= Linear Vector Spaces (LVS) =

<u>Def</u> : Objects in $\mathbb{V}$ form a LVS if they satisfy

1) Closure : $|A\rangle + |B\rangle \in \mathbb{V}$

2) Scalar multiplication is distributive in vectors :
$$a\big(|A\rangle + |B\rangle\big) = a|A\rangle + a|B\rangle$$

3) Scalar multiplication is distributive in scalars :
$(a+b)|A\rangle = a|A\rangle + b|A\rangle$ ~~$a(b|A\rangle) = ab|A\rangle$~~

4) Scalar multiplication is associative :
$$a\big(b|A\rangle\big) = ab|A\rangle$$

5) Addition is commutative :
$$|A\rangle + |B\rangle = |B\rangle + |A\rangle$$

6) Addition is associative :
$$|A\rangle + \big(|B\rangle + |C\rangle\big) = \big(|A\rangle + |B\rangle\big) + |C\rangle = \cdots$$

7) Null vector exists, s.t. :
$$|A\rangle + |0\rangle = |A\rangle \qquad (\text{"}|0\rangle\text{" or "}\phi\text{"})$$

8) Addition-inverse exists, s.t. :
$$|A\rangle + |-A\rangle = |0\rangle$$

<u>Def</u> : The <u>field</u> of the vector space is defined by the scalars $a, b, c, \ldots$

$a, b, c \ldots \in \mathbb{R}$ → real vector space (RVS)
$a, b, c \ldots \in \mathbb{C}$ → complex vector space (CVS)

2

<u>Linear Independence of a Vector Set</u> :

Consider the relation

$$\sum_{i=1}^{n} a_i |i\rangle = |\cancel{0}\rangle \qquad (1)$$

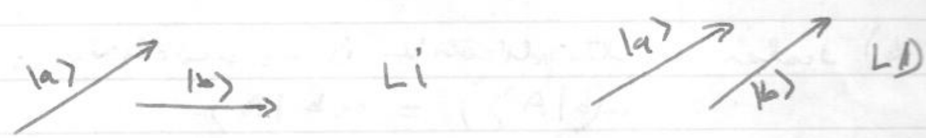
$\rightarrow$ null vector, or "0"

a) $\{|i\rangle\}_{i=\overline{1,n}}$ is a <u>linearly-independent (Li)</u> set iff

(1) is satisfied only for $a_i = 0$, $i = 1, \ldots, n$

b) otherwise $\{|i\rangle\}_{\overline{1,n}}$ is linearly dependent (LD)

Examples:



$|1\rangle = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$

$|2\rangle = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$

$|3\rangle = \begin{pmatrix} -2 & -1 \\ 0 & -2 \end{pmatrix} = -\left(2|2\rangle - |1\rangle\right) \Rightarrow \{|i\rangle\}_{i=1,2,3}$ is LD

$$\left.\begin{aligned} |1\rangle &= (1\,1\,0) \\ |2\rangle &= (1\,0\,1) \\ |3\rangle &= (3\,2\,1) \end{aligned}\right\} \text{LD} \qquad \begin{aligned} (3\,2\,1) &= 2(1\,1\,0) + (1\,0\,1) \\ |3\rangle &= 2|1\rangle + |2\rangle \end{aligned}$$

$$\left.\begin{aligned} |1\rangle &= (1\,1\,0) \\ |2\rangle &= (1\,0\,1) \\ |3\rangle &= (0\,1\,1) \end{aligned}\right\} \text{Li}$$

Dimension | A vector space has <u>dimension "n"</u> if it accommodates a maximum of <u>n linearly independent vectors</u>

$\mathbb{V}^n(\mathbb{R}) \rightarrow$ for real field

$\mathbb{V}^n(\mathbb{C}) \rightarrow$ for complex field

... $n = 3$; $2\times 2 \rightarrow n = 4$ Li vectors ...

Example

2×2:
$$|1\rangle = \begin{pmatrix}1&0\\0&0\end{pmatrix}$$
$$|2\rangle = \begin{pmatrix}0&1\\0&0\end{pmatrix} \quad \Rightarrow \text{LI, complete:}$$
$$|3\rangle = \begin{pmatrix}0&0\\1&0\end{pmatrix}$$
$$|4\rangle = \begin{pmatrix}0&0\\0&1\end{pmatrix} \qquad \begin{pmatrix}a&b\\c&d\end{pmatrix} = a|1\rangle + b|2\rangle + c|3\rangle + d|4\rangle$$

$a, b, c, d \in \mathbb{R} \rightarrow$ real 4-D space

" " $\in \mathbb{C} \rightarrow$ complex 4D space

BASIS

Theorem | Any vector $|v\rangle \in \mathbb{V}^n$ can be written as a LC of n LI vectors $\{|i\rangle\}_{i=\overline{1,n}} \in \mathbb{V}^n$

$$|v\rangle = \sum_{i=1}^{n} a_i |i\rangle$$

Basis

Definition | A set of n LI vectors in an n-D vector space $\mathbb{V}^n$ is called a basis.

a_i - components of $|v\rangle$ in the $\{|i\rangle\}_{i=\overline{1,n}}$ basis

* The expansion is unique.

