11 Theory of Angular Momenta:

Motivation:

Angular momenta are central for atomic physics:

- orbital angular momentum L
- spin angular momentum S
- nuclear angular momentum I

L, S: electronic angular momentum $J = |L-S|, \ldots, L+S$ (add successive a one)

J, I: total angular momentum of atom $F = |J-I|, \ldots, J+I$ (add successive a one)

Adding angular momenta leads to a shift of energies

LS-coupling ⇒ fine structure of energy levels — stems from Dirac equation by non-relativistic limit

JI-coupling ⇒ hyperfine structure of energy levels

another example: Zeeman effect → splitting of energy levels proportional to Landé factor:

$$g = \frac{\frac{\text{magnetic moment}}{\text{Bohr magneton}}}{\frac{\text{angular momentum}}{\hbar}}$$

Another application for adding angular momenta: scattering of atoms

atom with angular momentum F_1 + atom with angular momentum F_2 → compound with angular momentum $F = |F_1 - F_2|, \ldots, F_1 + F_2$ → atom with angular momentum F_1 + atom with angular momentum F_2

But here one has to discuss the scattering of both distinguishable and indistinguishable particles.

11.1 Commutation Relations:

angular momentum operators $\hat{J}_i$, $i = x, y, z$

- hermitian
- canonical commutation relations: $[\hat{J}_j, \hat{J}_k]_- = i \underbrace{\varepsilon_{jkl}}_{\text{Levi-Civita symbol}} \hat{J}_l$

$$\varepsilon_{ijk} = \varepsilon_{jki} = -\varepsilon_{kji} = -\varepsilon_{ikj} \quad ; \quad \varepsilon_{123} = +1$$

1. example: orbital angular momentum

$$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}} = \begin{pmatrix} \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \\ \hat{z}\hat{p}_x - \hat{x}\hat{p}_z \\ \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \end{pmatrix} ; \qquad [\hat{p}_j, \hat{x}_k]_- = \frac{\hbar}{i}\delta_{jk}$$

$$\left.\right\} [\hat{L}_j, \hat{L}_k]_- = i\varepsilon_{jkl}\hat{L}_l$$

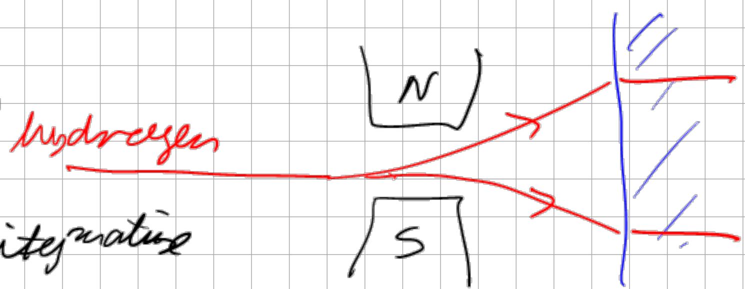
coordinate representation, $\hat{x}_j = x_j$; $\hat{p}_j = \frac{\hbar}{i}\frac{\partial}{\partial x_j}$

2. example: spin angular momentum

Pauli matrices $\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

Clifford algebra: $[\sigma^k, \sigma^l]_+ = 2\delta_{kl} \underbrace{I}_{2\times 2\text{-unit matrix}}$

Lie algebra: $[\sigma^k, \sigma^l]_- = 2i\varepsilon_{klm}\sigma^m$



Stern - Gerlach experiment

spin angular momentum operator $\hat{\vec{S}} = \frac{\hbar}{2}\vec{\sigma}$

$$[\hat{S}_k, \hat{S}_l]_- = \frac{\hbar^2}{4} 2i\varepsilon_{klm}\sigma^m = i\hbar\varepsilon_{klm}\hat{S}_m$$

back to general discussion:

$$[\hat{J}_j, \hat{J}_k]_- = i\,\varepsilon_{jkl}\,\hat{J}_l$$

$$\vec{\hat{J}}^2 = \sum_{k=1}^{3} \hat{J}_k^2 \,, \quad [\hat{J}_j, \vec{\hat{J}}^2]_- = \ldots = 0$$

$$[\hat{A}, \hat{B}\hat{C}]_- = [\hat{A},\hat{B}]_-\,\hat{C} + \hat{B}\,[\hat{A},\hat{C}]_-$$

