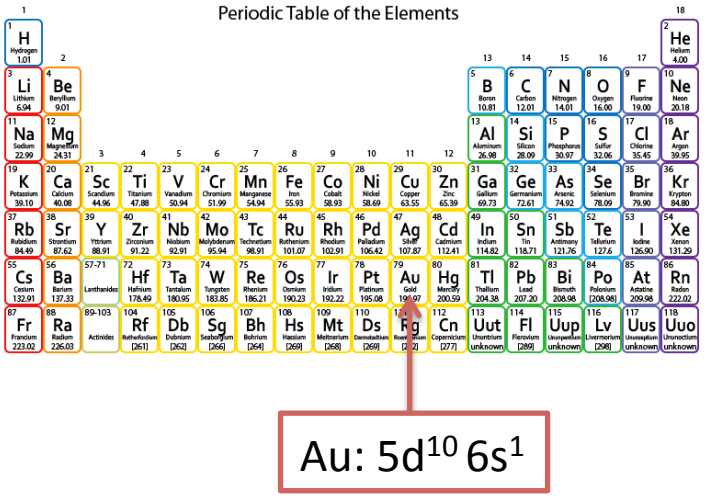
- The Hg-s state is lower in energy than Te-p states in HgTe (discuss later), giving rise to the topological insulator state.

Experimental consequence: *sp* contraction

Example 2: Au

- Why does Au have the golden color? (Known Al and Ag are white)





Small gap between filled 5d (expansion)
and empty 6s (contraction)

More examples:

atomic ground-state changes, such as Mo $4d^5 5s^1$ but W $5d^4 6s^2$

CsAu is a relativistic semiconductor, and CsAu(NR) would be a metal (Au^{-1})

Two types of SOC in solids

Symmetry-independent:

exists in all types of crystals

stem from SOC in atomic orbitals, similar to that in atoms.

Symmetry-dependent:

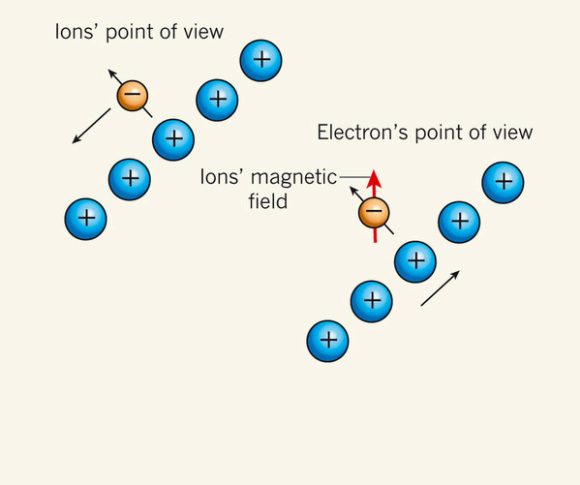
exists only in crystals without inversion symmetry

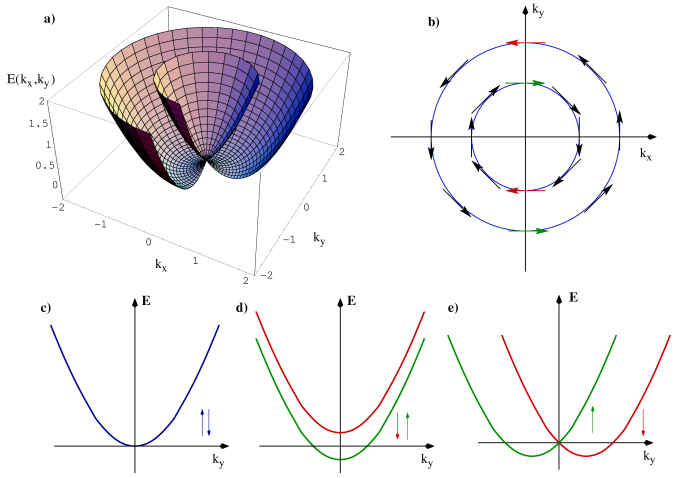
(a) Bychkov-Rashba (surface): usually referred to Surface-Induced-Asymmetry (SIA)

(b) Dresselhaus interaction (bulk): Bulk-Induced-Assymetry (BIA)

