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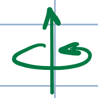
Chapter 5: Spin 1/2



→ Elementary particles can have an intrinsic angular momentum ("spin") that is not related to an internal circular motion of subparts of the elementary particle, but an intrinsic property of the particle.

<u>Example:</u> Electron, quarks, proton, neutron, ... (all belong to the particle class "spin-½ fermions")

The spin of a particle is physically like an angular momentum, i.e. it has the same dimension (unit) as angular momentum: Recall de Broglie free particle eigen function to energy $E = \frac{\vec{p}^2}{2m}$: $\psi(x) = e^{\pm i \vec{p}\vec{x}/\hbar}$

$$\Rightarrow [\vec{L}] = [\vec{x} \times \vec{p}] = [\hbar]$$

→ In a measurement of the spin of a spin-½ fermion one can only obtain the values $+\frac{\hbar}{2}$ ("spin up") or $-\frac{\hbar}{2}$ ("spin down").

→ The spin state of spin-½ particles are described by a 2-dimensional complex space as discussed in Chap. 4.4.

5.1. Spin Operators

→ The three spatial components of the 3-dimensional Spin-½ **operator** have the form:

$$\vec{S} = \begin{pmatrix} S_x \\ S_y \\ \ldots \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \ldots \end{pmatrix}$$

↳ Only possible non-trivial <u>vector operator</u> with each component

→ The three spatial components of the 3-dimensional spin-½ operator have the form:

$$\boxed{\vec{S} = \begin{pmatrix} S_x \\ S_y \\ S_z \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \end{pmatrix}}$$

↳ Only possible non-trivial <u>vector operator</u> with each component being an operator having eigenvalues $\pm\frac{\hbar}{2}$.

The operator for the measurement of the spin (projection) in spatial direction $\vec{a}$ $(|\vec{a}| = 1)$ has the form

$$\vec{a}\,\vec{S} = \frac{\hbar}{2}\sum_{k=1}^{3} a_k \sigma_k = \frac{\hbar}{2}\begin{pmatrix} a_3 & a_1 - i a_2 \\ a_1 + i a_2 & -a_3 \end{pmatrix}$$

The components of the spin-½ vector operator $\vec{S}$ do not commute with each other:

$$[S_k, S_l] = i\hbar\, \epsilon_{klm} S_m \quad \Rightarrow \quad \boxed{\text{A state can be eigenstate of at most one of the } S_i \ (i=1,2,3).}$$

→ Examples for pure spin-½ eigenstates (complete list): → $\boxed{S_i \ (i=1,2,3) \text{ has only eigenvalues } \pm\frac{\hbar}{2}.}$

* **<u>Spin in z direction</u>:** $\vec{e}_z \vec{S} = S_z = \frac{\hbar}{2}\sigma_3 = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

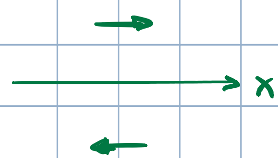
spin-up: eigenstate in z direction → $S_z \chi_{z,+} = +\frac{\hbar}{2}\chi_{z,+}$, $\chi_{z,+} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

spin-down: eigenstate in −z direction → $S_z \chi_{z,-} = -\frac{\hbar}{2}\chi_{z,-}$, $\chi_{z,-} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

* **<u>Spin in x direction</u>:** $\vec{e}_x \vec{S} = S_x = \frac{\hbar}{2}\sigma_1 = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

spin-up: $S_x \chi_{x,+} = +\frac{\hbar}{2}\chi_{x,+}$, $\chi_{x,+} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$

spin-down: $S_x \chi_{x,-} = -\frac{\hbar}{2}\chi_{x,-}$, $\chi_{x,-} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$



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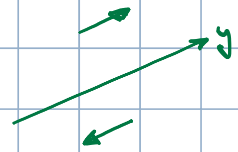
* **Spin in y direction:** $\vec{e}_y \vec{S} = S_y = \frac{\hbar}{2}\sigma_2 = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$



spin-up: $S_y \chi_{y,+} = +\frac{\hbar}{2}\chi_{y,+}\,,\quad \chi_{y,+} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}$

spin-down: $S_y \chi_{y,-} = -\frac{\hbar}{2}\chi_{y,-}\,,\quad \chi_{y,-} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$

* **Spin in $\vec{n}$ direction:** $\vec{n}\vec{S} = n_x S_x + n_y S_y + n_z S_z = \frac{\hbar}{2}\begin{pmatrix} n_3 & n_1 - i n_2 \\ n_1 + i n_2 & -n_3 \end{pmatrix}$

with solid angle in spherical angular coordinates $\vec{n} = \begin{pmatrix} n_1 \\ n_2 \\ n_3 \end{pmatrix} = \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix}\,,\quad |\vec{n}| = 1$

spin-up: $\vec{n}\vec{S}\,\chi_{\vec{n},+} = +\frac{\hbar}{2}\chi_{\vec{n},+}\,,\quad \chi_{\vec{n},+} = \begin{cases} \frac{1}{\sqrt{2(1+n_3)}}\begin{pmatrix} 1+n_3 \\ n_1 + i n_2 \end{pmatrix}\,, & n_3 \neq -1 \\ \begin{pmatrix} 0 \\ 1 \end{pmatrix}\,, & n_3 = -1 \end{cases}$
(in $\vec{n}$ direction)

$\vec{n} \to -\vec{n}$

spin-down: $\vec{n}\vec{S}\,\chi_{\vec{n},-} = -\frac{\hbar}{2}\chi_{\vec{n},-}\,,\quad \chi_{\vec{n},-} = \begin{cases} \frac{1}{\sqrt{2(1-n_3)}}\begin{pmatrix} 1-n_3 \\ -n_1 - i n_2 \end{pmatrix}\,, & n_3 \neq 1 \\ \begin{pmatrix} 1 \\ 0 \end{pmatrix}\,, & n_3 = 1 \end{cases}$
(in $-\vec{n}$ direction)

> We call $\chi_{\vec{n},\pm}$ the "spin-$\frac{1}{2}$ state with the spin pointing into the $\pm\vec{n}$ direction."

→ Corresponding density matrix (pure spin-$\frac{1}{2}$ state)

spin-up ($\vec{n}$ direction): $\rho_{\vec{n},+} = \frac{1}{2}\begin{pmatrix} 1+n_3 & n_1 - i n_2 \\ n_1 + i n_2 & 1 - n_3 \end{pmatrix} = \frac{1}{2}\left(\mathbb{1} + \vec{n}\vec{\sigma}\right) = \chi_{\vec{n},+}\chi_{\vec{n},+}^{\dagger}$

spin-up ($\vec{n}$ direction): $\rho_{\vec{n},+} = \frac{1}{2}\begin{pmatrix} 1+n_3 & n_1-in_2 \\ n_1+in_2 & 1-n_3 \end{pmatrix} = \frac{1}{2}(\mathbb{1}+\vec{n}\vec{\sigma}) = \chi_{\vec{n},+}\chi_{\vec{n},+}^{+}$

spin-down ($-\vec{n}$ direction): $\rho_{\vec{n},-} = \frac{1}{2}\begin{pmatrix} 1-n_3 & -n_1+in_2 \\ -n_1-in_2 & 1+n_3 \end{pmatrix} = \frac{1}{2}(\mathbb{1}-\vec{n}\vec{\sigma}) = \chi_{\vec{n},-}\chi_{\vec{n},-}^{+}$

