Rashba effect in the 2D system

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The Rashba effect, also called Bychkov-Rashba effect, is a momentum-dependent splitting of spin bands in bulk crystals and low-dimensional condensed matter systems (such as heterostructures and surface states) similar to the splitting of particles and anti-particles in the Dirac Hamiltonian. The splitting is a combined effect of spin–orbit interaction and asymmetry of the crystal potential, in particular in the direction perpendicular to the two-dimensional plane (as applied to surfaces and heterostructures). This effect is named in honour of Emmanuel Rashba, who discovered it with Valentin I. Sheka in 1959 for three-dimensional systems and afterward with Yurii A. Bychkov in 1984 for two-dimensional systems.
https://en.wikipedia.org/wiki/Rashba_effect

The properties of a 2D electron gas in which the two-fold spin degeneracy of the spectrum has been lifted by the Hamiltonian of the spin-orbit interaction of an electron,

$$\hat{H}_1 = \alpha_R \boldsymbol{n}\cdot(\hat{\boldsymbol{\sigma}}\times\boldsymbol{k})$$

where α_R is a Rashba coupling. Here we discuss the eigenvalue problem of Rashba Hamiltoniam (and also Dresselhaus Hamiltonian) as exercises in Phys.421-521 (Quantum mechanics I).

1. Derivation of the spin-orbit interaction from Dirac theory of electron

We consider the origin of the spin-orbit interaction. In a relativistic quantum mechanics of the electron (Dirac theory), the Hamiltonian of the Dirac equation can be approximated by

$$H = \frac{1}{2m}\boldsymbol{p}^2 + eA_0 - \frac{\boldsymbol{p}^4}{8m^2c^2} - \frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times\boldsymbol{p}) - \frac{e\hbar^2}{8m^2c^2}\nabla\cdot\boldsymbol{E}$$

in the non-relativistic approximation (see the detail in the lecture note of Phys.524 and 525 Quantum Mechanics (graduate course), where e (<0) is the charge of electron.

$$E_r = -\frac{Ze}{r^2} = -\frac{\partial\phi_0}{\partial r}, \qquad \text{(electric field)}$$

$$A_0 = \phi_0 = -\frac{Ze}{r} \qquad \text{(electric potential)}$$

$$V(r) = eA_0 = e\phi_0 = -\frac{Ze^2}{r} \qquad \text{(potential energy)}$$

((Physical meaning))

Third term: relativistic correction

$$\sqrt{m^2c^4 + \boldsymbol{p}^2c^2} - mc^2 = mc^2\sqrt{1 + \frac{\boldsymbol{p}^2}{m^2c^2}} - mc^2$$

$$= mc^2[1 + \frac{\boldsymbol{p}^2}{2m^2c^2} - \frac{1}{8}\frac{\boldsymbol{p}^4}{m^4c^4} + ...] - mc^2$$

$$= \frac{\boldsymbol{p}^2}{2m} - \frac{1}{8}\frac{\boldsymbol{p}^4}{m^3c^2} + ...$$

The fourth term (Thomas correction)

$$\text{Thomas term} = -\frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times\boldsymbol{p})$$

For a central potential field,

$$eA_0 = V(r)$$

$$\boldsymbol{E} = -\nabla A_0 = -\frac{1}{r}\frac{dA_0}{dr}\boldsymbol{r}$$

$$\boldsymbol{E}\times\boldsymbol{p} = -\frac{1}{r}\frac{dA_0}{dr}(\boldsymbol{r}\times\boldsymbol{p}) = -\frac{1}{r}\frac{dA_0}{dr}\boldsymbol{L}$$

where $\boldsymbol{L}$ is an orbital angular momentum. Then the Thomas term is rewritten as

Thomas term :

$$-\frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times\boldsymbol{p}) = -\frac{e\hbar}{4m^2c^2}(-\frac{1}{r}\frac{dA_0}{dr})\boldsymbol{\sigma}\cdot\boldsymbol{L}$$

$$= \frac{e}{2m^2c^2}\frac{1}{r}\frac{dA_0}{dr}\boldsymbol{S}\cdot\boldsymbol{L}$$

$$= \frac{1}{2m^2c^2}\frac{1}{r}\frac{dV}{dr}\boldsymbol{S}\cdot\boldsymbol{L}$$

(Spin-orbit interaction)

When

$$V = eA_0 = -\frac{Ze^2}{r} \qquad \text{(attractive interaction)}$$

$$-\frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times\boldsymbol{p}) = Z\frac{e^2}{2m^2c^2}\left\langle\frac{1}{r^3}\right\rangle \boldsymbol{S}\cdot\boldsymbol{L}$$

The spin angular momentum is defined by

$$\boldsymbol{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$$

which is an automatic consequence of the Dirac theory.

The last term is called the Darwin term.

For a hydrogen atom,

$$\nabla\cdot\boldsymbol{E} = -\delta^{(3)}(\boldsymbol{r}) .$$

It gives rise to an energy shift

$$\int \frac{e^2\hbar^2}{8m^2c^2}\delta^{(3)}(\mathbf{r})\left|\psi(\mathbf{r})^{(Schrodinger)}\right|^2 d^3x = \frac{e^2\hbar^2}{8m^2c^2}\left|\psi(\mathbf{r})^{(Schrodinger)}\right|^2_{\mathbf{r}=0}$$

which is non-vanishing only for the *s* state.

We note that the spin orbit interaction becomes stronger as the atomic number *Z* increases. The fine structure factor α is defined by $\alpha = \frac{e^2}{\hbar c} = \frac{1}{137.035999139}$.

2. Spin-orbit interaction

$$H_{SO} = \frac{Ze^2}{2m^2c^2}\left\langle\frac{1}{r^3}\right\rangle_{av} \boldsymbol{S}\cdot\boldsymbol{L}$$

Using the formula

$$r_n = \frac{n^2\hbar^2}{mZe^2} \qquad \text{(Bohr radius)}$$

we can evaluate the magnitude of the spin-orbit coupling.

$$
\begin{aligned}
H_{SO} &\approx \frac{Ze^2}{2m^2c^2}\frac{1}{r_1^3}\boldsymbol{S}\cdot\boldsymbol{L} \\
&= \frac{Ze^2}{2m^2c^2}\left(\frac{mZe^2}{\hbar^2}\right)^3\boldsymbol{S}\cdot\boldsymbol{L} \\
&= \frac{Ze^2}{2m^2c^2}\frac{m^3Z^3e^6}{\hbar^6}\boldsymbol{S}\cdot\boldsymbol{L} \\
&= \frac{mc^2}{2\hbar^2}(Z\frac{e^2}{c\hbar})^4\boldsymbol{S}\cdot\boldsymbol{L} \\
&= \frac{mc^2}{2}(Z\alpha)^4\frac{\boldsymbol{S}\cdot\boldsymbol{L}}{\hbar^2}
\end{aligned}
$$

where the fine structure factor α is defined by $\alpha = \frac{e^2}{\hbar c} = \frac{1}{137.035999139}$.

We note that the lowest energy for the Bohr model is

$$
\left|E_{n=1}\right| = \frac{Z^2me^4}{2\hbar^2} = \frac{mc^2}{2}\left(\frac{Ze^2}{c\hbar}\right)^2 = \frac{mc^2}{2}(Z\alpha)^2
$$

Thus we have the ratio:

$$
\frac{H_{so}}{\left|E_{n=1}\right|} = \frac{\frac{mc^2}{2}(Z\alpha)^4\frac{\boldsymbol{S}\cdot\boldsymbol{L}}{\hbar^2}}{\frac{mc^2}{2}(Z\alpha)^2} = (Z\alpha)^2\frac{\boldsymbol{S}\cdot\boldsymbol{L}}{\hbar^2}
$$

So the spin orbit coupling is proportional to the factor $(Z\alpha)^2$. We note that the spin orbit coupling becomes important when the atomic number Z becomes large.

