Quantum Mechanics

Algebraic Methods

Harmonic Oscillator

▪ 1D Harmonic Oscillator

▪ Hamiltonian

Hamiltonian for the 1D harmonic oscillator

$$H = \frac{1}{2\,m}\,p^2 + \frac{1}{2}\,m\,\omega^2\,x^2. \tag{1}$$

- **Coordinate** operator x,
- **Momentum** operator p,

Defined by their commutation relation

$$[x,\,p] = i\,\hbar. \tag{2}$$

Let us **rescale the operators** p and x

$$p \to p\,\sqrt{\hbar\,m\,\omega}\,,\;\; x \to x\,\sqrt{\frac{\hbar}{m\,\omega}}\,, \tag{3}$$

then the Hamiltonian looks simpler

$$\boxed{H = \frac{1}{2}\,\hbar\,\omega\,\left(p^2 + x^2\right).} \tag{4}$$

- **Energy scale** set by $\hbar\,\omega$.
- New operators x and p are *dimensionless*.

- Commutation relation for the rescaled operators

$$\boxed{[x,\,p] = i.} \tag{5}$$

▪ The Idea of Boson

It turns out the eigen energies of the harmonic oscillator Eq. (4) is given by $E_n = \hbar\,\omega(n + 1/2)$

(accept it for now, and we will prove it later).

- Levels are equally spaced: **oscillator** can only absorb/emit energy in *integer* multiples of $\hbar\,\omega$.
- Each unit (quantum) of energy is a **boson**:
  - For *mechanical oscillation* (sound), the boson is also called a **phonon**.
  - For *electromagnetic oscillation* (light), the boson is also called a **photon**.
- Each boson carries energy $\hbar\,\omega \Rightarrow$ can be considered as a *particle*.

Interpretation of boson: **elementary excitation**

oscillator		boson
state $\lvert n\rangle$	$E_n / \hbar\,\omega$	
$\lvert 0\rangle$ (ground)	1 / 2	vacuum
$\lvert 1\rangle$	3 / 2	1 boson
$\lvert 2\rangle$	5 / 2	2 bosons
⋮	⋮	⋮

(6)

The boson can be

- *created* by the operator $a^\dagger$: $\lvert 0\rangle \to \lvert 1\rangle \to \lvert 2\rangle \to \ldots$,
- *annihilated* by the operator a: $\ldots \to \lvert 2\rangle \to \lvert 1\rangle \to \lvert 0\rangle$.

■ Annihilation and Creation Operator

Introduce the boson **annihilation** and **creation** operators

$$a = \frac{1}{\sqrt{2}}\,(x + i\,p),\;\; a^\dagger = \frac{1}{\sqrt{2}}\,(x - i\,p). \tag{7}$$

- a and $a^\dagger$ are *Hermitian conjugate* to each other.
- Analogy: complex numbers $z = x + i\,y$, $z^* = x - i\,y \Rightarrow$ coordinate ~ real part, momentum ~ imaginary part.

Commutation relation

$$\left[a,\, a^\dagger\right] = 1, \tag{8}$$

meaning $a\,a^\dagger = a^\dagger\,a + 1$.

■ Boson Number Basis

Let $\lvert n\rangle$ be the state of n boson excitations ($n = 0, 1, 2, \ldots$). They form a set of basis known as the **Fock state** basis or the boson number basis. Representation of a and $a^\dagger$ on this basis:

$$\boxed{\begin{aligned} a\,|n\rangle &= \sqrt{n}\;\,|n-1\rangle, \\ a^\dagger\,|n\rangle &= \sqrt{n+1}\;\,|n+1\rangle. \end{aligned}} \tag{9}$$

One can verify that

$$a^\dagger\,a\,|n\rangle = n\,|n\rangle,\;\; a\,a^\dagger\,|n\rangle = (n+1)\,|n\rangle, \tag{10}$$

- therefore $a\,a^\dagger = a^\dagger\,a + 1$ indeed holds for all states, as an operator identity.
- $a^\dagger\,a$ is the boson **number operator**, which counts the number of bosons in the Fock state.
- The Hilbert space spanned by Fock states is called the **Fock space**.

Can we construct the Fock space from scratch?

Define the operator $\hat{n} = a^\dagger\,a$,

- $\hat{n}$ is Hermitian ($\hat{n}^\dagger = \hat{n}$),
- $\hat{n}$ is positive (semi)definite: $\forall\,|\psi\rangle : \langle\psi|\,\hat{n}\,|\psi\rangle = \langle\psi|\,a^\dagger\,a\,|\psi\rangle \geq 0$,

$\Rightarrow$ $\hat{n}$ has a set of orthogonal eigenstates (denoted as $|n\rangle$, labeled by $n = 0, 1, 2, \ldots$)

$$\hat{n}\,|n\rangle = \lambda_n\,|n\rangle. \tag{11}$$

with $\lambda_n \geq 0$. Because the spectrum is bounded from below, we can always arrange the eigenvalues in ascending order $0 \leq \lambda_0 \leq \lambda_1 \leq \lambda_2 \leq \ldots$, $|0\rangle$ is the "ground state" of $\hat{n}$.

From the following operator identity (use Eq. (8))

$$\hat{n}\,a = a\,(\hat{n}-1),\;\; \hat{n}\,a^\dagger = a^\dagger\,(\hat{n}+1), \tag{12}$$

one can show that

$$\hat{n}(a\,|n\rangle) = (\lambda_n - 1)\,(a\,|n\rangle),\;\; \hat{n}\left(a^\dagger\,|n\rangle\right) = (\lambda_n + 1)\left(a^\dagger\,|n\rangle\right). \tag{13}$$

If $|n\rangle$ is an eigenstate of $\hat{n}$ with eigenvalue λ_n, then $a\,|n\rangle$ and $a^\dagger\,|n\rangle$ are also eigenstates of $\hat{n}$ with eigen values $\lambda_n \mp 1$. But there is a caveat: we must make sure that the state is normalizable (the sate has a finite norm). For example $a\,|0\rangle$ must have zero norm, otherwise $a\,|0\rangle$ would be an eigenstate of $\hat{n}$ with eigenvalue $\lambda_0 - 1 < \lambda_0$, which contradict the with the fact that λ_0 is the smallest eigenvalue, therefore $a\,|0\rangle = 0 \Rightarrow \hat{n}\,|0\rangle = 0 \Rightarrow \lambda_0 = 0$.

Then we consider $a\,|1\rangle$, it is an eigenstate with eigenvalue $\lambda_1 - 1$, but λ_0 is the only eigenvalue smaller than λ_1, so $\lambda_1 - 1 = \lambda_0 \Rightarrow \lambda_1 = 1$. Iteratively apply similar argument, one can build up the entire Fock state representation.

■ Energy Spectrum

In terms of a and $a^\dagger$, the oscillator Hamiltonian becomes

$$\boxed{H = \hbar\,\omega\left(a^\dagger\,a + \frac{1}{2}\right),} \tag{14}$$

So the eigen energies are given by

$$E_n = \hbar\,\omega\left(n + \frac{1}{2}\right). \tag{15}$$

The constant $\hbar\,\omega/2$ is known as the **zero-point energy** or the **vacuum energy**. The corresponding eigenstate $|n\rangle$ can be raised from the ground state by

$$|n\rangle = \frac{1}{\sqrt{n!}}\left(a^\dagger\right)^n |0\rangle. \tag{16}$$

■ Wave Functions

The ground state is defined by $a\,|0\rangle = 0 \Rightarrow (x + i\,p)\,|0\rangle = 0$, where $p = -i\,\partial_x$, so the ground state wave function $\psi_0(x)$ must satisfy the differential equation

$$(x + \partial_x)\,\psi_0(x) = 0, \tag{17}$$

the solution is

$$\psi_0(x) = \frac{1}{\pi^{1/4}}\,e^{-\frac{1}{2}x^2}. \tag{18}$$

The excited state can be raised from the ground state by applying $a^\dagger$. For example $|1\rangle = a^\dagger\,|0\rangle$ implies

$$\psi_1(x) = \frac{1}{\sqrt{2}}\,(x - \partial_x)\,\psi_0(x) = \frac{1}{\pi^{1/4}}\,\sqrt{2}\;x\,e^{-\frac{1}{2}x^2}. \tag{19}$$