$\hookrightarrow$ check: $(\vec{a}\vec{\sigma})(\vec{b}\vec{\sigma}) = (\vec{a}\vec{b})\mathbb{1} + i(\vec{a}\times\vec{b})\vec{\sigma}$ $\quad (\sigma_k\sigma_l = \delta_{kl}\mathbb{1} + i\epsilon_{klm}\sigma_m)$

$$\Rightarrow (\vec{n}\vec{\sigma})^2 = |\vec{n}|^2\mathbb{1} = \mathbb{1}$$

$$\Rightarrow \vec{n}\vec{S}\rho_{\vec{n}\pm} = \frac{\hbar}{2}\vec{n}\vec{\sigma}\,\frac{1}{2}(\mathbb{1}\pm\vec{n}\vec{\sigma}) = \frac{\hbar}{2}\,\frac{1}{2}(\vec{n}\vec{\sigma}\pm\overbrace{(\vec{n}\vec{\sigma})^2}^{=1}) = \pm\frac{\hbar}{2}\rho_{\vec{n}\pm} \quad ✓$$

→ **Density matrix (mixed spin-½ state): polarized states**

We can construct a mixed state that is with probability p_+ in $\vec{n}$ direction (spin-up) and with probability p_- in $-\vec{n}$ direction (spin-down), where $p_+ + p_- = 1$. Such a spin state is called **p_+-polarized in the $\vec{n}$ direction.**

$$\hookrightarrow \rho_{p\pm} = p_+\rho_{\vec{n},+} + p_-\rho_{\vec{n},-} = \frac{1}{2}(\mathbb{1} + \underbrace{(p_+-p_-)\vec{n}}_{=:\vec{n}'}\vec{\sigma})$$

$$= \frac{1}{2}(\mathbb{1} + \vec{n}'\vec{\sigma}) \qquad \text{with } |\vec{n}'| = |p_+-p_-| < 1$$

$\frac{\vec{n}'}{|\vec{n}'|}$: direction $\qquad\qquad |\vec{n}'| \leq 1$: degree of polarization

$$\boxed{\begin{array}{l}\text{An unpolarized spin state is one where } p_+ = p_- = 0.5 = 50\%. \Rightarrow \rho = \frac{1}{2}\mathbb{1} \\ \text{A spin state that is unpolarized in the } \vec{n} \text{ direction, is also unpolarized in any direction}\end{array}}$$

→ Measurement of the spin in $\vec{a}$-direction for spin state with $\rho_{\vec{n}} = \frac{1}{2}(\mathbb{1} + \vec{n}\vec{\sigma})$, $|\vec{n}| \leq 1$

We calculate the expectation values involving the following operators:

$A = \vec{a}\vec{S} = \frac{\hbar}{2}\vec{a}\vec{\sigma}$, $|\vec{a}| = 1$: Spin in the $\vec{a}$ direction

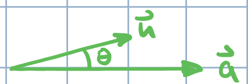
$A^2 = \frac{\hbar^2}{4}\mathbb{1}$: Modulus square of spin in $\vec{a}$ direction

$P_\pm = \frac{1}{2}(\mathbb{1} \pm \vec{a}\vec{\sigma})$: Projector on the eigenstates with eigenvalues $\pm\frac{\hbar}{2}$ (spin is in direction $\pm\vec{a}$)
Measurement: Does spin point in direction $\pm\vec{a}$ (Yes/No ?)

$\vec{S}^2 = S_x^2 + S_y^2 + S_z^2 = 3A^2 = \frac{3}{4}\hbar^2\mathbb{1}$: Total spin squared

↳ $\langle A \rangle = \mathrm{Tr}[\rho_{\vec{n}} A] = \mathrm{Tr}\left[\frac{\hbar}{4}\cancel{\vec{a}\vec{\sigma}} + \frac{\hbar}{4}(\vec{n}\vec{\sigma})(\vec{a}\vec{\sigma})\right] = \mathrm{Tr}\left[\frac{\hbar}{4}\vec{a}\vec{n}\cdot\mathbb{1}\right]$ $\quad \mathrm{Tr}[\mathbb{1}] = 2$

$= \frac{\hbar}{2}\vec{a}\vec{n} = \frac{\hbar}{2}|\vec{n}|\cos\theta$, $0 \leq \theta \leq \pi$



$\Rightarrow \langle \vec{S} \rangle = \frac{\hbar}{2}\vec{n} = \frac{\hbar}{2}\begin{pmatrix} n_1 \\ n_2 \\ n_3 \end{pmatrix}$

Result as expected.

We check: Assume pure spin-$\frac{1}{2}$ state in z-direction: $\chi_{z+} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $\quad (\vec{n} = (0,0,1))$

Eigenstate to A with eigenvalue $\pm\frac{\hbar}{2}$: $\chi_{\vec{a}\pm} = \frac{1}{\sqrt{2(1\pm a_3)}}\begin{pmatrix} 1 \pm a_3 \\ \pm a_1 \pm i a_2 \end{pmatrix}$ $\quad \vec{a} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix}$

Probability to measure $\pm\frac{\hbar}{2}$: $|\chi_{\vec{a}\pm}^\dagger \chi_{z+}|^2 = \frac{1}{2}(1 \pm \cos\theta)$

$\Rightarrow \langle A \rangle = +\frac{\hbar}{2}\frac{1}{2}(1+\cos\theta) - \frac{\hbar}{2}\frac{1}{2}(1-\cos\theta) = \frac{\hbar}{2}\cos\theta$

Probability to measure $\pm\frac{\hbar}{2}$: $|\chi_{\vec a\pm}^\dagger \chi_{z+}|^2 = \frac{1}{2}(1 \pm \cos\theta)$

$$\Rightarrow \langle A\rangle = +\frac{\hbar}{2}\,\frac{1}{2}(1+\cos\theta) - \frac{\hbar}{2}\,\frac{1}{2}(1-\cos\theta) = \frac{\hbar}{2}\cos\theta \checkmark$$

$$\langle A^2\rangle = \mathrm{Tr}\left[\rho_{\vec u} A^2\right] = \frac{\hbar^2}{4}\mathrm{Tr}\left[\rho_{\vec u}\right] = \frac{\hbar^2}{4} \neq \langle A\rangle^2 \qquad (\text{except for } \vec u = \vec a)$$

$$\langle \vec S^2\rangle = \frac{3}{4}\hbar^2 = s(s+1)\hbar^2 \quad \text{for } s = \frac{1}{2}$$

$$(\Delta A)^2 = \langle A^2\rangle - \langle A\rangle^2 = \frac{\hbar^2}{4}\left(1 - |\vec u|^2\cos^2\theta\right) \Rightarrow \Delta A = \frac{\hbar}{2}\sqrt{1-|\vec u|^2\cos^2\theta}$$

$$\rightarrow \Delta\vec S = \begin{pmatrix}\Delta S_x\\ \Delta S_y\\ \Delta S_z\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}\sqrt{1-u_x^2}\\ \sqrt{1-u_y^2}\\ \sqrt{1-u_z^2}\end{pmatrix}$$

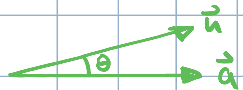
$$\langle P_\pm\rangle = \mathrm{Tr}\left[\rho_{\vec u} P_\pm\right] = \mathrm{Tr}\left[\frac{1}{2}(\mathbb{1}+\vec u\vec\sigma)\frac{1}{2}(\mathbb{1}\pm\vec a\vec\sigma)\right] = \mathrm{Tr}\left[\frac{1}{4}\mathbb{1} \pm \frac{1}{4}(\vec u\vec\sigma)(\vec a\vec\sigma)\right]$$

$$= \frac{1}{2}(1 \pm \vec a\vec u) = \frac{1}{2}(1 \pm |\vec u|\cos\theta) \qquad (P_\pm : 1 \text{ for } \vec u = \pm\vec a,\ 0 \text{ for } \vec u = \mp\vec a)$$

$\langle P_+\rangle + \langle P_-\rangle = 1$ ok! ✓

$$(\Delta P_\pm)^2 = \langle P_\pm^2\rangle - \langle P_\pm\rangle^2 = \langle P_\pm\rangle - \langle P_\pm\rangle^2 = \frac{1}{4}\left(1-|\vec u|^2\cos^2\theta\right) \Rightarrow \Delta P_\pm = \frac{1}{2}\sqrt{1-|\vec u|^2\cos^2\theta}$$

