

# Quantum Mechanics II.

Janos Polonyi

*University of Strasbourg*

(Dated: December 1, 2022)

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Quantum mechanics is usually taught on four different levels:

1. Basic ideas, simple examples for a one dimensional particle, particle in spherical potential
2. More realistic, three dimensional cases with few particles ←
3. Several particles, relativistic effects (Quantum Field Theory)
4. Fundamental issues, challenges, paradoxes and interpretation of the quantum world

## I. PERTURBATION EXPANSION

$$H = H_0 + gH_1$$

### A. Stationary perturbations

- **Example:** Atom in an EM field
- **Goal:** solve stationary Schrödinger equation,  $H|\psi_n\rangle = E_n|\psi_n\rangle$
- **Expansion in  $g$ :**

$$\begin{aligned} |\psi_n\rangle &= |\psi_n^{(0)}\rangle + g|\psi_n^{(1)}\rangle + g^2|\psi_n^{(2)}\rangle + \dots, \\ E_n &= E_n^{(0)} + gE_n^{(1)} + g^2E_n^{(2)} + \dots, \\ 0 &= (H_0 + gH_1 - E_n^{(0)} - gE_n^{(1)} - g^2E_n^{(2)} - \dots)(|\psi_n^{(0)}\rangle + g|\psi_n^{(1)}\rangle + g^2|\psi_n^{(2)}\rangle + \dots) \\ &= g^0 \left( H_0|\psi_n^{(0)}\rangle - E_n^{(0)}|\psi_n^{(0)}\rangle \right) \\ &\quad + g \left( H_0|\psi_n^{(1)}\rangle + H_1|\psi_n^{(0)}\rangle - E_n^{(1)}|\psi_n^{(0)}\rangle - E_n^{(0)}|\psi_n^{(1)}\rangle \right) \\ &\quad + g^2 \left( H_0|\psi_n^{(2)}\rangle + H_1|\psi_n^{(1)}\rangle - E_n^{(2)}|\psi_n^{(0)}\rangle - E_n^{(1)}|\psi_n^{(1)}\rangle - E_n^{(0)}|\psi_n^{(2)}\rangle \right) + \dots \end{aligned}$$

Orders one-by-one:

$$\begin{aligned} \mathcal{O}(g^0) : \quad H_0|\psi_n^{(0)}\rangle &= E_n^{(0)}|\psi_n^{(0)}\rangle \\ \mathcal{O}(g) : \quad (H_0 - E_n^{(0)})|\psi_n^{(1)}\rangle &= (E_n^{(1)} - H_1)|\psi_n^{(0)}\rangle \\ \mathcal{O}(g^2) : \quad (H_0 - E_n^{(0)})|\psi_n^{(2)}\rangle &= (E_n^{(1)} - H_1)|\psi_n^{(1)}\rangle + E_n^{(2)}|\psi_n^{(0)}\rangle \\ \mathcal{O}(g^k) : \quad (H_0 - E_n^{(0)})|\psi_n^{(k)}\rangle &= (E_n^{(1)} - H_1)|\psi_n^{(k-1)}\rangle + E_n^{(2)}|\psi_n^{(k-2)}\rangle + \dots + E_n^{(k)}|\psi_n^{(0)}\rangle \end{aligned}$$

- **Zeroth order:** unperturbed stationary states,  $|\psi_n^{(0)}\rangle$ ,  $\langle\psi_m^{(0)}|\psi_n^{(0)}\rangle = \delta_{mn}$
- **Higher order:** no unique solution

1.  $(H_0 - E_n^{(0)})^{-1}$  does not exist in the null space of  $H_0 - E_n^{(0)}$

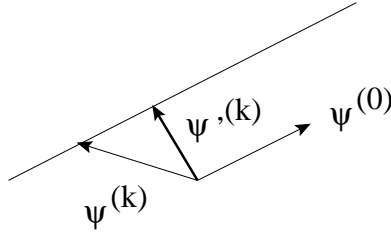


$$\mathcal{N}_A = \{|\psi\rangle | A|\psi\rangle = 0\}$$

2. Another way to see: if  $|\psi_n^{(k)}\rangle$  ( $k > 0$ ) is a solution  $\implies |\psi_n^{\prime(k)}\rangle = |\psi_n^{(k)}\rangle + c|\psi_n^{(0)}\rangle$  is another solution

$$\begin{aligned} (H_0 - E_n^{(0)})(|\psi_n^{(k)}\rangle + c|\psi_n^{(0)}\rangle) &= (H_0 - E_n^{(0)})|\psi_n^{(k)}\rangle \\ &= (E_n^{(1)} - H_1)|\psi_n^{(k-1)}\rangle + E_n^{(2)}|\psi_n^{(k-2)}\rangle + \dots + E_n^{(k)}|\psi_n^{(0)}\rangle \end{aligned}$$

3. Unique solution: choose  $c = -\langle\psi_n^{(0)}|\psi_n^{(k)}\rangle \implies \langle\psi_n^{(0)}|\psi_n^{\prime(k)}\rangle = \langle\psi_n^{(0)}|(|\psi_n^{(k)}\rangle - |\psi_n^{(0)}\rangle\langle\psi_n^{(0)}|\psi_n^{(k)}\rangle) = 0$



- **First order:** One writes  $|\psi_n^{(1)}\rangle = \sum_{\ell} c_{n,\ell} |\psi_{\ell}^{(0)}\rangle$

$$\begin{aligned} \langle\psi_k^{(0)}| (H_0 - E_n^{(0)})|\psi_n^{(1)}\rangle &= (E_n^{(1)} - H_1)|\psi_n^{(0)}\rangle \\ \sum_{\ell} c_{n,\ell} \langle\psi_k^{(0)}|(H_0 - E_n^{(0)})|\psi_{\ell}^{(0)}\rangle &= \langle\psi_k^{(0)}|(E_n^{(1)} - H_1)|\psi_n^{(0)}\rangle \\ \sum_{\ell} c_{n,\ell} \langle\psi_k^{(0)}|(E_k^{(0)} - E_n^{(0)})|\psi_{\ell}^{(0)}\rangle &= \langle\psi_k^{(0)}|(E_n^{(1)} - H_1)|\psi_n^{(0)}\rangle \\ \langle\psi_k^{(0)}|\psi_{\ell}^{(0)}\rangle = \delta_{k,\ell} \quad \rightarrow \quad (E_k^{(0)} - E_n^{(0)})c_{n,k} &= E_n^{(1)}\delta_{k,n} - H_{1kn} \quad \leftarrow \quad \langle\psi_k^{(0)}|H_1|\psi_n^{(0)}\rangle \end{aligned}$$

Solution:

$$c_{n,k} = \begin{cases} \frac{H_{1kn}}{E_n^{(0)} - E_k^{(0)}}, & k \neq n \\ 0 & k = n, \end{cases}$$

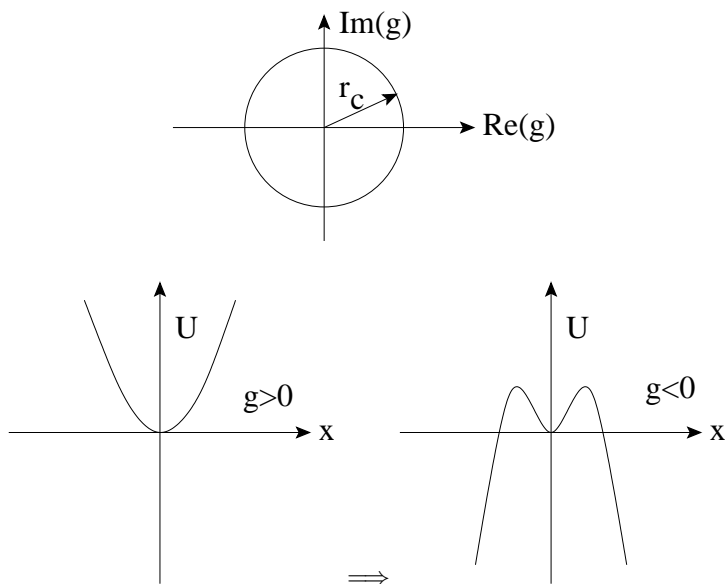
$$E_n^{(1)} = H_{1nn}$$

- **Necessary conditions:**

$$\begin{aligned} g\langle\psi_n^{(0)}|H_1|\psi_n^{(0)}\rangle &\ll E_n^{(0)} \\ g|\langle\psi_k^{(0)}|H_1|\psi_n^{(0)}\rangle| &\ll |E_n^{(0)} - E_k^{(0)}|. \end{aligned}$$

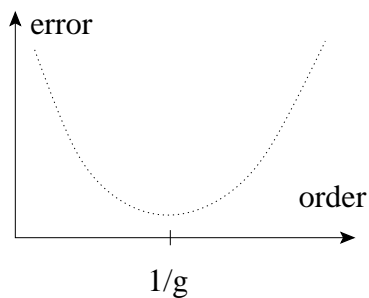
- **Convergence radius:**  $r_c = 0$

$$H = \frac{p^2}{2m} + U(x), \quad U(x) = \frac{m\omega^2}{2}x^2 + \frac{g}{4!}x^4, \quad g \rightarrow -g ?$$



• **Asymptotic convergence:**

1. Definition:  $f_N(g) = \sum_{n=0}^N f_n g^n \rightarrow_{as} f(g)$  if  $\frac{f_N(g) - f(g)}{g^N} \rightarrow 0$  as  $g \rightarrow 0$
2. Quantum mechanical systems:  $|f_N(g) - f(g)|$  starts to grow at  $N = \mathcal{O}\left(\frac{1}{g}\right)$  (QED:  $g = \frac{1}{137}$ )



• **Degenerate perturbations:**

1. *Problem:*

- (a)  $H_0|\psi_n^{(0)}\rangle = E_n^{(0)}|\psi_n^{(0)}\rangle \implies |\psi_n^{(0)}\rangle$  is ill defined within the degenerate subspace
- (b) *The higher orders* in  $|\psi_n\rangle = |\psi_n^{(0)}\rangle + g|\psi_n^{(1)}\rangle + g^2|\psi_n^{(2)}\rangle + \dots$  are not small
- (c) *Singularity* at  $g = 0$
- (d)  $g|\langle\psi_k^{(0)}|H_1|\psi_n^{(0)}\rangle| \ll |E_n^{(0)} - E_k^{(0)}|$  is violated

2. *Solution:* diagonalize  $H_1$  within the degenerate subspace

3. *Degeneracy:*  $E_k^{(0)} = E_\ell^{(0)}$  for  $1 \leq k, \ell \leq N \ll \dim(H)$

$$H_1 = \begin{pmatrix} \begin{pmatrix} H_{1,1,1} & 0 & \cdots & 0 \\ 0 & H_{1,2,2} & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & 0 & \cdots & H_{1,N,N} \end{pmatrix} & B \\ B^\dagger & H'_1 \end{pmatrix},$$

and suppose that  $H_{1,j,j} \neq H_{1,k,k}$  for  $j \neq k$ .

4. *Secular equation:*

- Eigenvalues:  $A|\psi\rangle = a|\psi\rangle \leftrightarrow (A - a\mathbb{1})|\psi\rangle = 0 \leftrightarrow \det(A - a\mathbb{1}) = 0$
- $\det[H_{1,k\ell} - \delta_{k,\ell}E_k^{(1)}] = 0 \leftrightarrow E_k^{(1)} = H_{1,kk}$

5. *Higher orders are regular:*

$$\begin{aligned} |\psi_k\rangle &= |\psi_k^{(0)}\rangle + \mathcal{O}(g) \\ E_k &= E_k^{(0)} + gH_{1kk} + \mathcal{O}(g^2) \end{aligned}$$

6. *Physical importance:*

(a) The increased sensitivity of the eigenfunctions on the perturbations: large  $\left| \frac{\langle \psi_n^{(0)} | H_1 | \psi_k^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}} \right|$

Weak interactions become more important for exact or approximate degeneracy

(b) An atom interacting with an ideal gas in box  $L$ :

- Typical level spacing of the gas:  $\Delta E \sim \frac{\hbar^2}{mL^2}$
- "Small" parameter of the perturbation expansion:

$$\frac{gH_{1kn}}{\frac{\hbar^2}{mL^2}} \sim 10^{54} mL^2 g H_{1kn} > 1$$

( $m, L$  expressed gram and centimeter)

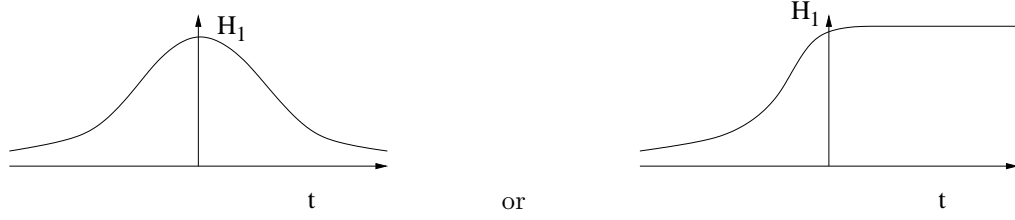
- Classical limit in quantum mechanics
- Relaxation in statistical physics (starting point of Statistical Mechanics)

## B. Time dependent perturbations

1. **Example:** Atom in time-dependent EM field

2. **Goal:**

$$i\hbar\partial_t|\psi\rangle = H|\psi\rangle, \quad H = H_0 + gH_1(t),$$



### 3. Typical problem:

Initial condition:  $|\psi(t = t_i)\rangle = e^{-i\frac{t_i}{\hbar}E_k^{(0)}}|\psi_n^{(0)}\rangle$ ,  $H_0|\psi_k^{(0)}\rangle = E_k^{(0)}|\psi_k^{(0)}\rangle$

Transition probability:

$$P_{n \rightarrow k}(t) = |\langle \psi_k^{(0)} | \psi(t) \rangle|^2$$

### 4. Time-dependence of the state:

$$|\psi(t)\rangle = \sum_k c_k(t) |\psi_k^{(0)}(t)\rangle$$



interaction



unperturbed dynamics

Time dependent basis:

$$\begin{aligned} i\hbar \partial_t |\psi_k^{(0)}(t)\rangle &= H_0 |\psi_k^{(0)}(t)\rangle \\ H_0 |\psi_k^{(0)}(0)\rangle &= E_k^{(0)} |\psi_k^{(0)}(0)\rangle \\ |\psi_k^{(0)}(t)\rangle &= e^{-i\frac{t}{\hbar}E_k^{(0)}} |\psi_k^{(0)}(0)\rangle \end{aligned}$$

### 5. Schrödinger equation:

$$\begin{aligned} i\hbar \partial_t |\psi(t)\rangle &= [H_0 + gH_1(t)] |\psi(t)\rangle \\ i\hbar \sum_k (\partial_t c_k(t) |\psi_k^{(0)}(t)\rangle + c_k(t) \underbrace{\partial_t |\psi_k^{(0)}(t)\rangle}_{\frac{1}{i\hbar} H_0 |\psi_k^{(0)}(t)\rangle}) &= [H_0 + gH_1(t)] \sum_k c_k(t) |\psi_k^{(0)}(t)\rangle \\ \langle \psi_\ell^{(0)} | i\hbar \sum_k \partial_t c_k(t) |\psi_k^{(0)}(t)\rangle &= gH_1(t) \sum_k c_k(t) \langle \psi_\ell^{(0)} | \psi_k^{(0)}(t)\rangle \\ i\hbar \partial_t c_\ell(t) &= g \sum_k \underbrace{\langle \psi_\ell^{(0)}(t) | H_1(t) | \psi_k^{(0)}(t)\rangle}_{H_{1\ell k}(t)} c_k(t) = g \sum_k H_{1\ell k}(t) c_k(t) \end{aligned}$$

Order by order:

$$\begin{aligned} c_\ell(t) &= \sum_k g^k c_\ell^{(k)}(t) \\ \mathcal{O}(g^0) : i\hbar \partial_t c_\ell^{(0)}(t) &= 0 \\ \mathcal{O}(g^m) : i\hbar \partial_t c_\ell^{(m)}(t) &= \sum_k H_{1\ell k}(t) c_k^{(m-1)}(t) \end{aligned}$$

6. **Factorizable interaction:**  $H_1(t) = f(t)H'$

$$\begin{aligned}
c_k^{(0)}(t) &= c_k^{(0)}(t_i) = \delta_{k,n} \quad \rightarrow \quad c_k^{(m)}(t_i) = \delta_{m,0}\delta_{k,n} \\
c_k^{(1)}(t) &= c_k^{(1)}(t_i) - \frac{i}{\hbar} \int_{-\infty}^t dt' H_{1kn}(t') = -\frac{i}{\hbar} \int_{-\infty}^t dt' H_{1kn}(t') \\
c_k(t) &= \delta_{k,n} - i \frac{g}{\hbar} \int_{-\infty}^t dt' H_{1kn}(t') + \mathcal{O}(g^2) \\
H_{1\ell k}(t) &= e^{i\frac{t}{\hbar}E_\ell^{(0)}} \langle \psi_\ell^{(0)}(0) | H' | \psi_k^{(0)}(0) \rangle e^{-i\frac{t}{\hbar}E_k^{(0)}} f(t) = H'_{\ell k} e^{i\omega_{\ell k} t} f(t) \\
\hbar\omega_{\ell k} &= E_\ell^{(0)} - E_k^{(0)}, \quad H'_{\ell k} = \langle \psi_\ell^{(0)}(0) | H' | \psi_k^{(0)}(0) \rangle \\
c_k(t) &= \delta_{k,n} - i \frac{gH'_{kn}}{\hbar} \int_{-\infty}^t dt' f(t') e^{i\omega_{k,n}t'} + \mathcal{O}(g^2)
\end{aligned}$$

7. Transition probability:

$$P_{n(\neq k) \rightarrow k}(t) = |c_k(t)|^2 = \left| \frac{gH'_{kn}}{\hbar} \int_{-\infty}^t dt' f(t') e^{i\omega_{kn}t'} \right|^2 + \mathcal{O}(g^3)$$

8. **Example:** Sinusoidal perturbation is turned on suddenly

- Transition amplitude:

$$\begin{aligned}
f(t) &= \begin{cases} 2 \cos \omega t, & \omega > 0 \quad t > 0 \\ 0 & t < 0, \end{cases} \\
c_{k \neq n} &= -\frac{igH'_{kn}}{\hbar} \int_0^t dt' e^{i\omega_{k,n}t'} \left( e^{i\omega t'} + e^{-i\omega t'} \right) \\
&= -\frac{gH'_{kn}}{\hbar} \left( \frac{e^{i(\omega_{k,n}-\omega)t} - 1}{\omega_{k,n} - \omega} + \frac{e^{i(\omega_{k,n}+\omega)t} - 1}{\omega_{k,n} + \omega} \right) \quad \left[ \int dt e^{i\omega t} = \frac{e^{i\omega t}}{i\omega} \right] \\
e^{i\phi} - 1 &= e^{i\frac{\phi}{2}} \left( e^{i\frac{\phi}{2}} - e^{-i\frac{\phi}{2}} \right) = 2ie^{i\frac{\phi}{2}} \sin \frac{\phi}{2} \\
c_{k \neq n} &= -\frac{2igH'_{k,n}}{\hbar} \left( \frac{e^{\frac{i}{2}(\omega_{kn}-\omega)t} \sin \frac{\omega_{kn}-\omega}{2} t}{\omega_{kn} - \omega} + \frac{e^{\frac{i}{2}(\omega_{kn}+\omega)t} \sin \frac{\omega_{kn}+\omega}{2} t}{\omega_{kn} + \omega} \right)
\end{aligned}$$

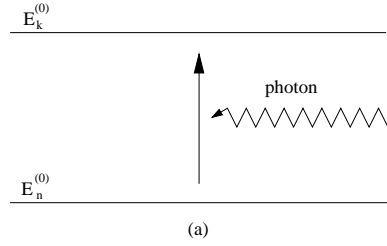
- Transition probability for  $\omega \approx |\omega_{kn}|$ :

$$\begin{aligned}
P &\approx \begin{cases} P^+ & \omega_{kn} > 0 \text{ (absorption)}, \\ P^- & \omega_{kn} < 0 \text{ (emission)}, \end{cases} \\
P_{n \rightarrow k}^\pm &= \frac{4g^2 |H'_{k,n}|^2}{\hbar^2 (\omega_{kn} \mp \omega)^2} \sin^2 \frac{1}{2} (\omega_{kn} \mp \omega) t.
\end{aligned}$$

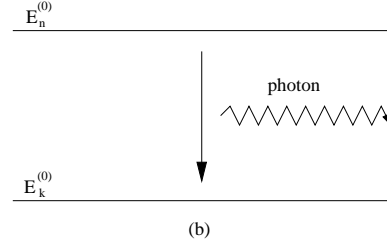
- Small and large  $t$  asymptotics:

$$\begin{aligned}
t \approx 0 : P_{n \rightarrow k}^\pm &= t^2 \frac{|gH_{kn}|^2}{\hbar^2} \\
t \rightarrow \infty : w_{n \rightarrow k}^\pm &= \frac{P_{n \rightarrow k}^\pm}{t} = \frac{2\pi |gH'_{kn}|^2}{\hbar^2} \frac{2 \sin^2 \frac{t(\omega_{kn} \mp \omega)}{2}}{\pi t (\omega_{kn} \mp \omega)^2} = \frac{2\pi |gH'_{kn}|^2}{\hbar^2} \delta_t(\omega_{kn} \mp \omega)
\end{aligned}$$





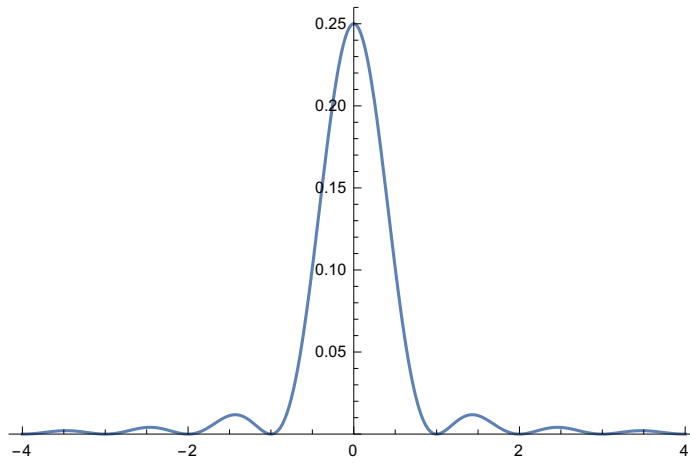
absorption:  $P_{n \rightarrow k}^+ = P(n + \gamma \rightarrow k)$



emission:  $P_{n \rightarrow k}^- = P(n \rightarrow k + \gamma)$

$$\delta(x) = \frac{2}{\pi} \lim_{\eta \rightarrow \infty} \frac{\sin^2 \frac{\eta x}{2}}{\eta x^2}$$

$$x = \frac{t(\omega_{kn} \mp \omega)}{2\pi}, \frac{\sin^2 \pi x}{(2\pi x)^2}:$$



### C. Non-exponential decay rate

#### 1. Time dependence:

- Initial state:  $|\psi_{in}\rangle$  at  $t = 0$ ,  $H|\psi_{in}\rangle \neq E|\psi_{in}\rangle$
- Time evolution:

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}Ht}|\psi_{in}\rangle$$

- Probability to preserve the initial state:

$$P_0(t) = |A(t)|^2$$

- Persistence amplitude:

$$A(t) = \langle \psi_{in} | e^{-\frac{i}{\hbar}Ht} | \psi_{in} \rangle.$$

- The decay is usually not exponential and has short, intermediate and long time regimes.