11.2 Ladder operators:

$$[\hat{J}_z, \vec{\hat{J}}^2]_- = 0 \quad \Rightarrow \quad \vec{\hat{J}}^2 |a,b\rangle = a\,|a,b\rangle$$

$$\hat{J}_z |a,b\rangle = b\,|a,b\rangle$$

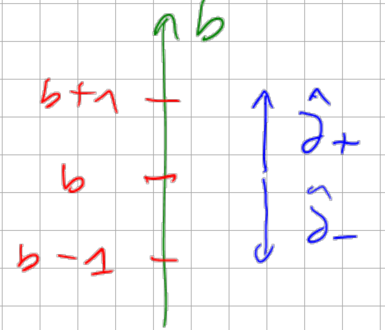
goal: determine a, b

Technique: introduce non-hermitian ladder operators $\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y = \hat{J}_\mp^+$

allows to determine a, b algebraically

1) $[\hat{J}_+, \hat{J}_-]_- = 2\hbar\,\hat{J}_z \neq 0 \Rightarrow$ ordering of $\hat{J}_+$ and $\hat{J}_-$ is important

2) $$[\hat{J}_z, \hat{J}_\pm]_- = \underbrace{[\hat{J}_z,\hat{J}_x]_-}_{=i\hbar\hat{J}_y} \pm \underbrace{[\hat{J}_z,\hat{J}_y]_-}_{=-i\hbar\hat{J}_x} = \pm\hbar\,\hat{J}_\pm$$



$$\hat{J}_z\{\hat{J}_\pm |a,b\rangle\} = (\hat{J}_\pm \hat{J}_- \pm \hbar\,\hat{J}_\pm)|a,b\rangle = (b \pm \hbar)\{\hat{J}_\pm |a,b\rangle\}$$

$\hat{J}_\pm$ represent ladder operators which increase / decrease b by $\hbar$

formal analogy to harmonic oscillator and its ladder operators

$$\hat{a}^+ |n\rangle \sim |n+1\rangle \,, \quad \hat{a}\,|n\rangle \sim |n-1\rangle$$

3) $$[\vec{\hat{J}}^2, \hat{J}_\pm]_- = \ldots = 0$$

$$\vec{\hat{J}}^2\{\hat{J}_\pm |a,b\rangle\} = \hat{J}_\pm\{\vec{\hat{J}}^2 |a,b\rangle\} = a\,\{\hat{J}_\pm |a,b\rangle\}$$

$\hat{J}_\pm$ does not change a

conclusion: $\hat{J}_\pm |a,b\rangle \sim |a, b \pm \hbar\rangle$

Note: normalization determined later. $\Rightarrow$ Thursday

11.3 Eigenvalues:

$$\hat{J}_+^n |a,b\rangle \sim |\underbrace{a}_{\text{unchanged}}, \underbrace{b + n\hbar}_{\text{increase}}\rangle$$

But: The limit of $n \to \infty$ does not exist as b has to fulfill an inequality

$$a \geq b^2$$

Let us prove this:

$$\hat{J}_+ \hat{J}_- = (\hat{J}_x + i\hat{J}_y)(\hat{J}_x - i\hat{J}_y) = \hat{J}_x^2 + i\underbrace{\cancel{(\hat{J}_y\hat{J}_x - \hat{J}_x\hat{J}_y)}}_{= -i\hbar\hat{J}_z} + \hat{J}_y^2 \qquad (**)$$

$$\hat{J}_- \hat{J}_+ = \_\ \_\ \_ = \hat{J}_x^2 \cancel{+ i\hbar\hat{J}_z} + \hat{J}_y^2 \qquad (*)$$

$$\hat{J}_x^2 + \hat{J}_y^2 = \frac{1}{2}(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+)$$