Special case : $|\vec u| = 1$ (pure state)



$$\langle A\rangle = \frac{\hbar}{2}\cos\theta \qquad \Delta A = \frac{\hbar}{2}\sin\theta$$

$$\langle\vec S\rangle = \begin{pmatrix}\langle S_x\rangle\\ \langle S_y\rangle\\ \langle S_z\rangle\end{pmatrix} = \frac{\hbar}{2}\vec u \qquad \Delta\vec S = \begin{pmatrix}\Delta S_x\\ \Delta S_y\\ \Delta S_z\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}\sqrt{1-u_x^2}\\ \sqrt{1-u_y^2}\\ \sqrt{1-u_z^2}\end{pmatrix}$$

$$\langle P_+\rangle = \frac{1}{2}(1+\cos\theta) = \cos^2\frac{\theta}{2} \qquad \langle P_-\rangle = \frac{1}{2}(1-\cos\theta) = \sin^2\frac{\theta}{2} \rightarrow \langle P_+\rangle + \langle P_-\rangle = 1$$

$$\Delta P_\pm = \frac{1}{2}\sin\theta$$

$\vec u = (0,0,1)$: $\langle\vec S\rangle = \frac{\hbar}{2}\begin{pmatrix}0\\0\\1\end{pmatrix}$, $\Delta\vec S = \frac{\hbar}{2}\begin{pmatrix}1\\1\\0\end{pmatrix}\Big\}$ maximal

Special case $\vec u = 0$ (unpolarized mixed state) → 50% up ⊕ 50% down

$\langle A\rangle = 0$, $\Delta A = \frac{\hbar}{2}$, $\langle P_\pm\rangle = \frac{1}{2}$, $\Delta P_\pm = \frac{1}{2}$, $\langle\vec S\rangle = \begin{pmatrix}0\\0\\0\end{pmatrix}$, $\Delta\vec S = \frac{\hbar}{2}\begin{pmatrix}1\\1\\1\end{pmatrix}\Big\}$ maximal

→ Characterization (naming) of spin-$\frac{1}{2}$ states

We want to uniquely name all spin states by their eigenvalues with respect to a minimal set of observables. In general, more than one observables are necessary due to the possibility of degenerate eigenvalues.

The set of quantum numbers that uniquely characterize a state are called "**quantum numbers**".

Due to the generalized uncertainty relation the observables used for naming must all commute with each other, because only then there exists a complete set of states (CONS) that consist of eigenstates to all of these observables.

Basis of the proof:

A, B observables with $[A, B] = 0$

Let $\{\phi_i\}$ be CONS of eigenstates to A : $A\phi_n = a_n \phi_n$ ($a_n \in \mathbb{R}$).

Let $\{\phi_i\}_{a_n}$ be a CONS of the eigenspace to eigenvalue $a_n \neq 0$

Take $\phi \in \{\phi_i\}_{a_n}$: $a_n B\phi = BA\phi = AB\phi$

↳ $B\phi$ is also $\in \{\phi_i\}_{a_n}$

↳ We can find a CONS of subspace $\{\phi_i\}_{a_n}$ made of eigenstates to B

⇒ **It is possible to construct a CONS of eigenstates to A and B.**

↳ One can go on the same way adding more observables that commute with all previous observables until each eigenstate of the resulting CONS can be uniquely identified by the eigenvalues of the commuting set of observables.

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> For spin-$\frac{1}{2}$ states the observables for uniquely characterizing a CONS are $\vec{S}^2$ and $\vec{a}\vec{S}$ (most frequently used is $\vec{a}=(0,0,1)$ with $\vec{a}\vec{S}=S_z$).

↳ Eigenstates : e.g. $|s,s_z\rangle$ with $s=\frac{1}{2}$ (for "spin-$\frac{1}{2}$" state) and $s_z=\pm\frac{1}{2}$ (for "spin up/down")

$$\left.\begin{aligned} \vec{S}^2|s,s_z\rangle &= \hbar^2 s(s+1)|s,s_z\rangle \\ S_z|s,s_z\rangle &= \hbar s_z|s,s_z\rangle \end{aligned}\right\} \quad \text{CONS}: \left\{|\tfrac{1}{2},+\tfrac{1}{2}\rangle, |\tfrac{1}{2},-\tfrac{1}{2}\rangle\right\}$$

In the context of problems where it is obvious that we only deal with $s=\frac{1}{2}$ particles we can also drop the s quantum number.

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5.2. Spatial Rotations

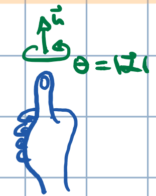
→ Recall: Spatial translations $\psi(\vec{x}) \to \psi(\vec{x}-\vec{a}) = \psi(\vec{x}) - \vec{a}\vec{\nabla}\,\psi(\vec{x}) + \frac{1}{2!}(\vec{a}\vec{\nabla})^2\psi(\vec{x}) + \dots$

Spatial translations are generated by the momentum operator $\vec{P}$.
Translation operator : $T_a = \exp(-i\vec{a}\vec{P}/\hbar) = \exp(-\vec{a}\vec{\nabla}) = 1 - \vec{a}\vec{\nabla} + \frac{1}{2}(\vec{a}\vec{\nabla})^2 - \dots$

→ The logical generalization to rotations is that they are generated by the angular momentum operator, which is the spin operator $\vec{S}$ for spin-$\frac{1}{2}$ states.

$$\boxed{\text{Spin-}\tfrac{1}{2}\text{ rotation operator}: \quad U(\vec{\alpha}) = \exp(-i\vec{\alpha}\vec{S}/\hbar) = \exp(-i\vec{\alpha}\vec{\sigma}/2), \quad \vec{\alpha} \in \mathbb{R}^3}$$

↳ $U(\vec{\alpha})$ generates an active rotation of a spin-$\frac{1}{2}$ state around the axis $\vec{n} = \frac{\vec{\alpha}}{|\vec{\alpha}|}$ by the angle $|\vec{\alpha}|$ in mathematically positive direction :



"right-handed rotation"
$\hat{=}$ mathematically positive

$$|\psi\rangle \leftrightarrow \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} : \quad \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \to U(\vec{\alpha})\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

↳ $U(\vec{\alpha})$ can be written in terms of $\mathbb{1}$ and the $\sigma_{1,2,3}$:
use $(\vec{\alpha}\vec{\sigma})^2 = |\vec{\alpha}|^2\,\mathbb{1}$

$$\Rightarrow (\vec{\alpha}\vec{\sigma})^{2n} = |\vec{\alpha}|^{2n}\,\mathbb{1}, \quad (\vec{\alpha}\vec{\sigma})^{2n+1} = |\vec{\alpha}|^{2n+1}\left(\frac{\vec{\alpha}\vec{\sigma}}{|\vec{\alpha}|}\right) \quad \text{for } n \in \mathbb{N}_0$$

$$\Rightarrow U(\vec{\alpha}) = \exp(-i\vec{\alpha}\vec{\sigma}/2) = \sum_{k=0}^{\infty} (-i)^k \frac{1}{k!}(\vec{\alpha}\vec{\sigma}/2)^k$$

$$\Rightarrow \quad U(\vec{\alpha}) = \exp(-i\vec{\alpha}\vec{\sigma}/2) = \sum_{k=0}^{\infty} (-i)^k \frac{1}{k!} (\vec{\alpha}\vec{\sigma}/2)^k$$

$$= \sum_{n=0}^{\infty} (-i)^{2n} \frac{1}{(2n)!} \left(\frac{|\vec{\alpha}|}{2}\right)^{2n} \mathbb{1} + \sum_{n=0}^{\infty} (-i)^{2n+1} \frac{1}{(2n+1)!} \left(\frac{|\vec{\alpha}|}{2}\right)^{2n+1} \left(\frac{\vec{\alpha}\vec{\sigma}}{|\vec{\alpha}|}\right)$$

$$= \underbrace{\sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} \left(\frac{|\vec{\alpha}|}{2}\right)^{2n}}_{=\cos(|\vec{\alpha}|/2)} \mathbb{1} - i \underbrace{\sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} \left(\frac{|\vec{\alpha}|}{2}\right)^{2n+1}}_{=\sin(|\vec{\alpha}|/2)} \left(\frac{\vec{\alpha}\vec{\sigma}}{|\vec{\alpha}|}\right)$$

$$\boxed{\text{Alternative form: } U(\vec{\alpha}) = \cos\left(\frac{|\vec{\alpha}|}{2}\right) \mathbb{1} - i \sin\left(\frac{|\vec{\alpha}|}{2}\right) \frac{\vec{\alpha}\vec{\sigma}}{|\vec{\alpha}|}}$$

↳ Very peculiar: $U(2\pi \vec{n}) = -\mathbb{1} = e^{i\pi}$ ← unit vector , $U(4\pi\vec{n}) = +\mathbb{1}$

A rotation by 2π ($=360°$) transforms a spin-$\frac{1}{2}$ state into (-1) times that state, both of which are, however, physically equivalent. Only a rotation by 4π transforms back to exactly the same state.

