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Spin dynamics in relativistic light-matter interaction

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Relativistic spin operators

A fundamental postulate of quantum mechanics:

To every observable of a physical system a Hermitian operator is associated allowing a complete set of eigenfunctions.

⟹ What is the operator of spin?

- total relativistic angular momentum (generating element of rotations)

$$\hat{\boldsymbol{J}} = \hat{\boldsymbol{r}} \times \hat{\boldsymbol{p}} + \frac{1}{2}\boldsymbol{\Sigma}$$

  with $\hat{\boldsymbol{r}} = \boldsymbol{r}$, $\hat{\boldsymbol{p}} = -\mathrm{i}\boldsymbol{\nabla}$, the matrices $\boldsymbol{\Sigma} = (\Sigma_1, \Sigma_2, \Sigma_3)^\mathsf{T}$ and $\Sigma_i = \begin{pmatrix}\sigma_i & 0\\ 0 & \sigma_i\end{pmatrix}$

- in analogy to the nonrelativistic Pauli theory split $\hat{\boldsymbol{J}}$ into orbital angular momentum and spin angular momentum:

$$\hat{\boldsymbol{L}}_\mathrm{P} = \hat{\boldsymbol{r}} \times \hat{\boldsymbol{p}} \qquad \hat{\boldsymbol{S}}_\mathrm{P} = \boldsymbol{\Sigma}/2$$

- *problem:* $\hat{\boldsymbol{L}}_\mathrm{P}$ and $\hat{\boldsymbol{S}}_\mathrm{P}$ not conserved under free motion ⟹ unphysical results
  - Zitterbewegung (trembling motion) of spin
  - no sharp spin state in the positive-energy subspace
- *aim:* find splitting $\hat{\boldsymbol{J}} = \hat{\boldsymbol{L}} + \hat{\boldsymbol{S}}$ such that $\hat{\boldsymbol{S}}$ is a meaningful spin operator, i. e.,

$$\hat{\boldsymbol{S}} = \hat{\boldsymbol{S}}^\dagger \qquad [\hat{H}_0, \hat{\boldsymbol{S}}] = 0 \qquad \operatorname{spec}\hat{\boldsymbol{S}} = \pm\frac{1}{2} \qquad [\hat{S}_i, \hat{S}_j] = \mathrm{i}\varepsilon_{i,j,k}\hat{S}_k$$

- angular momentum algebra for $\hat{\boldsymbol{S}}$ implies

$$[\hat{L}_i, \hat{L}_j] = \mathrm{i}\varepsilon_{i,j,k}\hat{L}_k \qquad [\hat{L}_i, \hat{S}_j] = 0$$

- each splitting $\hat{\boldsymbol{J}} = \hat{\boldsymbol{L}} + \hat{\boldsymbol{S}}$ ⟹ new position operator $\hat{\boldsymbol{r}}$ via $\hat{\boldsymbol{L}} = \hat{\boldsymbol{r}} \times (-\mathrm{i}\boldsymbol{\nabla})$
- relativistic spin operators proposed by mathematical reasoning ⟹ decide on relativistic spin operator via experiment
- energy eigenstates of highly charged hydrogen-like ions as a test case for spin operators
- degenerated ground state of hydrogen-like ions: $\psi_\uparrow$, $\psi_\downarrow$

Table 1: Brief summary of in the literature proposed spin operators' definitions and their mathematical properties, adopted from [1]. The table indicates from left to right the name and the definition of the various spin operators, if they are Hermitian, if they commute with the free Dirac Hamiltonian, if eigenvalues are ±1/2, and if they obey the angular momentum algebra.