## 2. Short time regime:

- Persistence amplitude:

$$\begin{aligned}
A(t) &= 1 - \frac{it}{\hbar} \langle \psi_{in} | H | \psi_{in} \rangle - \frac{t^2}{2\hbar^2} \langle \psi_{in} | H^2 | \psi_{in} \rangle + \mathcal{O}(t^3) \\
P_0(t) &= \left( 1 - \frac{it}{\hbar} \langle \psi_{in} | H | \psi_{in} \rangle - \frac{t^2}{2\hbar^2} \langle \psi_{in} | H^2 | \psi_{in} \rangle \right) \left( 1 + \frac{it}{\hbar} \langle \psi_{in} | H | \psi_{in} \rangle - \frac{t^2}{2\hbar^2} \langle \psi_{in} | H^2 | \psi_{in} \rangle \right) + \mathcal{O}(t^3) \\
&= 1 + \frac{t^2}{\hbar^2} \langle \psi_{in} | H | \psi_{in} \rangle^2 - \frac{t^2}{\hbar^2} \langle \psi_{in} | H^2 | \psi_{in} \rangle + \mathcal{O}(t^3) \\
&= 1 - \frac{t^2}{t_Z^2} + \mathcal{O}(t^3), \quad t_Z = \frac{\hbar}{\sqrt{\langle \psi_{in} | (H - \langle \psi_{in} | H | \psi_{in} \rangle)^2 | \psi_{in} \rangle}} \leftarrow \text{Zeno time}
\end{aligned}$$

## 3. Intermediate time regime:

- Projection operators:  $P^\dagger = P$ ,  $P^2 = P$  (spectrum =  $\{0, 1\}$ )

- (a) Longitudinal:

$$\begin{aligned}
L &= |\psi_{in}\rangle \langle \psi_{in}|, \quad \langle \psi_{in} | \psi_{in} \rangle = 1 \\
L|\psi\rangle &= |\psi_{in}\rangle \langle \psi_{in} | \psi \rangle \\
L^2|\psi\rangle &= |\psi_{in}\rangle \langle \psi_{in} | \psi_{in} \rangle \langle \psi_{in} | \psi \rangle = |\psi_{in}\rangle \langle \psi_{in} | \psi \rangle = L|\psi\rangle
\end{aligned}$$

- (b) Transverse:

$$\begin{aligned}
T &= \mathbb{1} - L \\
T^2 &= (\mathbb{1} - L)(\mathbb{1} - L) = \mathbb{1} - 2L + L^2 = T \\
\langle \psi_{in} | T | \psi \rangle &= \langle \psi_{in} | (\mathbb{1} - |\psi_{in}\rangle \langle \psi_{in}|) | \psi \rangle = 0
\end{aligned}$$

- Separation of the longitudinal and transverse parts of the state:

$$\begin{aligned}
|\psi(t)\rangle &= \underbrace{(\mathbb{1} + T)}_{\mathbb{1}} e^{-\frac{i}{\hbar} H t} |\psi_{in}\rangle \\
&= |\psi_{in}\rangle \langle \psi_{in} | e^{-\frac{i}{\hbar} H t} | \psi_{in} \rangle + T e^{-\frac{i}{\hbar} H t} |\psi_{in}\rangle \\
&= |\psi_{in}\rangle A(t) + |\phi(t)\rangle
\end{aligned}$$

↗

decay product,  $\langle \psi_{in} | \phi(t) \rangle = 0$

- Functional equation for the persistence amplitude:

$$\begin{aligned}
\langle \psi_{in} | e^{-\frac{i}{\hbar} H t'} | \psi(t) \rangle &= \langle \psi_{in} | e^{-\frac{i}{\hbar} H t'} | \psi_{in} \rangle A(t) + \langle \psi_{in} | e^{-\frac{i}{\hbar} H t'} | \phi(t) \rangle \\
A(t+t') &= A(t)A(t') + \underbrace{\langle \psi_{in} | e^{-\frac{i}{\hbar} H t'} | \phi(t) \rangle}_{\text{re-excitation}}
\end{aligned}$$

- Without re-excitation:  $A(t + t') = A(t)A(t') \implies A(t) = A(0)e^{-\frac{t}{\tau}}$
- Evolution of the decay product back to the undecayed state: deviation from the exponential decay
- Irreversibility:

(a)  $H^\dagger = H \implies$  there is always a regenerated undecayed state component:

$$\begin{aligned} P_{n \rightarrow k}^\pm &= \frac{4g^2 |H'_{k,n}|^2}{\hbar^2 (\omega_{kn} \mp \omega)^2} \sin^2 \frac{1}{2} (\omega_{kn} \mp \omega) t \\ P_{n \rightarrow k}^+ &= P_{k \rightarrow n}^- \end{aligned}$$

(b) Irreversibility, non-unitary time evolution is needed to arrive at exponential decays

- Spectral representation:

(a) Spectral function:  $H|n\rangle = E_n|n\rangle$

$$\begin{aligned} |\psi_{in}\rangle &= \mathbb{1}|\psi_{in}\rangle = \sum_n |n\rangle \langle n|\psi_{in}\rangle \\ A(t) &= \sum_n |\langle n|\psi_{in}\rangle|^2 e^{-\frac{i}{\hbar} E_n t} \\ &= \sum_n |\langle n|\psi_{in}\rangle|^2 \int dE \delta(E - E_n) e^{-\frac{i}{\hbar} E t} \\ &= \int dE \underbrace{\sum_n |\langle n|\psi_{in}\rangle|^2 \delta(E - E_n)}_{\rho(E)} e^{-\frac{i}{\hbar} E t} = \int dE \rho(E) e^{-\frac{i}{\hbar} E t} \end{aligned}$$

(b)  $A(t)$  and  $\rho(E)$  are related by Fourier transformation

(c) ‘‘Uncertainty relation’’: the width of  $A(t)$  and  $\rho(E)$  are inversely proportional

(d) There is no universal decay law

(e) Exponential decay: Lorentzian spectral weight,

$$\rho(E) = \frac{\Delta E}{\pi[(E - E_0)^2 + \Delta E^2]} \quad \rightarrow \quad A(t) = e^{-i\frac{E_0}{\hbar}t} e^{-\frac{\Delta E}{\hbar}|t|}$$

(f) Natural line width of atomic spectra:

i. Partial resummation of the perturbation series of QED

ii. Decay of excited state  $\implies$  finite life-time  $\implies E \rightarrow E - i\frac{\hbar}{\tau}$ ,  $e^{-\frac{i}{\hbar}Et} \rightarrow e^{-\frac{i}{\hbar}(E - i\frac{\hbar}{\tau})t} = e^{-\frac{i}{\hbar}Et} e^{-\frac{t}{\tau}}$

#### 4. Long time regime:

(a) Boundedness of the Hamiltonian from below:  $\rho(E) = 0$  for  $E < E_0$

(b) Shrunk of the support of a Lorentzian spectral function  $\rho(E) = 0 \implies$  spread of  $A(t)$

(c) Slower than exponential decay rate for long time

### D. Quantum Zeno-effect

1. **Zeno:** (b. Elea, 488BC) Achilles can not pass a tortoise!
2. **Quantum Zeno effect:** (short time, the parabolic decay regime)

- We observe the system at times  $j\Delta t$ ,  $\Delta t = t/n$ ,  $j = 1, \dots, n$
- Schrödinger equation is local in time  $\implies$  the eventual decays are independent

$$\begin{aligned} i\hbar\partial_t|\psi(t)\rangle &= H|\psi(t)\rangle \\ |\psi((j+1)\Delta t)\rangle &= e^{-\frac{i}{\hbar}\Delta t H}|\psi(j\Delta t)\rangle \\ P_0(t+\Delta t) &= P_0(\Delta t)P_0(t) \end{aligned}$$

- Probability of not having decay:

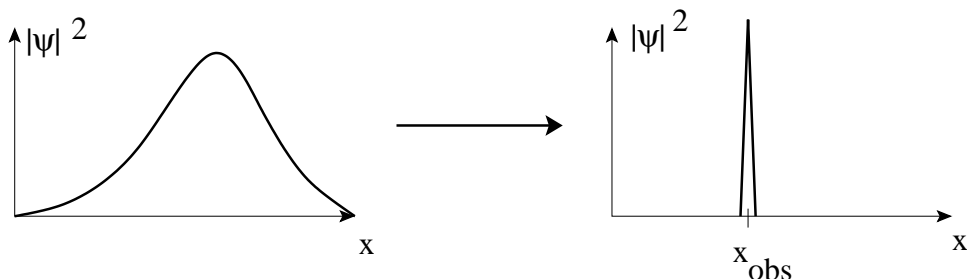
$$\begin{aligned} P_0(t) &= P_0^n(\Delta t) \\ &= \left[ 1 - \left( \frac{t}{nt_Z} \right)^2 + \mathcal{O}(n^{-3}) \right]^n \\ &= e^{n \ln[1 - (\frac{t}{nt_Z})^2 + \mathcal{O}(n^{-3})]} \rightarrow 1 \end{aligned}$$

- Continuously monitored radioactive atom does not decay:
  - (a) Undecayed state is completely regenerated by the collapse of the wave function (observations)
  - (b) Wave function has no time to spread, an  $\mathcal{O}(\Delta t^2)$  effect
- Watched pot paradox: (water does not boil in a continuously watched pot)

### 3. Measurement process:

- Microscopic  $\implies$  macroscopic transition (e.g. tracks in Wilson's cloud chamber)
- Selection of a spectral element of the observable,  $a_n$ 

$$A|n\rangle = a_n|n\rangle, |\psi\rangle = \sum_n c_n|n\rangle, \langle\psi|\psi\rangle = 1, \langle\psi|A|\psi\rangle = \sum_n |c_n|^2 a_n$$
- Collapse of the wave function



- Non-deterministic choice of  $x_{obs}$ 
  - QM: averages only.
  - No deterministic, causal theory for a single event
- Reality???
- Quantum Bar Kochba game
- Hidden parameter theories:
  - Classical description of each microscopical quantity by the help of so far unobserved classical degrees of freedom
  - Non-local  $\implies$  acausality
  - Contextuel  $\implies$  no mathematical structure
    - \* Three observables,  $A, B$  and  $C$ ,  $[A, B] = [A, C] = 0$ ,  $[B, C] \neq 0$
    - \* The value of  $A$  depends on whether we measure  $B$  or  $C$  simultaneously.

### E. Time-energy uncertainty principle

#### 1. Heisenberg's uncertainty principle:

(a) Algebraic derivation:

$$[A, B] = iC, \quad A = A^\dagger, \quad B = B^\dagger, \quad C = C^\dagger$$

$$A_0 = A - \langle A \rangle, \quad B_0 = B - \langle B \rangle, \quad \langle A \rangle = \begin{cases} \langle \psi | A | \psi \rangle & \text{pure state} \\ \text{Tr} \rho A & \text{mixed state} \end{cases}, \quad [A_0, B_0] = iC$$

$$\Delta A^2 = \langle A_0^2 \rangle = \langle A^2 \rangle - \langle A \rangle^2, \quad \Delta B^2 = \langle B_0^2 \rangle = \langle B^2 \rangle - \langle B \rangle^2$$

Non-negative norm:  $O = A_0 + ixB_0$ ,  $x \in \mathcal{R}$

$$\langle OO^\dagger \rangle = \langle A_0^2 \rangle - ix\langle [A_0, B_0] \rangle + x^2 \langle B_0^2 \rangle \geq 0$$

$$x_{min} = -\frac{\langle C \rangle}{2\langle B_0^2 \rangle}$$

Uncertainty:

$$\boxed{\Delta A \Delta B \geq \frac{1}{2} |\langle C \rangle|}$$

(b) Fourier transformation for  $x$  and  $p$ : Gaussian wave packet,

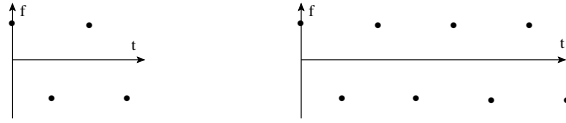
$$\psi(x) = \int \frac{dk}{2\pi} e^{ikx - \frac{k^2}{2\sigma^2}} = \frac{\sqrt{2\pi}}{\sigma} e^{-\frac{\sigma^2 x^2}{2}}$$

Uncertainty:

$$\psi(x) = e^{-\frac{x^2}{2\Delta x^2}}, \quad \tilde{\psi}(k) = e^{-\frac{k^2}{2\Delta k^2}} \implies \Delta x \Delta k = 1, \quad \Delta x \Delta p = \hbar$$

## 2. Frequency and observation time:

(a) Intuitive approach:  $T\Delta\omega \approx 1$ ,  $E = \hbar\omega$ ,  $T\Delta E \approx \hbar$



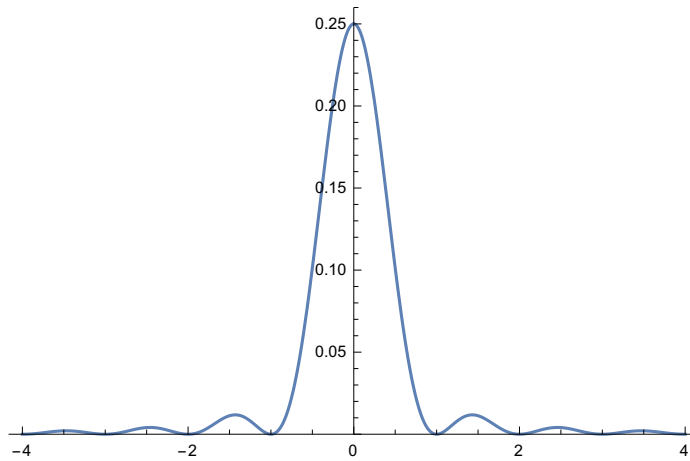
(b) Fourier transformation

(c) Width of the energy spread:

$$P_{n \rightarrow k \neq n}^{\pm} = \frac{4g^2 |H'_{k,n}|^2}{\hbar^2 (\omega_{kn} \pm \omega)^2} \sin^2 \frac{1}{2} (\omega_{kn} \pm \omega) t$$

$$t\Delta|\omega \pm \omega_{k,n}| \approx 2\pi, \quad \Delta E t \approx 2\pi\hbar.$$

$$\frac{\sin^2 \pi x}{(2\pi x)^2}.$$



## F. Fermi's golden rule

- Transition from discrete to continuous spectrum
- Final states are assumed to be decohered (no interference)

$$P_{\text{cont.} \leftarrow \text{discr.}} = \int dE g(E) \frac{|gH_{\text{cont.}, \text{discr.}}|^2}{\hbar^2} \frac{4 \sin^2 \frac{1}{2} (\omega_{\text{cont.}, \text{discr.}} \pm \omega) t}{(\omega_{\text{cont.}, \text{discr.}} \pm \omega)^2},$$

- Spectral density:  $g(E)$  the number of state in the energy interval  $[E, E + \Delta E]$
- Change of variable:  $E = \hbar\omega \rightarrow \beta = \frac{1}{2} (\omega_{\text{cont.}, \text{discr.}} \pm \omega) t$ ,  $d\beta = dE \frac{t}{2\hbar}$

$$P_{\text{cont.} \leftarrow \text{discr.}} = \frac{2t}{\hbar} \int d\beta g(E) |gH_{\text{cont.}, \text{discr.}}|^2 \frac{\sin^2 \beta}{\beta^2}.$$

- Assuming that  $t$  is large enough to keep  $g(E)$  approximately constant

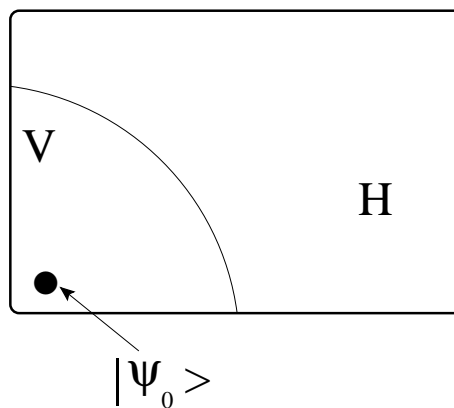
$$\int_{-\infty}^{\infty} d\beta \frac{\sin^2 \beta}{\beta^2} = \pi$$

$$P_{\text{cont.} \leftarrow \text{discr.}} \approx t \frac{2\pi}{\hbar} g(E) |g H_{\text{cont.,discr.}}|^2$$

### G. Variational method

- A non-perturbative and not completely systematic approximation
- An approach of the non-degenerate ground state:

- Hilbert space of states:  $H$
- Variational subset:  $V = \{|\psi(\alpha)\rangle\} \subset H$



- Minimization of the energy:

$$H|\psi_n\rangle = E_n|\psi_n\rangle, \quad E_0 \leq E_1 \leq E_2 \leq \dots$$

$$|\psi(\alpha)\rangle = \sum_n c_n(\alpha) |n\rangle$$

$$E(\alpha) = \frac{\langle \psi(\alpha) | H | \psi(\alpha) \rangle}{\langle \psi(\alpha) | \psi(\alpha) \rangle} = \frac{\sum_n |c_n(\alpha)|^2 E_n}{\sum_n |c_n(\alpha)|^2} \geq E_0$$

- Lower is  $E(\alpha)$ ,  $|\psi(\alpha)\rangle$  is a better approximation of  $|\psi_0\rangle$

$$E(\alpha) = E_0 \implies |\psi(\alpha)\rangle = |\psi_0\rangle$$

- Problems with degenerate ground state or spectrum with small gap ( $E_1 - E_0 \ll E_0$ )

## II. ROTATIONS

### A. Translations

1. **Classical physics:** coordinate space

$$\mathbf{r} \rightarrow T(\mathbf{a})\mathbf{r} = \mathbf{r} + \mathbf{a}.$$

2. **Functions in space:**

$$f(\mathbf{r}) \rightarrow f'(\mathbf{r}') = f(\mathbf{r}' - \mathbf{a}).$$

3. **Quantum mechanics:** Hilbert space

$$\psi(\mathbf{r}) \rightarrow U(T(\mathbf{a}))\psi(\mathbf{r}) = \psi(\mathbf{r} - \mathbf{a}).$$

4. **Representation:**  $T(\mathbf{a}) \rightarrow U(T(\mathbf{a}))$  preserves the algebraic structure

$$U(T(\mathbf{a}))U(T(\mathbf{b}))\psi(\mathbf{r}) = \psi(\mathbf{r} - \mathbf{a} - \mathbf{b}) = U(T(\mathbf{a} + \mathbf{b}))\psi(\mathbf{r})$$

5. **Unitary representation:**

$$\begin{aligned} \langle \psi | \phi \rangle &= \langle U\psi | U\phi \rangle = \langle \psi | \underbrace{U^\dagger U}_{U^\dagger U = \mathbb{1}} | \phi \rangle \\ \int d\mathbf{x} \psi^*(\mathbf{x} - \mathbf{a})\phi(\mathbf{x} - \mathbf{a}) &= \int d\mathbf{x} \psi^*(\mathbf{x})\phi(\mathbf{x}) \end{aligned}$$

6. **Infinitesimal translations:**

$$\begin{aligned} \mathbf{r} &\rightarrow \mathbf{r} + \delta\mathbf{r} \\ \psi(\mathbf{r}) &\rightarrow \psi(\mathbf{r}) - \delta\mathbf{r} \cdot \nabla \psi(\mathbf{r}) = \psi(\mathbf{r}) - \frac{i}{\hbar} \delta\mathbf{r} \cdot \vec{G} \psi(\mathbf{r}) \end{aligned}$$

$$\text{Generator: } \vec{G} = \frac{\hbar}{i} \nabla = \mathbf{p}$$

7. **Finite translations:**

$$\psi(\mathbf{r}) \rightarrow \psi(\mathbf{r} - \mathbf{a}) = \sum_{n=0}^{\infty} \frac{(-\mathbf{a} \cdot \nabla)^n}{n!} \psi(\mathbf{r}) = e^{-\mathbf{a} \cdot \nabla} \psi(\mathbf{r}) = e^{-\frac{i}{\hbar} \mathbf{a} \cdot \mathbf{p}} \psi(\mathbf{r})$$

$$\boxed{U(\mathbf{a}) = e^{-\frac{i}{\hbar} \mathbf{a} \cdot \mathbf{p}}}$$



## B. Rotations

### 1. Classical physics:

- *3x3 matrix:*

$$\mathbf{r} \rightarrow R_{\mathbf{n}}(\alpha)\mathbf{r}$$

$\nearrow$   
axis

$\nwarrow$   
angle

- *Orthogonality:*

$$(\mathbf{u}, \mathbf{v}) = \sum_j u_j v_j = (R\mathbf{u}, R\mathbf{v}) = \sum_j (R\mathbf{u})_j (R\mathbf{v})_j = \sum_{jkl} R_{jk} u_k R_{jl} v_l = \sum_{jkl} u_k \underbrace{R_{kj}^{\text{tr}} R_{jl}}_{R^{\text{tr}} R = \mathbb{1}} v_l$$

$$R_{\mathbf{n}}^{-1}(\alpha) = R_{\mathbf{n}}(-\alpha) = R_{\mathbf{n}}^{\text{tr}}(\alpha)$$

- *Rotation around the quantization axis  $\mathbf{z}$ :*

$$R_{\mathbf{z}}(\alpha) = \begin{pmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

- *Rotation around an arbitrary axis  $\mathbf{v} = A\mathbf{u}$ :*

$$R_{\mathbf{v}}(\alpha) = AR_{\mathbf{u}}(\alpha)A^{-1}$$

Proof:

- A rotation matrix has a single eigenvector with zero eigenvalue, the axis,  $R_{\mathbf{v}}(\alpha)\mathbf{v} = \mathbf{v}$

$$AR_{\mathbf{u}}(\alpha)A^{-1}\mathbf{v} = AR_{\mathbf{u}}(\alpha)\mathbf{u} = A\mathbf{u} = \mathbf{v}$$

- The rotation angle remains the same during basis transformation

In particular:  $\mathbf{n} = A\mathbf{z}$

$$R_{\mathbf{n}}(\alpha) = AR_{\mathbf{z}}(\alpha)A^{-1}$$

### 2. Functions in space:

$$f(\mathbf{r}) \rightarrow U(R)f(\mathbf{r}) = f(R^{-1}\mathbf{r}).$$

### 3. Quantum mechanics: Hilbert space

$$\psi(\mathbf{r}) \rightarrow U(R)\psi(\mathbf{r}) = \psi(R^{-1}\mathbf{r}).$$

#### 4. Representation:

$$\begin{aligned}
 U(R)U(R')\psi(\mathbf{r}) &= U(R)\psi(R'^{-1}\mathbf{r}) \\
 &= \psi(R'^{-1}R^{-1}\mathbf{r}) \\
 &= \psi((RR')^{-1}\mathbf{r}) \\
 &= U(RR')\psi(\mathbf{r}) \\
 U(R)U(R') &= U(RR')
 \end{aligned}$$

#### 5. Unitary representation:

$$\int d\mathbf{x}\psi^*(R\mathbf{x})\phi(R\mathbf{x}) = \int d\mathbf{x}\psi^*(\mathbf{x})\phi(\mathbf{x}) \implies U(R)U^\dagger(R) = \mathbb{1}$$

#### 6. Infinitesimal rotations:

$$\begin{aligned}
 \mathbf{r} &\rightarrow \mathbf{r} + \epsilon\mathbf{n} \times \mathbf{r} \\
 \psi(\mathbf{r}) &\rightarrow \psi(\mathbf{r}) - (\epsilon\mathbf{n} \times \mathbf{r})\nabla\psi(\mathbf{r}) = \psi(\mathbf{r}) - \epsilon\mathbf{n}(\mathbf{r} \times \nabla)\psi(\mathbf{r}) = \psi(\mathbf{r}) - \frac{i}{\hbar}\epsilon\mathbf{n}\mathbf{L}\psi(\mathbf{r}),
 \end{aligned}$$



Generator: angular momentum

#### 7. Finite rotations:

- (a) One dimensional subgroup of rotational around a fixed axis:  $\{R_{\mathbf{n}}(\alpha)\}$
- (b) Generator:  $\mathbf{n}\mathbf{L}$
- (c) Representation:

$$\boxed{U(R_{\mathbf{n}}(\alpha)) = e^{-\frac{i}{\hbar}\alpha\mathbf{n}\mathbf{L}}}$$