→ We want to cross check that $U(\vec{\alpha})$ really rotates a spin-$\frac{1}{2}$ state by angle $|\vec{\alpha}|$ around the axis $\vec{n} = \frac{\vec{\alpha}}{|\vec{\alpha}|}$.
Consider a spin-$\frac{1}{2}$ state represented by the density matrix $\quad \rho_{\vec{n}} = \frac{1}{2}(\mathbb{1} + \vec{n}\vec{\sigma})$ ← direction of spin
and a rotation around z-axis by angle θ $\quad U(\theta\hat{e}_z) = \cos(\frac{\theta}{2})\mathbb{1} - i\sin(\frac{\theta}{2})\sigma_3$

Rotation: $\rho_{\vec{n}} \to U(\theta\hat{e}_z)\,\rho_{\vec{n}}\,U^{+}(\theta\hat{e}_z)$

$$= \frac{1}{2}\mathbb{1} + U(\theta\hat{e}_z)(\vec{n}\vec{\sigma})U(-\theta\hat{e}_z) = \frac{1}{2}(\mathbb{1} + \vec{n}'\vec{\sigma}) =: \rho_{\vec{n}'}$$ → What is $\vec{n}'$?

We have: $U(\theta\hat{e}_z)(\vec{n}\vec{\sigma})U(-\theta\hat{e}_z) = \left(\cos(\tfrac{\theta}{2})\mathbb{1} - i\sin(\tfrac{\theta}{2})\sigma_3\right)\left(n_1\sigma_1 + n_2\sigma_2 + n_3\sigma_3\right)\left(\cos(\tfrac{\theta}{2})\mathbb{1} + i\sin(\tfrac{\theta}{2})\sigma_3\right)$

$$= (\vec{n}\vec{\sigma})\cos^2(\tfrac{\theta}{2}) - i\underbrace{\sigma_3(\vec{n}\vec{\sigma})}_{i\sigma_2 n_1 - i\sigma_1 n_2 + n_3\mathbb{1}}\sin(\tfrac{\theta}{2})\cos(\tfrac{\theta}{2}) + i\underbrace{(\vec{n}\vec{\sigma})\sigma_3}_{-i\sigma_2 n_1 + i\sigma_1 n_2 + n_3\mathbb{1}}\sin(\tfrac{\theta}{2})\cos(\tfrac{\theta}{2}) + \sin^2(\tfrac{\theta}{2})\underbrace{\sigma_3(\vec{n}\vec{\sigma})\sigma_3}_{-\sigma_1 n_1 - \sigma_2 n_2 + n_3\sigma_3}$$

use:
$\cos(2x) = \cos^2 x - \sin^2 x$
$\sin(2x) = 2\cos x \sin x$

(use: $\sigma_i^2 = \mathbb{1}$ (no sum) $\quad \sigma_i\sigma_j = i\epsilon_{ijm}\sigma_m \quad (i \neq j)$)

$$= \sigma_1(n_1\cos\theta - n_2\sin\theta) + \sigma_2(n_1\sin\theta + n_2\cos\theta) + \sigma_3 n_3$$

$$= \vec{n}'\vec{\sigma} \quad \text{with} \quad \vec{n}' = R(\theta\hat{e}_z)\vec{n}, \quad R(\theta\hat{e}_z) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$ spatial rotation matrix

So $\vec{n}'$ is obtained from rotation of $\vec{n}$ around $\hat{e}_z$ by angle $+\theta$.

To get the same result for $\langle\vec{a}'\vec{S}\rangle_{\vec{n}'}$ as for $\langle\vec{a}\vec{S}\rangle_{\vec{n}}$ (which is a function of $\vec{a}\vec{n}$) $\vec{a}'$ has to be obtained by rotation of $\vec{a}$ around $\hat{e}_z$ by angle $+\theta$. So $\vec{a}\vec{n} = \vec{a}'\vec{n}'$ for $\vec{a}' = R(\theta\hat{e}_z)\vec{a}$

$\Rightarrow$ **$U(\vec{\alpha})$ indeed rotates the physically observable spin around axis $\frac{\vec{\alpha}}{|\vec{\alpha}|}$ by the angle $|\vec{\alpha}|$.** ✓

→ Infinitesimal Rotations

One can construct a finite rotation $U(\vec{\alpha})$ from N ($\in \mathbb{N}$) successive rotations with angle $\theta = \frac{|\vec{\alpha}|}{N}$.

$$U(\vec{\alpha}) = U\left(\frac{\vec{\alpha}}{N}\right)^N$$

One can construct a finite rotation $U(\vec{\alpha})$ from N $(\in \mathbb{N})$ successive rotations with angle $\theta = \frac{\alpha}{N}$.

$$U(\vec{\alpha}) = U\left(\frac{\vec{\alpha}}{N}\right)^N$$

For $N \to \infty$ one the has : $U(\vec{\alpha}) = \exp(-i\vec{\alpha}\vec{\sigma}/2) = \lim_{N\to\infty} \Big(\underbrace{\mathbb{1} - i\frac{\vec{\alpha}}{N}\frac{\vec{S}}{\hbar}}_{\mathbb{1} - i\vec{\varepsilon}\vec{S}/\hbar}\Big)^N$

$\mathbb{1} - i\vec{\varepsilon}\vec{S}/\hbar \longrightarrow$ "infinitesimal rotation" by angle $\theta = |\vec{\varepsilon}| \ll 1$

Note that $\lim_{n\to\infty} \left(1 - \frac{a}{n} + \frac{b}{n^2}\right)^n = e^{-a}$ (!)

$\vec{S}$ "generates" rotations

$\Rightarrow$ Infinitesimal rotations already contain all relevant structural information on the complete set of finite rotations. The properties of the "generators" $\vec{S} = (S_x, S_y, S_z)$ fully determine the group structure of the rotations.

↳ Explicit form of infinitesimal rotation : → We calculate spin rotation for small angle $\theta \ll 1$.