exists only in crystals with/without inversion symmetry

(c) General SOC: Local-Space-Asymmetry (LSA), surface and bulk

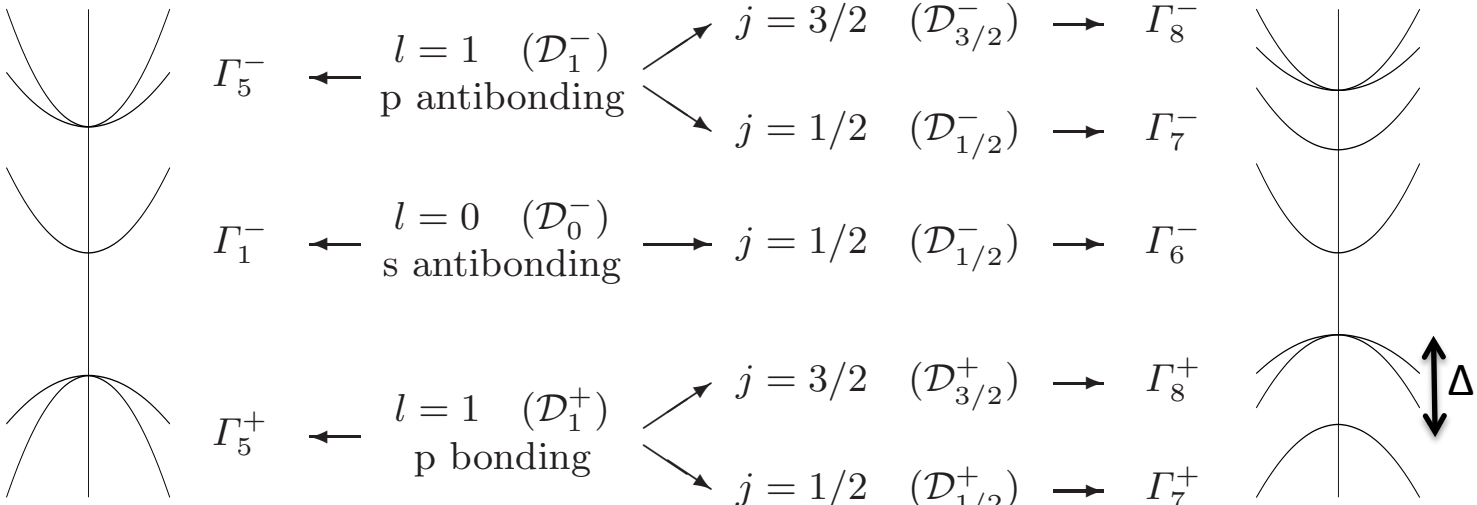




Symmetry-independent SOC

Table 3.1. Symmetry classification of the bands in the extended Kane model

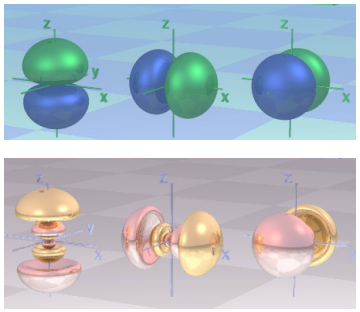
Single group			Double group	
O_h/T_d	Full rotation group $\mathcal{R}$			O_h/T_d
Γ_5^-	$l=1 \quad (\mathcal{D}_1^-)$ p antibonding		$j=3/2 \quad (\mathcal{D}_{3/2}^-)$	Γ_8^-
			$j=1/2 \quad (\mathcal{D}_{1/2}^-)$	Γ_7^-
Γ_1^-	$l=0 \quad (\mathcal{D}_0^-)$ s antibonding		$j=1/2 \quad (\mathcal{D}_{1/2}^-)$	Γ_6^-
Γ_5^+	$l=1 \quad (\mathcal{D}_1^+)$ p bonding		$j=3/2 \quad (\mathcal{D}_{3/2}^+)$	Γ_8^+
			$j=1/2 \quad (\mathcal{D}_{1/2}^+)$	Γ_7^+



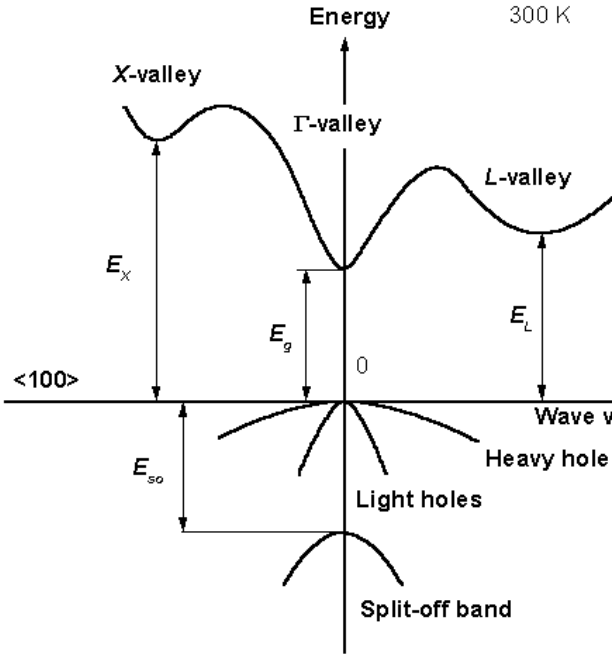
Zinc blend semiconductors
Si, Ge, GaAs, CdTe, HgTe

Winkler book 2003’

Symmetry-independent SOC



$\Delta \sim Z^2$ (outer p shell)



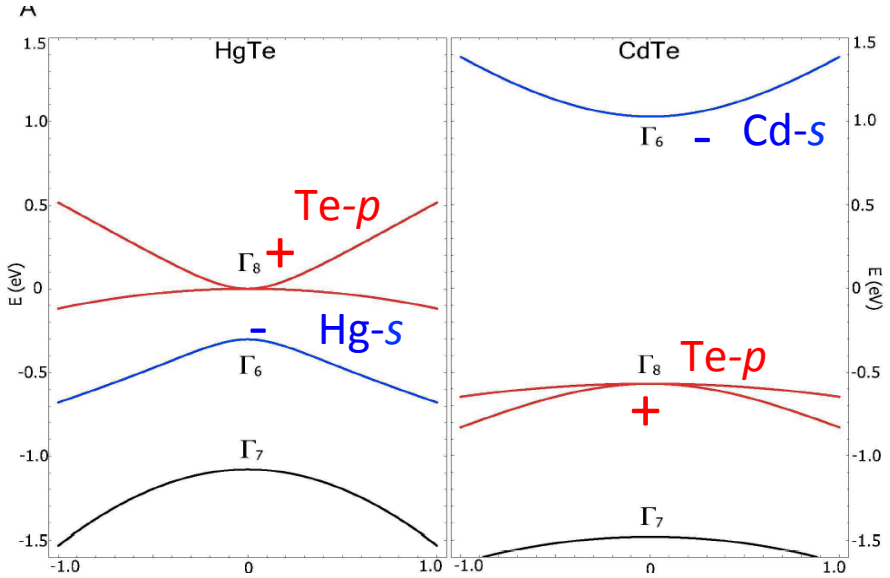
Compound	$\Delta_0^{\exp}$ (eV)
C	0.006
Si	0.044
Ge	0.29
α-Sn	
AlN	
AlP	
AlAs	
AlSb	0.75
GaN	0.011
GaP	0.127
GaAs	0.34
GaSb	0.80
InN	
InP	0.11
InAs	0.38
InSb	0.82
ZnO	−0.005
ZnS	0.07
ZnSe	0.43
ZnTe	0.93
CdS	0.066
CdSe	
CdTe	0.92
HgS	
HgSe	
HgTe	1.08