#### 8. $\mathbf{L}$ is a vector operator:

- (a) *Definition:* transforms under rotations as a vector and as an operator and the two transformations agree.
- (b)  $\mathbf{n}_j = A^{-1}\mathbf{e}_j$ ,

$$\begin{aligned}
 U(R_{\mathbf{n}_j}(\alpha)) &= U(A^{-1}R_{\mathbf{e}_j}(\alpha)A) \\
 &= U(A^{-1})U(R_{\mathbf{e}_j}(\alpha))U(A) \\
 &= U(A^{-1})e^{-\frac{i}{\hbar}\alpha\mathbf{e}_j\mathbf{L}}U(A) \\
 &= \sum_{n=0}^{\infty} \frac{(-\frac{i}{\hbar}\alpha)^n}{n!} U(A^{-1})(\mathbf{e}_j\mathbf{L})^n U(A) \\
 &= \sum_{n=0}^{\infty} \frac{(-\frac{i}{\hbar}\alpha)^n}{n!} [U(A^{-1})\mathbf{e}_j\mathbf{L}U(A)]^n \\
 &= e^{-\frac{i}{\hbar}\alpha U(A^{-1})\mathbf{e}_j\mathbf{L}U(A)}.
 \end{aligned}$$

(c) Another expression:  $\mathbf{n}_j = A^{-1}\mathbf{e}_j = A^{\text{tr}}\mathbf{e}_j = \mathbf{e}_j A$

$$\begin{aligned} U(R_{\mathbf{n}_j}(\alpha)) &= e^{-\frac{i}{\hbar}\alpha\mathbf{n}_j L} \\ &= e^{-\frac{i}{\hbar}\alpha\mathbf{e}_j A L} \end{aligned}$$

(d)

$$\boxed{AL = U^\dagger(A)L U(A)}$$

↗ ↖

vector       operator

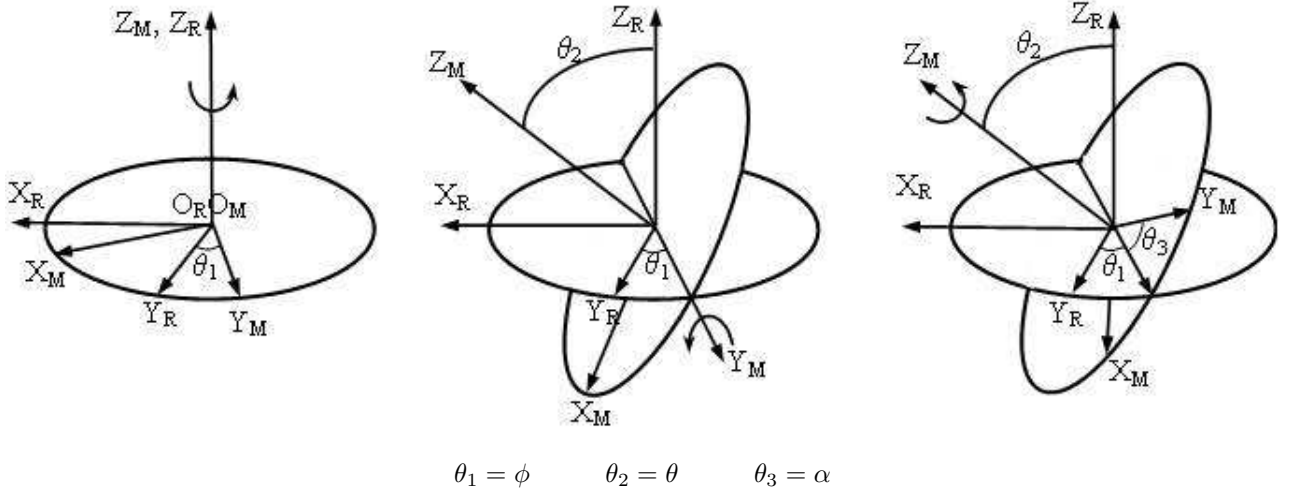
### C. Euler angles

#### 1. Definition:

$$R(\phi, \theta, \alpha) = R_{z''}(\alpha)R_{y'}(\theta)R_z(\phi)$$

↗ ↖

$$z'' = R_{y'}(\theta)R_z(\phi)z = R_{y'}(\theta)z \qquad y' = R_z(\phi)y$$



2. Another, equivalent expression:  $\mathbf{n} = Az, R_{\mathbf{n}}(\alpha) = AR_z(\alpha)A^{-1}$

$$\begin{aligned} R_{z''}(\alpha)R_{y'}(\theta)R_z(\phi) &= \underbrace{R_{y'}(\theta)R_z(\alpha)R_{y'}^{-1}(\theta)}_{R_{z''}(\alpha)} R_{y'}(\theta)R_z(\phi) \\ &= \underbrace{R_z(\phi)R_{y'}(\theta)R_z^{-1}(\phi)}_{R_{y'}(\theta)} R_z(\alpha)R_z(\phi) \\ &= R_z(\phi)R_{y'}(\theta)R_z(\alpha). \end{aligned}$$

### 3. Relation to the parameterization $R_{\mathbf{n}}(\alpha)$ :

$$\mathbf{n} = R(\phi, \theta, \chi)\mathbf{z} = R_z(\phi)R_y(\theta)R_z(\chi)\mathbf{z} = \begin{pmatrix} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{pmatrix}$$

$$R_{\mathbf{n}}(\alpha) = R(\phi, \theta, \chi)R_z(\alpha)R^{-1}(\phi, \theta, \chi)$$

Proof:  $\mathbf{v} = A\mathbf{u}$ ,  $R_{\mathbf{v}}(\alpha) = AR_u(\alpha)A^{-1}$

$$\begin{aligned} R(\phi, \theta, \chi)R_z(\alpha)R^{-1}(\phi, \theta, \chi) &= R_z(\phi)R_y(\theta)R_z(\chi)R_z(\alpha)R_z(-\chi)R_y(-\theta)R_z(-\phi) \\ &= R_z(\phi)R_y(\theta)R_z(\alpha)R_y(-\theta)R_z(-\phi), \quad R_y(\theta)\mathbf{z} = \mathbf{u} \\ &= R_z(\phi)R_u(\alpha)R_z(-\phi), \quad R_z(\phi)\mathbf{u} = \mathbf{v} \\ &= R_{\mathbf{v}}(\alpha), \quad \mathbf{n} = R_z(\phi)R_y(\theta)\mathbf{z} \end{aligned}$$

## D. Summary of the angular momentum algebra

### 1. Orbital angular momentum:

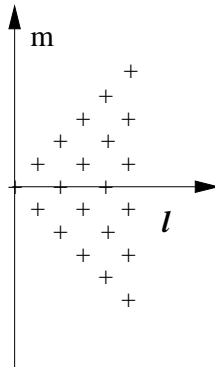
$$\mathbf{L} = \mathbf{r} \times \mathbf{p}$$

### 2. Commutation relations:

$$[L_a, L_b] = i\hbar \sum_c \epsilon_{abc} L_c.$$

### 3. Maximal set of commuting operators: $\{L_z, \mathbf{L}^2\} \implies$ eigenvalues to label the basis vectors,

$$\begin{aligned} L_z|\ell, m\rangle &= \hbar m|\ell, m\rangle, \quad \mathbf{L}^2|\ell, m\rangle = \hbar^2 \ell(\ell+1)|\ell, m\rangle \\ \ell &= 0, 1, \dots, \quad m \in \{-\ell, -\ell+1, \dots, \ell-1, \ell\} \end{aligned}$$



4. **Ladder operators:**  $L_{\pm} = L_x \pm iL_y$

$$\begin{aligned} [L_z, L_{\pm}] &= \pm \hbar L_{\pm}, & [L_+, L_-] &= 2\hbar L_z \\ L_{\pm}|\ell, m\rangle &= \hbar\sqrt{\ell(\ell+1) - m(m\pm 1)}|\ell, m\pm 1\rangle \end{aligned}$$

↗

to stop at the highest (lowest) state

5.  $\ell$  remains unvariant under  $\mathbf{L}$ :

$$\langle \ell, m | L_a | \ell', m' \rangle = \delta_{\ell, \ell'} F_a(\ell, m, m')$$

block diagonal structure  $\ell$

### E. Rotational multiplets

1. **Helicity basis:**

$$\begin{aligned} \mathbf{u} &= (u_x, u_y, u_z) \rightarrow (u_+, u_-, u_z), & u_{\pm} &= u_x \pm iu_y \\ \mathbf{nL} &= n_x L_x + n_y L_y + n_z L_z \\ &= \frac{1}{2}(n_+ L_+ + n_- L_-) + n_z L_z = \frac{1}{2}[(n_x - in_y)(L_x + iL_y) + (n_x + in_y)(L_x - iL_y)] + n_z L_z \end{aligned}$$

2. **Rotation of  $|\ell, m\rangle$ :**

$$\begin{aligned} e^{-\frac{i}{\hbar}\alpha\mathbf{nL}}|\ell, m\rangle &= \sum_{n=0}^{\infty} \frac{(-\frac{i}{\hbar}\alpha)^n}{n!} (\mathbf{nL})^n |\ell, m\rangle \\ &= \sum_{n=0}^{\infty} \frac{(-\frac{i}{\hbar}\alpha)^n}{n!} \left( n_3 L_3 + \frac{1}{2}n_+ L_- + \frac{1}{2}n_- L_+ \right)^n |\ell, m\rangle \\ &= \sum_{m'=-\ell}^{\ell} c_{m'}(\alpha, \mathbf{n}) |\ell, m'\rangle \end{aligned}$$

and all coefficients are non-vanishing if  $n_{\pm} \neq 0$

3. **Rotational multiplet:**  $\mathcal{H}_{\ell} = \{\sum_{m=-\ell}^{\ell} x_m |\ell, m\rangle\}$

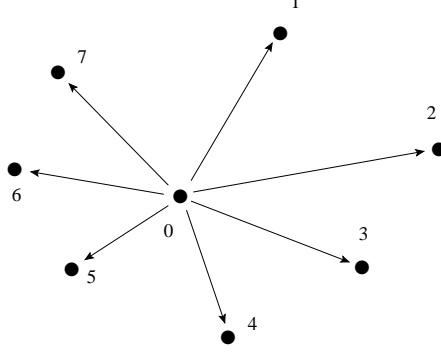
4. **Properties:**

(a) *Basis:*  $\{|\ell, m\rangle | -\ell \leq m \leq \ell\}$ ,  $\text{Dim}\mathcal{H}_{\ell} = 2\ell + 1$

(b)  $\mathcal{H}_{\ell}$  is closed with respect to rotations,  $e^{-\frac{i}{\hbar}\alpha\mathbf{nL}}\mathcal{H}_{\ell} \subset \mathcal{H}_{\ell}$ .

(c)  $\mathcal{H}_{\ell}$  is irreducible with respect to rotations.

i.  $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$  is reducible if each component is closed,  $e^{-\frac{i}{\hbar}\alpha\mathbf{nL}}\mathcal{H}_j \subset \mathcal{H}_j$ ,  $j = 1, 2$ .



- ii. Star condition of irreducibility of  $\mathcal{H}$ :  $\exists|\psi_0\rangle$  such that  $\forall|\psi\rangle \in \mathcal{H} \exists R$  such that  $\langle\psi|U(R)|\psi_0\rangle \neq 0$ .  
A suitable rotation of  $|\psi_0\rangle$  has a projection onto any state.

$$e^{-\frac{i}{\hbar}\alpha n\mathbf{L}}|\ell, m\rangle = \sum_{n=0}^{\infty} \frac{(-\frac{i}{\hbar}\alpha)^n}{n!} \left( n_z L_z + \frac{1}{2}n_+ L_- + \frac{1}{2}n_- L_+ \right)^n |\ell, m\rangle$$

$$\sum_{m'} c_{m'}^* \langle\ell, m'| e^{-\frac{i}{\hbar}\alpha n\mathbf{L}} |\ell, m\rangle = \sum_{n=0}^{\infty} \frac{(-\frac{i}{\hbar}\alpha)^n}{n!} \sum_{m'} c_{m'}^* \langle\ell, m'| \left( n_z L_z + \frac{1}{2}n_+ L_- + \frac{1}{2}n_- L_+ \right)^n |\ell, m\rangle = 0$$



$\infty$  equations for 3 variables (not a proof!)

## F. Wigner's $D$ matrix

1.  **$D$  matrix:** action of rotations within a rotational multiplet

2. **Definition:**  $\sum_{\ell', m'} |\ell', m'\rangle \langle\ell', m'| = \mathbb{1}$

$$\begin{aligned} U(R)|\ell, m\rangle &= \mathbb{1}U(R)|\ell, m\rangle = \sum_{\ell', m'} |\ell', m'\rangle \langle\ell', m'|U(R)|\ell, m\rangle \\ &= \sum_{m'} |\ell, m'\rangle \mathcal{D}_{m', m}^{(\ell)}(R) \end{aligned}$$

$$\boxed{\mathcal{D}_{m', m}^{(\ell)}(R) = \langle\ell, m'|U(R)|\ell, m\rangle}$$

3. **Euler angles:**

$$\begin{aligned} \mathcal{D}_{m', m}^{(\ell)}(R(\alpha, \beta, \gamma)) &= \mathcal{D}_{m', m}^{(\ell)}(R_z(\alpha)R_y(\beta))R_z(\gamma) \\ &= \sum_{m_1, m_2} \mathcal{D}_{m', m_1}^{(\ell)}(R_z(\alpha))\mathcal{D}_{m_1, m_2}^{(\ell)}(R_y(\beta))\mathcal{D}_{m_2, m}^{(\ell)}(R_z(\gamma)) \\ \langle\ell, m'|e^{-i\frac{\alpha}{\hbar}L_z}|\ell, m\rangle &= \mathcal{D}_{m', m}^{(\ell)}(R_z(\alpha)) = \delta_{m', m} e^{-i\alpha m} \\ \mathcal{D}_{m', m}^{(\ell)}(R_y(\beta)) &= \langle\ell, m'|e^{-i\frac{\beta}{\hbar}L_y}|\ell, m\rangle = d_{m', m}^{(\ell)}(\beta) \\ \mathcal{D}_{m', m}^{(\ell)}(R(\alpha, \beta, \gamma)) &= e^{-i\alpha m' - i\gamma m} d_{m', m}^{(\ell)}(\beta) \end{aligned}$$



Reduced  $d$ -matrix

4. **Block diagonal structure:** Basis:  $\underbrace{\{|0,0\rangle\}}_{\mathcal{H}_0}, \underbrace{\{|1,1\rangle, |1,0\rangle, |1,-1\rangle\}}_{\mathcal{H}_1}, \underbrace{\{|2,2\rangle, |2,1\rangle, |2,0\rangle, |2,-1\rangle, |2,-2\rangle\}}_{\mathcal{H}_2}, \dots\}$

$$U = \begin{pmatrix} \mathcal{D}^{(0)} & 0 & 0 & \dots \\ 0 & \mathcal{D}^{(1)} & 0 & \dots \\ 0 & 0 & \mathcal{D}^{(2)} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \quad \mathbf{L} = \begin{pmatrix} \mathbf{L}^{(0)} & 0 & 0 & \dots \\ 0 & \mathbf{L}^{(1)} & 0 & \dots \\ 0 & 0 & \mathbf{L}^{(2)} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

$$L_z^{(\ell)} = \hbar \begin{pmatrix} \ell & 0 & \dots & 0 & 0 \\ 0 & \ell-1 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & -\ell+1 & 0 \\ 0 & 0 & \dots & 0 & -\ell \end{pmatrix}, \quad L_+^{(\ell)} = \hbar \begin{pmatrix} 0 & \sqrt{2\ell} & \dots & 0 & 0 \\ 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & \sqrt{2\ell} \\ 0 & 0 & \dots & 0 & 0 \end{pmatrix}, \quad L_-^{(\ell)} = \hbar \begin{pmatrix} 0 & 0 & \dots & 0 & 0 \\ \sqrt{2\ell} & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & \dots & \sqrt{2\ell} & 0 \end{pmatrix}$$

5.  $S = \frac{1}{2}$ : Pauli matrices,

$$\langle \frac{1}{2}, m' | \mathbf{L} | \frac{1}{2}, m \rangle = \frac{\hbar}{2} \boldsymbol{\sigma} = \frac{\hbar}{2} \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\}$$

$$\left[ \frac{\hbar}{2} \sigma_j, \frac{\hbar}{2} \sigma_k \right] = i\hbar \sum_{\ell} \epsilon_{jkl} \frac{\hbar}{2} \sigma_{\ell} \iff [\sigma_j, \sigma_k] = 2 \sum_{\ell} \epsilon_{jkl} \sigma_{\ell}$$

6. **Two important relations:**

$$\sigma_a \sigma_b = \delta_{a,b} + i \sum_c \epsilon_{abc} \sigma_c \iff (\mathbf{u}\boldsymbol{\sigma}) \cdot (\mathbf{v}\boldsymbol{\sigma}) = \mathbf{1} \mathbf{u}\mathbf{v} + i(\mathbf{u} \times \mathbf{v})\boldsymbol{\sigma}$$

$$\sigma_y \boldsymbol{\sigma} \sigma_y = -\boldsymbol{\sigma}^*$$

7. **Finite rotation:**

• *Euler's relation:*

$$e^{i\alpha} = 1 + i\alpha + \frac{(i\alpha)^2}{2!} + \frac{(i\alpha)^3}{3!} + \frac{(i\alpha)^4}{4!} + \dots$$

$$= 1 + i\alpha + \frac{(i\alpha)^2}{2!} + \frac{(i\alpha)^3}{3!} + \frac{(i\alpha)^4}{4!} + \dots$$

$$= \frac{1}{2} (e^{i\alpha} + e^{-i\alpha}) + \frac{1}{2} (e^{i\alpha} - e^{-i\alpha})$$

$$= \cos \alpha + i \sin \alpha$$

• *Generalized Euler's relation:*

$$e^{i\alpha \mathbf{n}\boldsymbol{\sigma}} = \mathbf{1} + i\alpha \mathbf{n}\boldsymbol{\sigma} + \frac{(i\alpha)^2}{2!} (\mathbf{n}\boldsymbol{\sigma})^2 + \frac{(i\alpha)^3}{3!} (\mathbf{n}\boldsymbol{\sigma})^3 + \frac{(i\alpha)^4}{4!} (\mathbf{n}\boldsymbol{\sigma})^4 + \dots$$

$$\begin{aligned}
&= \mathbb{1} + i\alpha \mathbf{n}\boldsymbol{\sigma} + \mathbb{1} \frac{(i\alpha)^2}{2!} \mathbf{n}^2 + \frac{(i\alpha)^3}{3!} \mathbf{n}^2 \mathbf{n}\boldsymbol{\sigma} + \mathbb{1} \frac{(i\alpha)^4}{4!} \mathbf{n}^4 + \dots \\
&= \mathbb{1} \frac{1}{2} (e^{i\alpha} + e^{-i\alpha}) + \frac{\mathbf{n}\boldsymbol{\sigma}}{2} (e^{i\alpha} - e^{-i\alpha}) \\
&= \mathbb{1} \cos \alpha + i \mathbf{n}\boldsymbol{\sigma} \sin \alpha.
\end{aligned}$$

- *Reduced d matrix:*

$$\begin{aligned}
d_{m',m}^{(\frac{1}{2})}(\beta) &= \langle \frac{1}{2}, m' | e^{-i\frac{\beta\sigma_y}{2}} | \frac{1}{2}, m \rangle = \left( \mathbb{1} \cos \frac{\beta}{2} - i\sigma_y \sin \frac{\beta}{2} \right)_{m',m}, \\
d^{(\frac{1}{2})}(\beta) &= \begin{pmatrix} \cos \frac{\beta}{2} & -\sin \frac{\beta}{2} \\ \sin \frac{\beta}{2} & \cos \frac{\beta}{2} \end{pmatrix}.
\end{aligned}$$

## G. Invariant integration

### 1. Two sphere, $S_2$ :

- *Rotational invariance:*

$$\mathbf{n}(\theta, \phi) = \begin{pmatrix} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{pmatrix}, \quad d\Sigma = d\theta \sin \theta d\phi = d \cos \theta d\phi$$

↑

elementary area on the unit sphere

- *Invariant integral:*

$$\int_{\Sigma} d\phi d \cos \theta f(\mathbf{n}) = \int_{R\Sigma} d\phi d \cos \theta f(R^{-1}\mathbf{n})$$

### 2. Rotational group $SO(3)$ :

- *Invariant integral:*

$$\mathbf{n} = R(\phi, \theta, \chi)\mathbf{z} = R_z(\phi)R_y(\theta)R_z(\chi)\mathbf{z} = \begin{pmatrix} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{pmatrix}$$

$$\begin{aligned}
\int_V d\mathbf{n} d\chi f(R\mathbf{n}(\chi)) &= \int_V d\phi d \cos \theta d\chi f(R\mathbf{n}(\chi)) = \int_{R'V} d\phi d \cos \theta d\chi f(R'^{-1}R\mathbf{n}(\chi)) \\
\int_V d\phi d \cos \theta d\chi f(R(\phi, \theta, \chi)) &= \int_{R'V} d\phi d \cos \theta d\chi f(R'^{-1}R(\phi, \theta, \chi))
\end{aligned}$$

- *Equivalent form (Haar measure):*  $dR = d\phi d \cos \theta d\chi$

$$\int dR f(R) = \int d(R'R) f(R) = \int dR f(R'^{-1}R)$$

defined up to a normalization constant



- *Volumes:*

$$\int_{S_2} d\Sigma = \int_{-1}^1 dc \int_{-\pi}^{\pi} d\phi = 4\pi,$$

$$\int_{SO(3)} dR = \int_{-1}^1 dc \int_{-\pi}^{\pi} d\phi \int_{-\pi}^{\pi} d\chi = 8\pi^2$$

## H. Spherical harmonics

1. **Definition:** wave function of  $|\ell, m\rangle$ ,

$$\langle \mathbf{n} | \ell, m \rangle = Y_m^\ell(\mathbf{n}) = Y_m^\ell(\theta, \phi), \quad \leftarrow \quad \mathbf{n} = \begin{pmatrix} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{pmatrix}$$

determined by the structure of the rotation group.

2. **Normalization:**

$$1 = \int_{S_2} d^2n |Y_m^\ell(\mathbf{n})|^2,$$

3. **Defining relations:**

- *Necessary:* and sufficient condition

$$\begin{aligned} L_z Y_m^\ell(\mathbf{n}) &= L_z \langle \mathbf{n} | \ell, m \rangle = \langle \mathbf{n} | L_z | \ell, m \rangle = \hbar m \langle \mathbf{n} | \ell, m \rangle = \hbar m Y_m^\ell(\mathbf{n}), \\ L_\pm Y_m^\ell(\mathbf{n}) &= \langle \mathbf{n} | L_\pm | \ell, m \rangle \\ &= \hbar \sqrt{\ell(\ell+1) - m(m \pm 1)} \langle \mathbf{n} | \ell, m \pm 1 \rangle \\ &= \hbar \sqrt{\ell(\ell+1) - m(m \pm 1)} Y_{m \pm 1}^\ell(\mathbf{n}) \end{aligned}$$

- *Sufficient:*

- Eigenvectors of hermitian operators  $\implies$  basis set on the unit sphere
- Non-degeneracy in  $L_z$ : a set of functions on the unit sphere satisfying these eqs. are the spherical harmonics up to a constant

4. **Spherical harmonics in terms of  $\mathcal{D}$  matrices:**

- *Relation between the Euler angles and the polar angles:*

$$\mathbf{n} = \begin{pmatrix} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{pmatrix} = R(\phi, \theta, \chi) \mathbf{z}$$

$$|\mathbf{n}\rangle = U(R(\phi, \theta, \chi)) |z\rangle$$

with  $\mathbf{z} = (0, 0, 1)$  and  $\chi$  left arbitrary.