(1) $\vec{n} \to R(\theta\vec{e}_z)\vec{n} = (n_1\cos\theta - n_2\sin\theta,\ n_1\sin\theta + n_2\cos\theta,\ n_3)$ expand linear in θ

$\approx (n_1 - n_2\theta,\ n_1\theta + n_2,\ n_3) = \vec{n} + \theta(-n_2, n_1, 0)$

$= \vec{n} + \theta\,\vec{e}_z \times \vec{n}$

(2) $U(\theta\hat{e}_z)(\vec{n}\vec{\sigma})U(-\theta\hat{e}_z) = \left(\mathbb{1} - i\frac{\theta}{2}\sigma_3\right)(n_1\sigma_1 + n_2\sigma_2 + n_3\sigma_3)\left(\mathbb{1} + i\frac{\theta}{2}\sigma_3\right)$ expand linear in θ

$= \vec{n}\vec{\sigma} + \frac{\theta}{2}(n_1\sigma_2 - n_2\sigma_1 - in_3\mathbb{1}) - \frac{\theta}{2}(-n_1\sigma_2 + n_2\sigma_1 - in_3\mathbb{1})$

$= \vec{n}\vec{\sigma} + \theta(-n_2\sigma_1 + n_1\sigma_2)$

$= (\vec{n} + \theta\,\vec{e}_z \times \vec{n})\,\vec{\sigma}$ ✓

Rotation of a spatial vector $\vec{n}$ by infinitesimal angle $\theta = |\vec{\varepsilon}|$ around axis $\frac{\vec{\varepsilon}}{|\vec{\varepsilon}|}$:

$\vec{n} \longrightarrow \vec{n} + \vec{\varepsilon} \times \vec{n}$, $n_i \longrightarrow n_i + \epsilon_{ilk}\,\varepsilon_l\, n_k$

→ **Group Theory for Rotations** (only some very basic aspects)

$\vec{\alpha}\vec{\sigma}$ is Hermitian $\Rightarrow$ $U(\vec{\alpha})$ are unitary

$U^+(\vec{\alpha}) = \exp(+i\,\vec{\alpha}\vec{\sigma}/2) = U(-\vec{\alpha}) \Rightarrow U^+(\vec{\alpha})U(\vec{\alpha}) = \mathbb{1}$ ✓

Eigenvalues: $\vec{\alpha}\vec{S}$ has eigenvalues $\pm|\vec{\alpha}|\frac{\hbar}{2}$ $\Rightarrow$ $U(\vec{\alpha})$ has eigenvalues $e^{\pm i|\vec{\alpha}|/2}$ $\Rightarrow$ $\mathrm{Det}(U(\vec{\alpha})) = 1$

$$\boxed{\text{The complex matrices } U(\vec{\alpha}) \text{ with } \vec{\alpha}\in\mathbb{R}^3 \text{ form the group } SU(2) \text{ with respect to matrix multiplication. } SU(2) = \text{"unitary complex } 2\times 2 \text{ matrices with determinant} = 1\text{."}}$$

The Spin-$\frac{1}{2}$ (angular momentum) operator $\vec{S} = (S_1, S_2, S_3)$ is the generator of the $SU(2)$ spin-$\frac{1}{2}$ rotation group.

The operators S_i $(i=1,2,3)$ form the basis of the "Lie-algebra" of the spin-$\frac{1}{2}$ rotation group and their commutation relations $[S_k, S_\ell] = i\hbar\,\epsilon_{k\ell m} S_m$

completely determine the general properties of the $SU(2)$ group.

<u>Comment:</u> In mathematics the generators of $SU(2)$ are usually defined by $X_k := -\frac{i}{2}\sigma_k$

with $[X_k, X_\ell] = \epsilon_{k\ell m} X_m$.

The X_k, $k=1,2,3$, form the basis of the $SU(2)$ Lie-Algebra.

The constants $\epsilon_{k\ell m}$ $(k,\ell,m = 1,2,3)$ are called structure constants of $SU(2)$. $(\underset{\text{totally antisymmetric}}{\epsilon_{123}} = +1)$

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The X_k, $k=1,2,3$, form the basis of the SU(2) Lie-Algebra.

totally antisymmetric

The constants $\epsilon_{k\ell m}$ $(k,\ell,m = 1,2,3)$ are called structure constants of SU(2). $(\epsilon_{123} = +1)$

The Lie-Algebra itself is a real vector space (real-valued linear combinations of the X_k) on which the following operations are defined:

(a) addition $(X+Y)$

(b) multiplication by a (real) scalar (aX)

(c) a product $(X \circ Y)$ which here is $X \circ Y := [X, Y]$ for which the so-called Jacobi identity is valid:

$$(X \circ Y) \circ Z + (Y \circ Z) \circ X + (Z \circ X) \circ Y = 0 \quad \rightarrow \text{Automatically satisfied for } X \circ Y = [X, Y]$$

The exponentiation of members of the Lie-Algebra gives all members of the full SU(2) group.

Therefor SU(2) is also called a Lie-Group.

5.3. Motion of a Particle with Spin in a Magnetic Field

→ The spin angular momentum of a electrically charged particle is associated with a magnetic dipole moment :

$$\vec{\mu} = \gamma \vec{S} \qquad \gamma: \text{gyromagnetic ratio} \quad \leftarrow \text{explained more in T3}$$

In a magnetic field the magnetic dipole leads to an additional contribution in the Hamilton operator of the form :

$$\delta H = -\vec{\mu}\,\vec{B}(\vec{x})$$

General form of the Hamilton operator for a particle with spin-$\frac{1}{2}$ in a potential $V(\vec{x})$ and a magnetic field $\vec{B}(\vec{x})$

$$H = \left(\frac{\vec{p}^2}{2m} + V(\vec{x})\right)\mathbb{1}_{2\times 2} - \gamma\,\vec{S}\,\vec{B}(\vec{x})$$

The spin operator $\vec{S}$ is an operator that is completely independent of the location operator $\vec{X}$ and momentum operator $\vec{P}$:

$$[\vec{S},\vec{X}] = 0 \,, \quad [\vec{S},\vec{P}] = 0 \qquad (\text{also for Heisenberg operators})$$

↦ The basis to formulate spatial wave functions can be constructed from a direct product of location eigenstates $|\vec{x}\rangle$ and spin eigenstates, e.g. with respect to the z direction, $|\pm\frac{1}{2}\rangle$:

↳ $|\vec{x},+\frac{1}{2}\rangle = |\vec{x}\rangle \otimes |\frac{1}{2}\rangle \quad , \quad |\vec{x},-\frac{1}{2}\rangle = |\vec{x}\rangle \otimes |-\frac{1}{2}\rangle$

of location eigenstates $|\vec{x}\rangle$ and spin eigenstates, e.g. with respect to the z direction, $|\pm\frac{1}{2}\rangle$:

↳ $|\vec{x},+\frac{1}{2}\rangle = |\vec{x}\rangle \otimes |\frac{1}{2}\rangle$, $|\vec{x},-\frac{1}{2}\rangle = |\vec{x}\rangle \otimes |-\frac{1}{2}\rangle$

A general state $|\psi\rangle$ of a particle with spin-$\frac{1}{2}$ can the be described by a 2-component wave function:

$$|\psi\rangle \longrightarrow \begin{pmatrix} \psi_+(\vec{x}) \\ \psi_-(\vec{x}) \end{pmatrix} = \begin{pmatrix} \langle \vec{x},+\frac{1}{2}|\psi\rangle \\ \langle \vec{x},-\frac{1}{2}|\psi\rangle \end{pmatrix}$$

Schrödinger equation: $i\hbar \frac{d}{dt}|\psi\rangle = H|\psi\rangle$

$$\hookrightarrow \quad i\hbar \frac{\partial}{\partial t}\begin{pmatrix} \psi_+(\vec{x},t) \\ \psi_-(\vec{x},t) \end{pmatrix} = \left[\left(-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{x})\right)\mathbb{1}_{2\times 2} - \frac{\gamma\hbar}{2}\vec{\sigma}\,\vec{B}(\vec{x})\right]\begin{pmatrix} \psi_+(\vec{x},t) \\ \psi_-(\vec{x},t) \end{pmatrix}$$

→ From the Heisenberg equations we can quickly learn about the new basic effects that come from the interaction of the spin with the magnetic field:

$$\dot{\vec{X}}_H(t) = \frac{i}{\hbar}[H, \vec{X}_H(t)] = \left[\frac{\vec{P}_H^2(t)}{2m}, \vec{X}_H(t)\right] = \frac{\vec{P}_H(t)}{m}$$

→ unchanged to spin-less case

$$\dot{\vec{P}}_H(t) = \frac{i}{\hbar}[H, \vec{P}_H(t)] = \frac{i}{\hbar}\left[V(\vec{X}_H(t))\,\mathbb{1}_{2\times 2} - \gamma\,\vec{S}_H(t)\,\vec{B}(\vec{X}_H(t)),\, \vec{P}_H(t)\right]$$

$$= -\vec{\nabla}V(\vec{X}_H(t)) + \gamma\,\vec{\nabla}\left(\vec{S}_H(t)\,\vec{B}(\vec{X}_H(t))\right)$$

Additional force acts on particle if the $\vec{B}$ field is inhomogeneous.