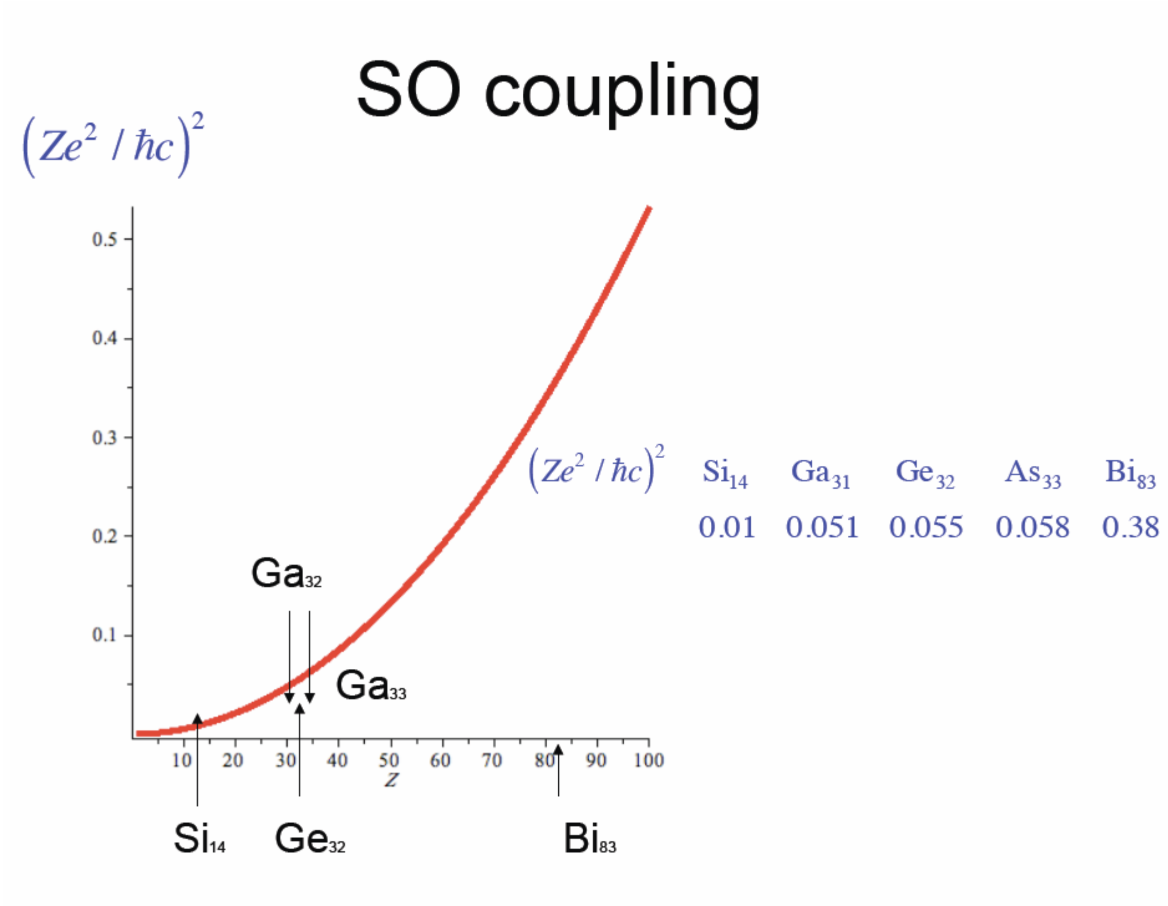


Fig. The factor $(Z\alpha)^2$ as a function of the atomic number Z.

3. Rashba Hamiltonian

The Rash Hamiltonian is given by

$$\hat{H} = \hat{H}_0 + \hat{H}_1$$

with

$$\hat{H}_0 = \frac{\hbar^2}{2m}k^2\hat{1} = \frac{\hbar^2}{2m}k^2\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

and

$$\hat{H}_1 = \alpha_R \boldsymbol{n}\cdot(\hat{\boldsymbol{\sigma}}\times\boldsymbol{k}) = \alpha_R(k_y\sigma_x - k_x\sigma_y)$$

with

$$[\hat{H}_0, \hat{H}_1] = 0$$

where $\boldsymbol{n}$ is the unit vector along the z axis. The Rashba field is defined by

$$\begin{aligned}\boldsymbol{B}_R &= \frac{2\alpha_R}{g\mu_B}\boldsymbol{k}\times\boldsymbol{n} \\ &= \frac{2\alpha_R}{g\mu_B}(k_y, -k_x, 0) \\ &= \frac{2\alpha_R k}{g\mu_B}(\sin\theta, -\cos\theta, 0)\end{aligned}$$

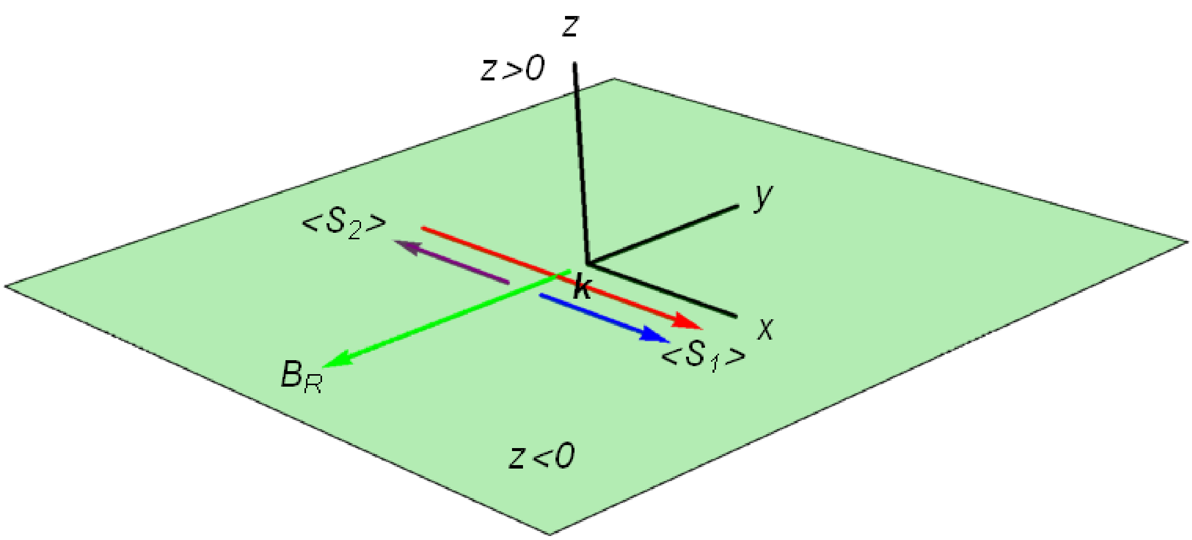


Fig. Rashba effect. $\boldsymbol{B}_R = \frac{2\alpha_R}{g\mu_B}\boldsymbol{k}\times\boldsymbol{n}$. $\boldsymbol{k} \perp \boldsymbol{n}$. $\boldsymbol{n}//z$. The spin orbit coupling and asymmetry of the potential in the z axis (half spaces with z>0 and z<0 are not equivalent), which is the surface induced asymmetry.

Using this field, the Rashba Hamiltonian can be rewritten as

$$
\begin{aligned}
\hat{H}_1 &= \alpha_R \boldsymbol{n}\cdot(\hat{\sigma}\times\boldsymbol{k}) \\
&= \alpha_R \hat{\sigma}\cdot(\boldsymbol{k}\times\boldsymbol{n}) \\
&= \frac{g\mu_B}{2}\frac{2\alpha_R}{g\mu_B}(\boldsymbol{k}\times\boldsymbol{n})\cdot\hat{\sigma} \\
&= \frac{g\mu_B}{2}\hat{\sigma}\cdot\boldsymbol{B}_R
\end{aligned}
$$

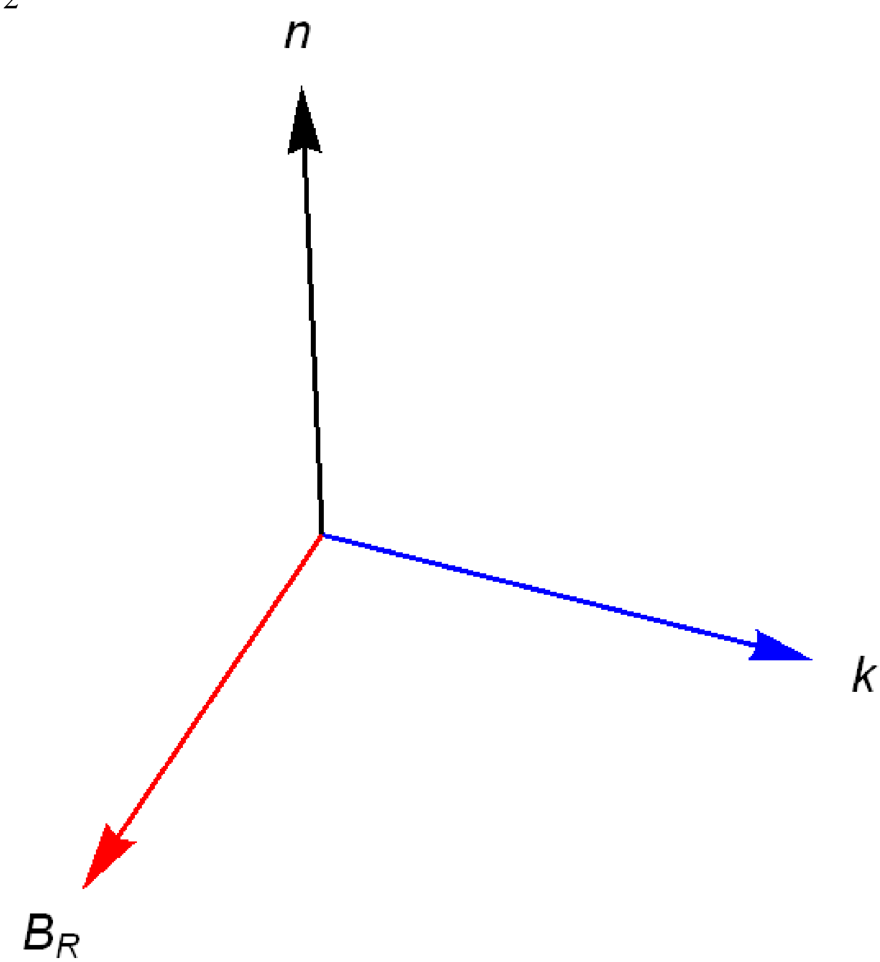


Fig. The effective magnetic field in the Rashba Hamiltonian. $\boldsymbol{B}_R = \dfrac{2\alpha_R}{g\mu_B}\boldsymbol{k}\times\boldsymbol{n}$. When $\boldsymbol{k}\perp\boldsymbol{n}$,

$$B_R = \frac{2\alpha_R k}{g\mu_B}$$

Using the Pauli matrices;