$$\left(\frac{Z_{Ge}}{Z_{Si}}\right)^2 = \left(\frac{(Z_{Ga}+Z_{As})/2}{Z_{Si}}\right)^2 = \left(\frac{32}{14}\right)^2 = 5.2$$

$$\frac{\Delta_{Ge}}{\Delta_{Si}} = 6.6 \qquad \frac{\Delta_{GaAs}}{\Delta_{Si}} = 7.7$$

SOC splits bands.

Symmetry-independent SOC



Due to the strong Hg-6s contraction, the Hg-6s band is lower than Te-5p bands.

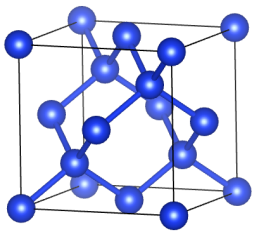
The relativistic terms induce a band inversion.

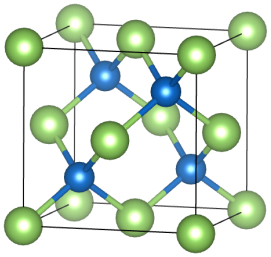
$$\hat{H} = \underbrace{\frac{\hat{p}^2}{2m} + eV}_{\text{non-relativistic}} + \underbrace{\frac{\hat{p}^4}{8m^2c^2}}_{\text{K.E. correction}} + \underbrace{\frac{\hbar^2}{8m^2c^2}\nabla^2 V}_{\text{Darwin term}} + \underbrace{\frac{\hbar}{4m^2c^2}\vec{\sigma}\bullet(\vec{\nabla}V \times \hat{\mathbf{p}})}_{\text{SOI}}$$

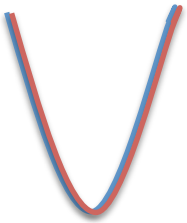
Symmetry and band splitting

Time reversal symmetry: $s \rightarrow -s,\ l \rightarrow -l,\ s.l \rightarrow s.l,\ k \rightarrow -k,\ E_n(s, k) = E_n(-s,-k)$

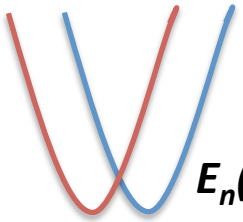
Inversion symmetry: $s \rightarrow s,\ l \rightarrow l,\ s.l \rightarrow s.l,\ k \rightarrow -k,\ E_n(s, k) = E_n(s,-k)$