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$$\dot{\vec{S}}_H(t) = \frac{i}{\hbar}\left[H, \vec{S}_H(t)\right] = \frac{i}{\hbar}(-\gamma)\underbrace{\left[S_{k,H}(t), \vec{S}_H(t)\right] B_k(\vec{x}_H(t))}_{i\hbar\, \vec{S}\times\vec{B}(\vec{x}_H(t))}$$

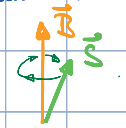
$$= \gamma\, \vec{S}_H(t)\times\vec{B}(\vec{x}_H(t))$$

$$= \vec{\mu}_H(t)\times\vec{B}(\vec{x}_H(t))$$ ← Torque force that leads to precession of spin ("Drehmoment")

$(\vec{A}\times\vec{B})_\ell = \varepsilon_{\ell k m} A_k B_m$

$\varepsilon_{\ell k m} = \varepsilon_{m \ell k}$ (cyclic permutation)

$[S_k, S_\ell] = i\hbar\, \epsilon_{k\ell m} S_m = i\hbar\, \epsilon_{\ell m k} S_m$



Note that solving the Schrödinger equation is completely equivalent to solving the problem in the Heisenberg picture. However in the Schrödinger picture it is much harder to see and identify the two new types of forces during the process of finding the energy eigenstates and eigen values.

__Comment:__

The Heisenberg equations are operator equations. Their solutions give time-dependent operators that describe how the observables (e.g. the possible measurable values, the expectation value in lots of measurements on same copies of the system). To get the time-dependent expectation value for making the measurement at a given time t one still has to calculate the average of them for the state at the initial time t_0. **In general the outcome of that might not look at all like a classical motion even though the Heisenberg equations look like the classic equations of motion.**

However, for the description of localized particles (described by localized wave packets that evolve in a localized manner in time*) the Heisenberg equations indeed describe classic behavior, up to the usual quantum mechanical issues (e.g. probability distribution in the localization measurement, broadening of wave packet, etc.).

evolve in a localized manner in time) the Heisenberg equations indeed describe classic behavior, up to the usual quantum mechanical issues (e.g. probability distribution in the localization measurement, broadening of wave packet, etc.).

* This means that the system, in which the wave packet is considered, should be such that the particle can behave essentially classically.

Example: Free particle wave packet that can traverse all space.
Counter example: Free particle in a impenetrable box (Chap. 3.1) which has similar size as the wave packet itself.

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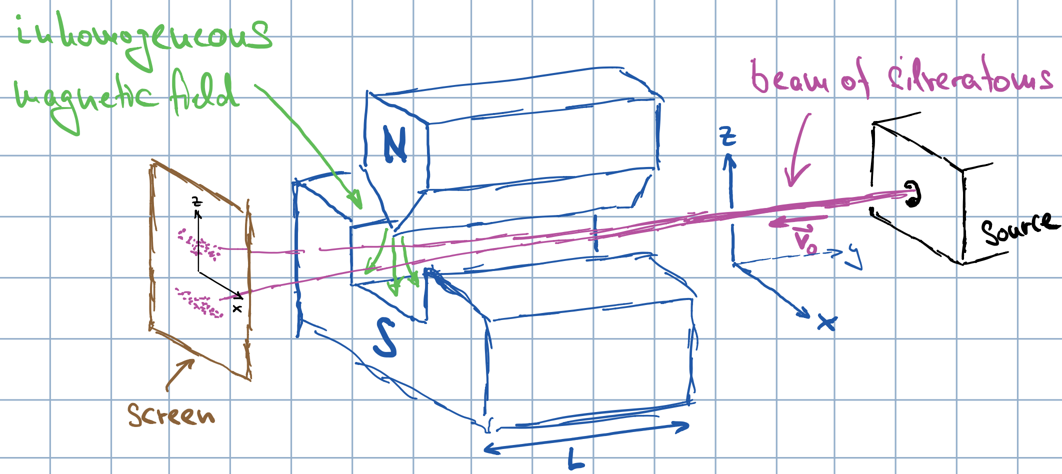
5.3. Stern - Gerlach Experiment

→ Experiment von Otto Stern und Walther Gerlach (1922) durch das die Existenz des Eigendrehimpulse (Spin) des Elektrons mit den beiden Werten $\pm \frac{\hbar}{2}$ nachgewiesen wurde.



Silver atoms have only 1 electron in the outer shell, so that they have the spin of this electron.
(Spins of all other electrons do not contribute.)

Source produces unpolarized silver atoms.

To understand quickly what is going on the Heisenberg picture is more suited than the Schrödinger picture because we have to consider a system (particles in a beam) that is classical up to the spin property.

The silver beam goes exactly along the fine blade of the north pole magnet and feels a magnetic field that has the approximate form

$$\vec{B}(\vec{x}) \approx (B_0 + a z)\,\vec{e}_z - a x\,\vec{e}_x \qquad a \ll B_0$$

Beam is located at $x \approx z \approx 0$ in the x-z plane.

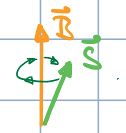
There are 2 main effects within the B-field:

Beam is located at $x = z = 0$ in the x-z plane.

There are 2 main effects within the B-field:

(a) The atoms experience a force: $\vec{F} = \vec{\nabla}(\vec{\mu}\cdot\vec{B}(\vec{x})) = a(\mu_z \vec{e}_z - \mu_x \vec{e}_x)$

(b) The spins in the atoms feel the torque caused by $\vec{B}(\vec{x})$ which, however, to a very good approximation is $\vec{B}(\vec{x}) \approx B_0 \vec{e}_z$



So the spins precess essentially around the z-axis following the equation of motion.

$$\dot{\vec{S}}(t) = \gamma \vec{S}(t) \times \vec{B} = \gamma B_0 \begin{pmatrix} S_y(t) \\ -S_x(t) \\ 0 \end{pmatrix}$$

$\hookrightarrow$ $\frac{d^2}{dt^2} S_x = \gamma B_0 \dot{S}_y = -(\gamma B_0)^2 S_x \Rightarrow$

$$\left.\begin{aligned} S_x(t) &= \cos(\omega t) S_x, \quad \omega = \gamma B_0 \\ S_y(t) &= -\sin(\omega t) S_y \end{aligned}\right\} \text{circular oszillation}$$

$S_z(t) = \text{const}$

Each silver atom feels a time-dependent force $\vec{F}(t) = a\gamma(\underbrace{S_z \vec{e}_z}_{\text{along } z \text{ axis}} - \underbrace{S_x(t)\vec{e}_x}_{\text{along } x \text{ axis}}) = \underbrace{m}_{\text{mass of silver atom}} \dot{\vec{v}}(t)$

The silver atoms have the initial velocity $\vec{v}_0 = \begin{pmatrix} 0 \\ -v \\ 0 \end{pmatrix}$ when they enter the magnet and we assume that the screen is located directly after the magnet.

$\hookrightarrow$ time each atom travels in the magnet: $\Delta t = \frac{L}{v}$, L: length of magnet

But note that Δt is not exactly the same for each silver atom because

(1) there is always some spread around some nominal value due to practical limitations,

(2) the particle wave packets broaden, so there is a quantum mechanical spread of Δt

$\rightarrow$ Typically (1) is a much larger effect, so that we can consider Δt a classic quantity with some statistical spread related to the quality of the source of the atoms.