operator name	definition	$\hat{\boldsymbol{S}} = \hat{\boldsymbol{S}}^\dagger$?	$[\hat{H}_0, \hat{\boldsymbol{S}}] = 0$?	eigenval. $= \pm 1/2$?	$[\hat{S}_i, \hat{S}_j] = \mathrm{i}\varepsilon_{i,j,k}\hat{S}_k$?
Pauli	$\hat{\boldsymbol{S}}_\mathrm{P} = \frac{1}{2}\hat{\boldsymbol{\Sigma}}$	✔	–	✔	✔
Foldy-Wouthuysen	$\hat{\boldsymbol{S}}_\mathrm{FW} = \frac{1}{2}\hat{\boldsymbol{\Sigma}} + \frac{\mathrm{i}\beta}{2\hat{p}_0}\hat{\boldsymbol{p}} \times \boldsymbol{\alpha} - \frac{\hat{\boldsymbol{p}}\times(\hat{\boldsymbol{\Sigma}}\times\hat{\boldsymbol{p}})}{2\hat{p}_0(\hat{p}_0+mc)}$	✔	✔	✔	✔
Czachor	$\hat{\boldsymbol{S}}_\mathrm{Cz} = \frac{m^2c^2}{2\hat{p}_0^2}\hat{\boldsymbol{\Sigma}} + \frac{\mathrm{i}mc\beta}{2\hat{p}_0^2}\hat{\boldsymbol{p}} \times \boldsymbol{\alpha} + \frac{\hat{\boldsymbol{p}}\cdot\hat{\boldsymbol{\Sigma}}}{2\hat{p}_0^2}\hat{\boldsymbol{p}}$	✔	✔	–	–
Frenkel	$\hat{\boldsymbol{S}}_\mathrm{F} = \frac{1}{2}\hat{\boldsymbol{\Sigma}} + \frac{\mathrm{i}\beta}{2mc}\hat{\boldsymbol{p}} \times \boldsymbol{\alpha}$	✔	✔	–	–
Chakrabarti	$\hat{\boldsymbol{S}}_\mathrm{Ch} = \frac{1}{2}\hat{\boldsymbol{\Sigma}} + \frac{\mathrm{i}}{2mc}\boldsymbol{\alpha} \times \hat{\boldsymbol{p}} + \frac{\hat{\boldsymbol{p}}\times(\hat{\boldsymbol{\Sigma}}\times\hat{\boldsymbol{p}})}{2mc(mc+\hat{p}_0)}$	–	–	✔	✔
Pryce	$\hat{\boldsymbol{S}}_\mathrm{Pr} = \frac{1}{2}\beta\hat{\boldsymbol{\Sigma}} + \frac{1}{2}\hat{\boldsymbol{\Sigma}}\cdot\hat{\boldsymbol{p}}(1-\beta)\frac{\hat{\boldsymbol{p}}}{\hat{\boldsymbol{p}}^2}$	✔	✔	✔	✔
Fradkin-Good	$\hat{\boldsymbol{S}}_\mathrm{FG} = \frac{1}{2}\beta\hat{\boldsymbol{\Sigma}} + \frac{1}{2}\hat{\boldsymbol{\Sigma}}\cdot\hat{\boldsymbol{p}}\left(\frac{\hat{H}_0}{c\hat{p}_0} - \beta\right)\frac{\hat{\boldsymbol{p}}}{\hat{\boldsymbol{p}}^2}$	✔	✔	✔	–

with the Dirac matrices $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)^\mathsf{T}$ and β, speed of light c, particle mass m, $\hat{H}_0 = c\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}} + mc^2\beta$, $\hat{p}_0 = (m^2c^2 + \hat{\boldsymbol{p}}^2)^{1/2}$, see [1]