$E_n(s, k) = E_n(-s,k)$

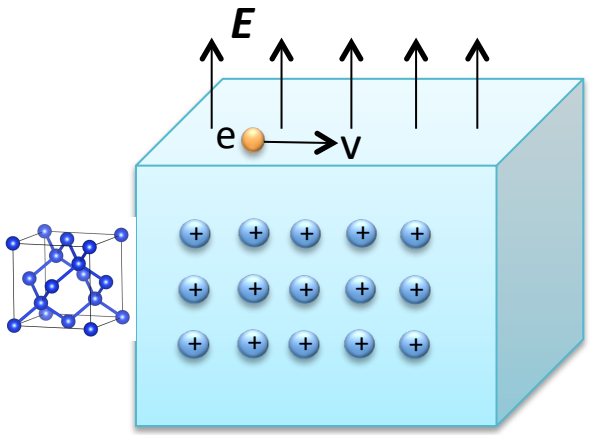


$E_n(s, k) \neq E_n(-s,k)$

TRS + Inversion symmetry

TRS + Inversion breaking

Rashba SOC



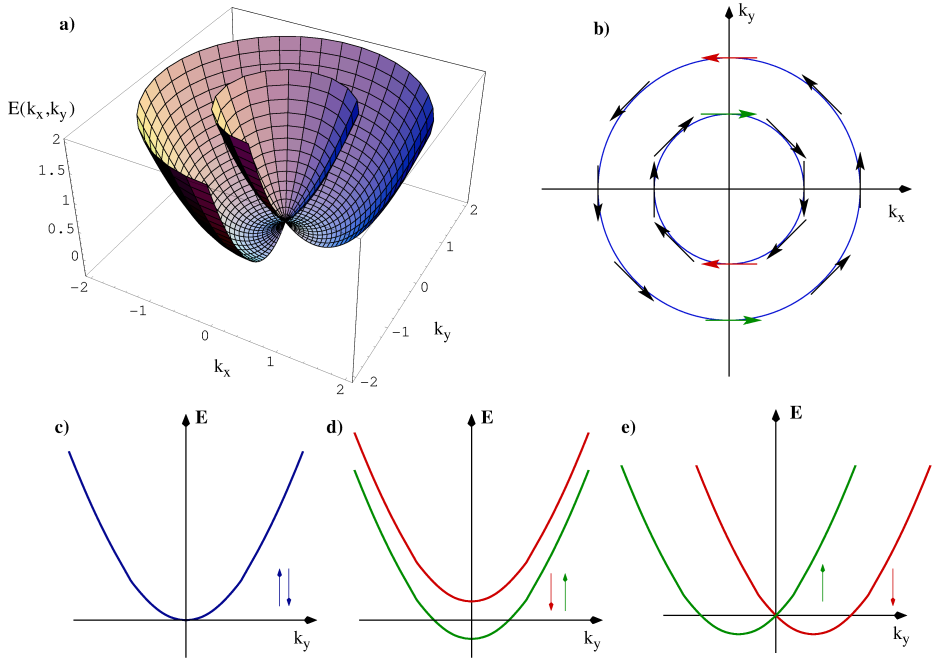
$$H_E = -E_0 z,$$

$$\mathbf{B} = \frac{1}{c^2}\mathbf{E} \times \mathbf{v}.$$

$$H_{SO} = \frac{g\mu_B}{2c^2}(\mathbf{v} \times \mathbf{E}) \cdot \sigma,$$

$$H_R = \alpha(\boldsymbol{\sigma} \times \mathbf{p}) \cdot \hat{z},$$

$$\alpha = \frac{g\mu_B E_0}{2mc^2} \qquad \alpha \sim E_0 Z^2$$

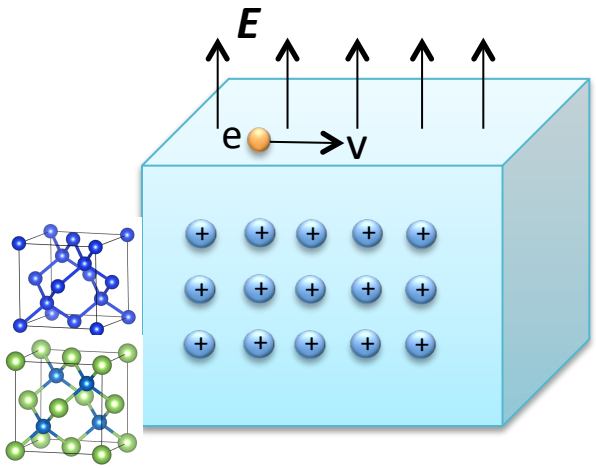


$$\hat{H}_R = \frac{k^2}{2m} + \alpha\hat{\mathbf{n}}\bullet(\vec{\sigma} \times \mathbf{k}) = \frac{k^2}{2m} + \alpha\left(\sigma^x k_y - \sigma^y k_x\right)$$

$$t \to -t : \mathbf{k} \to -\mathbf{k}, \sigma \to -\sigma$$

$$H_R = \begin{pmatrix} k^2/2m & \alpha\left(k_y + ik_x\right) \\ \alpha\left(k_y - ik_x\right) & k^2/2m \end{pmatrix} \Rightarrow \varepsilon_\pm = \frac{k^2}{2m} \pm \alpha k$$

Rashba SOC



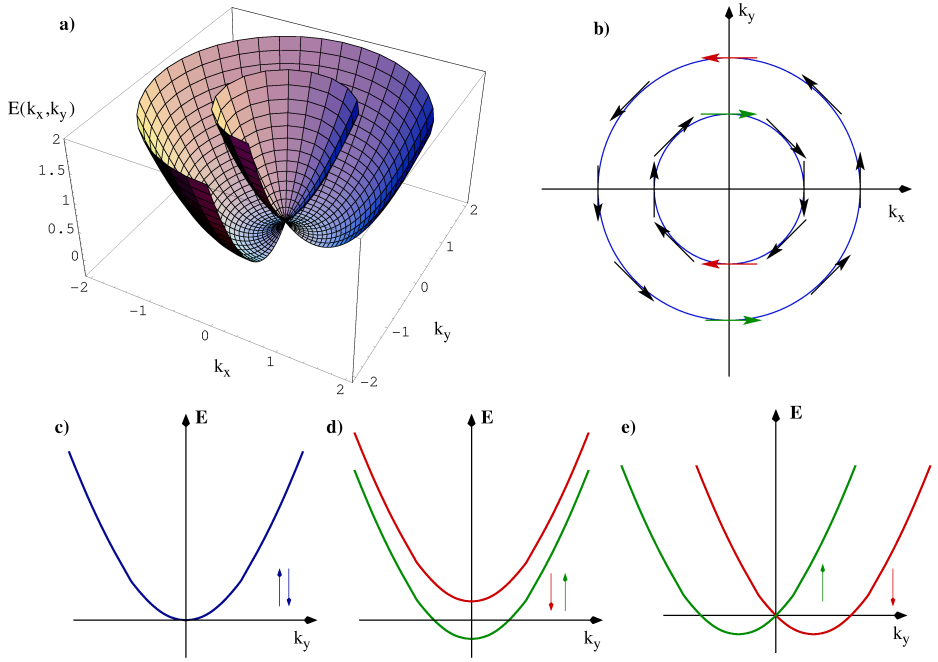
$$H_E = -E_0 z,$$

$$\mathbf{B} = \frac{1}{c^2}\mathbf{E} \times \mathbf{v}.$$

$$H_{SO} = \frac{g\mu_B}{2c^2}(\mathbf{v} \times \mathbf{E}) \cdot \sigma,$$

$$H_R = \alpha(\boldsymbol{\sigma} \times \mathbf{p}) \cdot \hat{z},$$

$$\alpha = \frac{g\mu_B E_0}{2mc^2} \qquad \alpha \sim E_0 Z^2$$



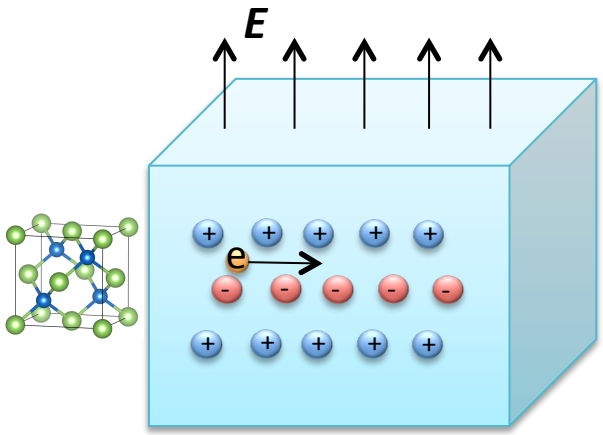
$$\varepsilon_{\pm} = \frac{k^2}{2m} \pm \alpha k \qquad \psi_{\pm} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \mp i e^{i\phi_k} \end{pmatrix}$$