↳ velocity as fct of time with $t_0 = 0$ being time of entrance of the atom:

$$\vec{v}(t) = \vec{v}_0 + \int_0^t dt\, \dot{\vec{v}}(t) = \vec{v}_0 + \frac{a\gamma}{m} \int_0^t dt \left(S_z \vec{e}_z - S_x(t) \vec{e}_x \right) \qquad S_x(t) = -\frac{1}{\gamma B_0} \dot{S}_y(t)$$

$$= \underbrace{\vec{v}_0 + \frac{a\gamma}{m} S_z t \vec{e}_z}_{\text{increase in z-direction}} + \underbrace{\frac{a}{m B_0} \left[S_y(t) - \overbrace{S_y(0)}^{=0} \right] \vec{e}_x}_{\text{oscillation in x-direction}} \qquad S_y(t) = \frac{1}{\gamma B} \dot{S}_x(t),$$

↳ location when silver atoms exit the magnet

$$\vec{x}(t) = \vec{x}_0 + \int_0^{\Delta t} dt\, \vec{v}(t)$$

$$= \vec{x}_0 + \vec{v}_0 \Delta t + \frac{a\gamma}{2m} (\Delta t)^2 S_z \vec{e}_z + \frac{a}{\gamma m B_0^2} \overbrace{\left(S_x(t) - S_x \right)}^{= (\cos(\omega t) - 1) S_x} \vec{e}_x$$

When the silver atom hits the screen the location measurement is carried out. The screen is located exactly at $\vec{x}_0 + \vec{v}_0 \Delta t$, so the Heisenberg operator for the measurement of the location on the screen is:

$$\vec{X}_H(\Delta t) = \frac{a\gamma}{2m} (\Delta t)^2 S_{z,H}(0) \vec{e}_z + \frac{a}{\gamma m B_0^2} (\cos(\omega \Delta t) - 1) S_{x,H}(0) \vec{e}_x \quad , \quad \Delta t : \text{distributed around } L/v$$

$$=: A(\Delta t) \vec{e}_z S_{z,S} + B(\Delta t) \vec{e}_x S_{x,S} \qquad \Delta t \gg 1/\omega$$

↑ increases like L^2 ↑ oscillates: $-\frac{2a}{\gamma m B_0^2} \le B(\Delta t) \le 0$

increases like L^2 oscillates: $-\frac{2a}{\gamma m B_0^2} \le B(\Delta t) \le 0$

The Heisenberg state is just the wave packet for the free silver atom with unpolarized spin when it enters the magnet at $t=0$:
So location measurement on the screen is just a measurement of the spin of each silver atom. (unpolarized spin $\Rightarrow \pm\frac{\hbar}{2}$ with each 50% probability for each spin component measurement)

For each silver atom we find the following outcomes:

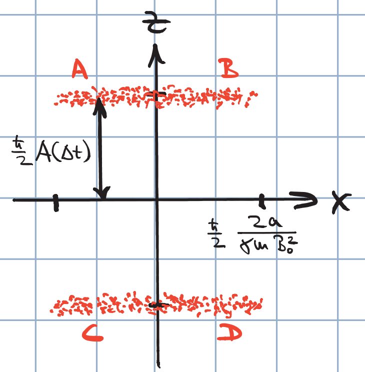
(A): $S_z = +\frac{\hbar}{2}$, $S_x = +\frac{\hbar}{2}$: 25% $\Rightarrow \tilde{x} = \left(B(\Delta t)\frac{\hbar}{2}, 0, A(\Delta t)\frac{\hbar}{2} \right)$

(B): $S_z = +\frac{\hbar}{2}$, $S_x = -\frac{\hbar}{2}$: 25% $\Rightarrow \tilde{x} = \left(-B(\Delta t)\frac{\hbar}{2}, 0, A(\Delta t)\frac{\hbar}{2} \right)$

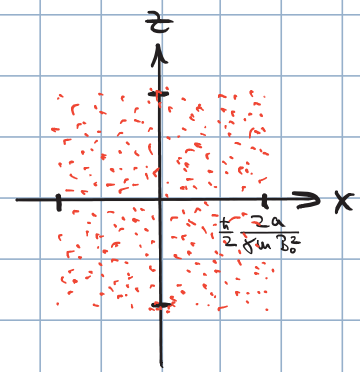
(C): $S_z = -\frac{\hbar}{2}$, $S_x = +\frac{\hbar}{2}$: 25% $\Rightarrow \tilde{x} = \left(B(\Delta t)\frac{\hbar}{2}, 0, -A(\Delta t)\frac{\hbar}{2} \right)$

(D): $S_z = -\frac{\hbar}{2}$, $S_x = -\frac{\hbar}{2}$: 25% $\Rightarrow \tilde{x} = \left(-B(\Delta t)\frac{\hbar}{2}, 0, -A(\Delta t)\frac{\hbar}{2} \right)$

Resulting hit pattern on the screen:



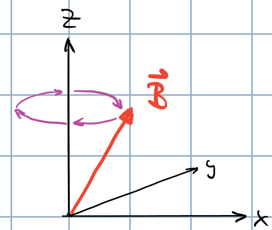
Classic expectation (assuming spin is not quantizes in $\pm\frac{\hbar}{2}$):



5.4. Rabi Spin Resonance

→ Method developed by Isidor Isaac Rabi to measure the nuclear spin.
The method is the basis of nuclear magnetic resonance (NMR) used e.g. for medical imaging.

→ The Rabi spin resonance considers spins (of atomic nuclei fixed in the molecules of some material, so that one does not have to treat any location dependence such as for the Stern-Gerlach experiment) in a **time-dependent magnetic field** of the form:



$$\vec{B}(t) = B_0 \vec{e}_z + B_\perp \left(\cos(\omega t)\, \vec{e}_x - \sin(\omega t)\, \vec{e}_y \right)$$

Hamilton operator : $H = -\gamma \vec{S}\, \vec{B}(t) \quad , \quad \vec{S} = \frac{\hbar}{2} \vec{\sigma}$

Note that in this system the Hamilton operator is time dependent, so that <u>energy is not conserved</u>. In fact, energy is exchanged between the $\vec{B}$ field and the spin.

This is an application where the Schrödinger picture is a bit more practical (also because there is no classical kind of motion to be considered here).

→ Schrödinger equation $i\hbar \dot{\psi}(t) = H(t)$ with $\psi(t) = \begin{pmatrix} a_+(t) \\ a_-(t) \end{pmatrix}$ gives

$$i\hbar \begin{pmatrix} \dot{a}_+(t) \\ \dot{a}_-(t) \end{pmatrix} = -\frac{\gamma\hbar}{2} \begin{pmatrix} B_0 & B_\perp e^{+i\omega t} \\ B_\perp e^{-i\omega t} & -B_0 \end{pmatrix} \begin{pmatrix} a_+(t) \\ a_-(t) \end{pmatrix}$$

$$i\hbar \begin{pmatrix} \dot{a}_+(t) \\ \dot{a}_-(t) \end{pmatrix} = -\frac{\gamma\hbar}{2} \begin{pmatrix} B_0 & B_1 e^{+i\omega t} \\ B_1 e^{-i\omega t} & -B_0 \end{pmatrix} \begin{pmatrix} a_+(t) \\ a_-(t) \end{pmatrix}$$

We define: $\omega_0 = \gamma B_0$, $\omega_1 = \gamma B_1$

$$\Rightarrow \quad i \begin{pmatrix} \dot{a}_+(t) \\ \dot{a}_-(t) \end{pmatrix} = -\frac{1}{2} \begin{pmatrix} \omega_0 & \omega_1 e^{+i\omega t} \\ \omega_1 e^{-i\omega t} & -\omega_0 \end{pmatrix} \begin{pmatrix} a_+(t) \\ a_-(t) \end{pmatrix}$$ $\leftarrow$ time-dependent eigenvalue problem