Iteratively, we can obtain the wave functions for all eigenstates

$$\psi_n(x) = \frac{1}{\pi^{1/4}\,\sqrt{2^n\,n!}}\,H_n(x)\,e^{-\frac{1}{2}x^2}, \tag{20}$$

where $H_n(x)$ is known as the **Hermite polynomial**.

n	$\psi_n(x)$	$H_n(x)$	plot of $\psi_n(x)$
0	$\frac{e^{-\frac{x^2}{2}}}{\pi^{1/4}}$	1	
1	$\frac{\sqrt{2}\, e^{-\frac{x^2}{2}} x}{\pi^{1/4}}$	$2x$	
2	$\frac{e^{-\frac{x^2}{2}} (-1+2x^2)}{\sqrt{2}\,\pi^{1/4}}$	$2(-1+2x^2)$	
3	$\frac{e^{-\frac{x^2}{2}} x (-3+2x^2)}{\sqrt{3}\,\pi^{1/4}}$	$4x(-3+2x^2)$	
4	$\frac{e^{-\frac{x^2}{2}} (3-12x^2+4x^4)}{2\sqrt{6}\,\pi^{1/4}}$	$4(3-12x^2+4x^4)$	
5	$\frac{e^{-\frac{x^2}{2}} x (15-20x^2+4x^4)}{2\sqrt{15}\,\pi^{1/4}}$	$8x(15-20x^2+4x^4)$	

Momentum space wave function

$$\tilde{\psi}_n(p) = \frac{1}{\pi^{1/4}\sqrt{2^n\, n!}} H_n(p)\, e^{-\frac{1}{2}p^2}. \tag{21}$$

- Comparing Eq. (20) and Eq. (21), there is an SO(2) *rotational* symmetry in the 2D **phase space** of (x, p), which is evident in Eq. (4).
  - This also corresponds to the **U(1) symmetry**:

    $$a \to e^{i\theta}\, a,\ \ a^\dagger \to e^{-i\theta}\, a^\dagger. \tag{22}$$

  - U(1) symmetry ⇒ *conservation* of the boson **number**.

3D Harmonic Oscillator

Hamiltonian

Hamiltonian of a 3D harmonic oscillator

$$H = \frac{\hbar\,\omega}{2}\left(\boldsymbol{p}^2 + \boldsymbol{x}^2\right). \tag{23}$$

- Coordinate $\boldsymbol{x} = (x_1, x_2, x_3)$,
- Momentum $\boldsymbol{p} = (p_1, p_2, p_3)$.

The boson now has three **polarizations**

- boson **annihilation** $\boldsymbol{a} = (a_1, a_2, a_3)$ and **creation** $\boldsymbol{a}^\dagger = \left(a_1^\dagger, a_2^\dagger, a_3^\dagger\right)$ operators

$$\boldsymbol{a} = \frac{1}{\sqrt{2}}(\boldsymbol{x} + i\,\boldsymbol{p}),\ \ \boldsymbol{a}^\dagger = \frac{1}{\sqrt{2}}(\boldsymbol{x} - i\,\boldsymbol{p}). \tag{24}$$

They satisfy the commutation relation

$$\left[a_a,\, a_b^\dagger\right] = \delta_{ab}, \tag{25}$$

In terms of the boson operators,

$$\boxed{H = \hbar\,\omega\left(\boldsymbol{a}^\dagger\,\boldsymbol{a} + \frac{3}{2}\right).} \tag{26}$$

■ Energy Levels

Each boson (regardless of polarization) carries the same energy $\hbar\,\omega$, so the total energy is proportional to the **total number** N of bosons.

$$\begin{aligned} &E = \hbar\,\omega\left(N + \frac{3}{2}\right), \\ &N = n_1 + n_2 + n_3. \end{aligned} \tag{27}$$

- Eigen state: $|n_1\; n_2\; n_3\rangle$
- Degeneracy

$$\sum_{n_1,n_2,n_3} \delta_{N=n_1+n_2+n_3} = \frac{1}{2}\,(N+1)\,(N+2). \tag{28}$$

	0	1	2	3	4	5
E	$\frac{3}{2}$	$\frac{5}{2}$	$\frac{7}{2}$	$\frac{9}{2}$	$\frac{11}{2}$	$\frac{13}{2}$
deg.	1	3	6	10	15	21

Questions: How are the *degenerate state* differed from each other?

Classical picture: they have the same energy ⇒ oscillation amplitude is the same, but oscillation direction can be different ⇒ *rotational degrees of freedom* may help to explain the degeneracy (but only partially).

■ Angular Momentum

The **angular momentum** $\boldsymbol{L} = (L_1,\, L_2,\, L_3)$ operators

$$\boldsymbol{L} = \boldsymbol{x} \times \boldsymbol{p}. \tag{29}$$

In component form, $L_a = \epsilon_{abc}\, x_b\, p_c$. ($\epsilon_{abc}$: Levi-Civita tensor, totally antisymmetric tensor) (Einstein summation is assumed here).

In terms of the boson operators,

$$\boxed{L_a = -i\,\epsilon_{abc}\, a_b^\dagger\, a_c.} \tag{30}$$

- The angular momentum operator generates the SO(3) *rotation* among different *polarization* modes.
- The (quadratic) **Casimir operator** (the square of angular momentum) $\boldsymbol{L}^2$.

$$\boldsymbol{L}^2 = L_1^2 + L_2^2 + L_3^2 = \sum_{i\neq j} \left(\hat{n}_i\left(\hat{n}_j + 1\right) - a_i^\dagger\, a_i^\dagger\, a_j\, a_j\right). \tag{31}$$

■ Fock State Basis

Represent the angular momentum operator in each subspace of fixed total boson number $N = n_1 + n_2 + n_3$.

$$\begin{aligned} L_1 &= -i\sqrt{(n_2+1)\,n_3}\;\left|n_1,\, n_2+1,\, n_3-1\right\rangle\left\langle n_1\; n_2\; n_3\right| + h.c.,\\ L_2 &= -i\sqrt{(n_3+1)\,n_1}\;\left|n_1-1,\, n_2,\, n_3+1\right\rangle\left\langle n_1\; n_2\; n_3\right| + h.c.,\\ L_3 &= -i\sqrt{(n_1+1)\,n_2}\;\left|n_1+1,\, n_2-1,\, n_3\right\rangle\left\langle n_1\; n_2\; n_3\right| + h.c.\,. \end{aligned} \tag{32}$$

For example in the $N = 1$ sector, we have 3 basis states

$$\{|100\rangle, |010\rangle, |001\rangle\}. \tag{33}$$

The angular momentum operators $L_{1,2,3}$ are represented as 3×3 matrices.

$$L_1 \doteq \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix},\; L_2 \doteq \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix},\; L_3 \doteq \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{34}$$

The $\boldsymbol{L}^2 = L_1^2 + L_2^2 + L_3^2$operator can be obtained by matrix square and summation,

$$\boldsymbol{L}^2 \doteq \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}. \tag{35}$$

HW 1 Show Eq. (34) and Eq. (35). Use the explicit matrix representation to verify the commutation relation $[L_a,\, L_b] = i\,\epsilon_{abc}\,L_c$.

Easy to see that $\boldsymbol{L}^2$ and L_3 commute ⇒ their simultaneous eigenstates span the degenerate subspace. Introduce l and m to label the common eigenstates.

$$\boxed{\begin{aligned} &\boldsymbol{L}^2\,|l,\, m\rangle = l(l+1)\,|l,\, m\rangle,\\ &L_3\,|l,\, m\rangle = m\,|l,\, m\rangle. \end{aligned}} \tag{36}$$

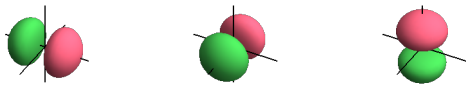
Diagonalize the matrices in Eq. (34),

$$\begin{aligned} |l=1,\, m=\pm 1\rangle &= \frac{1}{\sqrt{2}}\left(\left|100\right\rangle \pm i\,\left|010\right\rangle\right),\\ |l=1,\, m=0\rangle &= \left|001\right\rangle. \end{aligned} \tag{37}$$

- Classical picture:
  - $|l = 1,\ m = \pm 1\rangle$ - uniform circular rotation in the xy-plane, ± sign corresponds to counterclockwise or clockwise.
  - $|l = 1,\ m = 0\rangle$ - linear oscillation along the z-direction.
- Quantum wave function:
  - Fock state basis

$$\psi_{n_1\, n_2\, n_3}(x_1,\, x_2,\, x_3) = \psi_{n_1}(x_1)\, \psi_{n_2}(x_2)\, \psi_{n_3}(x_3). \tag{38}$$

$|100\rangle$ $|010\rangle$ $|001\rangle$



  - Angular momentum basis

$N = 1$ sector

l	m	state	
1	1	$\frac{i\,\lvert 010\rangle + \lvert 100\rangle}{\sqrt{2}}$	
1	0	$\lvert 001\rangle$	
1	−1	$\frac{-i\,\lvert 010\rangle + \lvert 100\rangle}{\sqrt{2}}$	

▫ More Examples

■ U(3) Symmetry

The SO(3) symmetry explains the 3-fold degeneracy of the *first* excited state. But the degeneracy of *higher* angular momentum states goes as $2\,l + 1$ (like 1, 3, 5, 7, ...), which is *smaller* than the observed degeneracies (1, 3, 6, 10, ...) in Eq. (28). This suggest the 3D harmonic oscillator has *more symmetry*!