- *Resolution of unity:*  $\sum_{\ell', m'} |\ell', m'\rangle \langle \ell', m'| = \mathbb{1}$

$$|\mathbf{n}\rangle = U(R(\phi, \theta, \chi))\mathbb{1}|\mathbf{z}\rangle = \sum_{\ell, m} U(R(\phi, \theta, \chi))|\ell, m\rangle \langle \ell, m|\mathbf{z}\rangle$$

- *Projection on  $\langle \ell, m'|$ :*

$$\langle \ell, m'|\mathbf{n}\rangle = Y_{m'}^{\ell*}(\mathbf{n}) = \sum_m \mathcal{D}_{m', m}^{(\ell)}(R(\phi, \theta, \chi)) \langle \ell, m|\mathbf{z}\rangle$$

- *Last factor in three steps:*

(a) Consider

$$\begin{aligned} \langle \ell, m|U(R_{\mathbf{z}}(\chi))|\mathbf{z}\rangle &= \sum_{\ell', m'} \langle \ell, m|U(R_{\mathbf{z}}(\chi))|\ell', m'\rangle \langle \ell', m'|\mathbf{z}\rangle \\ &= \sum_{m'} \mathcal{D}_{m, m'}^{(\ell)}(R_{\mathbf{z}}(\chi)) \langle \ell, m'|\mathbf{z}\rangle \\ &= e^{-im\chi} \langle \ell, m|\mathbf{z}\rangle \end{aligned}$$

(b)  $\mathbf{z} = R_{\mathbf{z}}(\chi)\mathbf{z} \implies$  no  $\chi$ -dependence,

$$\langle \ell, m|U(R_{\mathbf{z}}(\chi))|\mathbf{z}\rangle = \langle \ell, m|\mathbf{z}\rangle$$

(c) Hence

$$e^{-im\chi} \langle \ell, m|\mathbf{z}\rangle = \langle \ell, m|\mathbf{z}\rangle$$

acting on it by  $\frac{\partial}{\partial \chi}$  and setting  $\chi = 0$ :

$$-im \langle \ell, m|\mathbf{z}\rangle = 0 \implies \langle \ell, m|\mathbf{z}\rangle = \delta_{m,0} c_{\ell}$$

- *Normalization:*

– Resolution of unity:  $\mathbb{1} = \int_{S_2} d\mathbf{n} |\mathbf{n}\rangle \langle \mathbf{n}|$

– Integration over the unit sphere:

$$\begin{aligned} \int_{S_2} d\Omega f(\mathbf{n}) &= \int_{-1}^1 d\cos\theta \int_{-\pi}^{\pi} d\phi \underbrace{f(\theta, \phi)}_{\mathbf{n}}, \quad \mathbf{n} = \begin{pmatrix} \sin\theta \cos\phi \\ \sin\theta \sin\phi \\ \cos\theta \end{pmatrix} = R(\phi, \theta, \chi)\mathbf{z} \\ &= \underbrace{\int_{-1}^1 d\cos\theta \int_{-\pi}^{\pi} d\phi}_{\int_{S_2} d\mathbf{n}} f(R(\phi, \theta, \chi)\mathbf{z}) \\ &= \frac{1}{2\pi} \underbrace{\int_{-1}^1 d\cos\theta \int_{-\pi}^{\pi} d\phi \int_{-\pi}^{\pi} d\chi}_{\int_{SO(3)} dR} f(R(\phi, \theta, \chi)\mathbf{z}) \end{aligned}$$

– Normalization:

$$\begin{aligned}
1 &= \langle \ell, 0 | \ell, 0 \rangle \\
&= \langle \ell, 0 | \mathbb{1} | \ell, 0 \rangle \\
&= \int_{S_2} d\mathbf{n} \langle \ell, 0 | \mathbf{n} \rangle \langle \mathbf{n} | \ell, 0 \rangle \\
&= \frac{1}{2\pi} \int_{SO(3)} dR \langle \ell, 0 | U(R) | \mathbf{z} \rangle \langle \mathbf{z} | U^\dagger(R) | \ell, 0 \rangle
\end{aligned}$$

– Resolution of identity:  $\mathbb{1} = \sum_{\ell, m} |\ell, m\rangle \langle \ell, m|$

$$\begin{aligned}
1 &= \frac{1}{2\pi} \int_{SO(3)} dR \langle \ell, 0 | U(R) \mathbb{1} | \mathbf{z} \rangle \langle \mathbf{z} | \mathbb{1} U^\dagger(R) | \ell, 0 \rangle \\
&= \frac{1}{2\pi} \sum_{\ell', m'} \int_{SO(3)} dR \langle \ell, 0 | U(R) | \ell', m' \rangle \underbrace{\langle \ell', m' | \mathbf{z} \rangle}_{\delta_{m', 0} c_{\ell'}} \underbrace{\langle \mathbf{z} | \ell, m \rangle}_{\delta_{m, 0} c_\ell} \langle \ell, m | U^\dagger(R) | \ell, 0 \rangle \\
&= \frac{\langle \ell, 0 | \mathbf{z} \rangle^2}{2\pi} \underbrace{\int_{SO(3)} dR |\mathcal{D}_{0,0}^{(\ell)}(R)|^2}_{\frac{8\pi^2}{2\ell+1}} \implies c_\ell = \sqrt{\frac{2\ell+1}{4\pi}}
\end{aligned}$$

(assuming that  $c_\ell$  is real and positive)

• *Finally:*

$$\begin{aligned}
Y_m^\ell(\mathbf{n}) &= \sum_{m'} \mathcal{D}_{m,m'}^{(\ell)*}(R(\phi, \theta, \chi)) \langle \ell, m' | \mathbf{z} \rangle^* \\
&= \sqrt{\frac{2\ell+1}{4\pi}} \mathcal{D}_{m,0}^{(\ell)*}(R(\phi, \theta, \chi))
\end{aligned}$$

$$\boxed{Y_m^\ell(\mathbf{n}) = \sqrt{\frac{2\ell+1}{4\pi}} e^{im\phi} d_{m,0}^{(\ell)*}(\theta)}$$

5. **Example:**  $Y_m^1$  :

- Three functions on the unit sphere, transforming under rotations in an irreducible manner
- $\mathbf{n} = (\frac{x}{r}, \frac{y}{r}, \frac{z}{r})$  do the same
- Two different bases for  $\mathcal{H}_1$ :  $Y_m^1$  and  $\mathbf{n}$

–  $Y_0^1$ :  $L_z Y_0^1 = 0$ ,  $L_z z = 0$ , normalization:  $\int_{S_2} d\mathbf{n} |Y(\mathbf{n})|^2 = 1$ ,  $Y_0^1 = \sqrt{\frac{3}{4\pi}} \frac{z}{r}$

–  $Y_{\pm 1}^1$ :

$$\begin{aligned}
Y_{\pm 1}^1(\mathbf{n}) &= \frac{1}{\sqrt{2\hbar}} L_\pm Y_0^1(\mathbf{n}) \\
&= \frac{1}{\sqrt{2\hbar}} (L_z \pm iL_y) Y_0^1(\mathbf{n}) \\
&= \frac{1}{\sqrt{2\hbar r}} \sqrt{\frac{3}{4\pi}} [yp_z - zp_y \pm i(zp_x - xp_z)] z,
\end{aligned}$$

$\implies$

$$\begin{aligned} Y_1^1(\mathbf{n}) &= -\sqrt{\frac{3}{8\pi}} \frac{x+iy}{r} = -\sqrt{\frac{3}{8\pi}} \sin\theta e^{i\phi} \\ Y_0^1(\mathbf{n}) &= \sqrt{\frac{3}{4\pi}} \frac{z}{r} = \sqrt{\frac{3}{4\pi}} \cos\theta \\ Y_{-1}^1(\mathbf{n}) &= \sqrt{\frac{3}{8\pi}} \frac{x-iy}{r} = \sqrt{\frac{3}{8\pi}} \sin\theta e^{-i\phi}. \end{aligned}$$

### III. ADDITION OF ANGULAR MOMENTUM

#### A. Composite systems

1. **Two independent systems:** linear spaces  $\mathcal{H}_1$  and  $\mathcal{H}_2$

The two systems together: linear space consisting the pairs  $(|\psi_1\rangle, |\psi_2\rangle)$ ,  $|\psi_j\rangle \in \mathcal{H}_j$

Two widely used algebraic structures:

2. **Direct sum:**  $|\psi_1\rangle \oplus |\psi_2\rangle = |\psi_1\rangle + |\psi_2\rangle \in \mathcal{H}_1 \oplus \mathcal{H}_2 = \mathcal{H}_1 + \mathcal{H}_2$  treated as an orthogonal sum  $\mathcal{H}_1 \perp \mathcal{H}_2$

- (a) Multiplication:

$$(c|\psi_1\rangle) \oplus |\psi_2\rangle, |\psi_1\rangle \oplus (c|\psi_2\rangle) \in \mathcal{H}_1 \oplus \mathcal{H}_2$$

- (b) Addition:

$$(|\psi_1\rangle \oplus |\psi_2\rangle) + (|\psi'_1\rangle \oplus |\psi'_2\rangle) = (|\psi_1\rangle + |\psi'_1\rangle) \oplus (|\psi_2\rangle + |\psi'_2\rangle)$$

- (c) Scalar product:

$$(\langle\psi_1| \oplus \langle\psi_2|)(|\psi'_1\rangle \oplus |\psi'_2\rangle) = \langle\psi_1|\psi'_1\rangle + \langle\psi_2|\psi'_2\rangle \quad \leftarrow \text{sum}$$

- (d) Operators:  $A_j : \mathcal{H}_j \rightarrow \mathcal{H}_j \implies A_1 \oplus A_2 : \mathcal{H}_1 \oplus \mathcal{H}_2 \rightarrow \mathcal{H}_1 \oplus \mathcal{H}_2$

$$(\langle\psi_1| \oplus \langle\psi_2|)(A_1 \oplus A_2)(|\psi'_1\rangle \oplus |\psi'_2\rangle) = \langle\psi_1|A_1|\psi'_1\rangle + \langle\psi_2|A_2|\psi'_2\rangle \quad \leftarrow \text{sum}$$

- (e) Basis:  $\{|n_j\rangle\}$  a basis for  $\mathcal{H}_j$

i.  $\implies \{|n_1\rangle \oplus |n_2\rangle\}$  a basis for  $\mathcal{H}_1 \otimes \mathcal{H}_2$

ii.  $\dim \mathcal{H}_1 \oplus \mathcal{H}_2 = \dim \mathcal{H}_1 + \dim \mathcal{H}_2 \quad \leftarrow \text{sum}$

iii. Components:  $\langle j|(|\psi_1\rangle \otimes |\psi_2\rangle) = \langle j|\psi_1\rangle + \langle j|\psi_2\rangle \quad \leftarrow \text{sum}$

iv. Wave function:  $(\psi_1 \oplus \psi_2)(x) = \langle x|(|\psi_1 \oplus \psi_2\rangle) = \psi_1(x_1) + \psi_2(x_2) \quad \leftarrow \text{sum}$

3. **Direct product:**  $|\psi_1\rangle \otimes |\psi_2\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$  treated as a linear space generated by the pairs  $(\{\mathcal{H}_1\}, \{\mathcal{H}_2\})$

(a) Multiplication:

$$(c|\psi_1\rangle) \otimes |\psi_2\rangle = |\psi_1\rangle \otimes (c|\psi_2\rangle) = c(|\psi_1\rangle \otimes |\psi_2\rangle).$$

(b) Addition:

$$(|\psi_1\rangle \otimes |\psi_2\rangle) + (|\psi'_1\rangle \otimes |\psi'_2\rangle) \in \mathcal{H}_1 \otimes \mathcal{H}_2$$

(c) Scalar product:

$$(\langle\psi_1| \otimes \langle\psi_2|)(|\psi'_1\rangle \otimes |\psi'_2\rangle) = \langle\psi_1|\psi'_1\rangle\langle\psi_2|\psi'_2\rangle \quad \leftarrow \text{product}$$

(d) Operators:  $A_j : \mathcal{H}_j \rightarrow \mathcal{H}_j \implies A_1 \otimes A_2 : \mathcal{H}_1 \otimes \mathcal{H}_2 \rightarrow \mathcal{H}_1 \otimes \mathcal{H}_2$

$$(\langle\psi_1| \otimes \langle\psi_2|)(A_1 \otimes A_2)(|\psi'_1\rangle \otimes |\psi'_2\rangle) = \langle\psi_1|A_1|\psi'_1\rangle\langle\psi_2|A_2|\psi'_2\rangle \quad \leftarrow \text{product}$$

(e) Basis:  $\{|n_j\rangle\}$  a basis for  $\mathcal{H}_j$

i.  $\implies \{|n_1\rangle \otimes |n_2\rangle\}$  a basis for  $\mathcal{H}_1 \otimes \mathcal{H}_2$

ii.  $\dim \mathcal{H}_1 \otimes \mathcal{H}_2 = \dim \mathcal{H}_1 \dim \mathcal{H}_2 \quad \leftarrow \text{product}$

iii. Components:  $\langle j_1, j_2 | \psi_1 \rangle \otimes | \psi_2 \rangle = \langle j_1 | \psi_1 \rangle \langle j_2 | \psi_2 \rangle \quad \leftarrow \text{product}$

iv. Wave function:  $(\psi_1 \otimes \psi_2)(x_1, x_2) = \langle x_1, x_2 | (\psi_1 \otimes \psi_2) \rangle = \psi_1(x_1)\psi_2(x_2) \quad \leftarrow \text{product}$

#### 4. Usage:

(a) Direct sum: exclusively existing components

$$\text{example: s, p, d, etc, atomic shells, } \psi(\mathbf{x}) = \sum_{nml} c_{nml} \psi_{nml}(\mathbf{x})$$

(b) Direct product: simultaneously existing components

$$\text{example: two-particle state, } \psi(\mathbf{x}_1, \mathbf{x}_2) = \psi_1(\mathbf{x}_1)\psi_2(\mathbf{x}_2)$$

### B. Additive observables and quantum numbers

1. **Momentum:** Generator of translations,  $\mathbf{r} \rightarrow \mathbf{r} + \boldsymbol{\epsilon}$

$$\begin{aligned} \delta\psi(\mathbf{r}_1, \mathbf{r}_2) &= \psi(\mathbf{r}_1 - \boldsymbol{\epsilon}, \mathbf{r}_2 - \boldsymbol{\epsilon}) - \psi(\mathbf{r}_1, \mathbf{r}_2) \\ &= -\frac{i}{\hbar}\boldsymbol{\epsilon}(\mathbf{p}_1 + \mathbf{p}_2)\psi(\mathbf{r}_1, \mathbf{r}_2) \\ &= -\frac{i}{\hbar}\boldsymbol{\epsilon}\mathbf{P}\psi(\mathbf{r}_1, \mathbf{r}_2) \implies \mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2 \end{aligned}$$

2. **Angular momentum:** Generator of rotations,  $\mathbf{r} \rightarrow \mathbf{r} - \frac{i}{\hbar}\boldsymbol{\epsilon}\mathbf{nL}$

- An infinitesimal rotation around the  $z$  axis:

$$\mathbf{r} = \begin{pmatrix} r \sin \theta \cos \phi \\ r \sin \theta \sin \phi \\ r \cos \theta \end{pmatrix} \rightarrow \begin{pmatrix} r \sin \theta \cos(\phi + \epsilon) \\ r \sin \theta \sin(\phi + \epsilon) \\ r \cos \theta \end{pmatrix}$$

$$\begin{aligned} \delta\psi(\mathbf{r}_1, \mathbf{r}_2) &= -\epsilon(\partial_{\phi_1} + \partial_{\phi_2})\psi(\mathbf{r}_1, \mathbf{r}_2) \\ &= -\frac{i}{\hbar}\epsilon(L_{1z} + L_{2z})\psi(\mathbf{r}_1, \mathbf{r}_2) \\ &= -\frac{i}{\hbar}\epsilon L_z\psi(\mathbf{r}_1, \mathbf{r}_2) \end{aligned}$$

- General case:  $R_{\mathbf{n}}(\epsilon)$  is generated by  $\mathbf{n}(\mathbf{L}_1 + \mathbf{L}_2)$ ,  $\implies \mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2$
- Commutation relations:

$$\begin{aligned} [L_a, L_b] &= [L_{1a} + L_{2a}, L_{1b} + L_{2b}] \\ &= i\hbar \sum_c \epsilon_{a,b,c}(L_{1c} + L_{2c}) \\ &= i\hbar \sum_c \epsilon_{a,b,c}L_c. \end{aligned}$$

- But  $\mathbf{L}^2 = \mathbf{L}_1^2 + \mathbf{L}_2^2 + 2\mathbf{L}_1\mathbf{L}_2$  is not additive  $\implies \ell$  is not additive neither
- Allowed values of  $\ell$ ?
  - Classical mechanics

$$\left(\sqrt{\mathbf{L}_1^2} - \sqrt{\mathbf{L}_2^2}\right)^2 \leq \mathbf{L}^2 \leq \left(\sqrt{\mathbf{L}_1^2} + \sqrt{\mathbf{L}_2^2}\right)^2.$$

- Quantum mechanics?

### C. System of two particles

#### 1. System of two particles:

- States  $|\phi_1\rangle \in \mathcal{H}_{\ell_1}$ ,  $|\phi_2\rangle \in \mathcal{H}_{\ell_2}$
- Representation of rotations:  $e^{-\frac{i}{\hbar}\alpha\mathbf{n}\mathbf{L}}|\phi_1\rangle \otimes |\phi_2\rangle$  in  $\mathcal{H} = \mathcal{H}_{\ell_1} \otimes \mathcal{H}_{\ell_2}$ .
- Spectrum of  $\mathbf{L}^2 = (\mathbf{L}_1 + \mathbf{L}_2)^2$ :  $\{\ell_1, \ell_2, \dots, \ell_n\} \iff \mathcal{H} = \mathcal{H}_{\ell_1} \oplus \mathcal{H}_{\ell_2} \oplus \dots \oplus \mathcal{H}_{\ell_n}$
- A reducible unitary representation can always be broken up into the direct sum of irreducible representations

#### 2. Two different bases:

- (a) Decoupled basis:

$$|\ell_1, \ell_2, m_1, m_2\rangle = |\ell_1, m_1\rangle \otimes |\ell_2, m_2\rangle, \quad -\ell_j \leq m_j \leq \ell_j, \quad \dim\mathcal{H} = (2\ell_1 + 1)(2\ell_2 + 1)$$

(b) Coupled basis:  $\{|L, M\rangle\}$ :

$$L^2|L, M\rangle = \hbar^2 L(L+1)|L, M\rangle,$$

$$L_3|L, M\rangle = \hbar M|L, M\rangle,$$

### 3. Reduction (construction of the coupled basis):

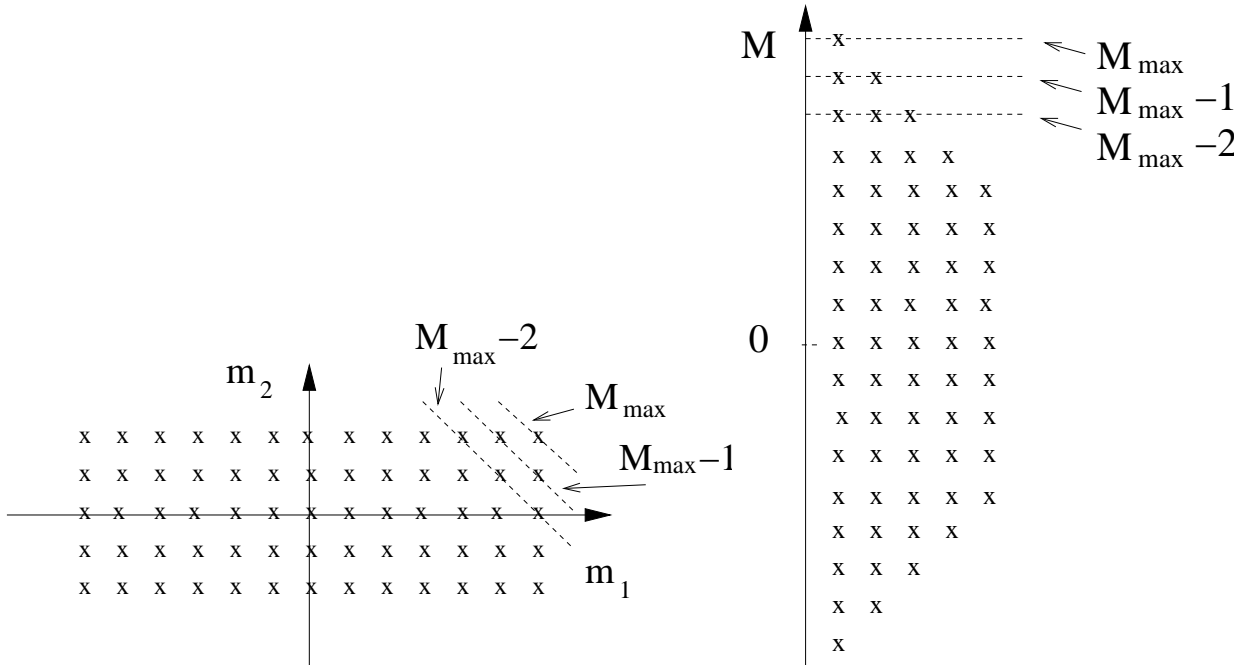
- $M = M_{max} = m_1 + m_2$ :

(a)  $|\ell_1, \ell_2, \ell_1, \ell_2\rangle = |M_{max}, M_{max}\rangle \in \mathcal{H}_{M_{max}} \subset \mathcal{H}$

(b)  $|\ell_1, \ell_2, \ell_1, \ell_2\rangle$  is unique  $\implies$  no other  $\mathcal{H}_{M_{max}} \subset \mathcal{H}$

(c) No  $\mathcal{H}_\ell \subset \mathcal{H}$  with  $\ell > M_{max}$

(d)  $U(R)\mathcal{H} \subset \mathcal{H} \implies \mathcal{H} = \mathcal{H}_{M_{max}} \oplus \dots$



- $M = M_{max} - 1 = m_1 + m_2 - 1$ :

(a) Application of  $L_- = L_{1-} + L_{2-}$ :

$$|M_{max}, M_{max} - 1\rangle = \frac{1}{\hbar\sqrt{2M_{max}}} L_- |M_{max}, M_{max}\rangle.$$

(b) Two decoupled basis elements with  $M = M_{max} - 1$ :  $|\ell_1, \ell_2, \ell_1 - 1, \ell_2\rangle$  and  $|\ell_1, \ell_2, \ell_1, \ell_2 - 1\rangle$

(c)  $S_{M_{max}-1} = \{c_1|\ell_1, \ell_2, \ell_1 - 1, \ell_2\rangle + c_2|\ell_1, \ell_2, \ell_1, \ell_2 - 1\rangle\}$   $\leftarrow$  dashed lines

–  $\dim(S_{M_{max}-1}) = 2$

–  $S_{M_{max}-1} \subset \mathcal{H}$

(d) Choose a basis vector  $|M_{max}, M_{max} - 1\rangle \in S_{M_{max}-1}$  such that  $|M_{max}, M_{max} - 1\rangle \in \mathcal{H}_{M_{max}}$

- (e) The other, orthogonal basis vector belongs to a new multiplet,  $|M_{max} - 1, M_{max} - 1\rangle \in S_{M_{max}-1}$ ,  
 $|M_{max} - 1, M_{max} - 1\rangle \in \mathcal{H}_{M_{max}-1}$
- (f)  $\in \mathcal{H}_{M_{max}-1} \subset \mathcal{H}$  comes with multiplicity one in  $\mathcal{H}$ .
- (g)  $U(R)\mathcal{H} \subset \mathcal{H} \implies \mathcal{H} = \mathcal{H}_{M_{max}} \oplus \mathcal{H}_{M_{max}-1} \oplus \dots$

- Iteration:

$$\mathcal{H} = \mathcal{H}_{|\ell_1 - \ell_2|} \oplus \dots \oplus \mathcal{H}_{\ell_1 + \ell_2}$$

or

$$\ell_1 \otimes \ell_2 = |\ell_1 - \ell_2| \oplus |\ell_1 - \ell_2| + 1 \oplus \dots \oplus \ell_1 + \ell_2 - 1 \oplus \ell_1 + \ell_2$$

- Sum rule:

$$\dim \mathcal{H} = (2\ell_1 + 1)(2\ell_2 + 1) = \sum_{|\ell_1 - \ell_2| \leq \ell \leq \ell_1 + \ell_2} (2\ell + 1),$$

- Resolution of the identity in  $\mathcal{H}$ :

$$\mathbb{1} = \sum_{m_1, m_2} |\ell_1, \ell_2, m_1, m_2\rangle \langle \ell_1, \ell_2, m_1, m_2| = \sum_{L, M} |L, M\rangle \langle L, M|$$

- Appears reasonable in the semiclassical limit,  $\ell_1, \ell_2 \rightarrow \infty$

#### 4. Clebsch-Gordan coefficients:

- Definition:

$$(\ell_1, \ell_2, m_1, m_2 | L, M) = \langle \ell_1, \ell_2, m_1, m_2 | L, M \rangle$$

- Decoupled  $\rightarrow$  coupled:

$$\begin{aligned} |L, M\rangle &= \sum_{m_1, m_2} |\ell_1, \ell_2, m_1, m_2\rangle \langle \ell_1, \ell_2, m_1, m_2 | L, M \rangle \\ &= \sum_{m_1, m_2} |\ell_1, \ell_2, m_1, m_2\rangle (\ell_1, \ell_2, m_1, m_2 | L, M) \end{aligned}$$

- Additivity of  $L_z$ :

$$(\ell_1, \ell_2, m_1, m_2 | L, M) = \delta_{m_1 + m_2, M} (\ell_1, \ell_2, m_1, M - m_1 | L, M)$$

- Theorem: One can choose the phase of  $|\ell, m\rangle$  in such a manner that Clebsch-Gordan coefficients become real.