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_x = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$\hat{H}_1$ can be expressed as

$$\hat{H}_1 = \alpha_R \begin{pmatrix} 0 & -i(k_x + ik_y) \\ i(k_x - ik_y) & 0 \end{pmatrix}$$

We use

$$\boldsymbol{k} = (k_x, k_y, 0)$$

With

$$k_x = k\cos\theta, \qquad k_y = k\sin\theta$$

or

$$k_x + ik_y = k(\cos\theta + i\sin\theta) = ke^{i\theta}$$

$$k_x - ik_y = k(\cos\theta - i\sin\theta) = ke^{-i\theta}$$

Using this notation, we have

$$\hat{H}_1 = \alpha_R k \begin{pmatrix} 0 & -ie^{i\theta} \\ ie^{i\theta} & 0 \end{pmatrix}$$

((**Eigenvalue problem**)) We solve the eigenvalue problems using the Mathematica.

We have

$$\hat{H}_1 |\psi_1\rangle = \alpha_R k |\psi_1\rangle, \qquad \hat{H}_1 |\psi_2\rangle = -\alpha_R k |\psi_2\rangle$$

where the eigenkets of $\hat{H}_1$ are given by

$$|\psi_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ ie^{-i\theta} \end{pmatrix} \qquad \text{(eigenvalue: } \alpha k \text{)}$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -ie^{-i\theta} \end{pmatrix} \qquad \text{(eigenvalue } -\alpha k\text{)}$$

Note that

$$\hat{H}_0|\psi_1\rangle = \alpha_R k|\psi_1\rangle, \qquad \hat{H}_0|\psi_2\rangle = -\alpha_R k|\psi_2\rangle$$

and

$$[\hat{H}_0, \hat{H}_1] = 0$$

So $|\psi_1\rangle$ and $|\psi_2\rangle$ are simultaneous eigenkets of $\hat{H}_0$ and $\hat{H}_1$. In other words, $|\psi_1\rangle$ and $|\psi_2\rangle$ are the eigenkets of $\hat{H}$. Then we have

$$\hat{H}|\psi_1\rangle = (\frac{\hbar^2 k^2}{2m} + \alpha_R k)|\psi_1\rangle = E_1(k)|\psi_1\rangle,$$

$$\hat{H}|\psi_2\rangle = (\frac{\hbar^2 k^2}{2m} - \alpha_R k)|\psi_2\rangle = E_2(k)|\psi_2\rangle$$

Note that

$$E_1(k) = \frac{\hbar^2 k^2}{2m} + \alpha_R k = \frac{\hbar^2}{2m}(k + \frac{m\alpha_R}{\hbar^2})^2 - \frac{m\alpha_R}{2\hbar^2}.$$

$$E_2(k) = \frac{\hbar^2 k^2}{2m} - \alpha_R k = \frac{\hbar^2}{2m}(k - \frac{m\alpha_R}{\hbar^2})^2 - \frac{m\alpha_R}{2\hbar^2}$$

We note that

$$E_2(-k) = E_1(k), \qquad E_1(-k) = E_2(k)$$

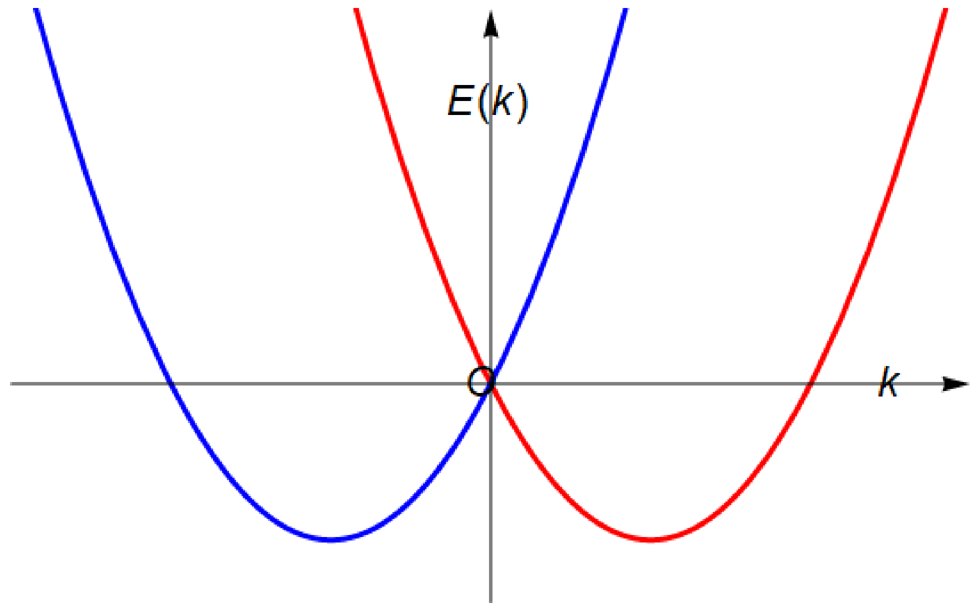


Fig. $E_1(k)$ for the state $|\psi_1\rangle$ (red) and $E_2(k)$ for the state $|\psi_2\rangle$ (blue). Symmetry: $E_2(-k)=E_1(k)$, $E_1(-k)=E_2(k)$

The average values of spin operators are given by

$$\begin{aligned}\langle \boldsymbol{S}_1\rangle &= \frac{\hbar}{2}\langle\psi_1|\hat{\boldsymbol{\sigma}}|\psi_1\rangle \\ &= \frac{\hbar}{2}(\langle\psi_1|\hat{\sigma}_x|\psi_1\rangle, \langle\psi_1|\hat{\sigma}_y|\psi_1\rangle, \langle\psi_1|\hat{\sigma}_z|\psi_1\rangle) \\ &= \frac{\hbar}{2}(\sin\theta, \cos\theta, 0)\end{aligned}$$

$$\begin{aligned}\langle \boldsymbol{S}_2\rangle &= \frac{\hbar}{2}\langle\psi_2|\hat{\boldsymbol{\sigma}}|\psi_2\rangle \\ &= \frac{\hbar}{2}(\langle\psi_2|\hat{\sigma}_x|\psi_2\rangle, \langle\psi_2|\hat{\sigma}_y|\psi_2\rangle, \langle\psi_2|\hat{\sigma}_z|\psi_2\rangle) \\ &= -\frac{\hbar}{2}(\sin\theta, \cos\theta, 0)\end{aligned}$$

We note that

$$\langle \boldsymbol{S}_2\rangle = -\langle \boldsymbol{S}_1\rangle \qquad \text{(which is always true)}$$

and

$$\langle \boldsymbol{S}_1 \rangle \cdot \boldsymbol{B}_R = \frac{2\alpha_R k}{g\mu_B} \cos(2\theta)$$

$$\langle \boldsymbol{S}_1 \rangle \cdot \boldsymbol{k} = \frac{\hbar k}{2} \sin(2\theta) \,.$$