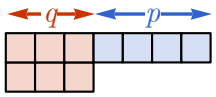
In fact, the following $U \in$U(3) transformation leaves the Hamiltonian invariant,

$$\boldsymbol{a} \to U\, \boldsymbol{a}. \tag{39}$$

So the 3D harmonic oscillator actually has **U(3) symmetry**.

- The Abelian U(1) subgroup does not leads to degeneracy.

- The non-Abelian **SU(3) subgroup** ⇒ irreducible representations D_{pq} are labeled by two quantum numbers p, $q = 0, 1, 2, \ldots$



and their dimensions are

$$\dim D_{pq} = \frac{1}{2}(p+1)(q+1)(p+q+2). \tag{40}$$

For bosonic systems, only $q = 0$ representations can appear, the corresponding dimensions $\dim D_{p0} = \frac{1}{2}(p+1)(p+2)$ (for $p = 0, 1, 2, \ldots$) fully explain the degeneracies of the entire spectrum, as in Eq. (28).

Angular Momentum

■ Operator Algebra

■ Definition

Motivation: classical mechanics: *orbital* angular momentum $\boldsymbol{L} = (L_1, L_2, L_3)$

$$\boxed{\boldsymbol{L} = \boldsymbol{x} \times \boldsymbol{p}.} \tag{41}$$

In component form, $L_a = \epsilon_{abc}\, x_b\, p_c$. ($\epsilon_{abc}$: Levi-Civita tensor, totally antisymmetric tensor) (Einstein summation is assumed here). From

$$[x_a, p_b] = i\,\delta_{ab}, \tag{42}$$

(set $\hbar = 1$ for simplicity) ⇒ the angular momentum operators satisfy

$$[L_a, L_b] = i\,\epsilon_{abc}\, L_c. \tag{43}$$

We may treat this *commutation relation* as the definition for angular momentum.

Definition: the **angular momentum** operator $\boldsymbol{J} = (J_1, J_2, J_3)$ consist of three Hermitian operators, satisfying

$$\boxed{[J_a, J_b] = i\,\epsilon_{abc}\, J_c.} \tag{44}$$

- Equivalently, in vector form, $\boldsymbol{J} \times \boldsymbol{J} = i\,\boldsymbol{J}$.
- This general definition applies to **orbital** and **spin** angular momenta. The spin angular momentum goes beyond the classical definition of $\boldsymbol{x} \times \boldsymbol{p}$.
- The Hermitian operators $\boldsymbol{J}$ generate a unitary group - the SU(2) group.

■ Casimir Operator

A **Casimir operator** is a operator that commutes with all components of $\boldsymbol{J}$. It turns out that for SU(2) group, there is only one such operator: the **squared angular momentum** $\boldsymbol{J}^2 = \boldsymbol{J} \cdot \boldsymbol{J}$,

$$\boxed{\boldsymbol{J}^2 = J_1^2 + J_2^2 + J_3^2.} \tag{45}$$

- $\boldsymbol{J}^2$ is Hermitian.
- By Eq. (44), one can verify that (for $a = 1, 2, 3$)

$$\left[\boldsymbol{J}^2, J_a\right] = 0. \tag{46}$$

■ Common Eigenstates

$\boldsymbol{J}^2$ and J_3 commute ⇒ they share the same set of eigenstates, which can be labeled by two independent quantum number: $|j, m\rangle$ ⇒ as a common eigenstate, $|j, m\rangle$ must satisfy the eigen equation for both operators

$$\begin{aligned} \boldsymbol{J}^2 |j, m\rangle &= \lambda_j |j, m\rangle, \\ J_3 |j, m\rangle &= m |j, m\rangle, \end{aligned} \tag{47}$$

where λ_j is a function of j (to be determined later).

- λ_j is the the eigenvalue of $\boldsymbol{J}^2$ on $|j, m\rangle$,
- m is the the eigenvalue of J_3 on $|j, m\rangle$.

■ Raising and Lowering Operators

Define the **raising** J_+ and **lowering** J_- operators

$$\boxed{J_\pm = J_1 \pm i\, J_2.} \tag{48}$$

- In analogy to $e^{\pm i\,\theta} = \cos\theta \pm i \sin\theta$.
- $J_\pm$ are *not* Hermitian. Under Hermitian conjugate: $J_\pm^\dagger = J_\mp$.
- Raising and lowering.

$$J_3\, J_\pm = J_\pm (J_3 \pm 1). \tag{49}$$

  - From Eq. (49), $J_3\, J_\pm |j, m\rangle = J_\pm (J_3 \pm 1) |j, m\rangle = (m \pm 1)\, J_\pm |j, m\rangle$ ⇒ the state $J_\pm |j, m\rangle$ (as long as it is not zero) is also an eigenstate of J_3 but with the eigenvalue $(m \pm 1)$ ⇒ $J_\pm |j, m\rangle$ is just the $|j, m \pm 1\rangle$ state (up to overall coefficient)

$$J_\pm |j, m\rangle = c_m^\pm |j, m \pm 1\rangle. \tag{50}$$

    Therefore $J_\pm$ is called the *raising/lowering* operator.

  - Also note that, under the action of $J_\pm$, the quantum number m can only change by 1 (not change continuously) ⇒ *angular momentum quantization*.

- Bounds on quantum numbers.

$$J_+ J_- = J^2 - J_3^2 + J_3,$$
$$J_- J_+ = J^2 - J_3^2 - J_3. \tag{51}$$

- $|j, m\rangle$ is also the eigenstate of $J_+ J_-$ and $J_- J_+$.

$$\langle j, m| J_+ J_- |j, m\rangle = \lambda_j - m^2 + m,$$
$$\langle j, m| J_- J_+ |j, m\rangle = \lambda_j - m^2 - m. \tag{52}$$

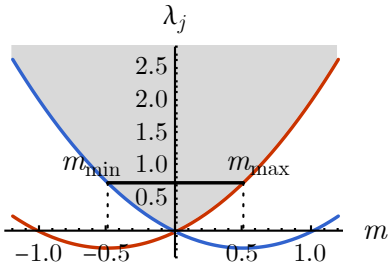
- On the other hand

$$\langle j, m| J_+ J_- |j, m\rangle = \langle j, m| J_-^\dagger J_- |j, m\rangle = |c_m^-|^2 \geq 0,$$
$$\langle j, m| J_- J_+ |j, m\rangle = \langle j, m| J_+^\dagger J_+ |j, m\rangle = |c_m^+|^2 \geq 0. \tag{53}$$

- Combining Eq. (52) and Eq. (53),

$$\lambda_j - m(m \pm 1) \geq 0 \Rightarrow$$
$$-\frac{1}{2}\left(\sqrt{1+4\lambda_j} - 1\right) \leq m \leq \frac{1}{2}\left(\sqrt{1+4\lambda_j} - 1\right). \tag{54}$$

So m is bounded from both above and below ⇒ denote the upper (lower) bound as $m_{\max}$ ($m_{\min}$).



Representation Theory

Highest and Lowest Weight State

Denote:

- **Highest weight state**: $|j, m_{\max}\rangle$, corresponds to $m = m_{\max}$. It can not be further raised by J_+ ⇒ $J_+ |j, m_{\max}\rangle = 0$.
- **Lowest weight state**: $|j, m_{\min}\rangle$, corresponds to $m = m_{\min}$. It can not be further lowered by J_- ⇒ $J_- |j, m_{\min}\rangle = 0$.