OPERATIONS

Adding vectors = adding components:

$$|v\rangle = \sum_i a_i |i\rangle \ (\in \mathbb{V}^n)$$
$$|w\rangle = \sum_i b_i |i\rangle \ (\in \mathbb{V}^n)$$
$$\Rightarrow |v\rangle + |w\rangle = \sum_i (a_i + b_i)|i\rangle \ (\in \mathbb{V}^n)$$

Multiplying by scalars:

$$|v\rangle = \sum_i a_i |i\rangle \ (\in \mathbb{V}^n)$$
$$b|v\rangle = b\sum_i a_i|i\rangle = \sum_i (b a_i)|i\rangle \in \mathbb{V}^n$$

Inner Product of Vectors

→ generalization of the 2D, 3D dot product.

* Axioms of iP :

A1) Skew-symmetry : $\langle A|B\rangle = \langle B|A\rangle^*$
A2) Positive definiteness : $\langle A|A\rangle \geq 0$; 0 iff $|A\rangle = |0\rangle$
A3) Linearity : $\langle V|\big(a|A\rangle + b|B\rangle\big) = a\langle V|A\rangle + b\langle V|B\rangle$
$\big(\equiv \langle V|\, aA + bB\rangle\big)$

$$\langle aA + bB|V\rangle = \langle V|aA+bB\rangle^*$$
$$\equiv \Big[\langle V|\big(a|A\rangle + b|B\rangle\big)\Big]^*$$
$$= a^*\langle V|A\rangle^* + b^*\langle V|B\rangle^*$$
$$= a^*\langle A|V\rangle + b^*\langle B|V\rangle$$

⇒ iP is antilinear in the first factor

orthogonal — $|A\rangle$ & $|B\rangle$ are <u>orthogonal</u> if $\langle A|B\rangle \big(= \langle B|A\rangle\big) = 0$

Norm — $|A| = \sqrt{\langle A|A\rangle}$ is the <u>norm</u> of $|A\rangle$. If $|A| = 1$, $|A\rangle$ is "normalized to unity"

orthogonal basis — A set of unit-norm orthogonal basis vectors $(|i\rangle)$ is called an <u>orthogonal basis</u>.

$\langle | \rangle$ in an ortho basis — If $|A\rangle = \sum_i a_i|i\rangle$, $|B\rangle = \sum_i b_i|i\rangle$, then

$$\langle A|B\rangle = \sum_i\sum_j a_i^* b_j \langle i|j\rangle \quad ; \quad \langle i|j\rangle = \delta_{ij} = \begin{cases} 1, & i=j \\ 0, & i\neq j\end{cases}$$

$$\Rightarrow \boxed{\langle A|B\rangle = \sum_i a_i^* b_i} \; ; \; \boxed{\langle A|A\rangle = \sum_i |a_i|^2} \geq 0$$

$\boxed{\text{Matrix representation}}$

$$|A\rangle = \sum_{i=1}^{n} a_i |i\rangle \doteq \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ a_n \end{bmatrix} \quad \text{in the } \{|i\rangle\}_{i=\overline{1,n}}$$

$$\langle A| = \sum_{i=1}^{n} a_i^* \langle i| \doteq (a_1^* \, a_2^* \, a_3^* \dots a_n^*)$$

$$\langle A|B\rangle = (a_1^* \dots a_n^*) \begin{pmatrix} b_1 \\ \vdots \\ b_n \end{pmatrix} = \sum_i a_i^* b_i$$

Dirac Notation and Dual Spaces

$| \ \rangle \doteq \begin{pmatrix} \vdots \end{pmatrix}$ ket

dual spaces

$\langle \ | \doteq (\cdots)$ bra

$$|A\rangle \doteq \begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix} \quad ; \quad \langle A| \doteq (a_1^* \dots a_n^*)$$

$\hookrightarrow$ adjoint (or transpose conjugate)

* Expansion in an orthonormal basis:

$$|A\rangle = \sum_i a_i |i\rangle \; ;$$
$$\langle j|A\rangle = \sum_i a_i \langle j|i\rangle = \sum_i a_i \delta_{ij} = a_j$$

j^{th} "component" of $|A\rangle$

$$\Rightarrow \quad |A\rangle = \sum_i a_i |i\rangle = \sum_i |i\rangle\langle i|A\rangle$$

Example:

$$|A\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} = a_1 \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + a_2 \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix} + \dots + a_n \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}$$

Adjoint operation : $a|V\rangle \longleftrightarrow a^*\langle V|$

$$a\begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix} \longleftrightarrow a^* \left(v_1^* \cdots v_n^*\right)$$

} transpose + conjugate

$$|A\rangle = \sum_{i=1}^{n} a_i |i\rangle \longleftrightarrow \langle A| = \sum_{i=1}^{n} \langle i| a_i^*$$

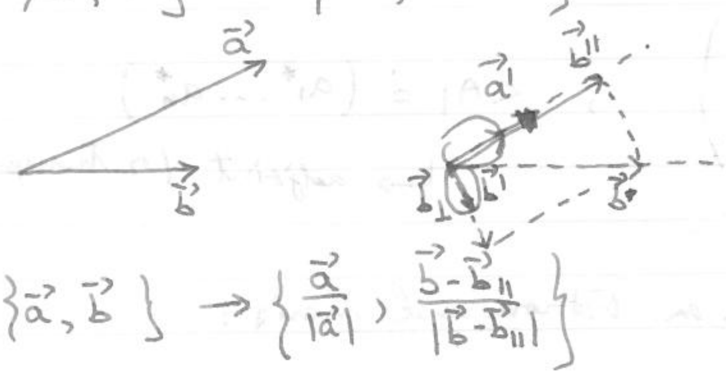
$$a_i = \langle i|A\rangle \longleftrightarrow a_i^* = \langle A|i\rangle$$

$$|A\rangle = \sum_i |i\rangle\langle i|A\rangle \longleftrightarrow \langle A| = \sum_i \langle A|i\rangle\langle i|$$