$$\hat{\vec{J}}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2 \Rightarrow \hat{\vec{J}}^2 - \hat{J}_z^2 = \frac{1}{2}(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+)$$

$$\langle a,b| \hat{\vec{J}}^2 - \hat{J}_z^2 |a,b\rangle = \frac{1}{2}\left\{\langle a,b|\underbrace{\hat{J}_+}_{=\hat{J}_-^+}\hat{J}_-|a,b\rangle + \langle a,b|\underbrace{\hat{J}_-}_{=\hat{J}_+^+}\hat{J}_+|a,b\rangle\right\}$$

$$= \frac{1}{2}\left\{\hat{J}_-|a,b\rangle\right\}^+ \hat{J}_-|a,b\rangle + \frac{1}{2}\left\{\hat{J}_+|a,b\rangle\right\}^+ \hat{J}_+|a,b\rangle \geq 0$$

$\rightarrow (a - b^2) \underbrace{\langle a,b|a,b\rangle}_{=1} \geq 0 \Rightarrow a \geq b^2 \Rightarrow \boxed{-\sqrt{a} \leq b \leq +\sqrt{a}}$

There must be a b_{max} such that $\hat{J}_+ |a, b_{max}\rangle = 0 \quad | \hat{J}_- \cdot$

$\hat{J}_- \hat{J}_+ |a, b_{max}\rangle \overset{(**)}{=} (\underbrace{\hat{\vec{J}}^2 - \hat{J}_z^2}_{= \hat{J}_x^2 + \hat{J}_y^2} - \hbar \hat{J}_z) |a, b_{max}\rangle = 0$

$\Rightarrow (a - b_{max}^2 - \hbar b_{max}) = 0 \Rightarrow \underline{a = b_{max}^2 + \hbar b_{max}}$ (1)

Similarly: $\hat{J}_- |a, b_{min}\rangle = 0 \quad | \hat{J}_+ \cdot$

$\underbrace{\hat{J}_+ \hat{J}_-} |a, b_{min}\rangle = 0$

$\overset{(**)}{=} (\hat{\vec{J}}^2 - \hat{J}_z^2 + \hbar \hat{J}_z) |a, b_{min}\rangle = 0 \Rightarrow a = b_{min}^2 - \hbar b_{min}$ (2)

observation: $b_{max} = -b_{min} \;\hat{=}\; (1) \Leftrightarrow (2)$

$-\sqrt{a} \leq b \leq +\sqrt{a} \Rightarrow -b_{max} \leq b \leq b_{max}$ $(b_{max} > 0)$

$\hat{J}_+^n |a, \underbrace{-b_{max}}_{=b_{min}}\rangle \sim |a, b_{max}\rangle$

must exist

$-b_{max} + n\hbar = b_{max} \Rightarrow b_{max} = \frac{n}{2} \hbar$

convenient notation: $j = \frac{b_{max}}{\hbar} \Rightarrow j = \frac{n}{2} \quad n \in \mathbb{N}$

angular momentum quantum number

n integer implies j either integer (n even) or half-integer (n odd)

$a = b_{max}^2 + \hbar\, b_{max} = \hbar^2 j(j+1)$: eigenvalue of $\vec{J}^2$

new definition: $m = \frac{b}{\hbar}$, $b = m\hbar$

magnetic quantum number

j integer $\hat{=}$ m integer , j half-integer $\hat{=}$ m half integer

allowed m values : $-j, -j+1, \dots, j-1, j$

$\hat{\vec{J}}^2 |j, m\rangle = \hbar^2 j(j+1) |j, m\rangle$, $\hat{J}_z = m\hbar\, |j, m\rangle$

Note: All these results only followed from commutation relations of angular momentum operators

Aim 1: $|j, m\rangle \Rightarrow \langle j', m'| \begin{pmatrix} \hat{J}_x \\ \hat{J}_y \\ \hat{J}_z \end{pmatrix} |j, m\rangle \Rightarrow$ matrix representation for $(2j+1)\times(2j+1)$ matrices

Aim 2: spin 1/2 representation matrices $\hat{=}$ Pauli matrices