Therefore

$$0 = \langle j, m_{\min}| J_+ J_- |j, m_{\min}\rangle = \lambda_j - m_{\min}^2 + m_{\min},$$
$$0 = \langle j, m_{\max}| J_- J_+ |j, m_{\max}\rangle = \lambda_j - m_{\max}^2 - m_{\max}. \tag{55}$$

Eliminate λ_j,

$$(m_{\max} + m_{\min})\,(m_{\max} - m_{\min} + 1) = 0, \tag{56}$$

As $m_{\max} \geq m_{\min} \Rightarrow m_{\max} - m_{\min} + 1 \geq 1 > 0 \Rightarrow$ to satisfy Eq. (56), we must have $m_{\max} + m_{\min} = 0$, i.e. $m_{\max} = -m_{\min}$.

We have not specify the meaning of the quantum number j yet. According to the convention, we give j such a physical meaning that j is the maximal value that $|m|$ can take, i.e.

$$m_{\max} = j,\ \ m_{\min} = -j \ \Rightarrow\ -j \leq m \leq j. \tag{57}$$

Then by Eq. (55)

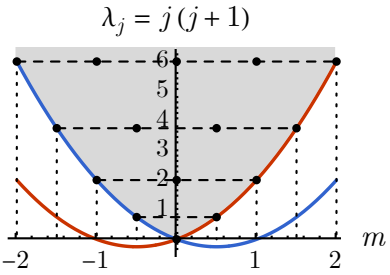
$$\lambda_j = j(j+1). \tag{58}$$

This also makes Eq. (57) consistent with Eq. (54).

■ Angular Momentum Quantization

Because m can only change by $\pm 1 \Rightarrow$ the difference between $m_{\max}$ and $m_{\min}$ must be an integer $\Rightarrow m_{\max} - m_{\min} = 2\,j = 0, 1, 2, \ldots$, therefore

- j can only be integer or half-integer: $j = 0, 1/2, 1, 3/2, 2, \ldots$
- m takes values in $m = -j, -j+1, \ldots, j-1, j$.
- For **orbital** angular momentum j takes *integer* values. For **spin** angular momentum j can also be *half-integer*.



■ Representation

Now we want to determine the coefficients $c_m^{\pm}$ in Eq. (50). From Eq. (52) and Eq. (53), $|c_m^{\pm}|^2 = j(j+1) - m(m \pm 1)$. It is a gauge choice to fix $c_m^{\pm}$to be real and positive, so we take

$$c_m^{\pm} = \sqrt{j(j+1) - m(m \pm 1)}\ . \tag{59}$$

In conclusion, we have obtained the following representations for angular momentum operators (from Eq. (47) and Eq. (50))

$$\boxed{\begin{aligned}&\boldsymbol{J}^2\,|j,\,m\rangle = j(j+1)\,|j,\,m\rangle,\\&J_3\,|j,\,m\rangle = m\,|j,\,m\rangle,\\&J_\pm\,|j,\,m\rangle = \sqrt{j(j+1)-m(m\pm 1)}\;\;|j,\,m\pm 1\rangle.\end{aligned}} \tag{60}$$

Induction implies that all basis states can be

- either *raised* from the *lowest weight* state,

$$|j,\,m\rangle = \left(\frac{(j-m)!}{(2\,j)!\,(j+m)!}\right)^{1/2}\;J_+^{j+m}\,|j,\,-j\rangle, \tag{61}$$

- or *lowered* from the *highest weight* state,

$$|j,\,m\rangle = \left(\frac{(j+m)!}{(2\,j)!\,(j-m)!}\right)^{1/2}\;J_-^{j-m}\,|j,\,j\rangle. \tag{62}$$

This is just like the Harmonic oscillator.

To make the analogy more precise, take the large-j limit,

$$\begin{aligned}&\frac{J_+}{\sqrt{2\,j}}\,|j,\,-j+n\rangle = \sqrt{n+1}\;\;|j,\,-j+n+1\rangle + O\big(j^{-1/2}\big),\\&\frac{J_-}{\sqrt{2\,j}}\,|j,\,-j+n\rangle = \sqrt{n}\;\;|j,\,-j+n-1\rangle + O\big(j^{-1/2}\big).\end{aligned} \tag{63}$$

Under the following correspondence

$$\begin{aligned}&|j,\,-j+n\rangle \to |n\rangle,\\&(2\,j)^{-1/2}\,J_-\to a,\;(2\,j)^{-1/2}\,J_+\to a^\dagger,\end{aligned} \tag{64}$$

the boson creation/annihilation algebra Eq. (9) can be reproduced approximately (to the leading order). In this sense, *spin excitations* can also be treated as bosons, called **magnons**.

■ Spin-1/2

In the $j = 1/2$ subspace, the (spin) angular momentum operators $\boldsymbol{S} = (S_1,\,S_2,\,S_3)$ can be represented as **Pauli matrices**,

$$\boxed{\boldsymbol{S} = \frac{1}{2}\,\boldsymbol{\sigma}.} \tag{65}$$

- Basis: $\{|\uparrow\rangle = |1/2,\,+1/2\rangle,\,|\downarrow\rangle = |1/2,\,-1/2\rangle\}$.
- Matrix representations:

$$S_1 \doteq \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ S_2 \doteq \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ S_3 \doteq \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{66}$$

- Eigenstates and eigenvalues

$$\begin{aligned} S_1 &: \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \to +\frac{1}{2},\ \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \to -\frac{1}{2}, \\ S_2 &: \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} \to +\frac{1}{2},\ \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} \to -\frac{1}{2}, \\ S_1 &: \begin{pmatrix} 1 \\ 0 \end{pmatrix} \to +\frac{1}{2},\ \begin{pmatrix} 0 \\ 1 \end{pmatrix} \to -\frac{1}{2}. \end{aligned} \tag{67}$$

■ Spin-1

The $j = 1$ subspace: dimension = 3 ⇒ 3 basis states, and angular momentum operator represented as 3×3 matrices.

- Basis: $\{|1, +1\rangle, |1, 0\rangle, |1, -1\rangle\}$.
- Matrix representations (the same matrices also represent spin-1)

$$L_1 \doteq \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},\ L_2 \doteq \frac{1}{\sqrt{2}\ i}\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix},\ L_3 \doteq \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{68}$$

Switch to another set of basis (p-wave orbitals)

- Basis transformation

$$\begin{pmatrix} |1, +1\rangle \\ |1, 0\rangle \\ |1, -1\rangle \end{pmatrix} = \begin{pmatrix} \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & -i \\ \frac{-i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}\begin{pmatrix} |x\rangle \\ |y\rangle \\ |z\rangle \end{pmatrix}. \tag{69}$$

- Denote the transformation matrix by U, the operators transform as $L_a \to U^\dagger\, L_a\, U$,

$$L_1 \doteq \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix},\ L_2 \doteq \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix},\ L_3 \doteq \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{70}$$

■ Rotation Operators

Rotation operators are generated **angular momentum operators** by

$$\boxed{R(\boldsymbol{\theta}) = e^{i\,\boldsymbol{\theta}\cdot\boldsymbol{L}}.} \tag{71}$$

The physical meaning of $\boldsymbol{\theta} = (\theta_1, \theta_2, \theta_3)$

- **direction** of $\boldsymbol{\theta}$: the direction of the rotational *axis* (following the *right-handed* rule),
- **magnitude** of $\boldsymbol{\theta}$: the amount of *angle* to rotate.
  Examples: rotate along (0, 0, 1) axis by $\theta \Rightarrow \boldsymbol{\theta} = (0, 0, \theta)$.
- Spin-1/2 representation, in the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis,

$$R_{1/2}(\boldsymbol{\theta}) \doteq \begin{pmatrix} e^{i\,\theta/2} & 0 \\ 0 & e^{-i\,\theta/2} \end{pmatrix}. \tag{72}$$

- Spin-1 representation, in the $\{|x\rangle, |y\rangle, |z\rangle\}$ basis,

$$R_1(\boldsymbol{\theta}) \doteq \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{73}$$

When $\theta = 2\,\pi$, a rotation by $2\,\pi$ should do nothing,

- This is indeed the case for spin-1 representation

$$R_1(0, 0, 2\,\pi) \doteq \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \doteq \mathbb{1}. \tag{74}$$

- But not for spin-1/2,

$$R_{1/2}(0, 0, 2\,\pi) \doteq \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \doteq -\mathbb{1}, \tag{75}$$

  The extra minus sign means that spin-1/2 is a **projective representation** of SO(3). Nevertheless, it is a **linear representation** of SU(2).