The Gram - Schmidt orthogonalization Theorem

2D Example: Transform a two-vector unorthogonal (LI) basis into an ~~orthogonal~~ orthogonal basis:

$$\{\vec{a}, \vec{b}\} \rightarrow \{\vec{a}', \vec{b}' \perp \vec{a}'\}$$



1) $\vec{a}' = \dfrac{\vec{a}}{|\vec{a}|}$ unit vect

$\vec{b} = \vec{b}_{\parallel} + \vec{b}_{\perp}$

2) $\vec{b}_{\perp} = \vec{b} - \vec{b}_{\parallel} = \vec{b} - \vec{a}'|\vec{b}''|$

3) $\vec{b}' = \dfrac{\vec{b}_{\perp}}{|\vec{b}_{\perp}|}$ unit vect

$$\Rightarrow \{\vec{a}, \vec{b}\} \rightarrow \left\{\frac{\vec{a}}{|\vec{a}|}, \frac{\vec{b} - \vec{b}_{\parallel}}{|\vec{b} - \vec{b}_{\parallel}|}\right\}$$

General vector space: Start with LI basis $\{|a\rangle, |b\rangle, |c\rangle, \ldots\}$, not-orthonormal.

Gram - Schmidt

$$|\alpha\rangle = \frac{|a\rangle}{|a|} = \frac{|a\rangle}{\sqrt{\langle a|a\rangle}}$$

$$|\beta\rangle = \frac{|b\rangle - |\alpha\rangle\langle\alpha|b\rangle}{\sqrt{\left(\langle b| - \langle\alpha|\langle b|\alpha\rangle\right)\left(|b\rangle - |\alpha\rangle\langle\alpha|b\rangle\right)}} \qquad \left(|\beta\rangle \perp |\alpha\rangle\right)$$

$$|\gamma\rangle = \frac{|c\rangle - |\alpha\rangle\langle\alpha|c\rangle - |\beta\rangle\langle\beta|c\rangle}{\sqrt{\left(\langle c| - \langle\alpha|\langle c|\alpha\rangle - \langle\beta|\langle c|\beta\rangle\right)\left(|c\rangle - |\alpha\rangle\langle\alpha|c\rangle - |\beta\rangle\langle\beta|c\rangle\right)}} \qquad \left(|\gamma\rangle \perp |\alpha\rangle \perp |\beta\rangle\right)$$

Try at home :

$$|a\rangle = \begin{pmatrix} 3 \\ 0 \\ 0 \end{pmatrix}, \quad |b\rangle = \begin{pmatrix} 0 \\ 1 \\ 2 \end{pmatrix}, \quad |c\rangle = \begin{pmatrix} 0 \\ 2 \\ 5 \end{pmatrix}$$ L i not-orthogonal basis

go to the orthonormal basis

$$|\alpha\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\beta\rangle = \begin{pmatrix} 0 \\ 1/\sqrt{5} \\ 2/\sqrt{5} \end{pmatrix}, \quad |\gamma\rangle = \begin{pmatrix} 0 \\ -2/\sqrt{5} \\ 1/\sqrt{5} \end{pmatrix}$$

Dimensionality of a space ($n_\perp$) is given by the maximum number of mutually orthogonal vectors.

Important Vector Inequalities :

* Schwarz :

$$|\langle A|B\rangle| \leq |A| \cdot |B|$$

* Triangle :

$$|A+B| \leq |A| + |B|$$

Subspaces

Def. A subspace is a subset of the elements of a given vector space $\mathbb{V}$, which forms a space in itself. Call subspace "i" of dimensionality "n_i", $\mathbb{V}_i^{n_i}$

Def II For two subspaces $\mathbb{V}_i^{n_i}$ and $\mathbb{V}_j^{n_j}$ (of $\mathbb{V}$), their sum is $\mathbb{V}_i^{n_i} \oplus \mathbb{V}_j^{n_j} = \mathbb{V}_k^{n_k}$ as the set containing

1) all elements of $\mathbb{V}_i^{n_i}$
2) all elements of $\mathbb{V}_j^{n_j}$
3) all linear combinations of 1 & 2 (for closure)

Linear Operators

→ Transformations on vectors: $\hat{\Omega}|V\rangle = |V'\rangle$

(→ consider ops that keep vectors within a given LVS)

$$\langle V|\hat{\Omega} = \langle V'| \quad \text{in the bra-space}$$

* Linear operations:

$$\hat{\Omega}\big(\alpha|A\rangle\big) = \alpha\,\hat{\Omega}|A\rangle$$

$$\hat{\Omega}\big(\alpha|A\rangle + \beta|B\rangle\big) = \alpha\,\hat{\Omega}|A\rangle + \beta\,\hat{\Omega}|B\rangle$$

and similar in dual (bra) space ...