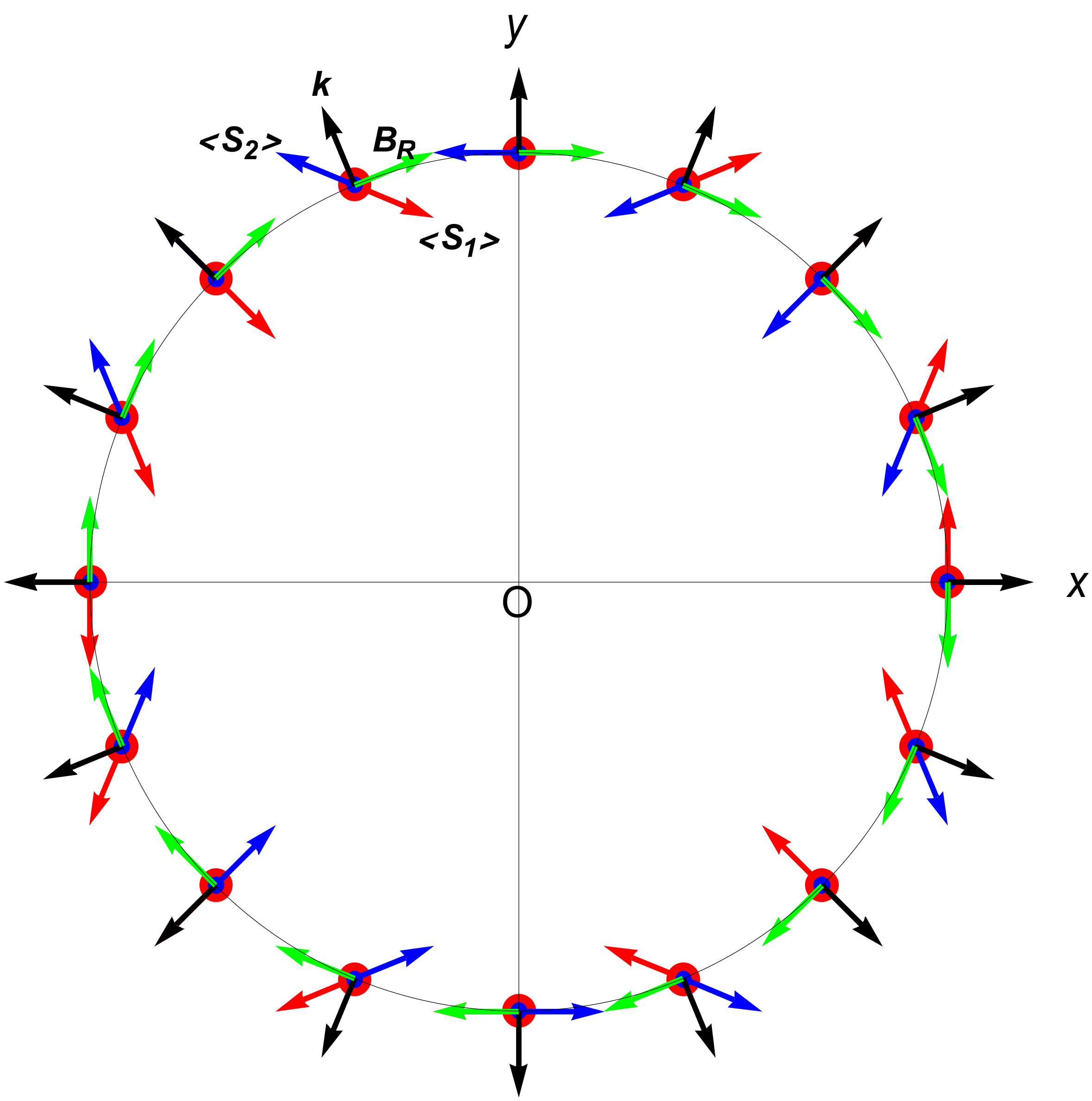


Fig. *x*-*y* plane. ***k***: black arrow [wave vector, (k_x, k_y)]. $\langle \boldsymbol{S}_1 \rangle$: red arrow. $\langle \boldsymbol{S}_2 \rangle$: blue arrow. $\boldsymbol{B}_R$: green arrow.

4 Effect of external magnetic field: Zeeman effect

In the presence of an external magnetic field

$$\hat{H}_1 = \frac{g\mu_B}{2}\hat{\boldsymbol{\sigma}}\cdot(\boldsymbol{B}_R + \boldsymbol{B})$$
$$= \alpha_R \boldsymbol{n}\cdot(\hat{\boldsymbol{\sigma}}\times\boldsymbol{k}) + \frac{g\mu_B}{2}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{B}$$

or

$$\hat{H}_1 = \alpha_R(k_y\sigma_x - k_x\sigma_y) + \frac{g\mu_B}{2}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{B}$$

Here we define a new parameter x as

$$x = \frac{B}{B_R} = \frac{B}{\frac{2\alpha_R k}{g\mu_B}} = \frac{g\mu_B B}{2\alpha_R k}$$

where

$$B_R = \frac{2\alpha_R k}{g\mu_B}.$$

We consider the two cases for the direction of $\boldsymbol{B}$.

(a) $\boldsymbol{B}\,//\,z$

We solve this eigenvalue problem using the Mathematica.

$$\hat{H}_1 = \alpha_R(k_y\sigma_x - k_x\sigma_y) + \frac{g\mu_B}{2}\sigma_z\cdot B$$
$$= \alpha_R k\begin{pmatrix} 0 & -ie^{i\theta} \\ ie^{-i\theta} & 0 \end{pmatrix} + \frac{g\mu_B}{2}B\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Note that

$$\frac{B}{B_R} = x$$

The eigenvalue: $\alpha_R k\sqrt{1+x^2}$

$$|\psi_1\rangle = \begin{pmatrix} \dfrac{x+\sqrt{1+x^2}}{\sqrt{2}\sqrt{1+x^2+x\sqrt{1+x^2}}} \\ \dfrac{ie^{-i\theta}}{\sqrt{2}\sqrt{1+x^2+x\sqrt{1+x^2}}} \end{pmatrix}$$

The eigenvalue: $-\alpha_R k\sqrt{1+x^2}$

$$|\psi_2\rangle = \begin{pmatrix} \dfrac{-x+\sqrt{1+x^2}}{\sqrt{2}\sqrt{1+x^2-x\sqrt{1+x^2}}} \\ \dfrac{-ie^{-i\theta}}{\sqrt{2}\sqrt{1+x^2-x\sqrt{1+x^2}}} \end{pmatrix}$$

The average values of spin operators are given by

$$\begin{aligned}\langle \boldsymbol{S}_1\rangle &= \frac{\hbar}{2}\langle\psi_1|\hat{\boldsymbol{\sigma}}|\psi_1\rangle \\ &= \frac{\hbar}{2}(\langle\psi_1|\hat{\sigma}_x|\psi_1\rangle, \langle\psi_1|\hat{\sigma}_y|\psi_1\rangle, \langle\psi_1|\hat{\sigma}_z|\psi_1\rangle) \\ &= \frac{\hbar}{2}(\frac{\sin\theta}{\sqrt{1+x^2}}, \frac{\cos\theta}{\sqrt{1+x^2}}, \frac{x}{\sqrt{1+x^2}})\end{aligned}$$

and

$$\begin{aligned}\langle \boldsymbol{S}_2\rangle &= \frac{\hbar}{2}\langle\psi_2|\hat{\boldsymbol{\sigma}}|\psi_2\rangle \\ &= \frac{\hbar}{2}(\langle\psi_2|\hat{\sigma}_x|\psi_2\rangle, \langle\psi_2|\hat{\sigma}_y|\psi_2\rangle, \langle\psi_2|\hat{\sigma}_z|\psi_2\rangle) \\ &= \frac{\hbar}{2}(-\frac{\sin\theta}{\sqrt{1+x^2}}, -\frac{\cos\theta}{\sqrt{1+x^2}}, -\frac{x}{\sqrt{1+x^2}})\end{aligned}$$

Thus we have

$$\langle \boldsymbol{S}_1 \rangle = -\langle \boldsymbol{S}_2 \rangle$$

Thus we have

$$\hat{H}|\psi_1\rangle = E_1|\psi_1\rangle, \qquad \hat{H}|\psi_2\rangle = E_2|\psi_2\rangle$$

with

$$E_1 = \frac{\hbar^2 k^2}{2m} + \alpha_R k\sqrt{1+x^2}, \qquad E_2 = \frac{\hbar^2 k^2}{2m} - \alpha_R k\sqrt{1+x^2}$$

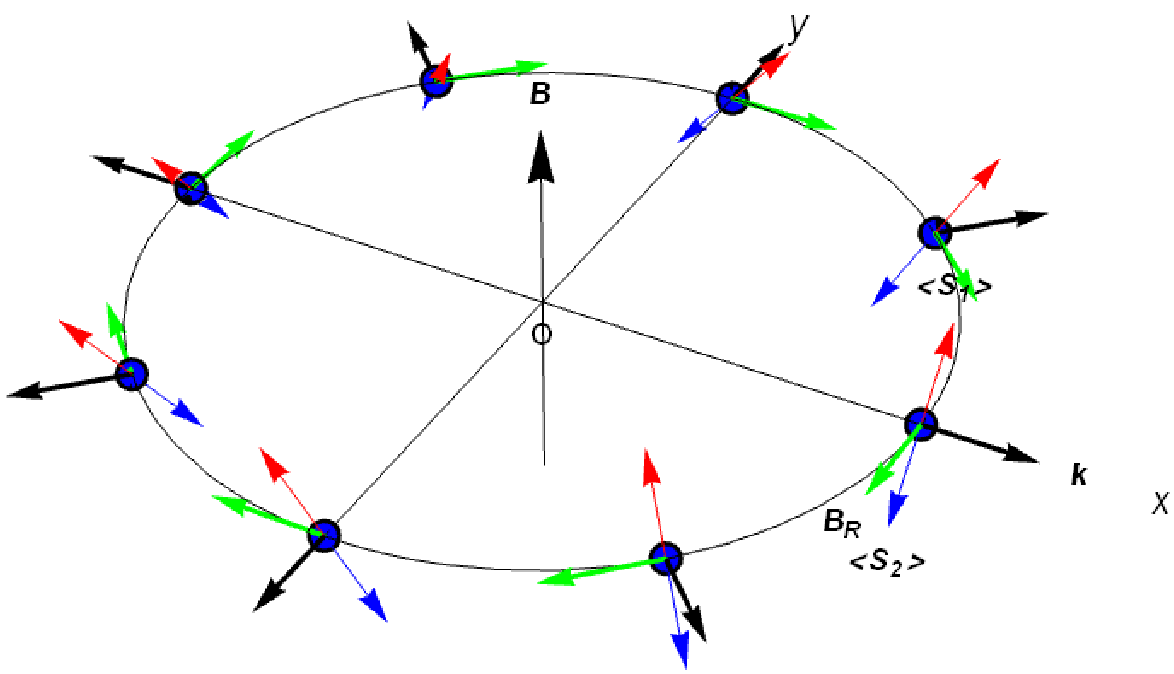


Fig. $B \neq 0$. *B//z*. *3D* plane. ***k***: black arrow [wave vector, (k_x, k_y)]. $\langle \boldsymbol{S}_1 \rangle$: red arrow. $\langle \boldsymbol{S}_2 \rangle$: blue arrow. $\boldsymbol{B}_R$: green arrow.