Addition of Angular Momentum

Example: Fusion of Spins

Combine two spin-1/2 systems together,

- **State** tensor products:

$$\{|\uparrow\rangle, |\downarrow\rangle\}_A \times \{|\uparrow\rangle, |\downarrow\rangle\}_B = \{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}. \tag{76}$$

- **Angular momentum** adds:

$$\boxed{\boldsymbol{S} = \boldsymbol{S}_A + \boldsymbol{S}_B,} \tag{77}$$

  where $\boldsymbol{S}_A$ and $\boldsymbol{S}_B$ are represented as

$$\begin{aligned} \boldsymbol{S}_A &= \frac{1}{2}\,\boldsymbol{\sigma}_A \otimes \mathbb{1}_B \doteq \frac{1}{2}\,(\sigma^{10}, \sigma^{20}, \sigma^{30}), \\ \boldsymbol{S}_B &= \frac{1}{2}\,\mathbb{1}_A \otimes \boldsymbol{\sigma}_B \doteq \frac{1}{2}\,(\sigma^{01}, \sigma^{02}\,\sigma^{03}). \end{aligned} \tag{78}$$

The operator $\boldsymbol{S}$ qualifies as an *angular momentum* operator, because it satisfies the defining relation $\boldsymbol{S} \times \boldsymbol{S} = i\,\boldsymbol{S}$ ⇒ In fact, $\boldsymbol{S}$ corresponds to the **total angular momentum** of the combined system. ⇒ They are **generators** of the *global* SU(2) symmetry.

$$\begin{aligned} \boldsymbol{S}^2 &= (\boldsymbol{S}_A + \boldsymbol{S}_B)^2 = \boldsymbol{S}_A^2 + \boldsymbol{S}_B^2 + 2\,\boldsymbol{S}_A \cdot \boldsymbol{S}_B \\ &= \frac{3}{2}\,\mathbb{1} + 2\,\boldsymbol{S}_A \cdot \boldsymbol{S}_B. \end{aligned} \tag{79}$$

The operator $\boldsymbol{S}_A \cdot \boldsymbol{S}_B$ describes the *spin coupling*.

$$\boldsymbol{S}_A \cdot \boldsymbol{S}_B \doteq \frac{1}{4}\left(\sigma^{11} + \sigma^{22} + \sigma^{33}\right) = \frac{1}{4}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{80}$$

Diagonalize $\boldsymbol{S}_A \cdot \boldsymbol{S}_B$:

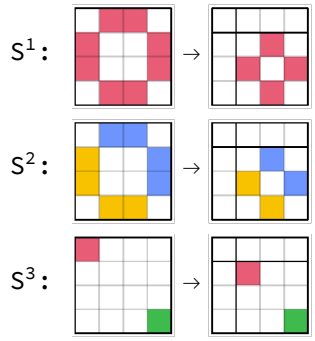
- Spin **singlet** state, $\boldsymbol{S}_A \cdot \boldsymbol{S}_B = -3/4 \Rightarrow \boldsymbol{S}^2 = 0$ $(s = 0)$:

$$|0, 0\rangle = \frac{1}{\sqrt{2}}\,(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle). \tag{81}$$

- Spin **triplet** states, $\boldsymbol{S}_A \cdot \boldsymbol{S}_B = 1/4 \Rightarrow \boldsymbol{S}^2 = 2$ $(s = 1)$:

$$\begin{aligned} &|1, +1\rangle = |\uparrow\uparrow\rangle, \\ &|1, 0\rangle = \frac{1}{\sqrt{2}}\,(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle), \\ &|1, -1\rangle = |\downarrow\downarrow\rangle. \end{aligned} \tag{82}$$

Under the basis transformation $\boldsymbol{S}$ is block diagonalized,



- The original basis $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$ form a **reducible representation** of SU(2).

- The new basis $\{|0,0\rangle\}$ and $\{|1,+1\rangle, |1,0\rangle, |1,-1\rangle\}$ respectively form **irreducible representations** of SU(2).

The two bases are related by basis transformations:

- $1/2 \otimes 1/2 \to 0$ channel:

$$(|0,0\rangle) = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix} \begin{pmatrix} |\uparrow\uparrow\rangle \\ |\uparrow\downarrow\rangle \\ |\downarrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \end{pmatrix}. \tag{83}$$

- $1/2 \otimes 1/2 \to 1$ channel:

$$\begin{pmatrix} |1,+1\rangle \\ |1,0\rangle \\ |1,-1\rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} |\uparrow\uparrow\rangle \\ |\uparrow\downarrow\rangle \\ |\downarrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \end{pmatrix}. \tag{84}$$

The matrix elements are called **Clebsch-Gordan coefficients**. They tell us how the composition of two spin-1/2 systems splits into a spin-0 and a spin-1 system.

■ Fusion Rules

Spins are irreducible representations of the SU(2) group. They are building blocks for more general (reducible) representations. All **representations** of SU(2) form a **category**:

- **Irreducible representations** are *simple objects* in the category, labeled by their spin quantum numbers $j = 0, 1/2, 1, \ldots$
- Other **reducible representations** are not simple. They can be considered as *spin systems*.
  - **Semisimple property**: each reducible representation (spin system) can split in to direct sum of irreducible representations (spins).

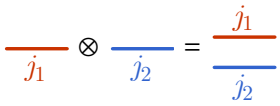
Each representation can be associated with a **representation space** (which is a Hilbert space). For example, spin-1/2 has a 2-dim representation space, spanned by $\{|\uparrow\rangle, |\downarrow\rangle\}$. For an irreducible representation of spin-j, the **representation dimension** is $2j+1$.

- Matrix representation of group element $g \in \mathrm{SU}(2)$ in representation j can be depicted as

Example: rotation $\boldsymbol{\theta} = (0, 0, \theta)$, c.f. Eq. (72) and Eq. (73)

$$\begin{aligned} &\tfrac{1}{2}\text{—}R(\boldsymbol{\theta})\text{—}\tfrac{1}{2} = \begin{pmatrix} e^{i\theta/2} & 0 \\ 0 & e^{-i\theta/2} \end{pmatrix}, \\ &1\text{—}R(\boldsymbol{\theta})\text{—}1 = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \end{aligned} \tag{85}$$

The representation category of SU(2) is actually a **tensor category**, i.e. a category equipped with **tensor product** structures, meaning that the tensor product two representations is still a representation (which can then be further decomposed into irreducible representations).



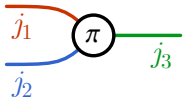
- The tensor structure specifies the **fusion rule**:

$$\boxed{j_1 \otimes j_2 \to |j_1 - j_2| \oplus (|j_1 - j_2| + 1) \oplus \ldots \oplus (j_1 + j_2 - 1) \oplus (j_1 + j_2).} \tag{86}$$

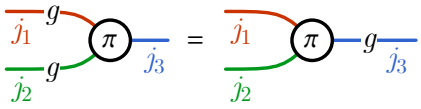
  - Composition of a spin-j_1 and a spin-j_2 systems is a spin system that contains irreducible representations ranging from $|j_1 - j_2|$ to $j_1 + j_2$ (each of them appear once).
  - Example: $1/2 \otimes 1/2 \to 0 \oplus 1$.
  - Notice that the *representation dimensions* add up correctly

$$\dim \mathcal{H}_{j_1 \otimes j_2} = \sum_{j_3 = |j_1 - j_2|}^{j_1 + j_2} (2\, j_3 + 1) = (2\, j_1 + 1)\,(2\, j_2 + 1). \tag{87}$$

- The decomposition is implemented by the **fusion vertex** (a *projective morphism*), which can be viewed as three-leg tensors preserving the SU(2) symmetry.



  such that $\forall\ g \in \mathrm{SU}(2)$:



  - Example: fusion of two spin-1/2s, c.f. Eq. (83) and Eq. (84)

$$\begin{aligned}
&\pi_0 : 1/2 \otimes 1/2 \to 0, \\
&\pi_0 \doteq \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}, \\
&\pi_1 : 1/2 \otimes 1/2 \to 1, \\
&\pi_1 \doteq \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.
\end{aligned} \tag{88}$$

  Tensor elements of the *fusion vertex* are **Clebsch-Gordan coefficients** (CG coefficients).

$$\left(\begin{array}{cc|c} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{array}\right) = \langle j_3,\, m_3 \mid j_1,\, m_1;\, j_2,\, m_2\rangle. \tag{89}$$

They can be used to implement basis transformations

$$\pi(j_1 \otimes j_2 \to j_3) = \sum_{m_1,m_2,m_3} |j_3,\, m_3\rangle \left(\begin{array}{cc|c} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{array}\right) \langle j_1,\, m_1;\, j_2,\, m_2|. \tag{90}$$

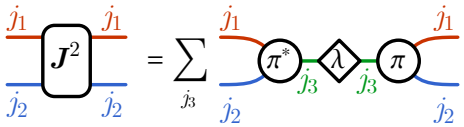
To obtain the CG coefficient,

- either look up in *Mathematica*:

```
ClebschGordan[{1 / 2, -1 / 2}, {1 / 2, 1 / 2}, {1, 0}]
```

$$\frac{1}{\sqrt{2}}$$

- or calculate as eigenbasis of the *Casimir operator* $\boldsymbol{J}^2$:

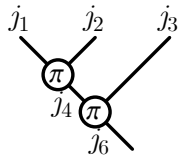


  - Represent $\boldsymbol{J}^2$ in the $j_1 \otimes j_2$ space.
  - Diagonalize $\boldsymbol{J}^2$, group eigenvectors by eigenvalues.
  - Within each degenerated subspace: the eigenvalue $\lambda_{j_3} = j_3(j_3+1)$ or the degeneracy $2\,j_3+1$ infers the spin quantum number j_3, the eigenvectors form the fusion vertex $\pi(j_1 \otimes j_2 \to j_3)$.

▫ Code Example

■ F-Symbols

Fusion vertices can be **composed** to fuse *multiple* spins.



- The composition follows from the *tensor network contraction*.

Given incoming representations j_1, j_2, j_3 and the outgoing representation j_6, there could still be multiple fusion channels, depending on the choice of j_4.

Example: $(1/2 \otimes 1/2) \otimes 1/2 \to 1/2$

- For $j_4 = 0$,

$\alpha_0 = \pi(1/2 \otimes 1/2 \to 0) \circ \pi(0 \otimes 1/2 \to 1/2)$

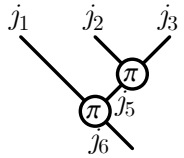
$$\doteq \begin{pmatrix} 0 & 0 & -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & 0 \end{pmatrix},$$

- For $j_4 = 1$,

$$\alpha_1 = \pi(1/2 \otimes 1/2 \to 1) \circ \pi(1 \otimes 1/2 \to 1/2)$$

$$\doteq \begin{pmatrix} 0 & -\sqrt{\frac{2}{3}} & \frac{1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{\sqrt{6}} & 0 & -\frac{1}{\sqrt{6}} & \sqrt{\frac{2}{3}} & 0 \end{pmatrix}. \tag{93}$$

However, we can also fuse the spin in a different order.



Now depending on j_5, there could be multiple fusion channels.

Example: $1/2 \otimes (1/2 \otimes 1/2) \to 1/2$

- For $j_5 = 0$,

$$\beta_0 = \pi(1/2 \otimes 1/2 \to 0) \circ \pi(1/2 \otimes 0 \to 1/2)$$

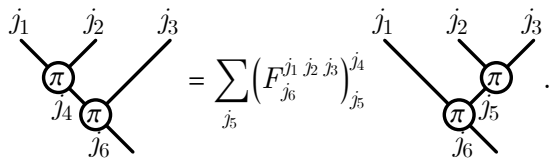
$$\doteq \begin{pmatrix} 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}, \tag{94}$$

- For $j_5 = 1$,

$$\beta_1 = \pi(1/2 \otimes 1/2 \to 1) \circ \pi(1/2 \otimes 1 \to 1/2)$$

$$\doteq \begin{pmatrix} 0 & -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{6}} & 0 & \sqrt{\frac{2}{3}} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\sqrt{\frac{2}{3}} & 0 & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & 0 \end{pmatrix}. \tag{95}$$

The incoming and outgoing representation remains the same, just by changing the fusion order, the resulting fusion tensors are different. For consistency, the two different **fusion trees** must be related. The relation is a *natural transformation* in category theory, which is a *linear transformation* among fusion trees,



$$= \sum_{j_5} \left(F_{j_6}^{j_1\, j_2\, j_3}\right)_{j_5}^{j_4}$$

. (96)

In the example of $1/2 \otimes 1/2 \otimes 1/2 \to 1/2$

$$\begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix}. \tag{97}$$

HW 2 Verify Eq. (92), Eq. (93), Eq. (94), Eq. (95), Eq. (97).

- The matrix $F_{j_6}^{j_1\, j_2\, j_3}$ is called ***F*-matrix**, whose elements are called ***F*-symbols**. The F-matrix is *unitary*.
- F-symbol is related to **Wigner 6 *j*-symbol** by a normalization factor

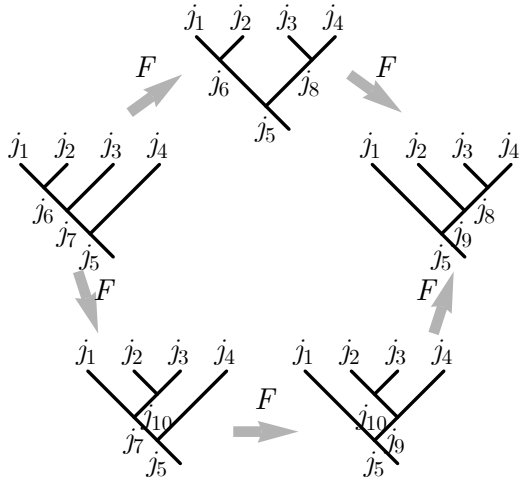
$$\left(F_{j_6}^{j_1\, j_2\, j_3}\right)_{j_5}^{j_4} = (-)^{j_1+j_2+j_3+j_6} \sqrt{(2\,j_4+1)\,(2\,j_5+1)} \begin{Bmatrix} j_1 & j_2 & j_4 \\ j_3 & j_6 & j_5 \end{Bmatrix}. \tag{98}$$

Mathematica knows how to calculate the 6 j-symbol.

```
SixJSymbol[{1 / 2, 1 / 2, 0}, {1 / 2, 1 / 2, 0}]
```

$$-\frac{1}{2}$$

Pentagon Relation: the consistency equation of F-symbols. The left-most and right-most fusion trees of four spins can be related to each other by F-moves in two different sequences. The diagram must commute.



$$\left(F_{j_5}^{j_6\, j_3\, j_4}\right)_{j_8}^{j_7} \left(F_{j_5}^{j_1\, j_2\, j_8}\right)_{j_9}^{j_6} = \sum_{j_{10}} \left(F_{j_7}^{j_1\, j_2\, j_3}\right)_{j_{10}}^{j_6} \left(F_{j_5}^{j_1\, j_{10}\, j_4}\right)_{j_9}^{j_7} \left(F_{j_9}^{j_2\, j_3\, j_4}\right)_{j_8}^{j_{10}}. \tag{99}$$

Fortunately, a mathematical theorem guarantees that the *pentagon relations* are all that need to be satisfied, i.e. all other consistencies are consequences of the pentagon relations.

▪ Wigner-Eckart Theorem

Hydrogen Atom

▪ Classical Mechanical Background

▪ Classical Equation of Motion

- A **hydrogen atom** is a bound state of a single **electron** and a single **proton**.
  - The proton is much *heavier* than the electron (mass ratio $m_p / m_e \approx 1836$), it is essentially pinned at the center of mass.
  - Consider electron moving in the *electric static potential* created by the proton.

$$V(r) = -\frac{k}{r}, \tag{100}$$

  where $k = e^2 / (4\pi\epsilon_0)$ describes the strength of the Coulomb force.