- Coupled  $\rightarrow$  decoupled:

$$\begin{aligned}
|\ell_1, \ell_2, m_1, m_2\rangle &= \sum_{L, M} |L, M\rangle \langle L, M | \ell_1, \ell_2, m_1, m_2\rangle \\
&= \sum_{L, M} |L, M\rangle \langle \ell_1, \ell_2, m_1, m_2 | L, M\rangle^* \\
&= \sum_{L, M} |L, M\rangle (\ell_1, \ell_2, m_1, m_2 | L, M)^* \\
&= \sum_{L, M} |L, M\rangle (\ell_1, \ell_2, m_1, m_2 | L, M)
\end{aligned}$$

5. **Simplest non-trivial example:**  $\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1$ :

- $M = \pm 1$ :

$$\begin{aligned}
|1, \pm 1\rangle &= |\pm \frac{1}{2}, \pm \frac{1}{2}\rangle \\
(\frac{1}{2}, \frac{1}{2}, \pm \frac{1}{2}, \pm \frac{1}{2} | 1, \pm 1) &= 1
\end{aligned}$$

- $M = 0$ :

(a)  $L = 1$ :

$$\begin{aligned}
|1, 0\rangle &= \frac{1}{\sqrt{2}\hbar} L_- |1, 1\rangle \\
&= \frac{1}{2\sqrt{2}} [\sigma_{1x} + \sigma_{2x} - i(\sigma_{1y} + \sigma_{2y})] |\frac{1}{2}, \frac{1}{2}\rangle \\
&= \frac{1}{\sqrt{2}} \left[ \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_1 + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_2 \right] |\frac{1}{2}, \frac{1}{2}\rangle \\
&= \frac{1}{\sqrt{2}} \left( |\frac{1}{2}, -\frac{1}{2}\rangle + |-\frac{1}{2}, \frac{1}{2}\rangle \right) \\
(\frac{1}{2}, \frac{1}{2}, \pm \frac{1}{2}, \mp \frac{1}{2} | 1, 0) &= \frac{1}{\sqrt{2}}
\end{aligned}$$

(b)  $L = 0$ :

$$\begin{aligned}
|0, 0\rangle &= \frac{1}{\sqrt{2}} \left( |\frac{1}{2}, -\frac{1}{2}\rangle - |-\frac{1}{2}, \frac{1}{2}\rangle \right) \\
(\frac{1}{2}, \frac{1}{2}, \pm \frac{1}{2}, \mp \frac{1}{2} | 0, 0) &= \pm \frac{1}{\sqrt{2}}
\end{aligned}$$

(c)  $\mathcal{H}_1$ : symmetric with respect to the exchange of the two particles

$\mathcal{H}_0$ : antisymmetric with respect to the exchange of the two particles

## IV. SELECTION RULES

### A. Tensor operators

1. **Definition:**  $\{T_m^{(\ell)}\}$ ,  $-\ell \leq m \leq \ell$ , transform according to two equivalent ways

- operators acting in the Hilbert space and
- as tensors, basis vectors of an irreducible multiplet in the linear space of operators,

$$\boxed{U^\dagger(R)T_m^{(\ell)}U(R) = \sum_{m'} T_{m'}^{(\ell)} \mathcal{D}_{m',m}^\ell(R^{-1})} = \sum_{m'} \mathcal{D}_{m,m'}^{\ell*}(R) T_{m'}^{(\ell)}$$

- $\ell = 1$ :

$$AL = LA^{-1} = U^\dagger(A)LU(A),$$

$$\nearrow \qquad \nwarrow$$

vector

operator

## 2. Invariance:

$$\sum_{m'} U^\dagger(R)T_{m'}^{(\ell)}U(R)\mathcal{D}_{m',m}^\ell(R) = T_m^{(\ell)}$$

## 3. Spherical harmonics:

(a) Transformation of kets and wave functions:

$$\begin{aligned} Y_m^\ell(R\mathbf{n}) &= U(R^{-1})Y_m^\ell(\mathbf{n}) = \langle \mathbf{n} | U(R^{-1}) | \ell, m \rangle = \langle \mathbf{n} | \mathbb{1} U(R^{-1}) | \ell, m \rangle \\ &= \sum_{m'} \langle \mathbf{n} | \ell, m' \rangle \underbrace{\langle \ell, m' | U(R^{-1}) | \ell, m \rangle}_{D_{m',m}^{(\ell)}(R^{-1})} = \sum_{m'} Y_{m'}^\ell(\mathbf{n}) D_{m',m}^{(\ell)}(R^{-1}) \end{aligned}$$

(b) Transformation of the spherical function of operators:  $Y_m^\ell(\hat{\mathbf{n}})$ ,  $R\hat{\mathbf{n}} = U^\dagger(R)\hat{\mathbf{n}}U(R)$

$$\nearrow$$

vector operator

$$\begin{aligned} Y_m^\ell(R\hat{\mathbf{n}}) &= \sum_{m'} Y_{m'}^\ell(\hat{\mathbf{n}}) D_{m',m}^{(\ell)}(R^{-1}) \\ &= Y_m^\ell(U^\dagger(R)\hat{\mathbf{n}}U(R)) = U^\dagger(R)Y_m^\ell(\hat{\mathbf{n}})U(R) \end{aligned}$$

## B. Orthogonality relations

1. **Orthogonality theorem:** The set of matrix elements of all irreducible representations of a group form a full, orthogonal basis for functions on the group.

2.  $SO(3)$ :

$$\begin{aligned} \mathcal{D}_{m',m}^{(\ell)}(R(\phi, \theta, \chi)) &= \langle \ell, m' | U(R_z(\phi))U(R_y(\theta))U(R_z(\chi)) | \ell, m \rangle \\ &= e^{-im'\phi - im\chi} d_{m',m}^{(\ell)}(\theta), \end{aligned}$$

is a basis for  $SO(3) = \{R(\phi, \theta, \chi)\}$  with the integral measure  $d\phi d(\cos \theta) d\chi$ ,

- *Orthogonality:*

$$\int dR \mathcal{D}_{m'_1, m_1}^{(\ell_1)*}(R) \mathcal{D}_{m'_2, m_2}^{(\ell_2)}(R) = \frac{8\pi^2}{2\ell_1 + 1} \delta_{\ell_1, \ell_2} \delta_{m'_1, m'_2} \delta_{m_1, m_2}$$

- *Completeness:*

$$f(\phi, \theta, \chi) = \sum_{\ell, m, m'} f_{\ell, m, m'} \mathcal{D}_{m, m'}^{(\ell)}(R(\phi, \theta, \chi))$$

where

$$f_{\ell, m, m'} = \frac{2\ell_1 + 1}{8\pi^2} \int_{-\pi}^{\pi} d\phi \int_{-1}^1 d(\cos \theta) \int_{-\pi}^{\pi} d\chi \mathcal{D}_{m, m'}^{(\ell)*}(\phi, \theta, \chi) f(\phi, \theta, \chi)$$

for square integrable functions over  $SO(3)$ .

- *Hand waving argument:*  $\mathcal{D}_{m, m'}^{\ell}(\phi, \theta, \chi) = d_{m, m'}^{(\ell)}(\theta) e^{-im\phi - im'\chi}$

- Set of spherical harmonics,

$$Y_m^{\ell}(\theta, \phi) = \sqrt{\frac{2\ell + 1}{4\pi}} d_{m, 0}^{(\ell)*}(\theta) e^{im\phi}$$

is a basis over  $\theta, \phi$  ( $S_2$ ) with the integral measure  $d\phi d(\cos \theta)$ .

- $\chi$ -dependence:  $\{e^{-im'\chi}\}$  is a basis for  $S_1 = U(1)$  with the integral measure  $d\chi$
- Normalization:

$$\int_{SO(3)} dR |\mathcal{D}_{0,0}^{(\ell)}(R)|^2 = \frac{8\pi^2}{2\ell + 1}$$

### 3. Applied for the addition of angular momentum:

- *Clebsch-Gordan coefficient are real*  $\implies$  the basis transformation from the decoupled to the coupled basis is not only unitary but orthogonal,

$$\begin{aligned} |L, M\rangle &= \sum_{m_1, m_2} |\ell_1, m_1\rangle \otimes |\ell_2, m_2\rangle (\ell_1, \ell_2, m_1, m_2 | L, M) \\ |\ell_1, m_1\rangle \otimes |\ell_2, m_2\rangle &= \sum_{L, M} |L, M\rangle (\ell_1, \ell_2, m_1, m_2 | L, M) \end{aligned}$$

- *Two ways of calculating the result of a rotation:*

(a) Commutative diagram:

$$\begin{array}{ccc} |\ell_1, m_1\rangle \otimes |\ell_2, m_2\rangle & \xrightarrow{U} & U|\ell_1, m_1\rangle \otimes |\ell_2, m_2\rangle \\ \text{C.G.} \downarrow & & \uparrow \text{C.G.} \\ |L, M\rangle & \xrightarrow{U} & U|L, M\rangle \end{array}$$

$$\begin{aligned}
U(R)|\ell_1, m_1\rangle \otimes |\ell_2, m_2\rangle &= \sum_{m'_1, m'_2} |\ell_1, m'_1\rangle \otimes |\ell_2, m'_2\rangle \mathcal{D}_{m'_1, m_1}^{(\ell_1)}(R) \mathcal{D}_{m'_2, m_2}^{(\ell_2)}(R) \\
&= \sum_{L, M, M'} |L, M'\rangle \mathcal{D}_{M', M}^{(L)}(R) \underbrace{(\ell_1, \ell_2, m_1, m_2 | L, M)}_{\langle L, M | \ell_1, \ell_2, m_1, m_2 \rangle} \\
&= \sum_{L, M, M', m'_1, m'_2} \underbrace{|\ell_1, m'_1\rangle \otimes |\ell_2, m'_2\rangle}_{|L, M'\rangle} (\ell_1, \ell_2, m'_1, m'_2 | L, M') \\
&\quad \mathcal{D}_{M', M}^{(L)}(R) (\ell_1, \ell_2, m_1, m_2 | L, M)
\end{aligned}$$

Projection on  $\langle \ell_1, m'_1 | \otimes \langle \ell_2, m'_2 |$ :

$$\begin{aligned}
\langle \ell_1, m'_1 | \otimes \langle \ell_2, m'_2 | U(R) |\ell_1, m_1\rangle \otimes |\ell_2, m_2\rangle &= \mathcal{D}_{m'_1, m_1}^{(\ell_1)}(R) \mathcal{D}_{m'_2, m_2}^{(\ell_2)}(R) \\
&= \sum_{L, M, M'} (\ell_1, \ell_2, m'_1, m'_2 | L, M') \mathcal{D}_{M', M}^{(L)}(R) (\ell_1, \ell_2, m_1, m_2 | L, M)
\end{aligned}$$

(b) Resolution of the identity:

i. Trivial (single basis):

$$\begin{aligned}
\mathbb{1} &= \sum_n |n\rangle \langle n| \\
\langle n | A | n' \rangle &= \langle n | \underbrace{\mathbb{1}}_{\sum_m |m\rangle \langle m|} A \underbrace{\mathbb{1}}_{\sum_{m'} |m'\rangle \langle m'|} | n' \rangle = \langle n | A | n' \rangle
\end{aligned}$$

ii. Less trivial (several bases):

$$\begin{aligned}
\mathbb{1}_d &= \sum_{m_1, m_2} |\ell_1, m_1\rangle \otimes |\ell_2, m_2\rangle \langle \ell_2, m_1 | \otimes \langle \ell_2, m_2 | \\
\mathbb{1}_c &= \sum_{L, M} |L, M\rangle \langle L, M| \\
\mathbb{1}_d U(R) \mathbb{1}_d &= \mathbb{1}_d \mathbb{1}_c U(R) \mathbb{1}_c \mathbb{1}_d \\
&= \mathbb{1}_d \sum_{L, M, M'} \underbrace{|L, M\rangle \langle L, M | U(R) | L, M'\rangle \langle L, M'|}_{\mathbb{1}_c U(R) \mathbb{1}_c} \mathbb{1}_d
\end{aligned}$$

and

$$\begin{aligned}
&\langle \ell_1, m'_1 | \otimes \langle \ell_2, m'_2 | U(R) |\ell_1, m_1\rangle \otimes |\ell_2, m_2\rangle = \\
&= \sum_{L, M, M'} \langle \ell_1, m'_1 | \otimes \langle \ell_2, m'_2 | L, M\rangle \langle L, M | U(R) | L, M'\rangle \langle L, M' | \ell_1, m_1\rangle \otimes |\ell_2, m_2\rangle \\
&= \sum_{L, M, M'} \langle \ell_1, \ell_2, m'_1, m'_2 | L, M'\rangle \mathcal{D}_{M', M}^{(L)}(R) \langle L, M | \ell_1, \ell_2, m_1, m_2\rangle \\
&= \sum_{L, M, M'} (\ell_1, \ell_2, m'_1, m'_2 | L, M') \mathcal{D}_{M', M}^{(L)}(R) (\ell_1, \ell_2, m_1, m_2 | L, M)
\end{aligned}$$

• Multiplication by  $\mathcal{D}_{M', M}^{(L)*}(R)$  and integration over  $R$ :

$$\begin{aligned}
\mathcal{D}_{m'_1, m_1}^{(\ell_1)}(R) \mathcal{D}_{m'_2, m_2}^{(\ell_2)}(R) &= \sum_{L, M, M'} (\ell_1, \ell_2, m'_1, m'_2 | L, M') \mathcal{D}_{M', M}^{(L)}(R) (\ell_1, \ell_2, m_1, m_2 | L, M) \\
\int dR \mathcal{D}_{M', M}^{(L)*}(R) \mathcal{D}_{m'_1, m_1}^{\ell_1}(R) \mathcal{D}_{m'_2, m_2}^{\ell_2}(R) &= \\
&\quad \int dR \mathcal{D}_{M', M}^{(L)*}(R) (\ell_1, \ell_2, m'_1, m'_2 | L, M') \mathcal{D}_{M', M}^{(L)}(R) (\ell_1, \ell_2, m_1, m_2 | L, M)
\end{aligned}$$

- *Orthogonality relation for Clebsch-Gordan coefficients:*

$$\int dR \mathcal{D}_{M',M}^{(L)*}(R) \mathcal{D}_{m'_1,m_1}^{(\ell_1)}(R) \mathcal{D}_{m'_2,m_2}^{(\ell_2)}(R) = \frac{8\pi^2}{2L+1} (\ell_1, \ell_2, m'_1, m'_2 | L, M') (\ell_1, \ell_2, m_1, m_2 | L, M)$$

$$\begin{array}{ccc} \nearrow & & \nwarrow \\ \langle \ell_1, \ell_2, m'_1, m'_2 | L, M' \rangle & & \langle L, M | \ell_1, \ell_2, m_1, m_2 \rangle \end{array}$$

### C. Wigner-Eckart theorem

1. **Selection rules for a tensor operator:** Rotational quantum numbers  $\{\ell, m\}$ , remaining quantum numbers  $n$

$$\mathcal{M} = \langle n_1, \ell_1, m_1 | T_m^{(\ell)} | n_2, \ell_2, m_2 \rangle$$

$$\begin{array}{ccc} \nearrow & & \nwarrow \\ \text{Rotational quantum numbers } \{\ell, m\} & & \text{remaining quantum numbers } n \end{array}$$

#### 2. Derivation:

- *Tensor operator invariance:*  $\sum_{m'} U^\dagger(R) T_{m'}^{(\ell)} U(R) \mathcal{D}_{m',m}^\ell(R) = T_m^{(\ell)}$

$$\begin{aligned} \mathcal{M} &= \langle n_1, \ell_1, m_1 | T_m^{(\ell)} | n_2, \ell_2, m_2 \rangle \\ &= \sum_{m'} \langle n_1, \ell_1, m_1 | U^\dagger(R) T_{m'}^{(\ell)} U(R) | n_2, \ell_2, m_2 \rangle \mathcal{D}_{m',m}^\ell(R) \\ &= \sum_{m'} \langle n_1, \ell_1, m_1 | U^\dagger(R) \mathbb{1} T_{m'}^{(\ell)} \mathbb{1} U(R) | n_2, \ell_2, m_2 \rangle \mathcal{D}_{m',m}^\ell(R) \quad \leftarrow \quad \mathbb{1} = \sum_m |\ell, m\rangle \langle \ell, m| \\ &= \sum_{m'_1 m'_2 m'} \underbrace{\langle n_1, \ell_1, m_1 | U^\dagger(R) | n_1, \ell_1, m'_1 \rangle}_{\langle n_1, \ell_1, m'_1 | U(R) | n_1, \ell_1, m_1 \rangle^*} \langle n_1, \ell_1, m'_1 | T_{m'}^{(\ell)} | n_2, \ell_2, m'_2 \rangle \underbrace{\langle n_2, \ell_2, m'_2 | U(R) | n_2, \ell_2, m_2 \rangle}_{\langle n_2, \ell_2, m'_2 | U(R) | n_2, \ell_2, m_2 \rangle} \\ &\quad \times \mathcal{D}_{m',m}^\ell(R) \end{aligned}$$

Integration over  $R$ :

$$\mathcal{M} \int dR = \sum_{m'_1, m'_2, m'} \langle n_1, \ell_1, m'_1 | T_{m'}^{(\ell)} | n_2, \ell_2, m'_2 \rangle \int dR \mathcal{D}_{m'_1, m_1}^{(\ell_1)*}(R) \mathcal{D}_{m', m}^{(\ell)}(R) \mathcal{D}_{m'_2, m_2}^{(\ell_2)}(R)$$

- *Orthogonality relation for Clebsch-Gordan coefficients:*

$$\underbrace{\int dR}_{8\pi^2} = \frac{8\pi^2}{2\ell_1+1} (\ell, \ell_2, m, m_2 | \ell_1, m_1) \sum_{m'_1, m'_2, m'} (\ell, \ell_2, m', m'_2 | \ell_1, m'_1) \langle n_1, \ell_1, m'_1 | T_{m'}^{(\ell)} | n_2, \ell_2, m'_2 \rangle.$$

- **Wigner-Eckart theorem:**

$$\boxed{\mathcal{M} = (\ell, \ell_2, m, m_2 | \ell_1, m_1) \ll n_1, \ell_1 | T^{(\ell)} | n_2, \ell_2 \gg}$$

Factorization of the rotational kinematics from the rest of the dynamics

$$\begin{array}{ccc}
 \nearrow & & \nwarrow \\
 (\ell, \ell_2, m, m_2 | \ell_1, m_1) & & \text{reduced matrix element:} \\
 \ll n_1, \ell_1 | T_m^{(\ell)} | n_2, \ell_2 \gg = \frac{1}{2\ell_1 + 1} \sum_{m'_1, m'_2, m'} (\ell, \ell_2, m', m'_2 | \ell_1, m'_1) \langle n_1, \ell_1, m'_1 | T_{m'}^{(\ell)} | n_2, \ell_2, m'_2 \rangle,
 \end{array}$$

3. **Selection rule:**  $\langle n_1, \ell_1, m_1 | T_m^{(\ell)} | n_2, \ell_2, m_2 \rangle$  is vanishing if  $(\ell, \ell_2, m, m_2 | \ell_1, m_1) = 0$

4. **Examples:**

(a)  $\ell = 0$ :

$$\begin{aligned}
 (\ell_2, 0, m_2, 0 | \ell_1, m_1) &= \delta_{\ell_1, \ell_2} \delta_{m_1, m_2} \\
 \langle n_1, \ell_1, m_1 | T_m^{(0)} | n_2, \ell_2, m_2 \rangle &= \delta_{\ell_1, \ell_2} \delta_{m_1, m_2} \ll n_1, \ell_1 | T^{(0)} | n_2, \ell_2 \gg
 \end{aligned}$$

Rotation invariant potential  $U(r) = r^p$

$$\langle n_1, \ell_1, m_1 | r^p | n_2, \ell_2, m_2 \rangle = \underbrace{\int d\phi \int d(\cos \theta) Y_{m_1}^{\ell_1*}(\theta, \phi) Y_{m_2}^{\ell_2}(\theta, \phi)}_{(\ell_2, 0, m_2, 0 | \ell_1, m_1)} \underbrace{\int dr r^{2+p} \eta_{n_1, \ell_1}^*(r) \eta_{n_2, \ell_2}(r)}_{\ll n_1, \ell_1 | r^p | n_2, \ell_2 \gg}$$

(b)  $\ell = 1$ : angular momentum

$$\langle n_1, \ell_1, m_1 | T_m^{(1)} | n_2, \ell_2, m_2 \rangle = (1, \ell_2, m, m_2 | \ell_1, m_1) \ll n_1, \ell_1 | T | n_2, \ell_2 \gg$$

To find the reduced matrix elements for the angular momentum  $T_0^{(1)} = L_z$ ,  $T_{\pm 1}^{(1)} = \mp \frac{1}{\sqrt{2}} L_{\pm}$ :

$$\begin{aligned}
 \langle n_1, \ell_1, \ell_1 | L_0 | n_2, \ell_2, \ell_2 \rangle &= (1, \ell_2, 0, \ell_2 | \ell_1, \ell_1) \ll n_1, \ell_1 | L | n_2, \ell_2 \gg \\
 \langle n_1, \ell_1, m | L_0 | n_2, \ell_2, m \rangle &= \hbar m \delta_{n_1, n_2} \delta_{\ell_1, \ell_2} \\
 (1, \ell_1, 0, \ell_1 | \ell_1, \ell_1) &= \sqrt{\frac{\ell_1}{\ell_1 + 1}} \\
 \Rightarrow \ll n_1, \ell_1 | L | n_2, \ell_2 \gg &= \frac{\langle n_1, \ell_1, \ell_1 | L_0 | n_2, \ell_2, \ell_2 \rangle}{(1, \ell_2, 0, \ell_2 | \ell_1, \ell_1)} = \delta_{n_1, n_2} \delta_{\ell_1, \ell_2} \hbar \sqrt{\ell(\ell + 1)}.
 \end{aligned}$$

## V. RELATIVISTIC CORRECTIONS TO THE HYDROGEN ATOM

### A. Scale dependence of physical laws

1. **No "constants" in physics:** no truly isolate system

Measured results depend on the scale of observation (environment)