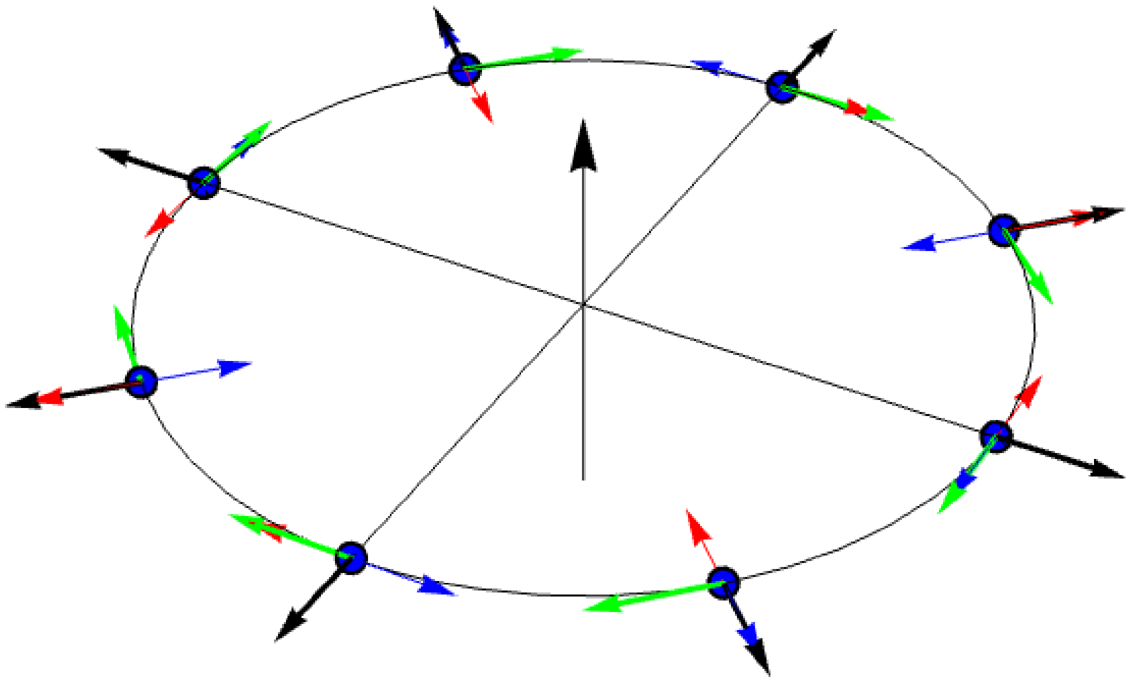


Fig. $B = 0$ for comparison. *3D* plane. $\boldsymbol{k}$: black arrow [wave vector, (k_x, k_y)]. $\langle \boldsymbol{S}_1 \rangle$: red arrow. $\langle \boldsymbol{S}_2 \rangle$: blue arrow. $\boldsymbol{B}_R$: green arrow.

Since

$$x = \frac{g\mu_B B}{2\alpha_R k}$$

we have

$$E_1 = \frac{\hbar^2 k^2}{2m} + \alpha_R k\sqrt{1+\left(\frac{g\mu_B B}{2\alpha_R k}\right)^2} = \frac{\hbar^2 k^2}{2m} + \alpha_R\sqrt{k^2+\left(\frac{g\mu_B B}{2\alpha_R}\right)^2},$$

$$E_2 = \frac{\hbar^2 k^2}{2m} - \alpha_R k\sqrt{1+\left(\frac{g\mu_B B}{2\alpha_R k}\right)^2} = \frac{\hbar^2 k^2}{2m} - \alpha_R\sqrt{k^2+\left(\frac{g\mu_B B}{2\alpha_R}\right)^2}$$

We assume that these energies can be expressed by

$$y_1 = x^2 + a\sqrt{x^2 + b^2}\,, \qquad y_2 = x^2 - a\sqrt{x^2 + b^2}$$

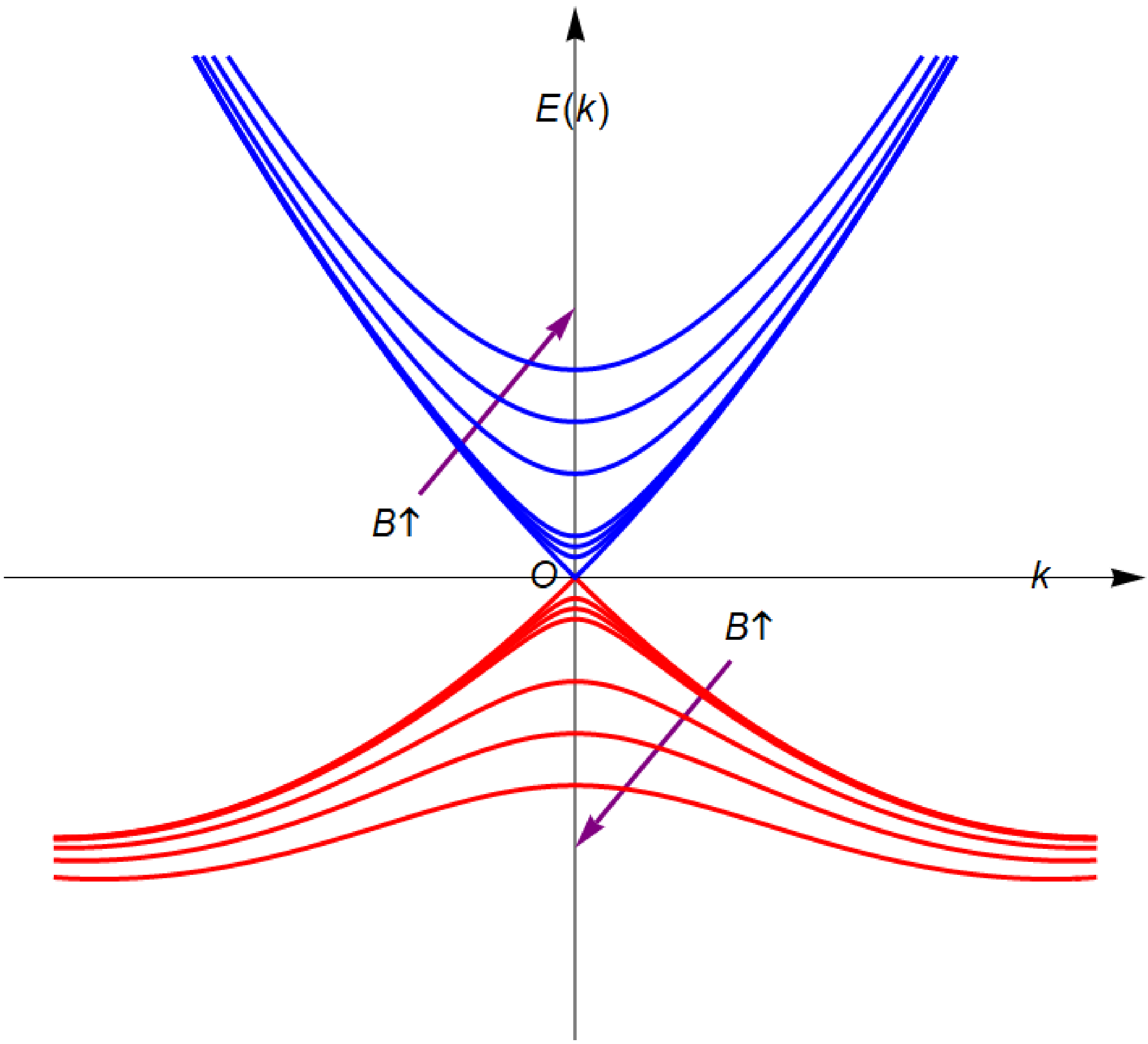


Fig. Energy dispersion E vs k for $\boldsymbol{B}//z$, where $\boldsymbol{B}$ is perpendicular to B_R.