$$S_{z,\pm} = \frac{1}{2}\bar{\psi}_{\pm}\sigma^z\psi_{\pm} = 0$$

$$S_{x,\pm} = \frac{1}{2}\bar{\psi}_{\pm}\sigma^x\psi_{\pm} = \pm\frac{1}{2}\sin\phi_k; \; S_{y,\pm} = \frac{1}{2}\bar{\psi}_{\pm}\sigma^y\psi_{\pm} = \mp\frac{1}{2}\cos\phi_k$$

$$\mathbf{k}\cdot\mathbf{S}_{\pm} = 0$$

Dresselhaus SOC



zincblende ($A_{III}B_V$) lattice

$$H_D = D\vec{\Omega}(\mathbf{k})\cdot\vec{\sigma}$$

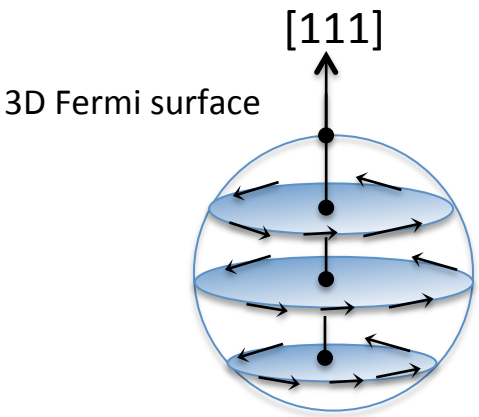
$$\vec{\Omega} = \left(k_x\left(k_y^2 - k_z^2\right), k_y\left(k_z^2 - k_x^2\right), k_z\left(k_x^2 - k_y^2\right)\right)$$

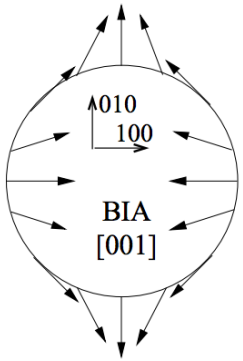
(001) surface (interface) of a $A_{III}B_V$ semiconductor

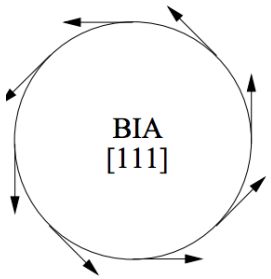
$$\left\langle k_z\right\rangle = 0, \left\langle k_z^2\right\rangle \sim 1/d^2$$

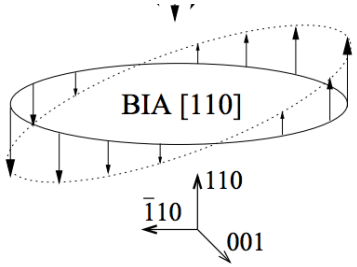
$$\left\langle\vec{\Omega}\right\rangle = \left(\underbrace{k_x k_y^2}_{\text{cubic}\to 0} - k_x\left\langle k_z^2\right\rangle, k_y\left\langle k_z^2\right\rangle - \underbrace{k_y k_x^2}_{\text{cubic}\to 0}, 0\right) = \left\langle k_z\right\rangle^2\left(-k_x, k_y, 0\right)$$

$$H_{DS} = \beta\left(\sigma^y k_y - \sigma^x k_x\right)$$





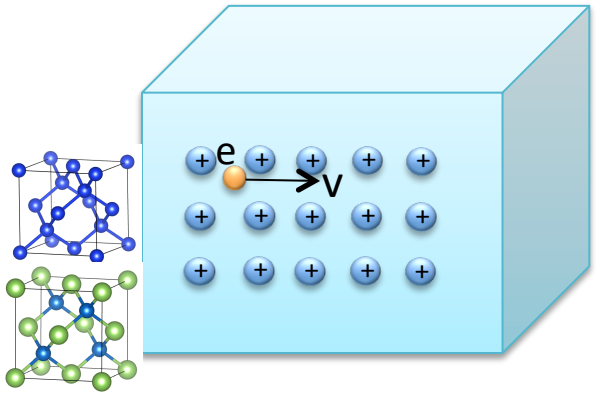


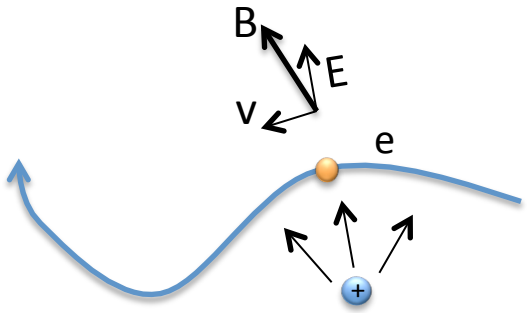


in general: Rashba+Dresselhaus

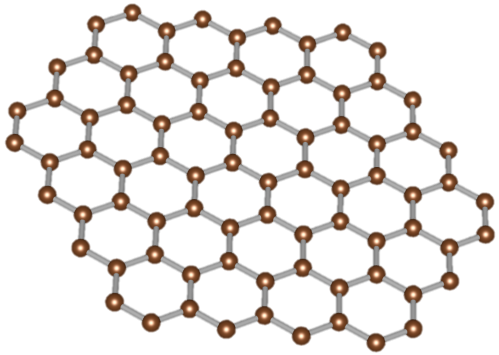
$$H = \frac{k^2}{2m} + \alpha\left(\sigma^x k_y - \sigma^y k_x\right) + \beta\left(\sigma^y k_y - \sigma^x k_x\right) = \frac{k^2}{2m} + \sigma^x\left(\alpha k_y - \beta k_x\right) + \sigma^y\left(\alpha k_x + \beta k_y\right)$$