- The **Energy** (Hamiltonian) of the *electron* is given by

$$\boxed{E = \frac{\boldsymbol{p}^2}{2m} - \frac{k}{r},} \tag{101}$$

  - $\boldsymbol{r}$ is the **displacement** from the proton and $r = |\boldsymbol{r}|$ is the electron-proton distance.
  - $\boldsymbol{p} = m\dot{\boldsymbol{r}}$ is the **momentum**.
  - m is the **mass** of electron (or more precisely the *reduced mass* of the electron in this two-body problem).

- The **angular momentum**

$$\boxed{\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}.} \tag{102}$$

- The **classical equation of motion**:

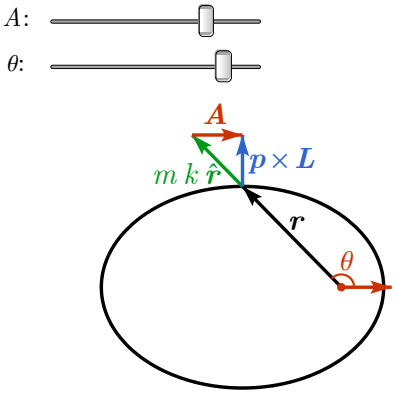
$$\dot{\boldsymbol{r}} = \frac{\boldsymbol{p}}{m}, \ \dot{\boldsymbol{p}} = -\frac{k\,\boldsymbol{r}}{r^3}. \tag{103}$$

  - $\dot{\boldsymbol{L}} = \dot{\boldsymbol{r}} \times \boldsymbol{p} + \boldsymbol{r} \times \dot{\boldsymbol{p}} = 0$ from Eq. (103) $\Rightarrow$ the angular momentum is *conserved*. ($\because$ the Hamiltonian has the SO(3) *rotation symmetry*)

■ Laplace-Runge-Lenz (LRL) Vector

- The **Laplace-Runge-Lenz** (LRL) vector is defined to be

$$\boxed{\boldsymbol{A} = \boldsymbol{p} \times \boldsymbol{L} - m\,k\,\frac{\boldsymbol{r}}{r}.} \tag{104}$$



- The LRL vector is *conserved* (there must be an *symmetry* associate to it, what is it?)

$$\boxed{\dot{\boldsymbol{A}} = 0.} \tag{105}$$

Using Eq. (103),

$$\begin{aligned}
\dot{\boldsymbol{A}} &= \dot{\boldsymbol{p}} \times \boldsymbol{L} - m\,k\,\frac{\dot{\boldsymbol{r}}}{r} + m\,k\,\frac{\boldsymbol{r}}{r^2}\,\dot{r} \\
&= -\frac{k}{r^3}\,\boldsymbol{r} \times (\boldsymbol{r} \times \boldsymbol{p}) - \frac{k}{r}\,\boldsymbol{p} + m\,k\,\frac{\boldsymbol{r}}{r^2}\,\dot{r} \\
&= -\frac{k}{r^3}\left(\boldsymbol{r}\,(\boldsymbol{r} \cdot \boldsymbol{p}) - r^2\,\boldsymbol{p}\right) - \frac{k}{r}\,\boldsymbol{p} + m\,k\,\frac{\boldsymbol{r}}{r^2}\,\dot{r} \\
&= -m\,k\,\frac{\boldsymbol{r}}{r^3}\,(\boldsymbol{r} \cdot \dot{\boldsymbol{r}}) + m\,k\,\frac{\boldsymbol{r}}{r^2}\,\dot{r} = 0
\end{aligned}$$

This conservation law can be used to derive the **Kepler orbit**. Consider

$$\boldsymbol{A} \cdot \boldsymbol{r} = A\,r\cos\theta = \boldsymbol{r} \cdot (\boldsymbol{p} \times \boldsymbol{L}) - m\,k\,r, \tag{106}$$

where θ is the angle between $\boldsymbol{r}$ and $\boldsymbol{A}$. Permuting the scalar triple product $\boldsymbol{r} \cdot (\boldsymbol{p} \times \boldsymbol{L}) = \boldsymbol{L} \cdot (\boldsymbol{r} \times \boldsymbol{p}) = L^2$, Eq. (106) ⇒ the orbit equation

$$\frac{1}{r} = \frac{m\,k}{L^2}\left(1 + \frac{A}{m\,k}\cos\theta\right). \tag{107}$$

- Conservation of the *magnitude* $A = |\boldsymbol{A}| \Rightarrow$ conservation of the *eccentricity* of the orbit (in fact $e \equiv c/a = A/mk$).
- Conservation of the *direction* of $\boldsymbol{A} \Rightarrow$ conservation of the *periapsis* (the point of closest approach) with respect to the force center.

So the LRL vector is conserved.

- $\boldsymbol{L}$ and $\boldsymbol{A}$ are always perpendicular ($\boldsymbol{L}\cdot\boldsymbol{A} = 0$), they fully specifies a *unique* Kepler orbit (shape and orientation are both determined).
- As the orbit is specified, its energy must be determined too $\Rightarrow$ so the energy E is *not* an independent conserved quantity, in fact

$$\boxed{A^2 = m^2 k^2 + 2\, m\, E\, L^2.} \tag{108}$$

- Given the *magnitude* of L and A,
  - All orbits of different orientations are *degenerated* in energy $\Rightarrow$ they are related by **symmetry**.
  - Each orbit orientation $\Leftrightarrow$ a pair of *perpendicular unit* vectors ($\boldsymbol{L}/L$, $\boldsymbol{A}/A$) $\Leftrightarrow$ a particular rotation in 3D space, i.e., a group element of SO(3) $\Leftrightarrow$ a point on (half of) a **4D sphere**! (more precisely a point on RP^3)
  - The symmetry that keeps the 4D sphere *invariant* is **SO(4)** (more precisely, to keep RP^3 invariant, the symmetry is actually $\mathrm{SO}(4)/\mathbb{Z}_2$).
  - SO(4) group has *six* generators, all of them must be *conserved* $\Rightarrow$ corresponding to the conservation of both $\boldsymbol{L}$ and $\boldsymbol{A}$.

HW 3

Let us represent the SO(4) group as 4×4 orthogonal matrices. (a) Show that orthogonal matrices $O = e^{i\theta A}$ are generated by imaginary antisymmetric matrices A (i.e., $A^{\mathsf{T}} = -A \in \mathbb{I}$). (b) Verify that the following six matrices form a complete basis of generators

$$T_1 = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix},\ T_2 = \frac{1}{2}\begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix},\ T_3 = \frac{1}{2}\begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \end{pmatrix};$$

$$S_1 = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix},\ S_2 = \frac{1}{2}\begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix},\ S_3 = \frac{1}{2}\begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix}.$$

(c) Verify the following commutation relations
$[T_i, T_j] = i\,\epsilon_{ijk}\, T_k$, $[S_i, S_j] = i\,\epsilon_{ijk}\, S_k$, $[T_i, S_j] = 0$.
Compare with Eq. (44), we learn that $\mathrm{so}(4) \cong \mathrm{su}(2) \times \mathrm{su}(2)$.

■ Quantum Mechanical Treatment

■ Operator Algebra

We promote *classical observables* to **Hermitian operators**:

- **Coordinate $\boldsymbol{r}$** and **momentum $\boldsymbol{p}$** operators, satisfying $[r_a, p_b] = i\,\delta_{ab}$. See Eq. (42).
- **Angular momentum** operator $\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}$. See Eq. (41).
- **Quantum LRL** operator

$$\boldsymbol{A} = \frac{1}{2}(\boldsymbol{p} \times \boldsymbol{L} - \boldsymbol{L} \times \boldsymbol{p}) - m\,k\,\frac{\boldsymbol{r}}{r}. \tag{109}$$

Compared with the classical case Eq. (104), the additional "anti-symmetrization" is to ensure $\boldsymbol{A}$ to be Hermitian.