(b) $\boldsymbol{B}//\boldsymbol{B}_R$

$$\hat{H}_1 = \frac{g\mu_B}{2}\hat{\boldsymbol{\sigma}}\cdot[\boldsymbol{B}_R + \frac{B}{k}(\boldsymbol{k}\times\boldsymbol{n})$$
$$= (\alpha_R + \frac{g\mu_B B}{2k})(\boldsymbol{k}\times\boldsymbol{n})\cdot\hat{\boldsymbol{\sigma}}$$
$$= (\alpha_R k + \frac{g\mu_B B}{2})(\frac{\boldsymbol{k}}{k}\times\boldsymbol{n})\cdot\hat{\boldsymbol{\sigma}}$$

where

$$\alpha_R \boldsymbol{n}\cdot(\hat{\boldsymbol{\sigma}}\times\boldsymbol{k}) = \alpha_R(\boldsymbol{k}\times\boldsymbol{n})\cdot\hat{\boldsymbol{\sigma}}$$

The energy eigenvalues are obtained as

$$E_1(k) = \frac{\hbar^2 k^2}{2m} + \alpha_R(k + \frac{g\mu_B B}{2\alpha_R})$$
$$= \frac{\hbar^2 k^2}{2m} + \alpha_R k + \frac{g\mu_B B}{2}$$

$$E_2(k) = \frac{\hbar^2 k^2}{2m} - \alpha_R(k + \frac{g\mu_B B}{2\alpha_R})$$
$$= \frac{\hbar^2 k^2}{2m} - \alpha_R k - \frac{g\mu_B B}{2}$$

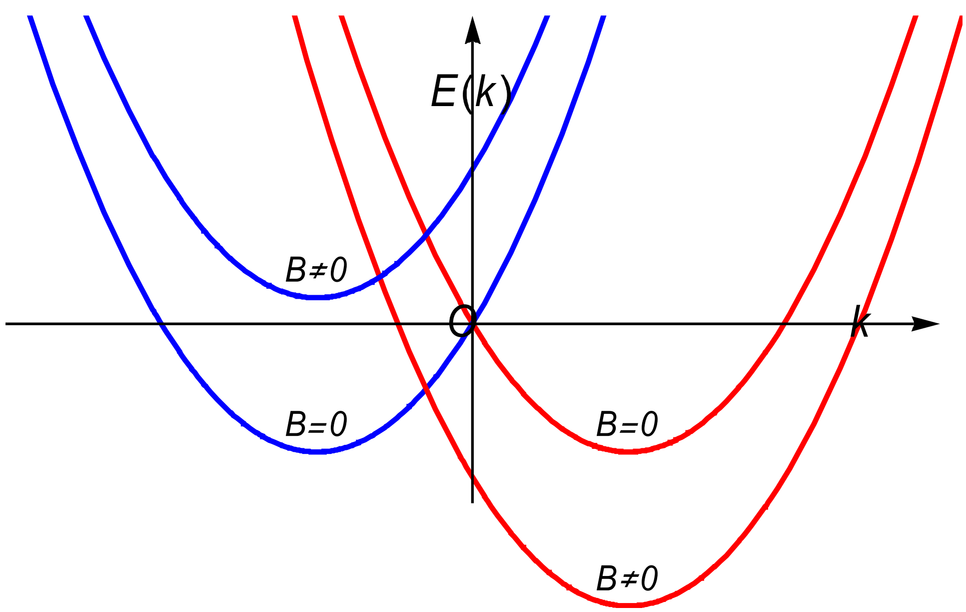


Fig. Energy dispersion E vs k for $\boldsymbol{B}//\boldsymbol{B}_{\mathrm{R}}$.

3. Dresselhaus Hamiltonian

We consider the eigenvalue problem for the Dresselhaus Hamiltonian

$$\begin{aligned}\hat{H}_{DS} &= \beta_{DS}(k_y\hat{\sigma}_y - k_x\hat{\sigma}_x) \\ &= \beta_{DS}k(\sin\theta\hat{\sigma}_y - \cos\theta\hat{\sigma}_x) \\ &= \beta_{DS}k\begin{pmatrix} 0 & -e^{i\theta} \\ -e^{-i\theta} & 0 \end{pmatrix}\end{aligned}$$

where β_{DS} is a Dresselhaus coupling. Eigenvalue problem

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -e^{-i\theta} \end{pmatrix}, \qquad \text{(eigenvalue: } \beta k\text{)}$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ e^{-i\theta} \end{pmatrix} \qquad \text{(eigenvalue: } -\beta k\text{)}$$

$$\begin{aligned}\langle \boldsymbol{S}_1\rangle &= \frac{\hbar}{2}\{\langle\psi_1|\hat{\sigma}_x|\psi_1\rangle, \langle\psi_1|\hat{\sigma}_y|\psi_1\rangle, \langle\psi_1|\hat{\sigma}_z|\psi_1\rangle\} \\ &= \frac{\hbar}{2}(-\cos\theta, \sin\theta, 0\}\end{aligned}$$

$$\begin{aligned}\langle \boldsymbol{S}_2\rangle &= \frac{\hbar}{2}\{\langle\psi_2|\hat{\sigma}_x|\psi_2\rangle, \langle\psi_2|\hat{\sigma}_y|\psi_2\rangle, \langle\psi_2|\hat{\sigma}_z|\psi_2\rangle\} \\ &= \frac{\hbar}{2}(\cos\theta, -\sin\theta, 0)\end{aligned}$$

$$\langle \boldsymbol{S}_2\rangle = -\langle \boldsymbol{S}_1\rangle$$

$$\langle \boldsymbol{S}_1\rangle\cdot\boldsymbol{k} = -\frac{\hbar}{2}\cos(2\theta), \qquad \langle \boldsymbol{S}_2\rangle\cdot\boldsymbol{k} = \frac{\hbar}{2}\cos(2\theta)$$

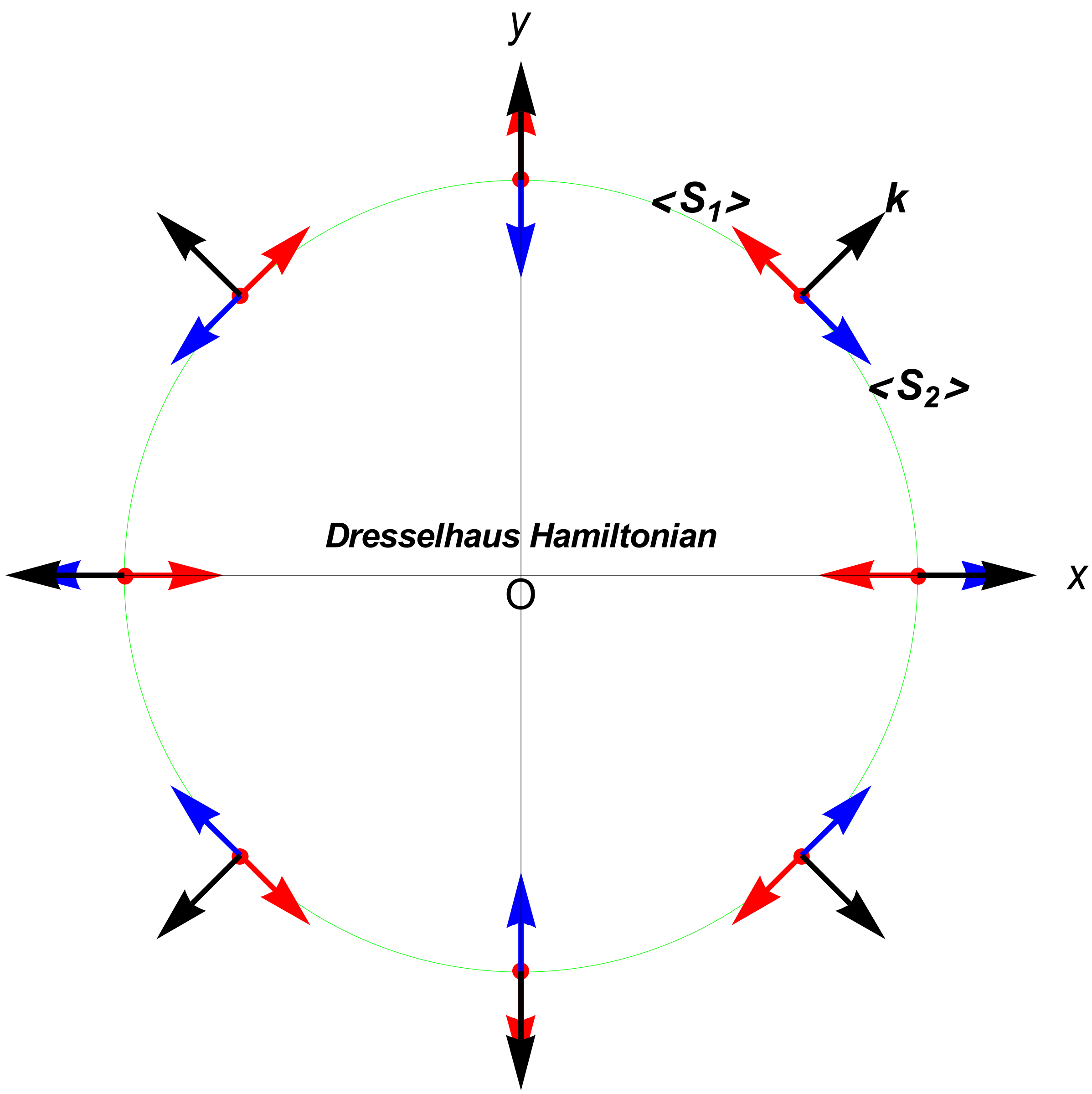


Fig. Dresselhaus interaction. x-y plane. $\boldsymbol{k}$: black arrow [wave vector, (k_x, k_y)]. $\langle \boldsymbol{S}_1 \rangle$: red arrow. $\langle \boldsymbol{S}_2 \rangle$.