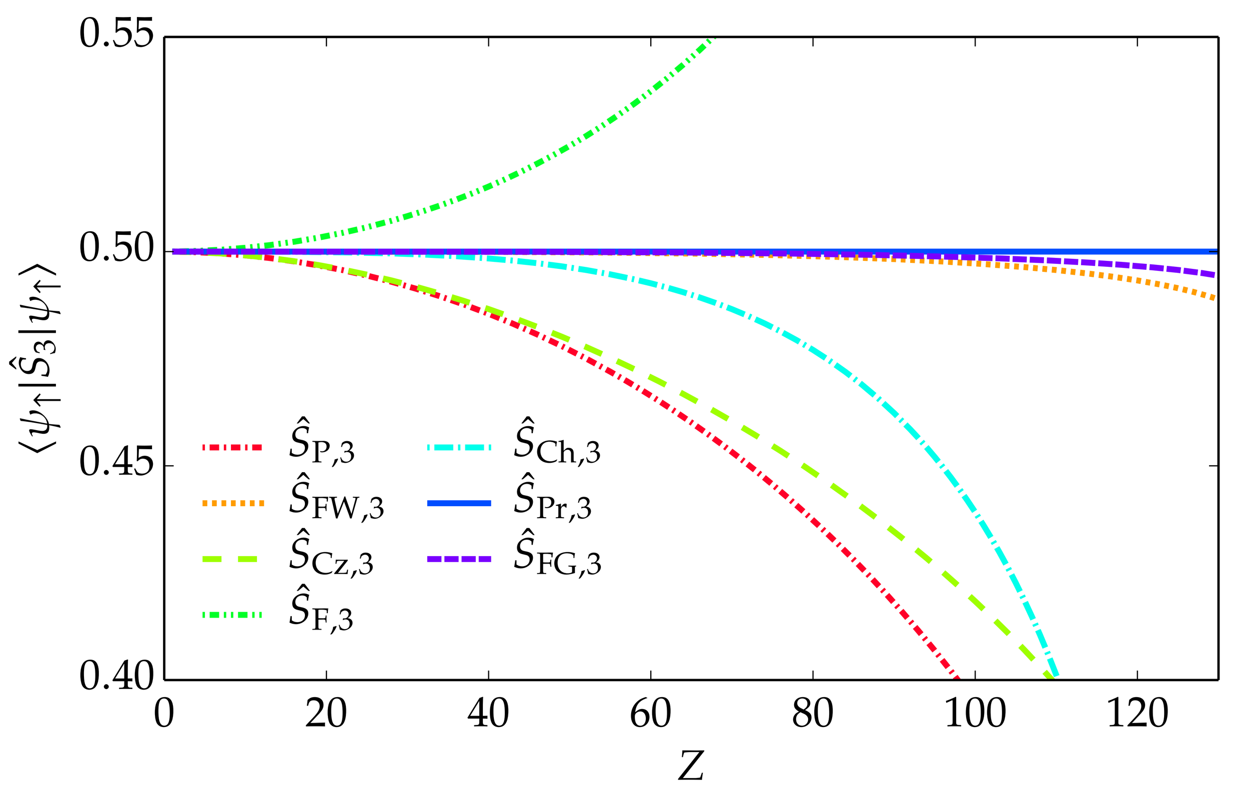

Figure 1: Spin expectation values of various relativistic spin operators for the hydrogenic ground state $\psi_\uparrow$ as a function of the atomic number Z, adopted from [2].

Coupling photonic spin to the electron spin

A fundamental property of light and matter:

Both electrons and light carry spin angular momentum.

⟹ Can electronic and photonic spin angular momentum interact?

- total spin angular momentum of light

$$\int \varepsilon_0 \boldsymbol{E}(\boldsymbol{r}, t) \times \boldsymbol{A}(\boldsymbol{r}, t)\,\mathrm{d}^3r$$

  with Coulomb gauge magnetic vector potential $\boldsymbol{A}(\boldsymbol{r}, t)$ such that

$$\boldsymbol{E}(\boldsymbol{r}, t) = -\partial_t \boldsymbol{A}(\boldsymbol{r}, t) \qquad \boldsymbol{B}(\boldsymbol{r}, t) = \boldsymbol{\nabla} \times \boldsymbol{A}(\boldsymbol{r}, t)$$

- counter-propagating laser beams with elliptical polarization

$$\boldsymbol{E}_{1,2}(\boldsymbol{r}, t) = \hat{E}\left(\cos\frac{2\pi(x \mp ct)}{\lambda}\boldsymbol{e}_y + \cos\left(\frac{2\pi(x \mp ct)}{\lambda} \pm \eta\right)\boldsymbol{e}_z\right)$$

$$\boldsymbol{B}_{1,2}(\boldsymbol{r}, t) = \frac{\hat{E}}{c}\left(\mp\cos\left(\frac{2\pi(x \mp ct)}{\lambda} \pm \eta\right)\boldsymbol{e}_y \pm \cos\frac{2\pi(x \mp ct)}{\lambda}\boldsymbol{e}_z\right)$$

- photonic spin density

$$\varrho_\sigma = \varepsilon_0 \boldsymbol{E}_{1,2} \times \boldsymbol{A}_{1,2} = \frac{\varepsilon_0 \hat{E}^2 \lambda \sin\eta}{2\pi c}\boldsymbol{e}_x$$