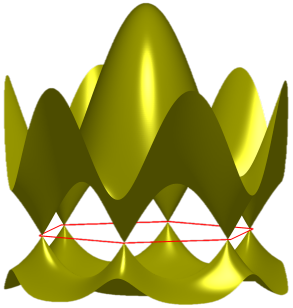
Non Rashba-Dresselhaus SOC



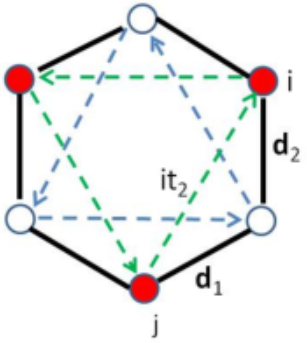


$$\mathbf{B} = \frac{1}{c^2}\mathbf{E} \times \mathbf{v}.$$



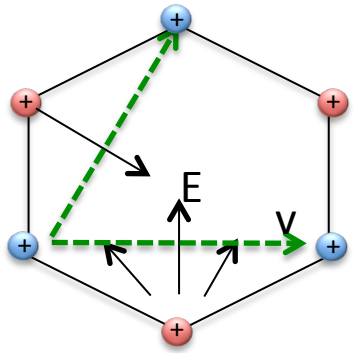


$$\mathcal{H} = \sum_{\langle ij \rangle \alpha} t c_{i\alpha}^{\dagger} c_{j\alpha}$$



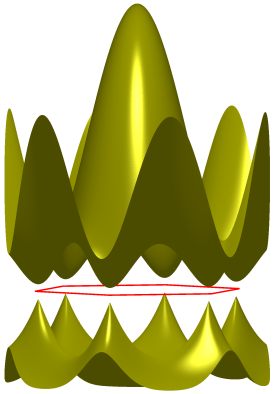
SOC in the graphene model

Refs:
C. L. Kane and E. J. Mele,
Phys. Rev. Lett. **95**, 226801 (2005).
F. D. M. Haldane,
Phys. Rev. Lett. **61**, 2015 (1988).

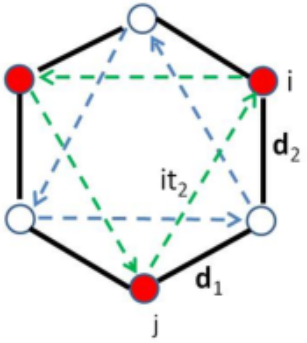


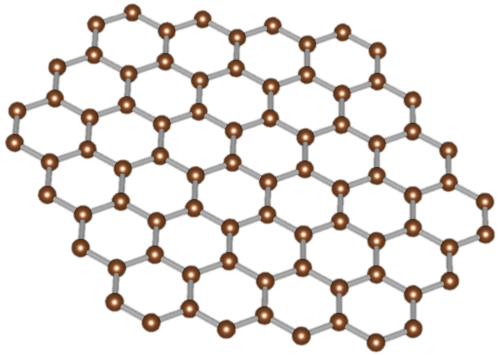
e

$$\mathbf{B} = \frac{1}{c^2}\mathbf{E} \times \mathbf{v}.$$



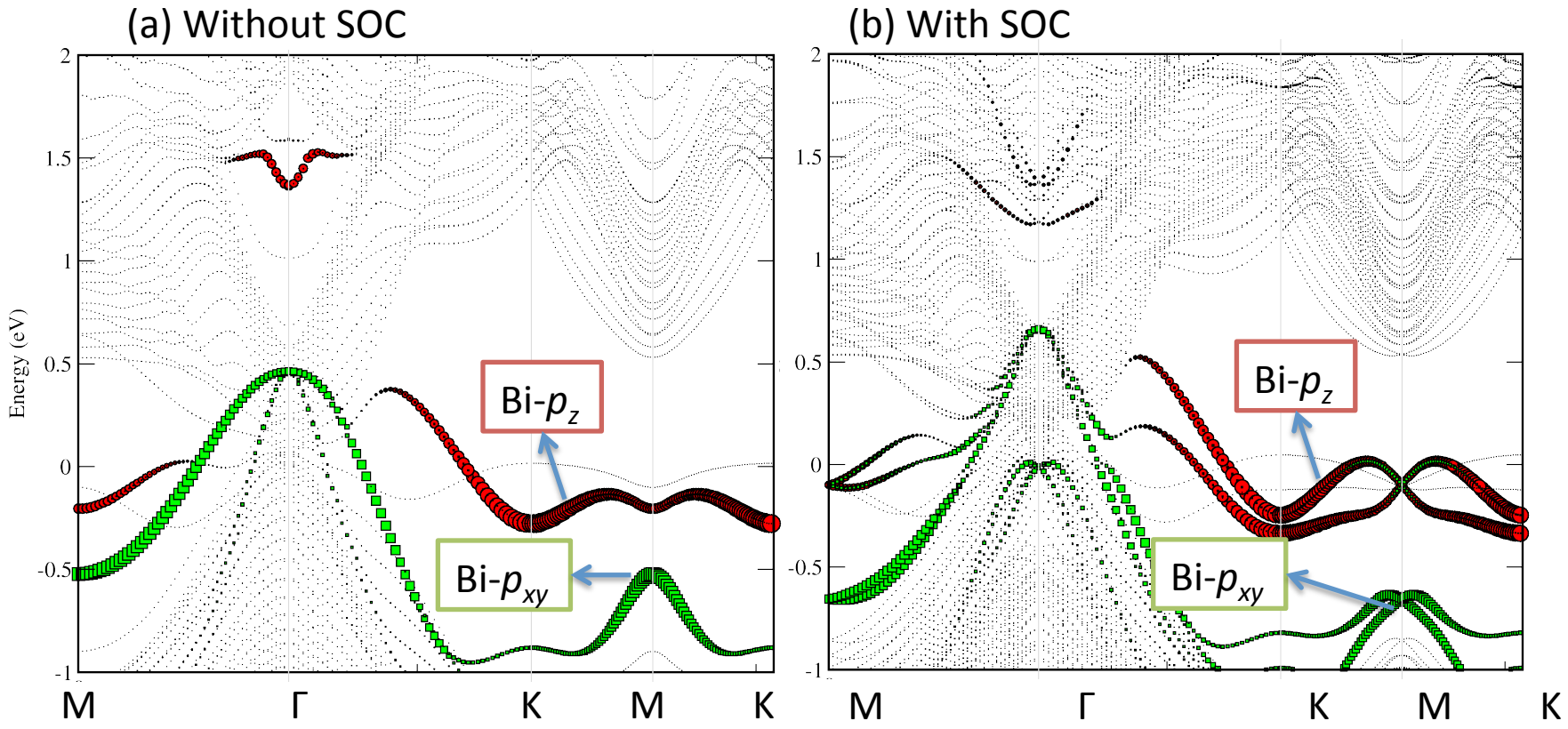
$v_{ij} = +1$ (-1) for left (right) turn hopping