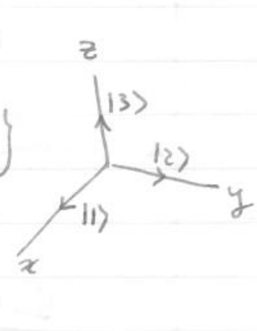
Examples

1) Identity op: $\hat{\mathbb{1}}|A\rangle = |A\rangle$, $\langle A|\hat{\mathbb{1}} = \langle A|$

2) Spatial Rotation by $\pi/2$ rad about axis $\hat{z}$:

$$\hat{R}(\tfrac{\pi}{2}\hat{z})|1\rangle = |2\rangle \qquad \text{for } \{|1\rangle, |2\rangle, |3\rangle\} \text{ as in the figure}$$

$$\hat{R}(\tfrac{\pi}{2}\hat{z})|2\rangle = -|1\rangle = e^{i\pi}|1\rangle$$



$$\hat{R}(\tfrac{\pi}{2}\hat{z})|3\rangle = |3\rangle$$

↳ check linearity of $\hat{R}(\tfrac{\pi}{2}\hat{z})$

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* In a basis $\{|i\rangle\}_{i=\overline{1,n}}$: $|A\rangle = \sum_{i=1}^{n} a_i|i\rangle$

$$\hat{\Omega}|A\rangle = \hat{\Omega}\sum_i a_i|i\rangle$$

$$= \sum_i a_i\,\hat{\Omega}|i\rangle = \sum_i a_i|i'\rangle$$

if $\hat{\Omega}|i\rangle = |i'\rangle$ is known

$\hat{\Omega} = 1\!\!1 \Omega 1\!\!1 = \sum_i |i\rangle\langle i| \Omega \sum_j |j\rangle\langle j| = \sum_{ij} |i\rangle \Omega_{ij} \langle j|$ or $\sum_{ij} \Omega_{ij} |i\rangle\langle j|$

↳ expression of an operator in an orthonormal basis

$\boxed{\text{DF on p.10 for MR of ops}}$

* Product of operators:

$$\hat{\Lambda}\hat{\Omega}|A\rangle = \hat{\Lambda}\left(\hat{\Omega}|A\rangle\right) = \hat{\Lambda}\,|\Omega A\rangle$$

Just a "label" describing the effect of $\hat{\Omega}$ on $|A\rangle$

* Attention: in general

$$\hat{\Lambda}\hat{\Omega} - \hat{\Omega}\hat{\Lambda} \equiv [\hat{\Lambda}, \hat{\Omega}] \neq 0$$

$[\hat{\Lambda}, \hat{\Omega}]$ = commutator of $\hat{\Lambda}, \hat{\Omega}$

* Inverse operators:

$$\hat{\Omega}^{-1}\hat{\Omega} = \hat{\Omega}\hat{\Omega} = 1\!\!1$$

$$\left(\hat{\Lambda}\hat{\Omega}\right)^{-1} = \hat{\Omega}^{-1}\hat{\Lambda}^{-1} \quad ⚠$$

↳ show, by action on a vector (in a basis) or via $1\!\!1$.

$(\hat{\Lambda}\hat{\Omega})^{-1}(\hat{\Lambda}\hat{\Omega}) \overset{!}{=} \hat{1\!\!1} = \cancel{(\hat{\Lambda}\hat{\Omega})(\hat{\Lambda}\hat{\Omega})^{-1}} = \cancel{(\Lambda\Omega)(\Omega^{-1}\Omega)(\Lambda\Omega)^{-1}}$

$= \cancel{\hat{\Lambda}^{-1}(\hat{\Lambda}\hat{\Omega})\hat{\Omega}^{-1}} \Rightarrow \cancel{(\hat{\Lambda}\hat{\Lambda}^{-1})(\hat{\Omega}^{-1}\hat{\Omega})}$

$= \hat{\Omega}^{-1}\hat{\Lambda}^{-1}\hat{\Lambda}\Omega$

$(\hat{\Lambda}\hat{\Omega})^{-1}|A\rangle = (\hat{\Lambda}\hat{\Omega})^{-1}\sum_i a_i|i\rangle = \sum_i a_i (\hat{\Lambda}\hat{\Omega})^{-1}|i\rangle$

$(\hat{\Lambda}\hat{\Omega})\|\; (\hat{\Lambda}\hat{\Omega})(\hat{\Lambda}\hat{\Omega})^{-1}|A\rangle \overset{!}{=} \sum_i a_i \underbrace{(\hat{\Lambda}\hat{\Omega})(\hat{\Lambda}\hat{\Omega})^{-1}}_{1\!\!1}|i\rangle \overset{?}{=} \sum_i a_i \hat{1\!\!1}|i\rangle = |A\rangle$

$\langle A|\|\; \langle A|(\hat{\Lambda}\hat{\Omega})(\hat{\Lambda}\hat{\Omega})^{-1}|A\rangle \overset{!}{=} \sum_j\sum_i a_j^* a_i \langle j|\hat{\Lambda}\hat{\Omega}(\hat{\Lambda}\hat{\Omega})^{-1}|i\rangle$

$\overset{?}{=} \langle A|A\rangle = \sum_i |a_i|^2 = \sum_j\sum_i a_j^* a_i \langle j|1\!\!1|i\rangle \overset{!}{=} \sum_j\sum_i a_j^* a_i \langle j|\hat{\Lambda}\hat{\Omega}\hat{\Omega}^{-1}\hat{\Lambda}^{-1}|i\rangle$

$\Rightarrow \boxed{(\hat{\Lambda}\hat{\Omega})^{-1} \overset{!}{=} \Omega^{-1}\Lambda^{-1}}$ q.e.d.