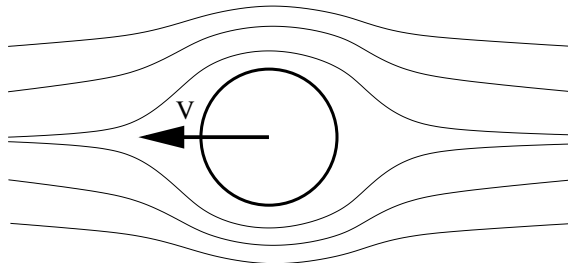
Scales in physics: dimensional quantities, M, L, T, and ...



to establish relation between physical quantities

Bureau of Standard: to assure unchanged environment

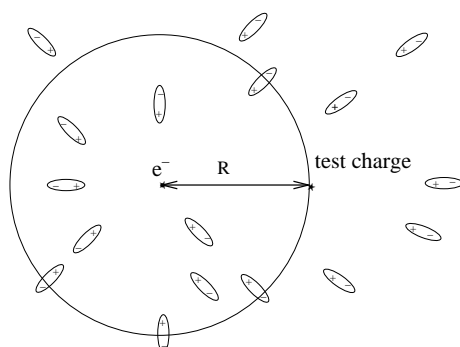
(a) *Mass*: a ball moving with velocity  $v$  in a viscous fluid



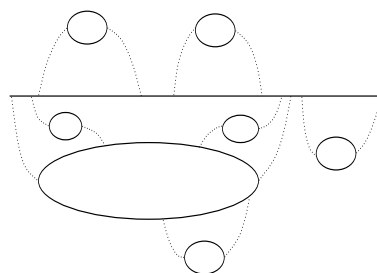
$$E_{tot}(v) = E_{ball}(v) + E_{fl}, \quad E_{ball} = \frac{m(v)}{2}v^2 \quad \Rightarrow \quad m(v) = \frac{d^2 E_{tot}(v)}{dv^2}$$

(b) *Charge*:

- Polarization:



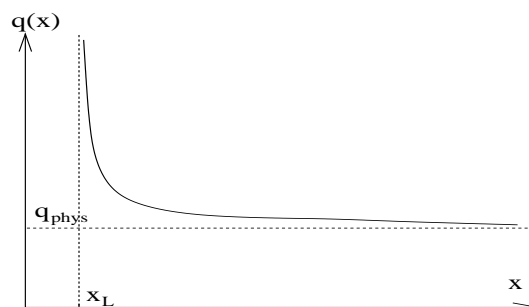
Classical polarizable medium



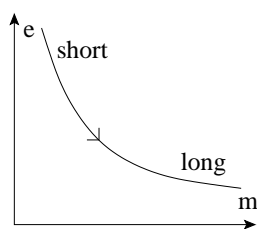
Vacuum polarization around a charge in QED

- Running electric charge:

$$F(R) \neq \frac{q_t q}{R^2} \quad \Rightarrow \quad F(R) = \frac{q_t q(R)}{R^2}$$



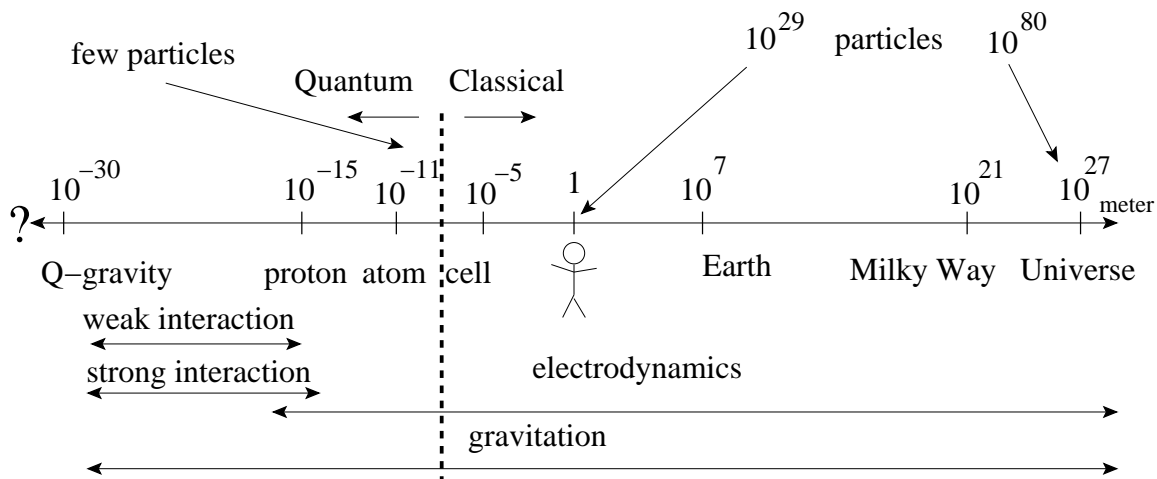
- Renormalized trajectory: Identical physics, changing resolution



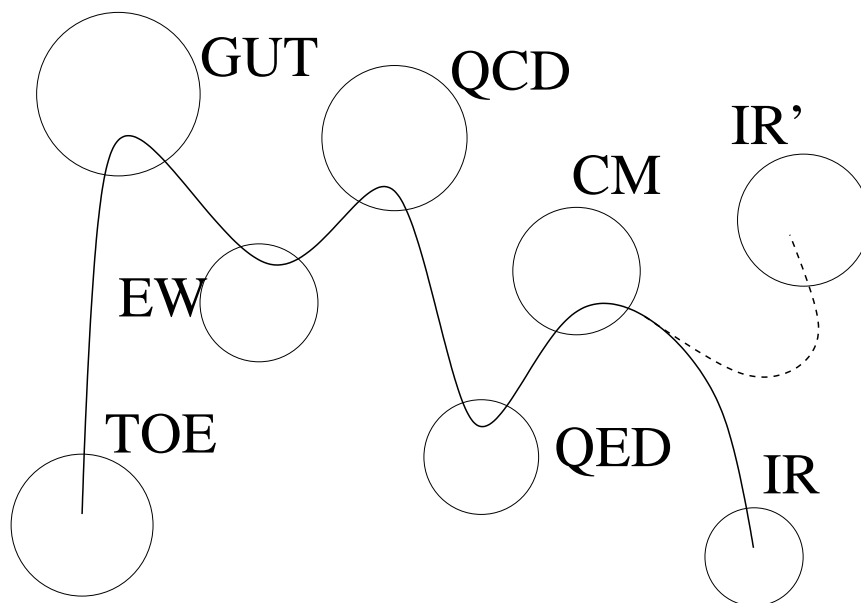
(c) *Speed of light:*

$$v = \frac{c}{\sqrt{\epsilon\mu}}$$

(d) *Relevant length scales:*



(e) *Theory Of Everything:* parameter space of all “constants”, a guided tour of physics

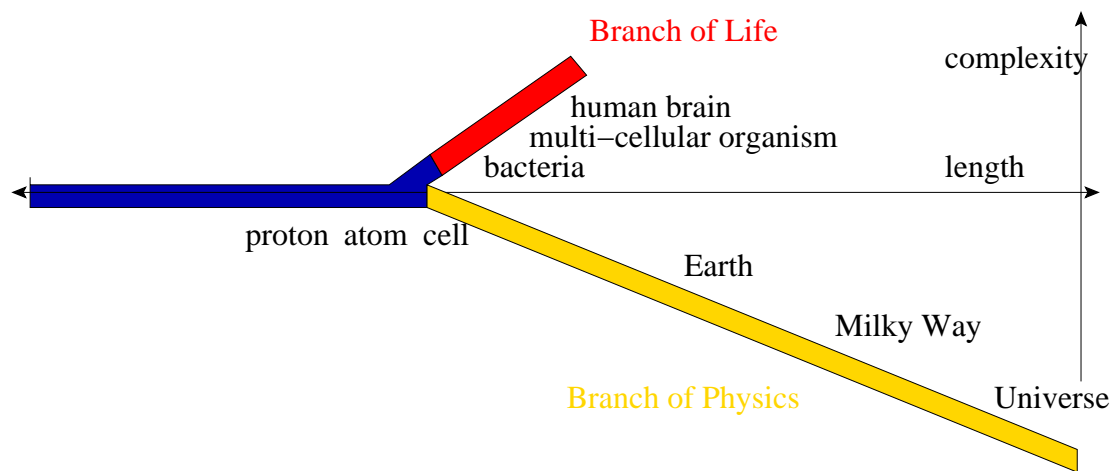




## 2. Why can not we understand Quantum Mechanics?

- The brain is a problem solver organ for the problems presented by the senses
- We learn about the classical world in childhood by playing with macroscopic objects
- Intuition, logics are based on macroscopic, classical physics,
- We have no clue to the quantum world
- What is left is the universal language of mathematics without “understanding“

## 3. Quantum Biology: Life = microscopic order enfolding on macroscopic level



- Average of micr. events
  - Photosynthesis (molecular antennas)
  - Electron transfer in proteins (transport at the micr-macr edge)
- A single micr. event
  - Rhodopsin in the retina (photon detector)
  - Olfaction (spectrum analyser)
  - Bird navigation by the Earth’s magnetic field (quantum measuring device)
  - Neuron dynamics (brain as an amplifier)
- Evolution:
  - $10^{60}$  possible proteins, 6225 appear in living organisms
  - How were they selected?
    - \* At least 165 nucleic acid bases in RNA for reproductibility
    - \*  $4^{165} \sim 10^{99}$  possibilities
    - \* One from each in a primordial soup:  $10^{25} \times M_{Univ}$ .

- \* “Survival of the fittest” is not enough
- Quantum criticality
  - \* 500 randomly chosen proteins function in between the micr. and the macr. domain
  - \* Life exploits the more efficient quantum transport processes on the macr. scale

## B. Hierarchy of scales in QED

### 1. Fine-structure constant:

$$\alpha = \frac{e^2}{\hbar c} \approx \frac{1}{137}$$

(a) *Relativistic effects in the hydrogen atom:*  $a_0 = \frac{\hbar^2}{me^2}$

$$\frac{v^2}{c^2} \approx \frac{\frac{\hbar^2}{m^2 a_0^2}}{c^2} = \frac{e^4}{\hbar^2 c^2} = \alpha^2.$$

(b) *Hierarchy of length scales:*

Bohr radius,  $a_0 \implies$  perturbation expansion  $\implies$  length scales  $r_n = a_0 \alpha^n$ ,  $n = 1, 2, \dots$   
 $\implies$  semiclassical expansion  $\implies$  length scales  $r_n = a_0 \alpha^{-n}$ ,  $n = 1, 2, \dots$

### 2. Bohr radius: $n = 0$ ,

- $a_0 = \frac{\hbar^2}{me^2} \approx 0.053nm$
- size of a hydrogen atom
- $\mathcal{O}(c^0) \implies$  non-relativistic physics

### 3. Compton wavelength: $n = 1$

- $\lambda_C = \frac{\hbar}{mc} \approx 3.86 \cdot 10^{-11}cm = 386fm$
- $\mathcal{O}(e^0) \implies$  relativistic dynamics of a neutral particle
- particle localized in a region of length  $\ell \lesssim \lambda_C \implies$  pair creation

$$E = c\sqrt{m^2c^2 + \mathbf{p}^2} \approx c\sqrt{m^2c^2 + \frac{\hbar^2}{\ell^2}}$$

### 4. Classical electron radius: $n = 2$

- electron-proton Coulomb energy creates electron-positron pairs
- $r_c$  :

$$\frac{e^2}{r_c} = mc^2 \implies r_c = \frac{e^2}{mc^2} \approx 2.8fm$$

- $\mathcal{O}(\hbar^0) \implies$  classical physics, embedded deeply into the quantum domain
- Abraham-Lorentz force, the last more or less open chapter of classical electrodynamics

### 5. Lamb shift: $n = 3$

- $\ell_L = \frac{e^4}{mc^3\hbar} \approx 0.02 fm$
- accidental degeneracy of the hydrogen atom spectrum

### 6. Beyond $n = 0, 1, 2, 3$ :

$$\underbrace{\dots - 2, -1}_{\uparrow} \quad \overbrace{0, 1, 2, 3}^{\text{visible}} \quad \underbrace{4, 5, 6, \dots}_{\uparrow}$$

Overwritten by classical physics

by the electro-weak interaction

## C. Unperturbed, non-relativistic dynamics

### 1. Hamiltonian: $\mathbf{P} = \mathbf{p}_e + \mathbf{p}_p$ , $\mathbf{p} = \mathbf{p}_e - \mathbf{p}_p$ , $\mathbf{r} = \mathbf{r}_e - \mathbf{r}_p$

$$H = \frac{\mathbf{P}^2}{2M} + \frac{\mathbf{p}^2}{2m} - \frac{e^2}{r}, \quad M = m_e + m_p, \quad \frac{1}{m} = \frac{1}{m_e} + \frac{1}{m_p} \approx \frac{1}{m_e}$$

### 2. Eigenstates: $\mathbf{P}$ free motion

$$\psi_{n,\ell,m,s_e,s_p}(r, \theta, \phi, \sigma, \Sigma) = \eta_{m,\ell}(r) Y_m^\ell(\theta, \phi) \chi_{s_e}(\sigma) \chi_{s_p}(\Sigma),$$

### 3. Eigenvalues: Rydberg constant: $R = \frac{\hbar^2}{2ma_0^2} \approx 13.6eV$

$$E_{n,\ell,m,s} = -\frac{R}{n^2}, \quad \ell = 0, \dots, n-1, \quad -\ell \leq m \leq \ell$$

(accidental) Degeneracy:  $(2S_p + 1)(2S_e + 1)n^2 = 4n^2$ -fold

## D. Fine structure

### 1. Relativistic effects:

- *Kinetic energy*: relativistic free particle
- *Interactions*: dynamical degrees of freedom of the E.M. field are resolved

### 2. Kinetic energy

(a) *Origin:*

$$E = c\sqrt{m^2c^2 + \mathbf{p}^2} = mc^2 + \frac{\mathbf{p}^2}{2m} - \frac{\mathbf{p}^4}{8m^3c^2} + \mathcal{O}\left(\left(\frac{v}{c}\right)^6\right)$$

(b) *Form:*

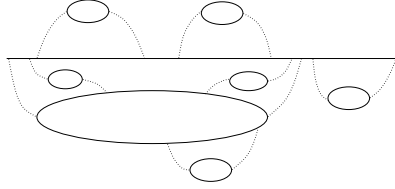
$$H_0 = \frac{\mathbf{p}^2}{2m} - \frac{\mathbf{p}^4}{8m^3c^2} = \frac{\mathbf{p}^2}{2m} + H_m.$$

(c) *Magnitude:*

$$\frac{|H_m|}{\frac{\mathbf{p}^2}{2m}} \approx \frac{\frac{\mathbf{p}^4}{m^3c^2}}{\frac{\mathbf{p}^2}{m}} = \frac{v^2}{c^2} = \alpha^2$$

### 3. Darwin term:

(a) *Origin:* cloud of virtual electron-positron pairs, the vacuum polarization of the Dirac-see



(b) *Form:* Smearing,  $\rho(\mathbf{r}) = \delta(\mathbf{r}) \rightarrow \rho(\mathbf{r})$ ,  $\int d\mathbf{r}\rho(\mathbf{r}) = 1$ ,  $U_C(r) = \frac{e^2}{r} \rightarrow U(\mathbf{r}) = U_C(\mathbf{r}) + U_D(\mathbf{r})$

Multipole expansion:

$$\begin{aligned} U(\mathbf{r}) &= \int d\mathbf{r}'\rho(\mathbf{r}')U_C(\mathbf{r} + \mathbf{r}') \\ &= \int d\mathbf{r}'\rho(\mathbf{r}') \left[ U_C(\mathbf{r}) + \mathbf{r}'\nabla U_C(\mathbf{r}) + \frac{1}{2}r'_j r'_k \partial_j \partial_k U_C(\mathbf{r}) + \dots \right] \\ \int d\mathbf{r}'\mathbf{r}' &= 0, \quad \int d\mathbf{r}'\rho(\mathbf{r}')r'_j r'_k = \frac{1}{3}\delta_{jk} \underbrace{\int d\mathbf{r}'\mathbf{r}'^2 \rho(\mathbf{r}')}_{\frac{3}{4}\lambda_C^2} \end{aligned}$$

$$= U_C(\mathbf{r}) + \frac{\lambda_C^2}{4}\nabla^2 U_C(\mathbf{r})$$

$$H_D = -U_D = \frac{1}{8}\lambda_C^2\nabla^2 U_C(\mathbf{r}) = -\frac{1}{2}\pi e^2\lambda_C^2\delta(\mathbf{r}) = -\frac{\pi\hbar^2 e^2}{2m^2 c^2}\delta(\mathbf{r})$$

↑

$$\nabla_x^2 \frac{1}{|\mathbf{x}-\mathbf{y}|} = -4\pi\delta(\mathbf{x}-\mathbf{y})$$

(c) *Magnitude:*

$$-\langle U_D \rangle = \frac{\pi\hbar^2 e^2}{2m^2 c^2} \underbrace{|\psi(0)|^2}_{\approx \frac{1}{a_0^3}} \approx \frac{e^2\hbar^2}{m^2 c^2} \frac{m^3 e^6}{\hbar^6} = mc^2 \frac{e^8}{\hbar^4 c^4} = mc^2 \alpha^4$$

$$\langle H_0 \rangle \approx R = \frac{\hbar^2}{2ma_0^2} = \frac{\hbar^2}{2m} \frac{m^2 e^4}{\hbar^4} = \frac{me^4}{2\hbar^2} = \frac{1}{2}mc^2 \alpha^2$$

$$\frac{|\langle H_D \rangle|}{\langle H_0 \rangle} \approx \alpha^2$$

#### 4. Spin-orbit coupling:

(a) *Origin:* spin  $\implies$  magnetic moment & moving charge (proton!)  $\implies$  current  $\implies$  magnetic field

- *Form:*

$$\boxed{H_i = -\mathbf{m}\mathbf{B}}$$

- *E.M. field in quantum mechanics:* canonical quantization

$$\begin{aligned} L &= \frac{m}{2}\dot{\mathbf{x}}^2 - e\phi(t, \mathbf{x}) + \frac{e}{c}\dot{\mathbf{x}}\mathbf{A}(t, \mathbf{x}) \\ \mathbf{p} &= \frac{\partial L(\dot{\mathbf{x}}, \mathbf{x})}{\partial \dot{\mathbf{x}}} = m\dot{\mathbf{x}} + \frac{e}{c}\mathbf{A}(t, \mathbf{x}) \implies \dot{\mathbf{x}} = \frac{1}{m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right) \\ [x_j, p_k] &= i\hbar\delta_{j,k} \implies \mathbf{p} = \frac{i}{\hbar}\nabla \\ H &= \mathbf{p}\dot{\mathbf{x}} - L = \mathbf{p}\dot{\mathbf{x}} - \frac{m}{2}\dot{\mathbf{x}}^2 + e\phi(t, \mathbf{x}) - \frac{e}{c}\dot{\mathbf{x}}\mathbf{A}(t, \mathbf{x}) \\ &= \mathbf{p}\frac{1}{m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right) - \frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2 + e\phi - \frac{e}{cm}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)\mathbf{A} = \frac{(\mathbf{p} - \frac{e}{c}\mathbf{A})^2}{2m} + e\phi, \end{aligned}$$

- *Magnetic moment of the orbital angular momentum:*

– Homogeneous magnetic field

$$\begin{aligned} A^\mu &= (0, \mathbf{A}), \quad A_\mu = (0, -\mathbf{A}), \quad \mathbf{A} = -\frac{1}{2}\mathbf{r} \times \mathbf{B} \\ B_i &= (\nabla \times \mathbf{A})_i = -\frac{1}{2}\epsilon_{ijk}\nabla_j\epsilon_{klm}x_l B_m = -\frac{1}{2}\epsilon_{ijk}\epsilon_{klm}B_m = \frac{1}{2}\underbrace{\epsilon_{ijk}\epsilon_{klm}}_{2\delta_{im}}B_m = B_i \end{aligned}$$

– Hamiltonian:

$$\begin{aligned} H &= \frac{\mathbf{p}^2}{2m} - \frac{e}{2mc}(\mathbf{p}\mathbf{A} + \mathbf{A}\mathbf{p}) + \frac{e^2}{2mc^2}\mathbf{A}^2 \\ &= \frac{\mathbf{p}^2}{2m} - \frac{e}{mc}\mathbf{A}\mathbf{p} + i\frac{e\hbar}{2mc}\nabla\mathbf{A} + \frac{e^2}{2mc^2}\mathbf{A}^2 \\ &= \frac{\mathbf{p}^2}{2m} + \frac{e}{2mc}(\mathbf{r} \times \mathbf{B})\mathbf{p} + \frac{e^2}{2mc^2}\mathbf{A}^2 \\ &= \frac{\mathbf{p}^2}{2m} - \frac{e}{2mc}\mathbf{L}\mathbf{B} + \frac{e^2}{2mc^2}\mathbf{A}^2 \end{aligned}$$

– Magnetic moment:

$$\boxed{\mathbf{m} = \frac{e}{2mc}\mathbf{L} = \mu_B\frac{\mathbf{L}}{\hbar}, \quad \mu_B = \frac{e\hbar}{2mc}}$$

- *Magnetic moment of the spin:* Pauli 1927, Dirac 1928

– Pauli:  $\mathbf{P} = \mathbf{p} - \frac{e}{c}\mathbf{A} \rightarrow \boldsymbol{\sigma}\mathbf{P}$ ,

$$\begin{aligned} H &= \frac{\mathbf{P}^2}{2m} \rightarrow \frac{(\boldsymbol{\sigma}\mathbf{P})^2}{2m} = \frac{\{\sigma_j, \sigma_k\}\{P_j, P_k\} + [\sigma_j, \sigma_k][P_j, P_k]}{8m} \\ \sigma_a\sigma_b &= \delta_{a,b} + i\sum_c \epsilon_{abc}\sigma_c \implies \{\sigma_j, \sigma_k\} = 2\delta_{jk}, \quad [\sigma_j, \sigma_k] = 2i\epsilon_{jkl}\sigma_l \\ H &= \frac{2\delta_{jk}\{P_j, P_k\} + 2i\epsilon_{jkl}\sigma_l[P_j, P_k]}{8m} = \frac{\mathbf{P}^2}{2m} + i\frac{\epsilon_{jkl}\sigma_l[P_j, P_k]}{4m} \end{aligned}$$

$$\begin{aligned}
[\nabla_j + f_j, \nabla_k + f_k]h &= [\nabla_j, \nabla_k]h + [f_j, f_k]h + \underbrace{[\nabla_j, f_k]h}_{\nabla_j(f_k h) - f_k \nabla_j h} + [f_j, \nabla_k]h = (\nabla_j f_k - \nabla_k f_j)h \\
\frac{(\boldsymbol{\sigma} \mathbf{P})^2}{2m} &= \frac{\mathbf{P}^2}{2m} - \frac{i}{4m} \epsilon_{jkl} \sigma_\ell \frac{\hbar e}{i c} (\nabla_j A_k - \nabla_k A_j) = \frac{\mathbf{P}^2}{2m} - \frac{\hbar e}{2mc} \epsilon_{jkl} \nabla_j A_k \sigma_\ell \\
&= \frac{\mathbf{P}^2}{2m} - \frac{\hbar e}{2mc} B_\ell \sigma_\ell = \frac{\mathbf{P}^2}{2m} - \mathbf{m} \mathbf{B} \implies \mathbf{m} = \frac{\hbar e}{2mc} \boldsymbol{\sigma} = \frac{\hbar e}{mc} \frac{\mathbf{s}}{\hbar}
\end{aligned}$$

$$\boxed{\mu = g_S \mu_B, \quad g_S = 2}$$

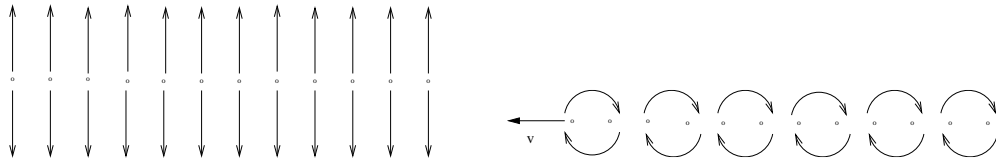
– Magnetic moment of a composite particle:  $\mathbf{J} = \mathbf{L} + \mathbf{S}$

$$\mathbf{m} = \mu_B \frac{\mathbf{L} + g_S \mathbf{S}}{\hbar} = \mu_B \frac{\mathbf{J} + (g_S - 1) \mathbf{S}}{\hbar} \approx g_P \mu_B \frac{\mathbf{J}}{\hbar}, \quad g_P \neq 1$$