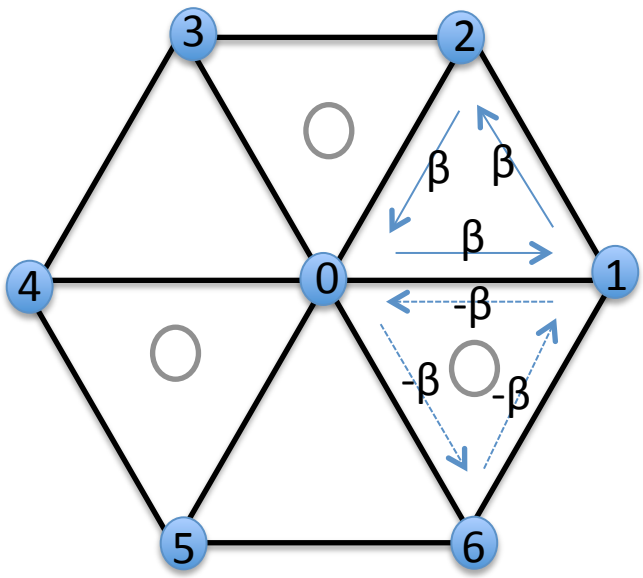


$$\mathcal{H} = \sum_{\langle ij\rangle\alpha} t c^{\dagger}_{i\alpha} c_{j\alpha} + \sum_{\langle\langle ij\rangle\rangle\alpha\beta} i t_2 \nu_{ij} s^{z}_{\alpha\beta} c^{\dagger}_{i\alpha} c_{j\beta}.$$

More general than graphene



We confirm that the surface state near -100 meV is indeed the Bi-pz state.
Next, we will fit above ab inito results using a simple TB model in the 2D triangular lattice.



Top Bi atoms form a triangular lattice.
The underlying Pt atom.

The Bi layer exhibits C_3 symmetry, rather than $C_{6,}$ due to the Pt layer below it.

Lattice constant: a = 4.6513 Å

Besides the common Rashba effect, there is a spin-dependent hopping term along a Bi-Bi bond, like the Kane-Mele term in grapehene.

The Hamiltonian can be written as

$$H = H^0 + H^R + H^{KM}$$

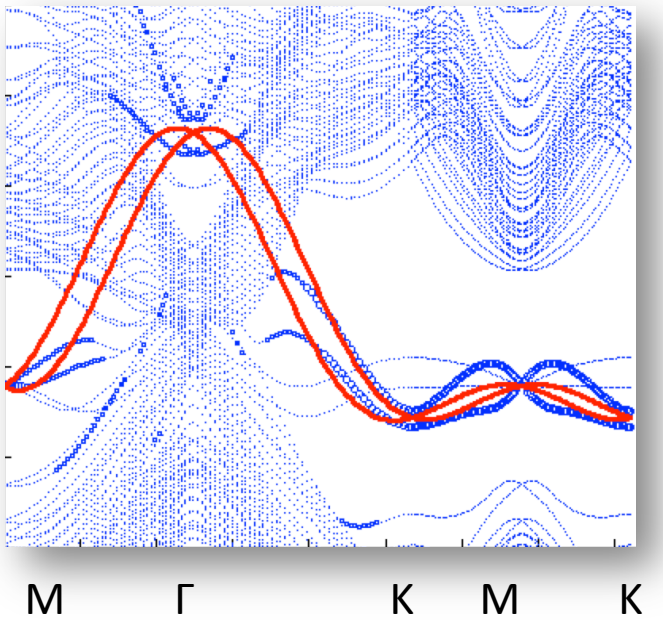
$$H^0 = -t\Sigma_{<ij>\sigma} c^+_{i\sigma} c_{j\sigma}$$

$$H^R = \frac{\alpha}{2} \sum_{<ij>\sigma\sigma'} \left(\boldsymbol{\sigma} \times \frac{\widehat{\boldsymbol{e_{ij}}}}{i} \right)_{z,\sigma\sigma'} c^+_{i\sigma}\, c_{j\sigma'}$$

$$H^{KM} = \frac{\beta}{2i} \sum_{<ij>\sigma\sigma'} \nu_{ij} \sigma_z\, c^+_{i\sigma}\, c_{j\sigma'}$$