- expand electron's wave function into free-particle eigenstates $\psi_n^\gamma(\boldsymbol{r})$ with
  - definite momentum (multiples of photon momentum $2\pi\hbar/\lambda\boldsymbol{e}_x$) and
  - definite (Foldy-Wouthuysen) spin
  - definite energy sign

$$\Psi(\boldsymbol{r}, t) = \sum_{n,\gamma} c_n^\gamma(t)\psi_n^\gamma(\boldsymbol{r}) \qquad \text{with integer } n \text{ and } \gamma \in \{+\uparrow, -\uparrow, +\downarrow, -\downarrow\}$$

- with initial condition $c_0^{+\uparrow}(0) = 1$, $c_n^\gamma(0) = 0$ else, calculate $c_n^\gamma(t)$ via Dirac equation

$$\mathrm{i}\hbar\dot{\Psi}(\boldsymbol{r}, t) = \left(c\boldsymbol{\alpha}\cdot\left(-\mathrm{i}\hbar\boldsymbol{\nabla} - qw(t)\boldsymbol{A}(\boldsymbol{r}, t)\right) + mc^2\beta\right)\Psi(\boldsymbol{r}, t)$$

- spin expectation value precesses with angular frequency

$$\Omega = \frac{q^4\hat{E}^4\lambda^5}{(2\pi)^5\hbar^2m^2c^5}\sin\eta = \varrho_\sigma I \lambda^4 \frac{\alpha_\mathrm{el}^2}{2\pi^2m^2c^3}$$