Matrix Representations of an Operator

$|A\rangle = \sum_{i=1}^{n} a_i |i\rangle \doteq (a_1, \dots, a_n)$ in $\{|i\rangle\}_{i=\overline{1,n}}$ basis K

What are the matrix elements of an operator $\hat{\Omega}$ in the same basis?

$$\hat{\Omega}|A\rangle = \sum_{i=1}^{n} a_i \underbrace{\hat{\Omega}|i\rangle}_{\substack{\| \\ |i'\rangle}} = \sum_{i=1}^{n} a_i |i'\rangle$$

basis change by $\hat{\Omega}$. How does the ~~state~~ vector $|A\rangle$'s representation change?

$$\underbrace{\langle j|\hat{\Omega}|A\rangle}_{\substack{\| \\ \langle j|A'\rangle \equiv a'_j}} = \langle j|\sum_{i=1}^{n} a_i \hat{\Omega}|i\rangle = \sum_{i=1}^{n} a_i \langle j|\hat{\Omega}|i\rangle$$

$$\left(= \sum_{i=1}^{n} a_i \langle j|i'\rangle \right)$$

$$\equiv \sum_{i=1}^{n} a_i \Omega_{ji}$$

jth component of transformed ket $|A'\rangle$

where $\Omega_{ji} \equiv \langle j|\hat{\Omega}|i\rangle$ is the ji^{th} matrix element of $\hat{\Omega}$ in the basis $\{|i\rangle\}_{i=\overline{1,n}}$

So $\boxed{a'_j = \sum_{i=1}^{n} a_i \Omega_{ji}}$ or in MR:

$$\begin{pmatrix} a'_1 \\ a'_2 \\ \vdots \\ a'_n \end{pmatrix} = \begin{pmatrix} \Omega_{11} & \Omega_{12} \cdots & \Omega_{1n} \\ \Omega_{21} & \Omega_{22} \cdots & \Omega_{2n} \\ \cdots & & \\ \Omega_{n1} & \Omega_{n2} \cdots & \Omega_{nn} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}$$

new vector components (in original basis $\{|i\rangle\}$)

matrix elements of operator $\hat{\Omega}$. that changes the basis from $|i\rangle$ to $|i'\rangle = \hat{\Omega}|i\rangle$

old vector components (in original basis $\{|i\rangle\}$)

$$|A'\rangle = \hat{\Omega}|A\rangle$$

$$\hat{\Omega} = \sum_{ij} |i\rangle \Omega_{ij} \langle j| = \sum_{ij} \Omega_{ij} |i\rangle\langle j|$$

Projection Operators

$$|A\rangle = \sum_{i=1}^{n} a_i |i\rangle = \sum_{i=1}^{n} |i\rangle\langle i|A\rangle \equiv \sum_{i=1}^{n} \hat{\mathbb{P}}_i |A\rangle$$

$\hat{\mathbb{P}}_i \equiv |i\rangle\langle i|$ - projection operator that "projects" vector $|A\rangle$ onto basis ~~....~~ vector $|i\rangle$

⚠ $$\boxed{\hat{\mathbb{1}} = \sum_{i=1}^{n} |i\rangle\langle i| = \sum_{i=1}^{n} \hat{\mathbb{P}}_i \quad \text{- Completeness relation}}$$

$$\hat{\mathbb{P}}_i |A\rangle = |i\rangle\langle i|A\rangle = a_i |i\rangle$$

$$\langle A|\hat{\mathbb{P}}_i = \langle A|i\rangle\langle i| = a_i^* \langle i|$$

$$\hat{\mathbb{P}}_i \hat{\mathbb{P}}_j = |i\rangle\langle i|j\rangle\langle j| = |i\rangle \delta_{ij} \langle j| \quad \text{for orthonormal basis } \{|i\rangle\}_{i=\overline{1,n}}$$

$$= \delta_{ij} \hat{\mathbb{P}}_{ij} \quad \text{(check it!)}$$

* MR of $\hat{\mathbb{P}}_i$:

- "kl" matrix element of $\hat{\mathbb{P}}_i$: $\left(\hat{\mathbb{P}}_i\right)_{kl} = \langle k|i\rangle\langle i|l\rangle = \delta_{ki}\delta_{li}$

$$= \delta_{ik}\delta_{il} = \begin{cases} 0, & i\neq k \text{ OR } i\neq l \\ 1, & i=k=l \end{cases}$$

~~Example:) Let $|i\rangle = (0\,0\,0 \ldots 1 \ldots 0) \Rightarrow \langle i| = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}$~~

~~$\Rightarrow \hat{\mathbb{P}}_i = |i\rangle\langle i| = (0 \ldots 1 \ldots 0) \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}$~~

Let $|i\rangle = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}$
$$\Rightarrow \hat{\mathbb{P}}_i = |i\rangle\langle i| = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} (0 \ldots 1 \ldots 0)$$

$\langle i| \hat{=} (0 \ldots 1 \ldots 0)$

$$= \begin{pmatrix} 0 & \cdots & 0 \\ \vdots & \ddots\, ^{0}\,_{1}\,_{0} & \vdots \\ 0 & \cdots & 0 \end{pmatrix}$$

$$\hat{\mathbb{P}}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} (0\,1\,0) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$\mathbb{R}^2 \times 2$