APPENDIX
Mathematica

```
Clear["Global`*"];
σx = PauliMatrix[1]; σy = PauliMatrix[2];
σz = PauliMatrix[3];
exp_* := exp /. {Complex[re_, im_] :→ Complex[re, -im]};
```

$$A = \begin{pmatrix} 0 & -i\, e^{i\theta} \\ i\, e^{-i\theta} & 0 \end{pmatrix};$$

```
Eigensystem[A] // Simplify[#, θ > 0] &
```

$$\{\{1, -1\}, \{\{-i\, e^{i\theta}, 1\}, \{i\, e^{i\theta}, 1\}\}\}$$

$$\psi1 = \frac{1}{\sqrt{2}}\{1,\ i\, e^{-i\theta}\};\ \psi2 = \frac{1}{\sqrt{2}}\{1,\ -i\, e^{-i\theta}\};$$

```
{ψ1*.σx.ψ1, ψ1*.σy.ψ1, ψ1*.σz.ψ1} // FullSimplify
```

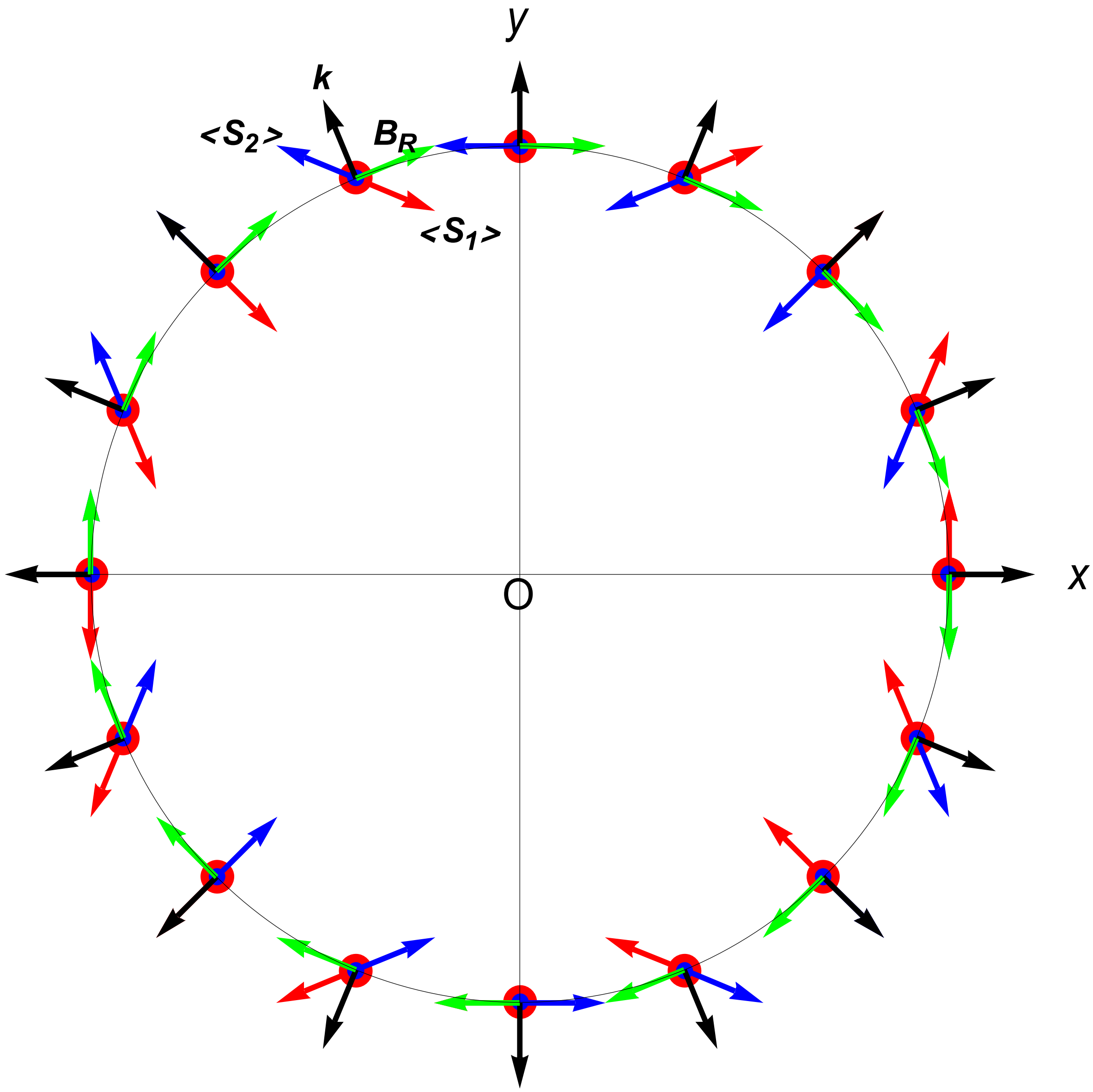
{Sin[θ], Cos[θ], 0}

```
{ψ2*.σx.ψ2, ψ2*.σy.ψ2, ψ2*.σz.ψ2} // FullSimplify
```

{-Sin[θ], -Cos[θ], 0}

```
P1 = 8;
R1[θ_] := {Cos[θ], Sin[θ]};
BR1[θ_] := {Sin[θ], -Cos[θ]};
S1[θ_] := 0.2 {Sin[θ], Cos[θ]};
S2[θ_] := -0.2 {Sin[θ], Cos[θ]};
s1 = Graphics[{Red, Thick, Arrowheads[0.03],
    Table[Arrow[{R1[θ], R1[θ] + S1[θ]}],
     {θ, 0, 2 π, π / P1}], PointSize[0.03],
    Table[Point[R1[θ]], {θ, 0, 2 π, π / P1}]}] ;

s2 = Graphics[{Blue, Thick, Arrowheads[0.03],
   Table[Arrow[{R1[θ], R1[θ] + S2[θ]}],
    {θ, 0, 2 π, π / P1}], PointSize[0.015],
   Table[Point[R1[θ]], {θ, 0, 2 π, π / P1}]}] ;
s3 = Graphics[{Black, Thick, Arrowheads[0.03],
   Table[Arrow[{ R1[θ], 1.2 R1[θ]}], {θ, 0, 2 π, π / P1}],
   Green, Table[Arrow[{ R1[θ], R1[θ] + 0.2 BR1[θ]}],
    {θ, 0, 2 π, π / P1}]}] ;
s4 = Graphics[{Black, Thin, Line[{{-1, 0}, {1, 0}}],
   Line[{{0, -1}, {0, 1}}],
   Text[Style["x", Black, 15, Italic], {1.3, 0}],
   Text[Style["y", Black, 15, Italic], {0, 1.3}],
   Text[Style["O", Black, 15], {0, -0.05}],
   Text[Style["BR", Black, Bold, 12, Italic],
    {-0.29, 1.03}],
   Text[Style["k", Black, Bold, 12, Italic],
    {-0.46, 1.16}],
   Text[Style["<S1>", Black, Bold, 12, Italic],
    {-0.14, 0.8}],
   Text[Style["<S2>", Black, Bold, 12, Italic],
    {-0.65, 1.03}]}];
s5 = Graphics[{Black, Thin, Circle[{0, 0}, 1]}];
Show[s1, s2, s3, s4, s5]
```



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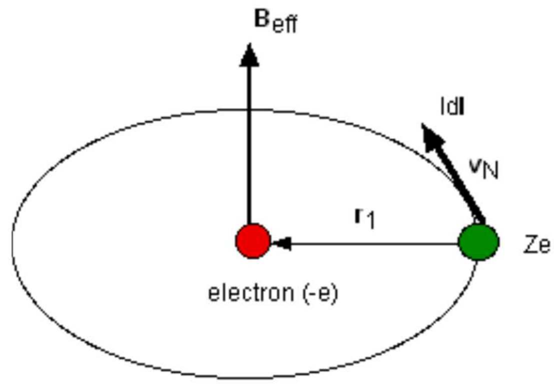
APPENDIX

Spin-orbit interaction

A.1. Biot-Savart law

The electron has an orbital motion around the nucleus. This also implies that the nucleus has an orbital motion around the electron. The motion of nucleus produces an orbital current. From the Biot-Savart's law, it generates a magnetic field on the electron.