• *Magnetic field in the hydrogen atom:*

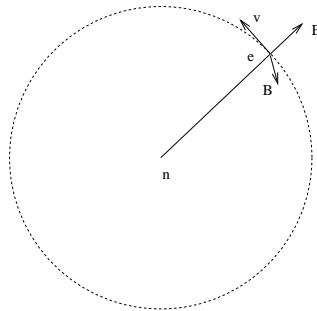
- The best frame: rest frame of the electron
- Homogeneous electric field  $\mathbf{E}$  seen by velocity  $\mathbf{v}$ :

$$\mathbf{B} = -\frac{1}{c} \mathbf{v} \times \mathbf{E}$$



– Magnetic field of the moving nucleus

$$\mathbf{E}(\mathbf{r}) = -\mathbf{e}_r \partial_r \frac{e}{r} = \frac{e}{r^2} \mathbf{e}_r \implies \mathbf{B} = \frac{1}{c} \partial_r \frac{e}{r} \mathbf{v} \times \mathbf{e}_r = \frac{1}{rc} \partial_r \frac{e}{r} \mathbf{v} \times \mathbf{r}$$



(b) *Form:*

$$\begin{aligned}
H_{so} &= -\mathbf{m}_s \mathbf{B} = -2\mu_B \frac{\mathbf{s}}{\hbar} \frac{1}{rc} \partial_r \frac{e}{r} \mathbf{v} \times \mathbf{r} = -2 \frac{e\hbar}{2mc} \frac{\mathbf{s}}{\hbar} \frac{1}{rc} \partial_r \frac{e}{r} \mathbf{v} \times \mathbf{r} = -\frac{e^2}{m^2 c^2} \frac{1}{r} \partial_r \frac{1}{r} \mathbf{s} (\mathbf{p} \times \mathbf{r}) \\
&= \frac{e^2}{m^2 c^2} \frac{1}{r} \partial_r \frac{1}{r} \mathbf{s} \mathbf{L}
\end{aligned}$$

(c) *Magnitude:*

$$\frac{\langle H_{so} \rangle}{\langle U_C \rangle} \approx \frac{\frac{e^2 \hbar^2}{m^2 c^2 a_0^3}}{\frac{e^2}{a_0}} = \frac{\hbar^2}{m^2 c^2 a_0^2} = \frac{\hbar^2}{m^2 c^2 \left(\frac{\hbar^2}{m e^2}\right)^2} = \frac{e^4}{\hbar^2 c^2} = \alpha^2$$

## E. Hyperfine structure

### 1. Origin:

(a)  $\mathbf{S}_e, \mathbf{L}_e \implies$  magnetic field for  $\mathbf{S}_p$

(b) suppressed by  $\frac{m_e}{m_p} \sim \frac{0.51 \text{ MeV}}{938 \text{ MeV}} \sim \frac{1}{2000}$  compared to the fine structure

### 2. Form:

$$H_{hf} = -\frac{1}{c^2} \left\{ \frac{e}{m_e R^3} \mathbf{L} \mathbf{m}_p + \frac{1}{R^3} [3(\mathbf{m}_e \mathbf{n})(\mathbf{m}_p \mathbf{n}) - \mathbf{m}_e \mathbf{m}_p] + \frac{8\pi}{3} \mathbf{m}_e \mathbf{m}_p \delta^{(3)}(R) \right\}$$

$$\mathbf{m}_e = 2 \frac{e \hbar}{2 m_e} \frac{\mathbf{s}_n}{\hbar}$$

$$\mathbf{m}_p = g_p \frac{e \hbar}{2 m_n} \frac{\mathbf{s}_n}{\hbar}, \quad g_p \approx 5.585 (\neq 2)$$

### 3. Magnitude:

$$\langle H_{hf} \rangle \approx \frac{e^2 \hbar^2}{m_e m_p c^2 a_0^3} \approx \langle H_{so} \rangle \frac{m_e}{m_p}$$

## F. Splitting of the fine structure degeneracy

### 1. Hamiltonian:

$$H_f = H_m + H_D + H_{so}$$

$\mathbf{Ls}$  in  $H_{so}$ :

$$\mathbf{J} = \mathbf{L} + \mathbf{s} \implies \mathbf{Ls} = \frac{1}{2}(\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{s}^2)$$

Coupled basis:

$$|n, J, M, \ell\rangle = \sum_{s_e} |n, \ell, M - s_e, s_e\rangle \left\langle \ell, \frac{1}{2}, M - s_e, s_e | J, M \right\rangle.$$

Spectroscopic quantum numbers:  $n \ell_J, \ell = 0, 1, 2, 3, \dots = s, p, d, f, g, \dots$

2.  $n = 1$ :  $1s$  level, 2 dimensional degeneracy ( $s_e$ )

- We seek  $E^{(1)} = \langle \psi^{(0)} | H_f | \psi^{(0)} \rangle$

$$E^{(1)} = \langle n, \ell, m, s_s | H_f | n, \ell, m, s_s \rangle$$

$$\langle r, \theta, \phi, s_s | n, \ell, m, s_s \rangle = R_{n,\ell}(r) Y_m^\ell(\theta, \phi) u(s_s), \quad R_{1,0}(r) = \frac{2}{a_0^{\frac{3}{2}}} e^{-\frac{r}{a_0}}, \quad Y_0^0 = \frac{1}{\sqrt{4\pi}}$$

- $H_m$ :

$$\mathbf{p}^4 = 4m^2 \left( H_0 + \frac{e^2}{r} \right)^2, \quad H_0 = \frac{\mathbf{p}^2}{2m} - \frac{e^2}{r}, \quad E_n = -\frac{\alpha^2 m c^2}{2n^2}$$

$$H_m = -\frac{\mathbf{p}^4}{8m^3 c^2} = -\frac{(H_0 + \frac{e^2}{r})^2}{2m c^2}$$

$$\langle H_m \rangle = -\frac{1}{2m c^2} \left( E_n^2 + 2E_n \langle \frac{e^2}{r} \rangle + \langle \frac{e^4}{r^2} \rangle \right)$$

Generator functional:

$$I(\kappa) = \int_0^\infty dr e^{-\kappa r} = \frac{1}{\kappa}$$

$$\langle \frac{1}{r^n} \rangle = \frac{4\pi}{4\pi} \int_0^\infty dr r^{2-n} \frac{4}{a_0^3} e^{-\frac{2r}{a_0}} = \frac{4}{a_0^3} (-1)^{2-n} \frac{d^{2-n} I(\kappa)}{d\kappa^{2-n}} \Big|_{\kappa=\frac{2}{a_0}}$$

$$\langle \frac{1}{r} \rangle = -\frac{4}{a_0^3} \frac{dI(\kappa)}{d\kappa} \Big|_{\kappa=\frac{2}{a_0}} = \frac{4}{a_0^3} \frac{a_0^2}{4} = \frac{1}{a_0}, \quad \langle \frac{1}{r^2} \rangle = \frac{4}{a_0^3} (-1)^{2-n} \frac{d^{2-n} I(\kappa)}{d\kappa^{2-n}} \Big|_{\kappa=\frac{2}{a_0}} = \frac{4}{a_0^3} \frac{a_0}{2} = \frac{2}{a_0^2}$$

$$\langle H_m \rangle = -\frac{1}{2m c^2} \left( \frac{\alpha^4 m^2 c^4}{4} - \frac{\alpha^2 m c^2 e^2}{a_0} + \frac{2e^4}{a_0^2} \right) = -\frac{5}{8} \alpha^4 m c^2$$

- $H_D$ :

$$\langle H_D \rangle = -\frac{\pi \hbar^2 e^2}{2m^2 c^2} \langle \delta(\mathbf{r}) \rangle = \frac{e^2 \hbar^2 \pi}{2m^2 c^2} |\psi_{n,\ell,m}(0)|^2 = \frac{e^2 \hbar^2}{8m^2 c^2} \underbrace{|R_{1,0}(0)|^2}_{4a_0^{-3} = 4(\frac{m e^2}{\hbar^2})^3} = \frac{1}{2} \alpha^4 m c^2.$$

- $H_{so} : \langle H_{so} \rangle \sim \langle \mathbf{sL} \rangle = 0$

- Finally:  $\Delta E = -\frac{1}{8} \alpha^4 m c^2$ , the spin degeneracy prevails in  $1s_{\frac{1}{2}}$

3.  $n = 2$ :

- Degeneracy:

$$\underbrace{2}_{2s_{\frac{1}{2}}} + \underbrace{2}_{2p_{\frac{1}{2}}} + \underbrace{4}_{2p_{\frac{3}{2}}} = 8$$

- Absence of mixing of  $2s$  and  $2p$ :

$$H_f = \begin{pmatrix} H_{2s} & 0 \\ 0 & H_{2p} \end{pmatrix}.$$



- $2s$ :

$$\begin{aligned}
 R_{2,0} &= \frac{2}{(2a_0)^{\frac{3}{2}}} \left(1 - \frac{r}{2a_0}\right) e^{-\frac{r}{2a_0}}, & R_{2,1} &= \frac{1}{\sqrt{2}(2a_0)^{\frac{3}{2}}} \frac{r}{a_0} e^{-\frac{r}{2a_0}} \\
 \langle 2s | \frac{1}{r} | 2s \rangle &= \frac{1}{4a_0}, & \langle 2s | \frac{1}{r^2} | 2s \rangle &= \frac{1}{12a_0^2}, & \langle 2s | \frac{1}{r^3} | 2s \rangle &= \frac{1}{24a_0^3} \\
 \langle H_m \rangle &= -\frac{13}{128} mc^2 \alpha^4 \\
 \langle H_D \rangle &= -\frac{1}{16} mc^2 \alpha^4 \\
 \langle H_{so} \rangle &= 0
 \end{aligned}$$

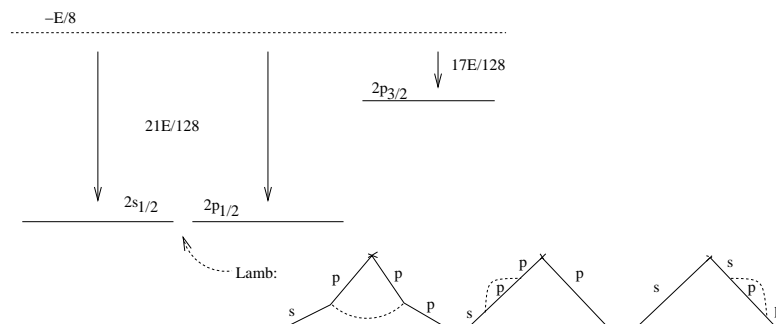
Energy shift: degeneracy remains

$$\Delta E_{2s_{\frac{1}{2}}} = -\frac{21}{128} \alpha^4 mc^2$$

- $2p$ :

$$\begin{aligned}
 \langle H_m \rangle &= -\frac{55}{384} mc^2 \alpha^4 \\
 \langle H_D \rangle &= 0 \quad \leftarrow \quad R_\ell = \mathcal{O}(r^\ell) \\
 \langle H_{so} \rangle &= \langle 2p, m, s_e | \frac{e^2}{2m^2 c^2} \frac{1}{r^3} \mathbf{SL} | 2p, m', s'_e \rangle = \underbrace{\frac{e^2}{2m^2 c^2} \int_0^\infty dr r^2 \frac{1}{r^3} |R_{2,1}(r)|^2}_{\frac{mc^2 \alpha^4}{48 \hbar^2}} \langle 1, m, s_e | \mathbf{SL} | 1, m', s'_e \rangle
 \end{aligned}$$

$$\begin{aligned}
 \mathbf{SL} | \ell, m, s \rangle &= \frac{1}{2} (\vec{J}^2 - \mathbf{L}^2 - \mathbf{S}^2) | \ell, m, s \rangle \\
 &= \frac{\hbar^2}{2} \left[ J(J+1) - \ell(\ell+1) - \frac{1}{2} \frac{3}{2} \right] | \ell, m, s \rangle \\
 &= \frac{\hbar^2}{2} \left[ J(J+1) - \frac{11}{4} \right] | \ell, m, s \rangle \\
 &= \begin{cases} -\hbar^2 | 1, m, s_e \rangle & J = \frac{1}{2} \\ \frac{\hbar^2}{2} | 1, m, s_e \rangle & J = \frac{3}{2} \end{cases} \\
 \langle H_{so} \rangle &= \begin{cases} -\frac{1}{48} mc^2 \alpha^4 & J = \frac{1}{2}, \\ \frac{1}{96} mc^2 \alpha^4 & J = \frac{3}{2}. \end{cases} \\
 \implies \Delta E_{2p_{\frac{1}{2}}} &= -\frac{21}{128} \alpha^4 mc^2, & \Delta E_{2p_{\frac{3}{2}}} &= -\frac{17}{128} \alpha^4 mc^2
 \end{aligned}$$

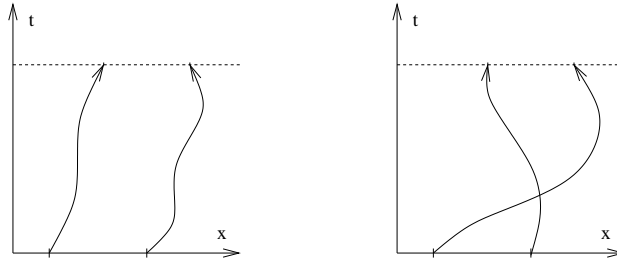


- (a) Degeneracy in  $J$  is split
- (b) Subspaces  $2s_{\frac{1}{2}}$  and  $2p_{\frac{1}{2}}$  remain degenerate, they split up in  $\mathcal{O}(\alpha^2)$  by photon emission and absorption processes (Lamb shift)

## VI. IDENTICAL PARTICLES

### 1. Macroscopic quantum effect

- *Classical physics:* trajectories distinguish the particles



- *Quantum physics:*

- Heisenberg's uncertainty principle  $\implies \nexists$  trajectories
- The difficulty of distinguishability is generalised to the principle of undistinguishability
- $\hbar$ -independent quantum effect
- Realization:

- \*  $\pi$ : exchange of two particles,  $|x_1, x_2\rangle \neq \pi|x_1, x_2\rangle = |x_2, x_1\rangle$

- \* Hilbert space: ray representation of physical states,  $|\psi\rangle_{phys} = \{e^{i\alpha}|\psi\rangle\}$

$$|x_2, x_1\rangle = e^{i\theta_e}|x_1, x_2\rangle$$

$$\psi(x_2, x_1) = e^{i\theta_e}\psi(x_1, x_2).$$

- Gibbs paradox: entropy of the ideal gas is non-extensive

Solution:  $N$  identical particles has  $N!$  identical rearrangements

### 2. Fermions and bosons:

- *Naive expectation:*

$$\pi^2 = 1 \implies e^{2i\theta_e} = 1 \implies e^{i\theta_e} = \pm 1$$

$$\text{However } \pi^2|x_1, x_2\rangle = e^{2i\theta_e}|x_1, x_2\rangle = e^{i\alpha}|x_1, x_2\rangle \implies 2\theta_e = \alpha \neq 2n\pi$$

- *Spin-statistic theorem:*

(a) Rotational phase:

$$U_j(R_n(2\pi))|x_1, x_2\rangle = e^{i\theta_r}|x_1, x_2\rangle,$$

(b) Exchange phase:

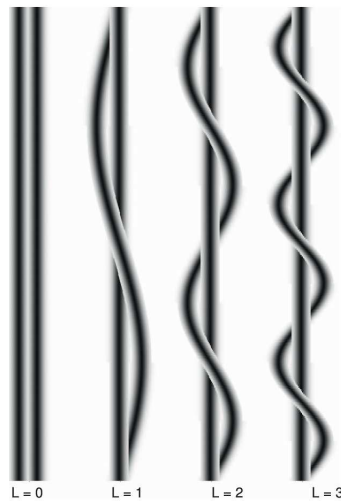
$$\psi(x_2, x_1) = e^{i\theta_e}\psi(x_1, x_2).$$

(c) Theorem:

$$\boxed{\theta_r = \theta_e}$$

(d) Topological proof:

- Twist number of a closed ribbon: number of rotation by  $2\pi$



$$\nu = \frac{1}{2\pi} \int_0^L dx \frac{d\alpha(x)}{dx}$$

- Ribbon, attached to each particle and to the wall
- Exchange of the ends of a ribbon generates  $2\pi$  rotation

(e) Fermions and bosons in three dimensions:

$$U(R_n(2\pi)) = \xi = \pm 1$$

(f) Anyons in two dimensions: phase (irreducible) representations of rotation group  $SO(2)$

$$U_\theta(2\pi)|x_1, x_2\rangle = e^{i\theta}|x_1, x_2\rangle, \quad -\pi < \theta \leq \pi$$

### 3. Superselection rule:

No mixing between fermions and bosons  $\iff$  classical physics has no fermionic coordinate

(a) Matrix element of a tensor operator of integer angular momentum:

$$\begin{aligned}
\langle \psi_{\xi'} | T_m^{(\ell)} | \phi_{\xi} \rangle &= \langle \psi_{\xi'} | U^\dagger(R_{\mathbf{n}}(2\pi)) U(R_{\mathbf{n}}(2\pi)) T_m^{(\ell)} U^\dagger(R_{\mathbf{n}}(2\pi)) U(R_{\mathbf{n}}(2\pi)) | \phi_{\xi} \rangle \\
T_m^{(\ell)} &= \sum_{m'} U^\dagger(R) T_{m'}^{(\ell)} U(R) \mathcal{D}_{m',m}^\ell(R) \\
\langle \psi_{\xi'} | T_m^{(\ell)} | \phi_{\xi} \rangle &= \sum_{m'} \mathcal{D}_{m',m}^\ell(R_{\mathbf{n}}(2\pi)) \langle \psi_{\xi'} | U^\dagger(R_{\mathbf{n}}(2\pi)) T_{m'}^{(\ell)} U(R_{\mathbf{n}}(2\pi)) | \phi_{\xi} \rangle \\
&= \xi' \xi \sum_{m'} \underbrace{\mathcal{D}_{m',m}^\ell(R_{\mathbf{n}}(2\pi))}_{\delta_{m,m'}} \langle \psi_{\xi'} | T_{m'}^{(\ell)} | \phi_{\xi} \rangle \\
&= \xi' \xi \langle \psi_{\xi'} | T_m^{(\ell)} | \phi_{\xi} \rangle \implies \langle \psi_{\xi'} | T_m^{(\ell)} | \phi_{\xi} \rangle = 0 \text{ for } \xi' \neq \xi
\end{aligned}$$

(b) Interactions do not mix fermionic and bosonic states (Hamiltonian is an  $\ell = 0$  tensor operator)

$$\begin{aligned}
\underbrace{\psi(1,2)}_{\mathcal{H}_{12}} &= \underbrace{\frac{1}{2}(\psi(1,2) + \psi(2,1))}_{\mathcal{H}_s} \oplus \underbrace{\frac{1}{2}(\psi(1,2) - \psi(2,1))}_{\mathcal{H}_a} \\
\mathcal{H}_{12} &= \mathcal{H}_s \oplus \mathcal{H}_a
\end{aligned}$$

#### 4. Several particles:

(a) *Exchange of two neighbouring particles:*

$$\psi(x_1, \dots, x_j, x_{j+1}, \dots, x_n) = \xi \psi(x_1, \dots, x_{j+1}, x_j, \dots, x_n)$$

(b) *Exchange a pair:*

$$\psi(x_1, \dots, x_j, \dots, x_k, \dots, x_n) = \xi \psi(x_1, \dots, x_k, \dots, x_j, \dots, x_n)$$

because each particle  $j+1, \dots, k-1$  are skipped twice by  $x_j$  and  $x_k$  producing  $\xi^{2|j-k-1|}$

(c) *Parity of a permutation:*

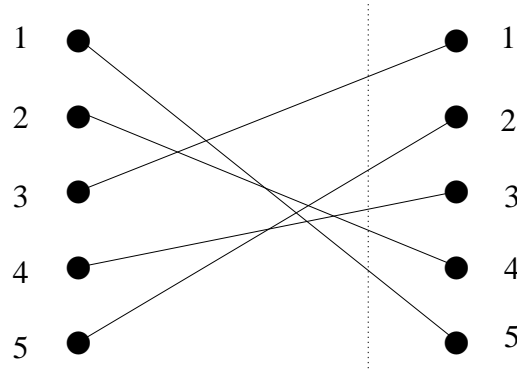
- Each permutation

$$\pi = \begin{pmatrix} 1, \dots, N \\ \pi(1), \dots, \pi(N) \end{pmatrix}$$

is the product of the exchange of neighbours

Example:

$$\begin{pmatrix} 1,2,3,4,5 \\ 3,5,4,2,1 \end{pmatrix} = (1,4)(1,5)(4,5)(2,3)(3,5)(2,4)(3,4)$$



- Number of exchanged neighbours,  $n(\pi)$ , is not unique but its parity

$$\sigma(\pi) = n(\pi) \pmod{2}$$

is unique and well defined

Proof: continuous deformation of the lines

- can reproduce any factorization
- changes the number of crossing in units of 2

- Each crossing generates a multiplicative factor  $\xi \implies$  total exchange factor is  $\xi^{\sigma(\pi)}$

Example:  $N = 3$

$$\begin{aligned} 1 &= \sigma\left(\begin{pmatrix} 1,2,3 \\ 1,2,3 \end{pmatrix}\right) = \sigma\left(\begin{pmatrix} 1,2,3 \\ 3,1,2 \end{pmatrix}\right) = \sigma\left(\begin{pmatrix} 1,2,3 \\ 2,3,1 \end{pmatrix}\right) \\ -1 &= \sigma\left(\begin{pmatrix} 1,2,3 \\ 1,3,2 \end{pmatrix}\right) = \sigma\left(\begin{pmatrix} 1,2,3 \\ 3,2,1 \end{pmatrix}\right) = \sigma\left(\begin{pmatrix} 1,2,3 \\ 2,1,3 \end{pmatrix}\right). \end{aligned}$$

(d)  $N$  particle ket state from  $N$  one-particle states  $\{|k\rangle\}$ :

$$\boxed{|k_1, \dots, k_N\rangle = \mathcal{N} \sum_{\pi \in S_N} \xi^{\sigma(\pi)} |k_{\pi(1)}\rangle \otimes \dots \otimes |k_{\pi(N)}\rangle}$$

Proof:

$$\sum_{\pi \in S_N} F(\pi) = \sum_{\pi \in S_N} F(\pi\pi') = \sum_{\pi \in S_N} F(\pi'\pi)$$

the maps  $\pi \rightarrow \pi\pi'$ ,  $\pi \rightarrow \pi'\pi$  are onto and one-to-one  $\implies$  same sums in different order

$$\begin{aligned} |k_{\pi'(1)}, \dots, k_{\pi'(N)}\rangle &= \mathcal{N} \sum_{\pi \in S_N} \xi^{\sigma(\pi)} |k_{\pi\pi'(1)}\rangle \otimes \dots \otimes |k_{\pi\pi'(N)}\rangle \\ \sigma(\pi\pi') &= \sigma(\pi) \pm \sigma(\pi') \quad \leftarrow \quad \xi^{2\sigma(\pi')} = 1 \\ |k_{\pi'(1)}, \dots, k_{\pi'(N)}\rangle &= \xi^{\sigma(\pi')} \mathcal{N} \sum_{\pi \in S_N} \xi^{\sigma(\pi\pi')} |k_{\pi\pi'(1)}\rangle \otimes \dots \otimes |k_{\pi\pi'(N)}\rangle = \xi^{\sigma(\pi')} |k_1, \dots, k_N\rangle \end{aligned}$$