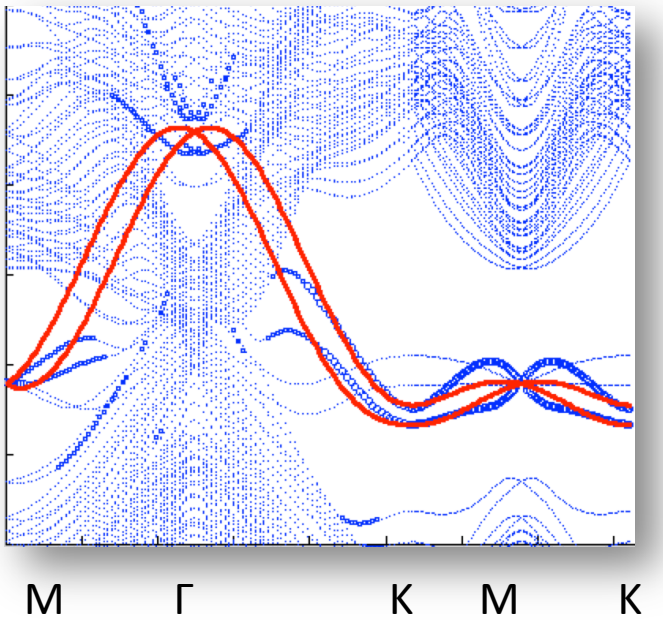
Where, ν_{ij}=-ν_{ji}=1, depends on the relative hopping direction with respect to the underlying Pt neighbor.

Fitting without H^{KM} term



t=0.35
α = 0.5
β = 0

Fitting with H^{KM} term



t=0.35
α = 0.5
β = 0.1

More examples:

ZK Liu, B. Yan et al, arXiv:1602.05633, Nature Comm. in press
K. Nakajin and S. Murakami, Physical Review B **91**, (2015).
X. Zhang, et al, Nature Physics **10**, 387 (2014).

Outline

Spin-orbit coupling in an atom

- Atom SOC
- Contraction of s and p shells

Spin-orbit coupling in solids

- Atomic SOC, such as HgTe
- Rashba effect
- Dresselhaus effect
- SOC in graphene

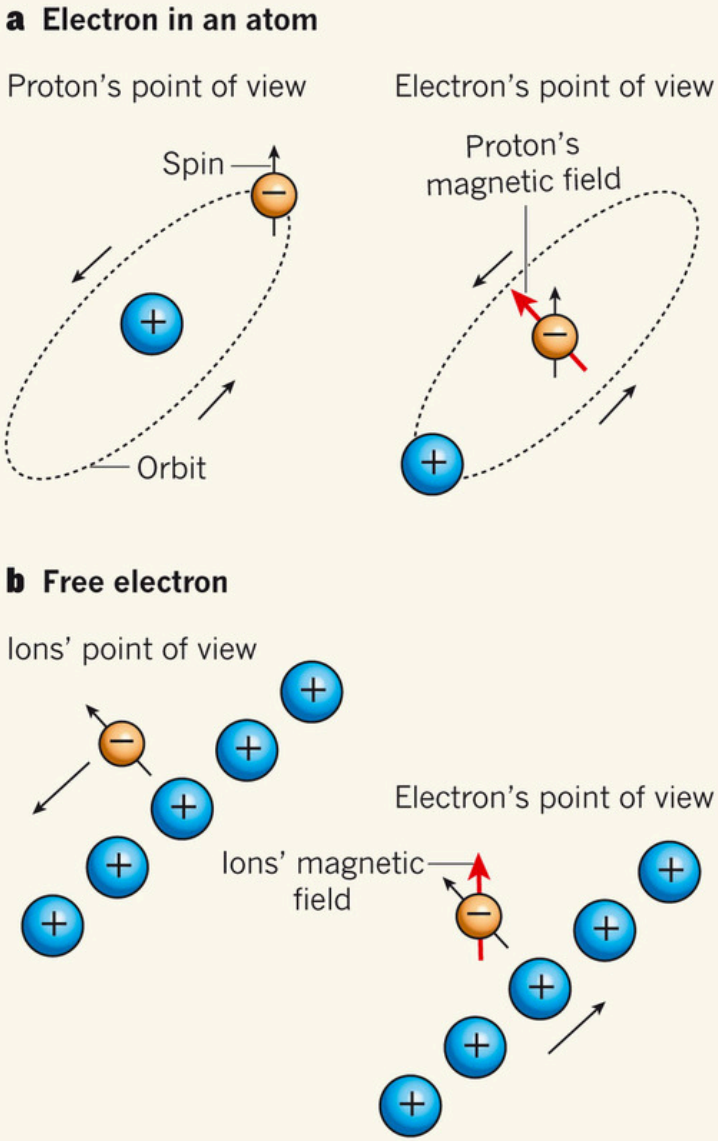
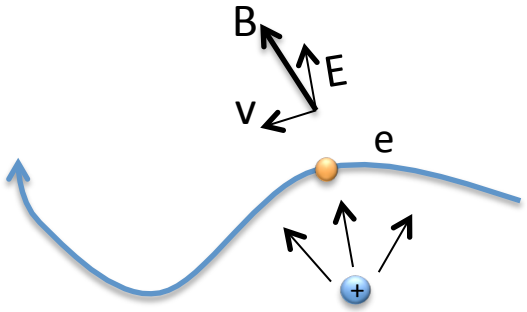


Figure credit: M. Chapman & C. Sá de Melo, Nature 471, 41–42 (2011)

Spin-orbit coupling:
a general relativistic effect in solids



$$\mathbf{B} = \frac{1}{c^2}\mathbf{E} \times \mathbf{v}.$$

Thanks for your attention!