We define: $b_\pm(t) = e^{\mp i\omega t/2} a_\pm(t) \Leftrightarrow a_\pm(t) = e^{\pm i\omega t/2} b_\pm(t)$

OR $$\begin{pmatrix} b_+(t) \\ b_-(t) \end{pmatrix} = \begin{pmatrix} e^{-i\omega t/2} & 0 \\ 0 & e^{+i\omega t/2} \end{pmatrix} \begin{pmatrix} a_+(t) \\ a_-(t) \end{pmatrix} \Leftrightarrow \begin{pmatrix} a_+(t) \\ a_-(t) \end{pmatrix} = \begin{pmatrix} e^{+i\omega t/2} & 0 \\ 0 & e^{-i\omega t/2} \end{pmatrix} \begin{pmatrix} b_+(t) \\ b_-(t) \end{pmatrix}$$

$$\Rightarrow \quad i \begin{pmatrix} \dot{b}_+(t) \\ \dot{b}_-(t) \end{pmatrix} = -\frac{1}{2} \underbrace{\begin{pmatrix} \omega_0 - \omega & \omega_1 \\ \omega_1 & \omega - \omega_0 \end{pmatrix}}_{=:\, A} \begin{pmatrix} b_+(t) \\ b_-(t) \end{pmatrix}$$ $\leftarrow$ time-independent eigenvalue problem

$=: A$ is Hermitian $\Rightarrow$ real eigenvalues!

Eigenvalues of A: $\mathrm{Tr}[A] = 0 \Rightarrow A$ has eigen values $\pm\Omega$ with $\Omega \geq 0$
$\mathrm{Det}(A) = -\Omega^2 = -(\omega-\omega_0)^2 - \omega_1^2$

$$\Rightarrow \quad \Omega = \sqrt{(\omega-\omega_0)^2 + \omega_1^2}$$

Spectral representation of matrix A: $A = \Omega\,(P_+ - P_-)$, $P_\pm$: projector on eigenspace to eigenvalue $\pm\Omega$

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Function of matrix A: use $P_+ + P_- = \mathbb{1}$

$$f(A) = f(\Omega)P_+ + f(-\Omega)P_- = \frac{1}{2}f(\Omega)\left(P_+ + \mathbb{1} - P_-\right) + \frac{1}{2}f(-\Omega)\left(P_- + \mathbb{1} - P_+\right)$$

$$= \frac{1}{2}\left(f(\Omega)+f(-\Omega)\right)\mathbb{1} + \frac{1}{2}\left(f(\Omega)-f(-\Omega)\right)\left(P_+ - P_-\right)$$

$$\Rightarrow \mathbf{f(A) = \frac{1}{2}\left(f(\Omega)+f(-\Omega)\right)\mathbb{1} + \frac{1}{2\Omega}\left(f(\Omega)-f(-\Omega)\right) A}$$ ← Applies also to $A = \vec{a}\vec{\sigma}$!

Solution for the $b_\pm(t)$:

$$\begin{pmatrix} b_+(t) \\ b_-(t) \end{pmatrix} = e^{iAt/2}\begin{pmatrix} b_+(0) \\ b_-(0) \end{pmatrix} \qquad e^{-ix} = \cos(x) - i\sin(x)$$

$$= \left(\cos\left(\frac{\Omega t}{2}\right)\mathbb{1} + \frac{i}{\Omega}\sin\left(\frac{\Omega t}{2}\right) A\right)\begin{pmatrix} b_+(0) \\ b_-(0) \end{pmatrix}$$

$$= \left(\cos\left(\frac{\Omega t}{2}\right)\mathbb{1} + \frac{i}{\Omega}\sin\left(\frac{\Omega t}{2}\right)\begin{pmatrix} \omega_0-\omega & \omega_1 \\ \omega_1 & \omega-\omega_0 \end{pmatrix}\right)\begin{pmatrix} b_+(0) \\ b_-(0) \end{pmatrix}$$

→ Time-dependence of a spin state pointing in z direction at $t=0$: (eigenstate to S_z with eigenvalue $+\frac{\hbar}{2}$)

$$\begin{pmatrix} a_+(0) \\ a_-(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} b_+(0) \\ b_-(0) \end{pmatrix}$$

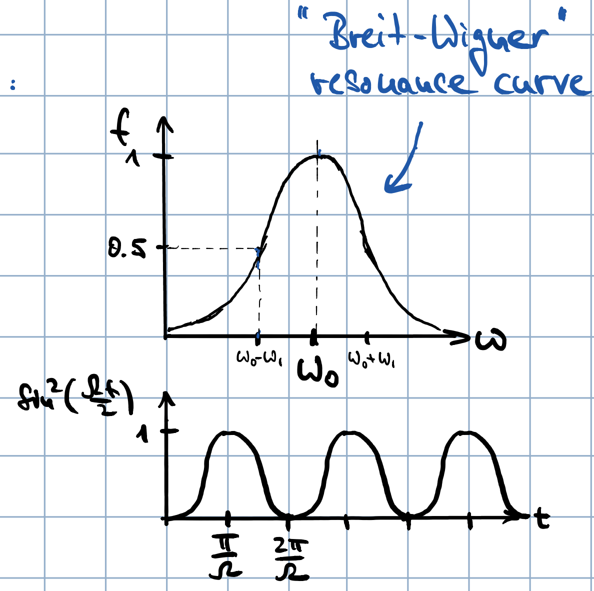
$$\Rightarrow b_+(t) = \cos\left(\frac{\Omega t}{2}\right) - i\,\frac{\omega-\omega_0}{\Omega}\sin\left(\frac{\Omega t}{2}\right), \quad b_-(t) = i\,\frac{\omega_1}{\Omega}\sin\left(\frac{\Omega t}{2}\right)$$

Probability to obtain at time t eigenvalue $-\frac{\hbar}{2}$ in a measurement of S_z: "Breit-Wigner" resonance curve

$$\Rightarrow \quad b_+(t) = \cos\left(\frac{\Omega t}{2}\right) - i\,\frac{\omega-\omega_0}{\Omega}\sin\left(\frac{\Omega t}{2}\right) \;, \quad b_-(t) = i\,\frac{\omega_1}{\Omega}\sin\left(\frac{\Omega t}{2}\right)$$

Probability to obtain at time t eigenvalue $-\frac{\hbar}{2}$ in a measurement of S_z:

$$|a_-(t)|^2 = |b_-(t)|^2 = \frac{\omega_1^2}{\Omega^2}\sin^2\left(\frac{\Omega t}{2}\right) = \underbrace{\frac{\omega_1^2}{(\omega-\omega_0)^2+\omega_1^2}}_{= f(\omega,\omega_0,\omega_1)}\sin^2\left(\frac{\Omega t}{2}\right)$$



When the rotation frequency ω is equal to ω_0 ("on resonance") the spin oscillates between the states "spin up in z-direction" $\binom{1}{0}$ and "spin-down in z-direction" $\binom{0}{1}$ with frequency $\frac{2\pi}{\Omega}$.

For $\omega \neq \omega_0$ the spin oscillates with the same frequency between "spin up" $\binom{1}{0}$ in z-direction and the state

$$\begin{pmatrix} a_+(t) \\ a_-(t) \end{pmatrix}\Bigg|_{t=\frac{\pi}{\Omega}} = \begin{pmatrix} i e^{-i\omega t}\,\frac{\omega-\omega_0}{\Omega} \\ -i e^{i\omega t}\,\frac{\omega_1}{\Omega} \end{pmatrix}$$

which is a spin pointing in a completely different direction.

The energy difference of the two states between which the spin oscillates is maximal on the resonance when $\omega = \omega_0$. The resonance frequency ω_0 can be experimentally measured because the energy exchange between magnetic field and the spins is maximal on the resonance. $(\omega_0 = \gamma B_0)$

$\Rightarrow$ This method allows to measure the gyromagnetic ratio γ that enters the relation between spin and magnetic moment:

$$\vec{\mu} = \gamma\,\vec{S}.$$