MR of Operator Products

$$\left(\hat{\Omega}\hat{\Lambda}\right)_{ij} = \langle i|\underset{\Uparrow\mathbb{1}}{\hat{\Omega}\hat{\Lambda}}|j\rangle = \langle i|\hat{\Omega}\,\mathbb{1}\,\hat{\Lambda}|j\rangle$$

$$= \langle i|\hat{\Omega}\sum_k |k\rangle\langle k|\hat{\Lambda}|j\rangle =$$

$$= \sum_k \langle i|\hat{\Omega}|k\rangle\langle k|\hat{\Lambda}|j\rangle = \sum_k \Omega_{ik}\Lambda_{kj}$$

n×n matrix multiplication rule

Adjoint of an Operator

Reminder: $\alpha|A\rangle \longleftrightarrow \langle A|\alpha^*$, α - scalar

Now with op: $\hat{\Omega}|A\rangle \longleftrightarrow \langle A|\hat{\Omega}^\dagger$, $\hat{\Omega}^\dagger$ is the adjoint of $\hat{\Omega}$

MR of $\hat{\Omega}^\dagger$: in $\{|i\rangle\}_{i=1..n}$ basis

$$\underbrace{\left(\hat{\Omega}^\dagger\right)_{ij}}_{\text{matrix of } \hat{\Omega}^\dagger} = \langle i|\hat{\Omega}^\dagger|j\rangle = \left(\langle j|\hat{\Omega}|i\rangle\right)^* = \Omega^*_{ji}$$

$$= \Omega^*_{ji}$$

transpose conjugate of matrix for $\hat{\Omega}$

Adjoint of operator product $\hat{\Lambda}\hat{\Omega}$

$$\hat{\Lambda}\hat{\Omega}|A\rangle = \hat{\Lambda}\left(\hat{\Omega}|A\rangle\right)$$

$$\langle A|\left(\hat{\Lambda}\hat{\Omega}\right)^\dagger = \left(\hat{\Lambda}\hat{\Omega}|A\rangle\right)^* = \left(\hat{\Lambda}\left(\underline{\hat{\Omega}|A\rangle}\right)\right)^*$$

$$= \left(\underline{\langle A|\hat{\Omega}^\dagger}\right)\hat{\Lambda}^\dagger = \langle A|\left(\hat{\Omega}^\dagger\hat{\Lambda}^\dagger\right)$$

$$\Rightarrow \boxed{\left(\hat{\Lambda}\hat{\Omega}\right)^\dagger = \hat{\Omega}^\dagger\hat{\Lambda}^\dagger}$$

Hermitian, Anti-Hermitian and Unitary Operators

(Anti-) Hermitian

Def.)
Hermitian : $\hat{\Omega}^\dagger = \hat{\Omega}$
Anti-hermitian : $\hat{\Omega}^\dagger = -\hat{\Omega}$

Usefulness : Any operator can be decomposed in a Hermitian part and an anti-Hermitian part :

$$\hat{\Omega} = \underbrace{\frac{\hat{\Omega}+\hat{\Omega}^\dagger}{2}}_{H.} + \underbrace{\frac{\hat{\Omega}-\hat{\Omega}^\dagger}{2}}_{a-H.}$$

(Analogy with complex numbers :

$$a = \underbrace{\frac{a+a^*}{2}}_{\text{purely real}} + \underbrace{\frac{a-a^*}{2}}_{\text{purely imaginary}}$$
)

Unitary

Def.)
Unitary operator : $\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = \mathbb{1}$
i.e. $\hat{U}^{-1} = \hat{U}^\dagger$

(Analogy with complex numbers :
for $a = e^{i\varphi}$, $a a^* = a^* a = 1$)

Properties :
1) if $\hat{A}$ and $\hat{B}$ are unitary, so is $\hat{A}\hat{B}$ or $\hat{B}\hat{A}$

2) unitary operators preserve the inner product between vectors on which they act (and their lengths)

$|A'\rangle = \hat{U}|A\rangle$
$|B'\rangle = \hat{U}|B\rangle$

$$\langle A'|B'\rangle = \langle A|\hat{U}^\dagger\hat{U}|B\rangle = \langle A|B\rangle$$

→ more important than it seems ⚠

Note: Unitary operators represent generalized rotations in n-dimensional spaces

(analogy with "rotations" in the complex plane $a = e^{i\varphi}$)

in orthonormal basis $\{|i\rangle\}_{i=1,n}$

$$\hat{U}^\dagger \hat{U} = \hat{\mathbb{1}} \Rightarrow \delta_{ij} = \langle i | j \rangle$$

$$= \langle i | \hat{\mathbb{1}} | j \rangle = \langle i | \hat{U}^\dagger \hat{U} | j \rangle$$

$$= \langle i | \hat{U}^\dagger \hat{\mathbb{1}} \hat{U} | j \rangle$$

$$= \langle i | \hat{U}^\dagger \left(\sum_{k=1}^{n} |k\rangle\langle k| \right) \hat{U} | j \rangle$$

$$= \sum_{k=1}^{n} \langle i | \hat{U}^\dagger | k \rangle \langle k | \hat{U} | j \rangle$$