- **Hamiltonian** operator

$$H = \frac{\boldsymbol{p}^2}{2\,m} - \frac{k}{r}. \tag{110}$$

One can verify the following commutation relations

$$\begin{aligned}
&[H, L_a] = 0,\\
&[H, A_a] = 0,\\
&[L_a, L_b] = i\,\epsilon_{abc}\,L_c,\\
&[L_a, A_b] = i\,\epsilon_{abc}\,A_c,\\
&[A_a, A_b] = -i\,2\,m\,\epsilon_{abc}\,L_c\,H,
\end{aligned} \tag{111}$$

and the following operator equations

$$\begin{aligned}
&\boldsymbol{A} \cdot \boldsymbol{L} = \boldsymbol{L} \cdot \boldsymbol{A} = 0,\\
&\boldsymbol{A}^2 = 2\,m\,H\big(\boldsymbol{L}^2 + 1\big) + m^2\,k^2.
\end{aligned} \tag{112}$$

■ SO(4) Generators

Suppose there exist *bound states* with energy $E < 0$. In the subspace of a *fixed eigen energy* E (i.e. replacing $H \to E$), it makes sense to rescale the quantum LRL operator $\boldsymbol{A}$ by a scalar

$$\tilde{\boldsymbol{A}} = \frac{1}{\sqrt{-2\,m\,E}}\,\boldsymbol{A}, \tag{113}$$

then Eq. (111) is simplified to

$$\begin{aligned}
&[H, L_a] = 0,\\
&[H, A_a] = 0,
\end{aligned}$$

$$[L_a,\, L_b] = i\,\epsilon_{abc}\,L_c,$$
$$\left[L_a,\, \tilde{A}_b\right] = i\,\epsilon_{abc}\,\tilde{A}_c,$$
$$\left[\tilde{A}_a,\, \tilde{A}_b\right] = i\,\epsilon_{abc}\,L_c.$$

Define the SO(4) generators

$$\boldsymbol{T} = \frac{1}{2}\left(\boldsymbol{L} + \tilde{\boldsymbol{A}}\right),\ \boldsymbol{S} = \frac{1}{2}\left(\boldsymbol{L} - \tilde{\boldsymbol{A}}\right). \tag{115}$$

- How do we know they form SO(4) generators? We check their commutation relations

$$\begin{aligned}
&[H,\, T_a] = 0,\\
&[H,\, S_a] = 0,\\
&[T_a,\, T_b] = i\,\epsilon_{abc}\,T_c,\\
&[S_a,\, S_b] = i\,\epsilon_{abc}\,S_c,\\
&[T_a,\, S_b] = 0.
\end{aligned} \tag{116}$$

- $\boldsymbol{A}\cdot\boldsymbol{L} = \boldsymbol{L}\cdot\boldsymbol{A} = 0$ further implies $\boldsymbol{T}^2 = \boldsymbol{S}^2$.
- $\boldsymbol{T}$ and $\boldsymbol{S}$ are two sets of independent "angular-momentum like" operators.
- Common eigen states of $\boldsymbol{T}$ and $\boldsymbol{S}$ are labeled by three quantum numbers t, m_t, m_s:

$$\begin{aligned}
&\boldsymbol{T}^2\,|t,\, m_t,\, m_s\rangle = \boldsymbol{S}^2\,|t,\, m_t,\, m_s\rangle = t(t+1)\,|t,\, m_t,\, m_s\rangle,\\
&T_3\,|t,\, m_t,\, m_s\rangle = m_t\,|t,\, m_t,\, m_s\rangle,\\
&S_3\,|t,\, m_t,\, m_s\rangle = m_s\,|t,\, m_t,\, m_s\rangle,
\end{aligned} \tag{117}$$

  - $t = 0,\ \frac{1}{2},\ 1,\ \frac{3}{2},\ 2,\ \ldots$. For each fixed $t \Rightarrow (2\,t+1)^2$ degeneracy.
  - $m_t,\, m_s = -t,\, -t+1,\, \ldots,\, t-1,\, t$.

■ Energy Levels

From Eq. (112), Eq. (113), Eq. (115),

$$\begin{aligned}
4\,\boldsymbol{T}^2 &= \boldsymbol{L}^2 + \tilde{\boldsymbol{A}}^2\\
&= \boldsymbol{L}^2 + \frac{1}{-2\,m\,E}\,\boldsymbol{A}^2\\
&= \boldsymbol{L}^2 - \frac{1}{2\,m\,E}\left(2\,m\,E\left(\boldsymbol{L}^2+1\right) + m^2\,k^2\right)\\
&= -1 - \frac{m\,k^2}{2\,E}.
\end{aligned} \tag{118}$$

- On the state $|t,\, m_t,\, m_s\rangle$, $\boldsymbol{T}^2 = t(t+1)$,

$$E = -\frac{m\,k^2}{2\left(4\,\boldsymbol{T}^2+1\right)} = -\frac{m\,k^2}{2\,(2\,t+1)^2}. \tag{119}$$

- Given $t = 0,\ \frac{1}{2},\ 1,\ \frac{3}{2},\ 2,\ \ldots$, define the **principal quantum number**

$$n = 2\,t+1 = 1,\ 2,\ 3,\ 4,\ 5,\ \ldots \tag{120}$$

The **energy levels** are given by $n \in \mathbb{Z}_+$

$$\boxed{E_n = -\frac{m\,k^2}{2\,n^2}.} \tag{121}$$

- The corresponding eigenstates $|t,\ m_t,\ m_s\rangle$ (with $t = (n-1)/2$) are labeled by $m_t,\ m_s = -t,\ -t+1,\ \ldots,\ t-1,\ t \Rightarrow$ level degeneracy: $(2\,t+1)^2 = n^2$.

■ Ground State

Which state is the ground state?

- The energy $E_n = -m\,k^2/\left(2\,n^2\right)$ is minimized when $n = 1$ (or $t = 0$).
- When $t = 0$, m_t and m_s has only one choice, i.e. $m_t = m_s = 0$.
- So the ground state corresponds to the $|0,\ 0,\ 0\rangle$ state.

How to find its wave function $\psi_{1\,s}(\boldsymbol{r})$? This amount to solve the differential equation $\boldsymbol{T}^2\,\psi_{1\,s} = 0$, which is equivalent to

$$H\,\psi_{1\,s} = E_1\,\psi_{1\,s}, \tag{122}$$

or more explicitly as

$$\left(\frac{\boldsymbol{p}^2}{2\,m} - \frac{k}{r}\right)\psi_{1\,s} = -\frac{m\,k^2}{2}\,\psi_{1\,s}. \tag{123}$$

We guess a trial wave function

$$\psi_{1\,s}(\boldsymbol{r}) \propto e^{-r/a}, \tag{124}$$

Eq. (123) implies $a\,k\,m - 1 = 0$, i.e. $a = 1/(k\,m)$.

In conclusion, the (normalized) **ground state wave function** of the electron in the hydrogen atom reads

$$\boxed{\psi_{1\,s}(\boldsymbol{r}) = \frac{2}{a^{3/2}}\,e^{-r/a},} \tag{125}$$

- $a = 1/(k\,m)$ is called the **Bohr radius**.
- The ground state energy is given by

$$\boxed{E_1 = -\frac{k}{2\,a},} \tag{126}$$

as if the electron in orbiting the proton in a circular orbital of radius a (the classical picture).

- The electron is observed randomly in a probability cloud, called the **electron cloud**.

$$p(\boldsymbol{r}) = |\psi(\boldsymbol{r})|^2 \propto e^{-2\,r/a}. \tag{127}$$

■ Excited States

Excited states are labeled by higher *principal quantum numbers* $n = 2, 3, \ldots$ (or $t = \frac{1}{2}, 1, \ldots$).

- States with the same principal quantum numbers are degenerated in energy.
- Within each degenerated sectors, the states $|t, m_t, m_s\rangle$ form a complete set of basis (with $m_t, m_s = -t, \ldots, t$), which can be viewed as a combined system of two "spins" of the same angular momentum t.

The *orbital* angular momentum $\boldsymbol{L}$ of electron is the total angular momentum of the fictitious spins,

$$\boxed{\boldsymbol{L} = \boldsymbol{T} + \boldsymbol{S}.} \tag{128}$$

According to the fusion rules of spins, we anticipate their total angular momentum to take $l = 0, 1, \ldots, 2\,t$ (each representation will appear once). So the excited states may as well be labeled by

$$|n, l, m\rangle \tag{129}$$

- n - **principal** quantum number ($n = 1, 2, \ldots$),
- l - **angular** quantum number ($l = 0, 1, \ldots, n-1$)
- m - **magnetic** quantum number ($m = -l, -l+1, \ldots, l-1, l$)

$|n, l, m\rangle$ and $|t, m_t, m_s\rangle$ are just differed by a basis transformation, but the former basis is more commonly used as **atomic orbitals**, because the electron-electron interaction will break the SO(4) symmetry down to SO(3).

Code