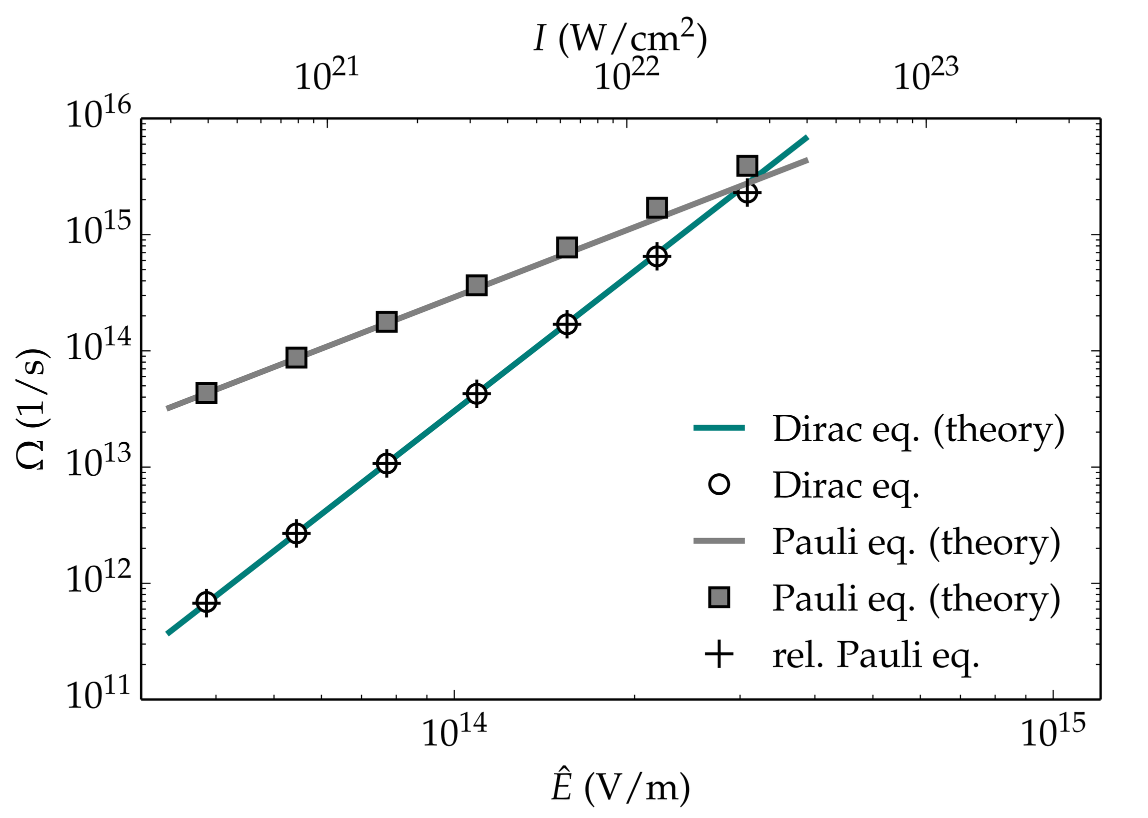

Figure 2: Angular frequency Ω of the spin precession as a function of the laser's electric field strength $\hat{E}$ and its intensity I for an electron in two counterpropagating circularly polarized light waves with wavelength $\lambda = 0.159\,\mathrm{nm}$. Depending on the applied theory the spin precession frequency scales with the second (Pauli equation) or the fourth power (Dirac equation, relativistic Pauli equation) of $\hat{E}$. Numerical data adopted from [3].

- coupling of photonic and electronic spin may becomes evident via Foldy-Wouthuysen expansion of Dirac equation leading to the relativistic Pauli equation [4]

$$\begin{aligned}\mathrm{i}\hbar\dot{\Psi}(\boldsymbol{r}, t) = \Bigg(&\frac{(-\mathrm{i}\hbar\boldsymbol{\nabla} - q\boldsymbol{A}(\boldsymbol{r}, t))^2}{2m} - \frac{q\hbar}{2m}\boldsymbol{\sigma}\cdot\boldsymbol{B}(\boldsymbol{r}, t) + q\phi(\boldsymbol{r}, t) - \frac{(-\mathrm{i}\hbar\boldsymbol{\nabla} - q\boldsymbol{A}(\boldsymbol{r}, t))^4}{8m^3c^2}\\ &- \frac{q^2\hbar^2}{8m^3c^4}(c^2\boldsymbol{B}(\boldsymbol{r}, t)^2 - \boldsymbol{E}(\boldsymbol{r}, t)^2) + \frac{q\hbar}{8m^3c^2}\left\{\boldsymbol{\sigma}\cdot\boldsymbol{B}(\boldsymbol{r}, t), (-\mathrm{i}\hbar\boldsymbol{\nabla} - q\boldsymbol{A}(\boldsymbol{r}, t))^2\right\}\\ &- \frac{q\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot\left(\boldsymbol{E}(\boldsymbol{r}, t) \times (-\mathrm{i}\hbar\boldsymbol{\nabla} - q\boldsymbol{A}(\boldsymbol{r}, t))\right) - \frac{q\hbar^2}{8m^2c^2}\boldsymbol{\nabla}\cdot\boldsymbol{E}(\boldsymbol{r}, t)\Bigg)\Psi(\boldsymbol{r}, t)\end{aligned}$$

  - Zeeman coupling and relativistic correction to Zeeman term
  - spin-orbit interaction: $\sim \boldsymbol{\sigma}\cdot\boldsymbol{E}(\boldsymbol{r}, t) \times \mathrm{i}\hbar\boldsymbol{\nabla}$
  - coupling of the photonic spin density to electron spin: $\sim \boldsymbol{\sigma}\cdot(\boldsymbol{E}(\boldsymbol{r}, t) \times \boldsymbol{A}(\boldsymbol{r}, t))$
- more complex spin dynamics may occur if electron meets Bragg condition of Kapitza Dirac scattering [5]

References

[1] H. Bauke, S. Ahrens, C. H. Keitel, R. Grobe, Relativistic spin operators in various electromagnetic environments, Phys. Rev. A 89 (2014) 052101.

[2] H. Bauke, S. Ahrens, C. H. Keitel, R. Grobe, What is the relativistic spin operator?, New J. Phys. 16 (2014) 043012.

[3] H. Bauke, S. Ahrens, C. H. Keitel, R. Grobe, Electron-spin dynamics induced by photon spins, New J. Phys. 16 (2014) 103028.

[4] H. Bauke, S. Ahrens, R. Grobe, Electron-spin dynamics in elliptically polarized light waves, Phys. Rev. A 90 (2014) 052101.

[5] S. Ahrens, H. Bauke, C. H. Keitel, C. Müller, Spin dynamics in the Kapitza-Dirac effect, Phys. Rev. Lett. 109 (2012) 043601.

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