$(\hat{U}^\dagger)_{ik} = U^*_{ki}$

$$\overset{1}{=} \sum_{k=1}^{n} (U^\dagger)_{ik} \, U_{kj}$$

or

$$\overset{2}{=} \sum_{k=1}^{n} \langle k | \hat{U} | i \rangle^* \langle k | \hat{U} | j \rangle$$

$$= \sum_{k=1}^{n} U^*_{ki} U_{kj}$$

for columns of $\begin{pmatrix} U_{11} \dots U_{1n} \\ \vdots \\ U_{n1} \dots U_{nn} \end{pmatrix}$

or, starting with

$$\hat{U} \hat{U}^\dagger = \hat{\mathbb{1}} \Rightarrow \delta_{ij} = \dots = \sum_{k=1}^{n} U_{ik} U^*_{jk}$$

for rows of $\begin{pmatrix} U_{11} \dots U_{1n} \\ \vdots \\ U_{n1} \dots U_{nn} \end{pmatrix}$

Active and Passive Transformations in a LVS

1) For all vectors $|v_i\rangle$, do $|v_i\rangle \rightarrow \hat{U}|v_i\rangle$ ← active transform.

Then, for any operator $\hat{\Omega}$ the matrix elements become:

$$\boxed{\langle v_i|\hat{\Omega}|v_j\rangle \longrightarrow \langle v_i|\hat{U}^\dagger \hat{\Omega} \hat{U}|v_j\rangle}$$

(active transformation) ← vectors affected

2) Same effect if $\boxed{\hat{\Omega} \rightarrow \hat{U}^\dagger \hat{\Omega} \hat{U}}$ (passive transf.)

vectors unaffected

Eigenvalue Problems

For any operator there exists a set of "proper" vectors such that

$$\hat{\Omega}|V\rangle = \omega|V\rangle$$

eigenvalue ("e-value") — eigenvector ("e-vector") or eigenket

Example

→ E-value problem for the identity operator $\hat{\mathbb{1}}$:

$$\hat{\mathbb{1}}|v\rangle = |v\rangle$$

↳ all kets are e-kets for $\hat{\mathbb{1}}$

↳ the only e-value is $= 1$

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Solution to E-value Problems. The Characteristic Eqn

$\hat{\Omega}|v\rangle = \omega|v\rangle \rightarrow (\hat{\Omega} - \hat{1}\omega)|v\rangle = |\phi\rangle$

$$|v\rangle = \underbrace{(\hat{\Omega} - \hat{1}\omega)^{-1}|\phi\rangle}_{\downarrow \triangle}$$

null vector

$$\underbrace{|\phi\rangle \overset{?}{=} \text{this is always } = |\phi\rangle}$$

$|v\rangle \neq |\phi\rangle$

$\Leftarrow$ The inverse $(\hat{\Omega} - \hat{1}\omega)^{-1}$ does not exist!

$\Rightarrow \ldots$ (matrix theory) $\boxed{\det(\hat{\Omega} - \omega\hat{1}) \overset{!}{=} 0}$

if nontrivial solutions to the e-value problem are needed

* Finding e-values *

$\langle i|(\hat{\Omega} - \omega\hat{1})|v\rangle = \langle i|\phi\rangle = 0$

basis bra

$\langle i|\hat{\Omega} - \omega\hat{1}|\hat{1}|v\rangle = \langle i|(\hat{\Omega} - \omega\hat{1})\sum_{k=1}^{n}|k\rangle\langle k|v\rangle$

$= \sum_{k}\langle i|\hat{\Omega} - \omega\hat{1}|k\rangle\langle k|v\rangle = \sum_{k}\left[\langle i|\hat{\Omega}|k\rangle - \omega\langle i|k\rangle\right]\underbrace{\langle k|v\rangle}_{v_k}$

MR $\rightarrow$ $= \sum_{k}(\Omega_{ik} - \omega\delta_{ik})v_k \overset{!}{=} 0$

v_k (k'th component)

Non-trivial solutions: $\underline{\det(\hat{\Omega} - \omega\hat{1}) \overset{!}{=} 0} \Leftrightarrow \boxed{\sum_{m=0}^{n} c_m\omega^m = 0}$ characteristic equation

characteristic polynomial

Do Ex. 1.8.4 / 33 Shankar

Theorem) The e-values of a Hermitian operators are real.

(easy to prove)

Theorem) To any Hermitian operator, there exists at least one orthonormal basis formed of the e-vectors of the operator. The operator is diagonal in this eigenbasis (with its e-values on the diagonal)

(~~[illegible]~~ lengthy proof)

Definition Degeneracy: More e-vectors for one e-value

$$\hat{\Omega}|\omega_1\rangle = \omega|\omega_1\rangle$$

$$\hat{\Omega}|\omega_2\rangle = \omega|\omega_2\rangle$$

Theorem) The e-values of a unitary operator are complex numbers of unit modulus

Theorem) The e-vectors of a unitary operator are mutually orthogonal. (no degeneracy is assumed)