(e) *N* particle function:

$$\begin{aligned}\psi_{k_1, \dots, k_n}^{(+)}(\mathbf{x}_1, \dots, \mathbf{x}_N) &= \mathcal{N} \sum_{\pi \in S_N} \psi_{k_1}(\mathbf{x}_{k_{\pi(1)}}) \cdots \psi_{k_N}(\mathbf{x}_{k_{\pi(N)}}) \\ \psi_{k_1, \dots, k_n}^{(-)}(\mathbf{x}_1, \dots, \mathbf{x}_N) &= \mathcal{N} \sum_{\pi \in S_N} (-1)^{\sigma(\pi)} \psi_{k_1}(\mathbf{x}_{k_{\pi(1)}}) \cdots \psi_{k_N}(\mathbf{x}_{k_{\pi(N)}}) \\ &= \mathcal{N} \det \begin{vmatrix} \psi_{k_1}(\mathbf{x}_1) & \psi_{k_1}(\mathbf{x}_2) & \cdots & \psi_{k_1}(\mathbf{x}_N) \\ \psi_{k_2}(\mathbf{x}_1) & \psi_{k_2}(\mathbf{x}_2) & \cdots & \psi_{k_2}(\mathbf{x}_N) \\ \vdots & \vdots & \cdots & \vdots \\ \psi_{k_N}(\mathbf{x}_1) & \psi_{k_N}(\mathbf{x}_2) & \cdots & \psi_{k_N}(\mathbf{x}_N) \end{vmatrix}\end{aligned}$$

↗

Slater determinant

(f) *Pauli's exclusion principle:*

Two fermions can not occupy the same quantum state

5. **Occupation number representation:** Counting the number of particles of different types

$$\begin{aligned}|k_1, k_2, \dots, k_N\rangle &\implies |n_k\rangle \\ N[n] &= \sum_k n_k, \quad \mathbf{P} = \sum_k n_k \mathbf{p}_k, \quad E[n] = \sum_k n_k E_k\end{aligned}$$

Does not contain unphysical information  $\implies$  no need of (anti)symmetrization

6. **Exchange interaction:** (wrong) historical name

(a) *Two particle state:*

$$\psi_{12}(\mathbf{x}_1, \sigma_1, \mathbf{x}_2, \sigma_2) = \frac{1}{\sqrt{2}} [\psi_1(\mathbf{x}_1, \sigma_1) \psi_2(\mathbf{x}_2, \sigma_2) + \xi \psi_2(\mathbf{x}_1, \sigma_1) \psi_1(\mathbf{x}_2, \sigma_2)].$$

(b) *Factorizable one- and two-particle wave functions:*

$$\begin{aligned}\psi_j(\mathbf{x}, \sigma) &= \chi_j(\mathbf{x}) \phi_j(\sigma) \\ \psi_{12}(\mathbf{x}_1, \sigma_1, \mathbf{x}_2, \sigma_2) &= \chi_{12}(\mathbf{x}_1, \mathbf{x}_2) \phi_{12}(\sigma_1, \sigma_2),\end{aligned}$$

(c) *Exchange statistics:*

$$\chi_{12}(\mathbf{x}_2, \mathbf{x}_1) = \xi_c \chi_{12}(\mathbf{x}_1, \mathbf{x}_2), \quad \chi_{12}(\mathbf{x}_2, \mathbf{x}_1) = \xi_s \phi_{12}(\sigma_1, \sigma_2) \implies \xi_c \xi_s = \xi$$

(anti)symmetrization of states may introduce correlations among quantum numbers

(d) *Bound states of two identical fermions:*

- Hamiltonian:

$$H = \frac{\mathbf{p}_1^2}{2m} + \frac{\mathbf{p}_2^2}{2m} + U(r_{12}).$$

↗

strongly attractive spherical symmetric potential at short distances

- New variables:

$$\begin{aligned} \mathbf{X} &= \frac{1}{2}(\mathbf{x}_1 + \mathbf{x}_2), & \mathbf{P} &= \frac{1}{2}(\mathbf{p}_1 + \mathbf{p}_2), & \mathbf{x} &= \mathbf{x}_1 - \mathbf{x}_2, & \mathbf{p} &= \mathbf{p}_1 - \mathbf{p}_2 \\ \chi(\mathbf{x}_1, \mathbf{x}_2) &= e^{-\frac{i}{\hbar}\mathbf{P}\cdot\mathbf{X}} \eta_{n,\ell}(r) Y_m^\ell(\theta, \phi) \end{aligned}$$

- Spatial inversion:

$$\mathbf{x} \rightarrow -\mathbf{x} \implies \xi_x = (-1)^\ell$$

- Correlation among quantum numbers for  $\xi = -1$ :

- $S = 0$ :  $\xi_s = -1 \implies \xi_c = 1 \implies \ell = 0$  in the bound state
- $S = 1$ :  $\xi_s = 1 \implies \xi_c = -1 \implies \ell = 1$  in the bound state
- $\eta_{n,\ell}(r) = \mathcal{O}(r^\ell)$
- Spin-dependent ground state energy:  $\int dr r^2 U(r) < \int dr r^4 U(r)$

## VII. DENSITY MATRIX

### A. Gleason theorem

#### 1. Classical probability:

- *Elementary events*:  $\mathcal{H}$
- *$\sigma$ -algebra*:  $\mathcal{M}$ , the measurable subsets of  $\mathcal{H}$ 
  - (a)  $a_n \in \mathcal{M} \implies \cup_n a_n \in \mathcal{M}$
  - (b)  $a \in \mathcal{M} \implies \mathcal{H} \setminus a \in \mathcal{M}$
- *Probability measure*:  $\mu : \mathcal{M} \rightarrow \mathbb{R}$ 
  - (a)  $0 \leq p(a) < \infty$  ( $p(a) < 1$  for discrete values of  $a$ )
  - (b)  $p(\emptyset) = 0$
  - (c)  $a_n \in \mathcal{M}$  and  $a_m \cap a_n = \emptyset \implies p(\cup_n a_n) = \sum_n p(a_n)$

#### 2. Quantum probability:

- *Elementary events:*  $\mathcal{H}$
- *$\sigma$ -algebra:*  $\mathcal{M}$ , the measurable linear subspaces of  $\mathcal{H}$

$$(a) a_n \in \mathcal{M} \implies \sum_n c_n a_n \in \mathcal{M}$$

$$(b) \forall a \in \mathcal{M}, \{v \in \mathcal{H} | \langle v | w \rangle = 0, \forall w \in a\} \in \mathcal{M}.$$

- *Probability measure:*  $\mu : \mathcal{M} \rightarrow R$

$$(a) 0 \leq p(a) < \infty$$

$$(b) p(\emptyset) = 0$$

$$(c) a_n \in \mathcal{M} \text{ and } a_m \perp a_n = 0 \implies p(\{\sum_n c_n a_n\}) = \sum_n p(a_n)$$

3. **Gleason's theorem:** Any measure  $p$  in a separable Hilbert space of at least 3 dimensions is of the form

$$\boxed{p(a) = \text{Tr}[\rho \Lambda(a)]}$$

- *Projector onto the subspace  $a$ :*  $\{|n\rangle\}$  is a basis for a linear subspace  $a \subset \mathcal{H}$

$$\Lambda(a) = \sum_n |n\rangle\langle n|,$$

- *Quantum state:*
  - collection of information about the system,
  - probability distribution for all subspaces
  - density matrix  $\rho$

4. **Expectation value of an observable:**

$$\begin{aligned} A &= \sum_n |\psi_n\rangle \lambda_n \langle \psi_n| = \sum_n \lambda_n |\psi_n\rangle \langle \psi_n| = \sum_n \lambda_n \Lambda(|n\rangle) & |\psi_n\rangle \leftrightarrow \lambda_n \\ \langle A \rangle &= \sum_n p_n \lambda_n \\ &= \sum_n \text{Tr}[\rho \Lambda(|n\rangle)] \lambda_n \\ &= \sum_n \text{Tr}[\rho \lambda_n \Lambda(|n\rangle)] \\ &= \text{Tr} \rho A \end{aligned}$$

$$\boxed{\langle A \rangle = \text{Tr}[\rho A]}$$



## B. Properties

### 1. Hermiticity:

$$\rho = \rho_h + \rho_{ah}, \quad \rho_h = \frac{1}{2}(\rho + \rho^\dagger), \quad \rho_{ah} = \frac{1}{2}(\rho - \rho^\dagger)$$

$$\text{Tr} P_\psi \rho = \langle \psi | \rho | \psi \rangle \in \mathbb{R} \implies \langle \psi | \rho | \psi \rangle = \langle \psi | \rho^\dagger | \psi \rangle \implies \rho_{ah} = 0$$

### 2. Positive operator:

$$\langle \psi | \rho | \psi \rangle = \text{Tr}[\Lambda(\psi)\rho] \geq 0$$

### 3. Unit trace:

$$\text{Tr} \rho = \text{Tr}[\rho \mathbb{1}] = 1$$

### 4. Diagonalizable: $\{|\psi_n\rangle\}$ is an orthonormal base

$$\rho = \sum_n |\psi_n\rangle p_n \langle \psi_n|, \quad 0 \leq p_n, \quad \sum_n p_n = 1$$

Interpretation:  $p_n$  is the probability of finding the system in  $|\psi_n\rangle$

### 5. Pure states: (factorizable density matrix)

$$\rho = |\psi\rangle \langle \psi| \quad \leftrightarrow \quad \text{Tr}[\rho^2] = \text{Tr}[\rho] = 1$$

### 6. Mixed states: (non-factorizable density matrix)

$$\rho = \sum_{n=1}^N |\psi_n\rangle p_n \langle \psi_n|, \quad (N \geq 2) \quad \leftrightarrow \quad \text{Tr} \rho^2 = \sum_n p_n^2 < \sum_n p_n = \text{Tr} \rho = 1$$

### 7. Degeneracy: non-unique decomposition

### 8. Example: Two-state system:

$$\rho = \frac{1}{2}(\mathbb{1} + \mathbf{p}\boldsymbol{\sigma}), \quad \boldsymbol{\sigma} = \left( \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right)$$

$$\langle \boldsymbol{\sigma} \rangle = \text{tr}[\rho \boldsymbol{\sigma}] = \mathbf{p}$$

## C. Physical origin

Two different(?) physical origins of the same mathematical structure:

1. **Loss of classical information:**  $|\psi_n\rangle \leftrightarrow p_n$

$$\rho = \sum_n |\psi_n\rangle p_n \langle\psi_n|$$

$$\langle A \rangle = \text{Tr} \rho A = \sum_n p_n \text{Tr} [|\psi_n\rangle \langle\psi_n| A] = \sum_n p_n \langle\psi_n| A |\psi_n\rangle$$

• *Expectation value:*

- quadratic in the wave function

$$\langle A \rangle = \langle \psi | A | \psi \rangle = \int dx dy \psi^*(x) \langle x | A | y \rangle \psi(y)$$

- linear in the density matrix

$$\rho(x, y) = \langle x | \rho | y \rangle$$

$$\text{Tr}[\rho A] = \int dx dy \langle x | \rho | y \rangle \langle y | A | x \rangle = \int dx dy \rho(x, y) \langle y | A | x \rangle$$

- no interference in  $\text{Tr}[\rho A] = \sum_n p_n \langle\psi_n| A |\psi_n\rangle$  between the eigenstate of  $\rho$

• *Coherent average in a pure state:*

$$|\psi\rangle = \sum_n \sqrt{p_n} |\psi_n\rangle$$

$$\langle\psi| A |\psi\rangle = \sum_{m,n} \sqrt{p_m p_n} \langle\psi_m| A |\psi_n\rangle \neq \sum_n p_n \langle\psi_n| A |\psi_n\rangle$$

$$\rho = \sum_{m,n} \sqrt{p_m p_n} |\psi_m\rangle \langle\psi_n| \neq \sum_n p_n |\psi_n\rangle \langle\psi_n|$$

- *Decoherence:* reduced coherence in the expectation values

$$\langle\psi| A |\psi\rangle = \text{Tr}[\rho A] = \sum_n p_n \langle\psi_n| A |\psi_n\rangle$$

2. **Entangled states:**

- *Bipartite system:*  $\mathcal{H} = \mathcal{H}_\phi \otimes \mathcal{H}_\chi$ , with bases  $\{|\phi_m\rangle\}$  and  $\{|\chi_n\rangle\}$



observed system

environment

- *Complete system:* pure state

$$|\psi\rangle = \sum_{m,n} c_{m,n} |\phi_m\rangle \otimes |\chi_n\rangle$$

- *Schmidt decomposition:*

$$|\psi\rangle = \sum_{n=1}^N c_n |u_n\rangle \otimes |v_n\rangle, \quad \langle u_m | u_{m'} \rangle = \delta_{m,m'}, \quad \langle v_n | v_{n'} \rangle = \delta_{n,n'}$$

- *Classification of pure states:*

(a)  $N = 1$ : factorisable state  $|\psi\rangle = |u\rangle \otimes |v\rangle$

(b)  $N \geq 2$ : entangled state

- *Properties of a sub-system are well defined in a factorisable state*

$$\langle\psi|A_1|\psi\rangle = \langle u| \otimes \langle v|A_1 \otimes \mathbb{1}_2|u\rangle \otimes |v\rangle = \langle u|A_1|u\rangle$$

- *Properties of a sub-system depend on the entangled environment*

$$\begin{aligned} |\psi\rangle &= |u_1\rangle \otimes |v_1\rangle + |u_2\rangle \otimes |v_2\rangle \\ \langle\psi|A_1|\psi\rangle &= \langle u_1|A_1|u_1\rangle\langle v_1|v_1\rangle + \langle u_2|A_1|u_2\rangle\langle v_2|v_2\rangle \\ &\quad + \langle u_1|A_1|u_2\rangle\langle v_1|v_2\rangle + \langle u_2|A_1|u_1\rangle\langle v_2|v_1\rangle \end{aligned}$$

- *No state vectors for an entangled subsystem:*

(a) Suppose the contrary,  $\exists |\phi_{obs}\rangle$ ,  $N \geq 2$

$$|\psi\rangle = \sum_{n=1}^N c_n |u_n\rangle \otimes |v_n\rangle$$

(b)  $P(|\phi_{obs}\rangle) = ?$  1. way:

$$p(|\phi_{obs}\rangle\langle\phi_{obs}|) = \langle\phi_{obs}|\phi_{obs}\rangle\langle\phi_{obs}|\phi_{obs}\rangle = 1$$

(c)  $P(|\phi_{obs}\rangle) = ?$  2. way:

$$\begin{aligned} \Lambda(|\phi_{obs}\rangle) &= |\phi_{obs}\rangle\langle\phi_{obs}| \otimes \mathbb{1}_\chi \\ p(|\phi_{obs}\rangle\langle\phi_{obs}|) &= \langle\psi|\Lambda(|\phi_{obs}\rangle\langle\phi_{obs}|)|\psi\rangle = \langle\psi||\phi_{obs}\rangle\langle\phi_{obs}| \otimes \mathbb{1}_2|\psi\rangle \\ &= \sum_{n,n'} c_n^* c_{n'} \langle u_n| \otimes \langle v_n| (|\phi_{obs}\rangle\langle\phi_{obs}| \otimes \mathbb{1}) |u_{n'}\rangle \otimes |v_{n'}\rangle \\ &= \sum_{n=1}^N \underbrace{|c_n|^2}_{<1} \underbrace{|\langle u_n|\phi_{obs}\rangle|^2}_{\leq 1} < 1 \end{aligned}$$

↗

$$\sum_{n=1}^N |c_n|^2 = 1, N \geq 2$$

(d) The state of an entangled subsystem is given by the (reduced) density matrix

- *Reduced density matrix:*

$$\langle A_\phi \rangle = \sum_{n,n'} c_n^* c_{n'} \langle u_n| \otimes \langle v_n|A_\phi \otimes \mathbb{1}_\chi|u_{n'}\rangle \otimes |v_{n'}\rangle$$

$$\begin{aligned}
&= \sum_n |c_n|^2 \langle u_n | A_\phi | u_n \rangle \\
&= \text{Tr}[\rho_\phi A_\phi], \quad \rho_\phi = \sum_{n=1}^N |u_n\rangle |c_n|^2 \langle u_n| \\
&\quad \nearrow
\end{aligned}$$

non-factorizable

General form:

$$\begin{aligned}
\rho_{tot} &= \sum_{n,n'} c_n c_{n'}^* |u_n\rangle \otimes |v_n\rangle \langle u_{n'}| \otimes \langle v_{n'}| \\
\rho_\phi &= \text{Tr}_\chi[\rho_{tot}] \\
&= \sum_{\bar{n}} \langle \chi_{\bar{n}} | \rho_{tot} | \chi_{\bar{n}} \rangle \\
&= \sum_{\bar{n},n,n'} c_n c_{n'}^* \langle \chi_{\bar{n}} | (|u_n\rangle \otimes |v_n\rangle \langle u_{n'}| \otimes \langle v_{n'}|) | \chi_{\bar{n}} \rangle \\
&= \sum_{\bar{n},n,n'} c_n c_{n'}^* |u_n\rangle \langle u_{n'}| \langle v_n | \chi_{\bar{n}} \rangle \langle \chi_{\bar{n}} | v_{n'} \rangle \\
&= \sum_{n,n'} c_n c_{n'}^* |u_n\rangle \langle u_{n'}| \underbrace{\langle v_n | \sum_{\bar{n}} | \chi_{\bar{n}} \rangle \langle \chi_{\bar{n}} | v_{n'} \rangle}_{\mathbb{1}} \\
&= \sum_{n,n'} c_n c_{n'}^* |u_n\rangle \langle u_{n'}| \langle v_n | v_{n'} \rangle \\
&= \sum_n |c_n|^2 |u_n\rangle \langle u_n|.
\end{aligned}$$

• *Lessons:*

- (a) An entangled sub-system has no individual properties
- (b) Entanglement and mixed states arise from interactions
- (c) Entanglement is more general than interactions (no interaction Hamiltonian needed)
- (d) Mathematical equivalence of points 1. and 2.:

Loss of classical information  $\longleftrightarrow$  observed system is entangled

## VIII. MEASUREMENT THEORY

### 1. Tripartite system:

- *Hamiltonian:*  $H_{s,a}(t) \neq 0$  for  $t_m - \tau_m < t < t_m + \tau_m$

$$H = \underbrace{H_s}_{\text{system}} + \underbrace{H_a + H_{s,a}(t)}_{\text{apparatus}} + \underbrace{H_e + H_{s,a,e}}_{\text{environment}}$$

- *Non-demolishing measurement:*

$$[H_s, H_{s,a}] = 0$$

- *Initial state:*

$$|\Psi(t_i)\rangle = \sum_n c_n |s_n\rangle \otimes |a_0\rangle \otimes |e_0\rangle$$

## 2. Measurement process:

(a) *Pre-measurement:*  $t_m - \tau_m < t < t_m + \tau_m$

- Environment ignored:  $2\tau_m H_{a,e} \ll \int dt H_{s,a}(t)$
- System-apparatus correlations:

$$|\Psi(t)\rangle = \sum_n c_n |s_n\rangle \otimes |a_0\rangle \otimes |e_0\rangle \rightarrow \sum_n c_n |s_n\rangle \otimes |a_n\rangle \otimes |e_0\rangle$$

- Interaction generates entanglement
- Microscopic information spreads over macroscopic size
- Understood

(b) *Decoherence*  $t_m + \tau_m < t < t_m + \tau_m + \tau_d$ :

- Apparatus-environment interaction

$$|\Psi(t)\rangle = \sum_n c_n |s_n\rangle \otimes |a_n\rangle \otimes |e_0\rangle \rightarrow \sum_n c_n |s_n\rangle \otimes |a_n\rangle \otimes |e_n\rangle$$

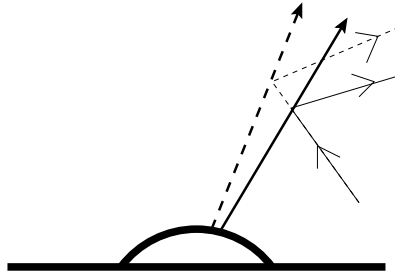
- Reduced density matrix:

$$\rho_{s,a} = \sum_{n,n'} c_n^* c_{n'} \langle e_n | e_{n'} \rangle |s_n\rangle \otimes |a_n\rangle \langle s_{n'}| \otimes \langle a_{n'}|$$

- Decoherence of the pointer of an ampermeter in an ideal gas environment:
  - Independent particles  $\implies$  factorizable pure state

$$|\chi\rangle = |\chi^{(1)}\rangle \otimes |\chi^{(2)}\rangle \otimes \dots$$

- Macroscopically different pointer states  $|a_n\rangle$  and  $|a_{n'}\rangle$



- The overlap of gas particle states after bouncing back from the pointer

$$\langle e_n^{(j)} | e_{n'}^{(j)} \rangle < 1 - \epsilon, \quad j = 1, \dots, N_p$$

– Macroscopical limit of the pointer

$$\lim_{N_p \rightarrow \infty} \langle e_n | e_{n'} \rangle = \lim_{N_p \rightarrow \infty} \prod_{j=1}^{N_s} \langle e_n^{(j)} | e_{n'}^{(j)} \rangle < \lim_{N_p \rightarrow \infty} (1 - \epsilon)^{N_p} = 0$$

- Macroscopically different apparatus states  $|a_n\rangle, |a_{n'}\rangle$   
 $\implies$  orthogonal environment states  $\langle e_n | e_{n'} \rangle = 0$
- Macroscopically off diagonal elements of the density matrix in the pointer basis are suppressed
- Requires non-unitary time evolution
- Loss of phase differences  $\implies$  irreversibility
- Understood

(c) *Collapse:*

- The result of the measurement is the apparatus state  $|\phi_{n_m}\rangle$

$$\begin{aligned} \rho_{s,a} &= \sum_{n,n'} c_n^* c_{n'} \langle \chi_n | e \chi_{n'} \rangle_e |\psi_n\rangle_s \otimes |\phi_n\rangle_a \langle \psi_{n'} |_s \otimes \langle \phi_{n'} | \\ &\rightarrow \frac{\Lambda(|\phi_{n_m}\rangle) \rho_{s,a} \Lambda(|\phi_{n_m}\rangle)}{\text{Tr}_{s,a}[\Lambda(|\phi_{n_m}\rangle) \rho_{s,a} \Lambda(|\phi_{n_m}\rangle)]} \\ &= |\psi_{n_m}\rangle_s \otimes |\phi_{n_m}\rangle_a \langle \psi_{n_m} |_s \otimes \langle \phi_{n_m} |_a \end{aligned}$$

- Collapse of a structure:  $c_n \rightarrow \delta_{n,n_m}$
- A complicated, fast many-body effect
- Nondeterministic, far from being understood
- Determinism emerges in macroscopic physics as thermodynamics appears in statistical physics

### 3. **Escape route:** Hidden variable theory

- Deterministic theory containing yet unresolved degrees of freedom
- The statistical treatment of the hidden variables reproduces the predictions of quantum theory
- It must be

(a) *Non-local*

– Entanglement is distance independent

– Einstein-Podolski-Rosen effect

$$* |S = 0\rangle = \frac{1}{\sqrt{2}} (|(\mathbf{x}, \uparrow), (\mathbf{y}, \downarrow)\rangle - |(\mathbf{x}, \downarrow), (\mathbf{y}, \uparrow)\rangle)$$

\* An interaction at  $\mathbf{x}$  influences the state at  $\mathbf{y}$

\* Such a correlation spreads with  $c + \epsilon$  (and infinite) speed (!!!)

(b) *Contextual*

- Three observable  $A$ ,  $B$  and  $C$
  - $[A, B] = [A, C] = 0 \neq [B, C]$
  - The result of a *single measurement* of  $A$  depends on whether  $B$  or  $C$  has been measured
- Is this an acceptable price to save microscopic determinism?
  - Why do we think that microscopic physics is deterministic?

**Oral exam topics:**

1. Time independent perturbation expansion
2. Time dependent perturbation expansion
3. Rotations
4. Addition of angular momentum
5. Relativistic corrections
6. Wigner's D-matrix, Indistinguishability of particles