The current I due to the movement of nucleus (charge Ze, e>0) is given by

$$I d\boldsymbol{l} = Ze\boldsymbol{v}_N ,$$

where $\vec{v}_N$ is the velocity of the nucleus and $\frac{d\boldsymbol{l}}{dt} = \boldsymbol{v}_N$. Note that

$$I d\boldsymbol{l} = \frac{\Delta q}{\Delta t} d\boldsymbol{l} = \Delta q \frac{d\boldsymbol{l}}{dt} = Ze\boldsymbol{v}_N .$$

The effective magnetic field at the electron at the origin is

$$\boldsymbol{B}_{eff} = \frac{I}{c}\frac{d\boldsymbol{l}\times\boldsymbol{r}_1}{|\boldsymbol{r}_1|^3}, \qquad \boldsymbol{v}_N = v\boldsymbol{e}_\theta$$

where v is the velocity of the electron. Then we have

$$\boldsymbol{B}_{eff} = \frac{Ze}{c}\frac{\boldsymbol{v}_N\times\boldsymbol{r}_1}{|\boldsymbol{r}_1|^3} = \frac{Ze}{c}\frac{v\boldsymbol{e}_\theta\times\boldsymbol{r}_1}{|\boldsymbol{r}_1|^3} .$$

Since $\boldsymbol{r}_1 = -\boldsymbol{r}$, $\boldsymbol{B}_{eff}$ can be rewritten as

$$\vec{\boldsymbol{B}}_{eff} = -\frac{Ze}{c}\frac{v\boldsymbol{e}_\theta\times\boldsymbol{r}}{|\boldsymbol{r}|^3} = \frac{Zev}{c}\frac{\boldsymbol{r}\times\boldsymbol{e}_\theta}{|\boldsymbol{r}|^3} = \frac{Zev}{c}\frac{\boldsymbol{e}_z}{|\boldsymbol{r}|^2} = \frac{Zem_e v}{m_e c|\boldsymbol{r}|^2}\boldsymbol{e}_z$$

where m_e is the mass of electron. The Coulomb potential energy is given by

$$V_c(r) = -\frac{Ze^2}{r}, \qquad \frac{dV_c(r)}{dr} = \frac{Ze^2}{r^2}.$$

Thus we have

$$\boldsymbol{B}_{eff} = \frac{Ze^2 rv}{cer^3}\boldsymbol{e}_z = \frac{1}{m_e cer}\frac{Ze^2}{r^2}m_e rv\boldsymbol{e}_z = \frac{1}{m_e cer}\frac{dV_c(r)}{dr}L_z\boldsymbol{e}_z,$$

or

$$\boldsymbol{B}_{eff} = \frac{1}{m_e ce}\frac{1}{r}\frac{dV_c(r)}{dr}L_z\boldsymbol{e}_z,$$

where L_z is the z-component of the orbital angular momentum, $L_z = m_e vr$.

A.2. Derivation of the expression for the spin-orbit interaction

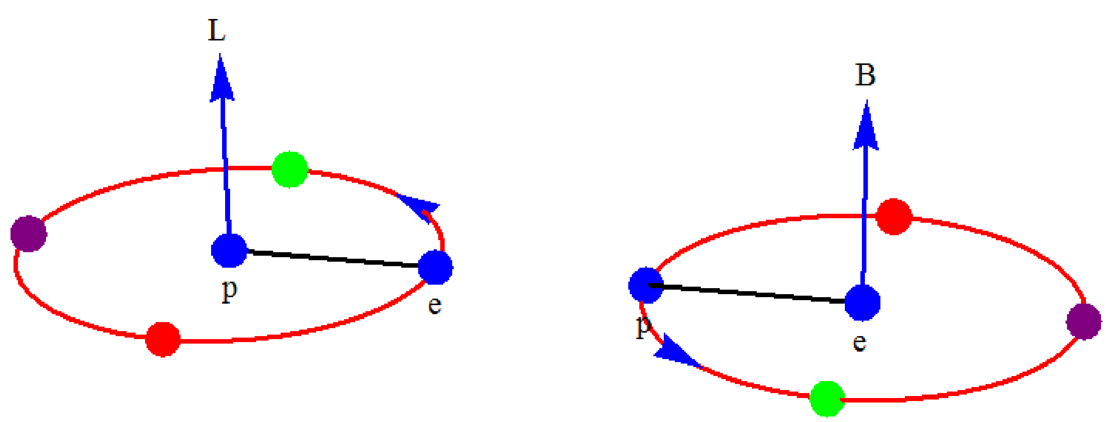


Fig. Electron in the proton frame, and proton in the electron frame. The direction of magnetic field ***B*** produced by the proton is the same as that of the orbital angular momentum ***L*** of the electron (the z axis in this figure).

We consider the circular motion of the nucleus (e) around an electron at the center. The nucleus rotates around the electron at the uniform velocity v. Note that the velocity of the proton in the electron frame is the same as the electron in the proton frame. The magnetic field (in cgs) at the center of the circle along with the current I flow.

$$B = \frac{2\pi I}{cr}.$$

according to the Biot-Savart law. The current I is given by

$$I = \frac{e}{T} = \frac{e}{\frac{2\pi r}{v}} = \frac{ev}{2\pi r},$$

where T is the period. Then the magnetic field $\boldsymbol{B}$ at the site of the electron (the proton frame) can be expressed as

$$\boldsymbol{B} = \frac{em_e v_N r}{m_e c r^3}\boldsymbol{e}_z = \frac{e\boldsymbol{L}}{m_e c r^3},$$

where $\boldsymbol{L}$ is the orbital angular momentum of the electron (the electron frame). Note that the direction of $\boldsymbol{B}$ is the same as that of $\boldsymbol{L}$. The spin magnetic moment is given by

$$\boldsymbol{\mu}_s = -\frac{2\mu_B}{\hbar}\boldsymbol{S},$$

where $\boldsymbol{S}$ is the spin angular momentum and μ_B is the Bohr magneton,

$$\mu_B = \frac{e\hbar}{2m_e c}.$$

Then the Zeeman energy of the electron is given by

$$H = -\frac{1}{2}\boldsymbol{\mu}_s \cdot \boldsymbol{B} = -\frac{1}{2}(-\frac{2\mu_B}{\hbar}\boldsymbol{S}) \cdot \left(\frac{e\boldsymbol{L}}{m_e c r^3}\right) = \frac{e^2}{2m_e{}^2 c^2 r^3}\boldsymbol{L} \cdot \boldsymbol{S},$$

where the factor (1/2) is the Thomas correction. In quantum mechanics we use the notation

$$\hat{H}_{so} = \frac{e^2}{2m_e{}^2 c^2}\left\langle \frac{1}{r^3} \right\rangle_{av} \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}.$$

A.3. Thomas correction

The spin magnetic moment is defined by

$$\boldsymbol{\mu}_s = -\frac{2\mu_B}{\hbar}\boldsymbol{S},$$

where $\boldsymbol{S}$ is the spin angular momentum. Then the Zeeman energy is given by

$$
\begin{aligned}
H_{so} &= -\frac{1}{2}\boldsymbol{\mu}_s \cdot \boldsymbol{B}_{eff} = -\frac{1}{2}\left(-\frac{2\mu_B}{\hbar}\boldsymbol{S}\right)\cdot\left(\frac{1}{m_e c e}\frac{1}{r}\frac{dV_c(r)}{dr}\boldsymbol{L}\right) \\
&= \frac{1}{2m_e{}^2c^2}\frac{1}{r}\frac{dV_c(r)}{dr}\boldsymbol{S}\cdot\boldsymbol{L} \\
&= \xi(\boldsymbol{S}\cdot\boldsymbol{L})
\end{aligned}
$$

where the factor 1/2 is the Thomas correction and the Bohr magneton μ_B is given by

$$\mu_B = \frac{e\hbar}{2m_e c}.$$

Thomas factor 1/2, which represents an additional relativistic effect due to the acceleration of the electron. The electron spin, magnetic moment, and spin-orbit interaction can be derived directly from the Dirac relativistic electron theory. The Thomas factor is built in the expression.

$$H_{so} = \xi\boldsymbol{S}\cdot\boldsymbol{L},$$

with

$$\xi = \left\langle \frac{1}{2m_e{}^2c^2}\frac{1}{r}\frac{dV_c(r)}{dr}\right\rangle = \frac{1}{2}\left(\frac{e}{m_e c}\right)^2\left\langle\frac{1}{r^3}\right\rangle_{av}.$$

When we use the formula

$$\left\langle r^{-3}\right\rangle = \frac{1}{n^3 a_B{}^3 l(l+1/2)(l+1)},$$

the spin-orbit interaction constant ξ is described by

$$\xi = \frac{e^2}{2m_e{}^2c^2n^3a_B{}^3l(l+1/2)(l+1)} = \frac{m_e e^8}{2c^2n^3\hbar^6 l(l+1/2)(l+1)}$$

where

$$a_B = \frac{\hbar^2}{m_e e^2} = 0.53 \text{ Å} \qquad \text{(Bohr radius).}$$

The energy level (negative) is given by

$$\left|E_n\right| = \frac{e^2}{2n^2a_B} = \frac{\Re_0}{n^2},$$

where

$$\Re_0 = \frac{m_e e^4}{2\hbar^2} = \frac{e^2}{2a_B}.$$

The ratio $\hbar^2\xi/|E_n|$ is

$$\frac{\hbar^2\xi}{|E_n|} = \frac{e^4}{c^2 n^2 \hbar^2 l(l+1/2)(l+1)} = \frac{\alpha^2}{n^2 l(l+1/2)(l+1)}$$

with

$$\alpha = \frac{e^2}{\hbar c} = \frac{1}{137.037}$$

((**Note**)) For $l = 0$ the spin-orbit interaction vanishes and therefore $\xi = 0$ in this case.

((**Summary**))

The spin-orbit interaction serves to remove the l degeneracy of the eigenenergies of hydrogen atom. If the spin-orbit interaction is neglected, energies are dependent only on n (principal quantum number). In the presence of spin-orbit interaction (n, l, s = 1/2; j, m) are good quantum numbers. Energies are dependent only on (n, l, j).