Proofs: $\hat{U}|u_i\rangle = u_i|u_i\rangle$, $\hat{U}|u_j\rangle = u_j|u_j\rangle$

$$\left.\begin{aligned}\langle u_j|\hat{U}^\dagger\hat{U}|u_i\rangle &\overset{1}{=} u_j^* u_i \langle u_j|u_i\rangle \\ &\overset{2}{=} \langle u_j|u_i\rangle\end{aligned}\right\} \Rightarrow$$

$$\Rightarrow (1-u_j^* u_i)\langle u_j|u_i\rangle = 0$$

- if $i=j$ $\rightarrow$ $u_i^* u_i = |u_i|^2 \overset{!}{=} 1$ (since $\langle u_j|u_i\rangle \neq 0$)
- if $i\neq j$ $\Rightarrow$ $\langle u_j|u_i\rangle \overset{!}{=} 0$ (since $|u_i\rangle \neq |u_j\rangle \Rightarrow u_i \neq u_j$ $\Rightarrow u_i u_j^* \neq u_i u_i^* \Rightarrow u_i u_j^* \neq 1$)

Commutator algebra

Commutator $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$

Def: If $[\hat{A},\hat{B}] = 0$ then "$\hat{A},\hat{B}$ commute"

Theorem: Hermitian operators commute if their product is also Hermitian.

$$\hat{A}^\dagger = \hat{A} \ , \ \hat{B}^\dagger = \hat{B} \ ; \ [\hat{A},\hat{B}] \stackrel{!}{=} 0 \Rightarrow \hat{A}\hat{B} \stackrel{!}{=} \hat{B}\hat{A} \ \Big|^\dagger$$

$$\left.\begin{array}{l} \Rightarrow (\hat{A}\hat{B})^\dagger \stackrel{!}{=} (\hat{B}\hat{A})^\dagger \\ (\hat{A}\hat{B})^\dagger \stackrel{?}{=} \hat{B}^\dagger\hat{A}^\dagger = \hat{B}\hat{A} \end{array}\right\} \Rightarrow \boxed{(\hat{B}\hat{A})^\dagger = \hat{B}\hat{A} \text{ and } (\hat{A}\hat{B})^\dagger = \hat{A}\hat{B}}$$

qed

Properties of commutators

1) $[\hat{A},\hat{B}] = -[\hat{B},\hat{A}]$ antisymmetry

2) $[\hat{A},\hat{B}+\hat{C}] = [\hat{A},\hat{B}] + [\hat{A},\hat{C}]$ linearity

3) $[\hat{A},\hat{B}]^\dagger = [\hat{B}^\dagger,\hat{A}^\dagger]$ Hermitian ~~a~~ conjugate (adjoint) of comm.

4) $[\hat{A},\hat{B}\hat{C}] = [\hat{A},\hat{B}]\hat{C} + \hat{B}[\hat{A},\hat{C}]$ distributivity
$[\hat{A}\hat{B},\hat{C}] = \hat{A}[\hat{B},\hat{C}] + [\hat{A},\hat{C}]\hat{B}$

5) $[\hat{A},[\hat{B},\hat{C}]] + [\hat{B},[\hat{C},\hat{A}]] + [\hat{C},[\hat{A},\hat{B}]] = 0$ Jacobi identity

6) $[\hat{A},\hat{B}^n] = \sum_{j=0}^{n-1} \hat{B}^j [\hat{A},\hat{B}] \hat{A}^{n-j-1}$

generalized distributivity

$$[\hat{A}^n,\hat{B}] = \sum_{j=0}^{n-1} \hat{A}^{n-j-1} [\hat{A},\hat{B}] \hat{B}^j$$

7) $[\hat{A},a] = 0$ where a = any scalar

⚠ ~~Commutators~~ do not (always) behave like numbers ⚠
Operators

Infinitesimal and Finite Unitary Transformations

Functions of Operators

$$f(\hat{A}) = \sum_{n=0}^{\infty} a_n \hat{A}^n$$ Taylor expansion, if $\hat{A}$ is a linear op.

Example: $f(\hat{A}) = e^{a\hat{A}} = \sum_{n=0}^{\infty} \frac{a^n}{n!} \hat{A}^n$

$$= \hat{\mathbb{1}} + a\hat{A} + \frac{a}{2!}\hat{A}\hat{A} + \frac{a^2}{3!}\hat{A}\hat{A}\hat{A} + \cdots$$

- commutators:

1) if $[\hat{A},\hat{B}] = 0 \Rightarrow [f(\hat{A}), \hat{B}] = 0$ where $f(\hat{A})$ is <u>any</u> function of $\hat{A}$.

2) $[\hat{A}, f(\hat{A})] = 0$; $[\hat{A}^n, f(\hat{A})] = 0$; $[f(\hat{A}), g(\hat{A})] = 0$

- Hermitian conjugates (adjoints):

$$[f(\hat{A})]^\dagger = f^*(\hat{A}^\dagger)$$

- for $\hat{A}^\dagger = \hat{A}$ (Hermitian), $f(\hat{A})$ is not always Hermitian (only if $f(\cdot)$ is a <u>real</u> function)

$$f(\hat{A}) = e^{\hat{A}} \Rightarrow [f(\hat{A})]^\dagger = \left(e^{\hat{A}}\right)^\dagger = \left(\sum_{n=0}^{\infty} \frac{a^n}{n!}\hat{A}^n\right)^\dagger$$

$$= \sum_{n=0}^{\infty} \frac{(a^*)^n}{n!}(\hat{A}^\dagger)^n$$

$$\doteq f(\hat{A})$$ iff $a^* = a$ i.e. $a \in \mathbb{R}$ and $\hat{A}^\dagger = \hat{A}$ i.e. Hermitian

$$f(\hat{A}) = e^{i\hat{A}} \Rightarrow [f(\hat{A})]^\dagger = e^{-i\hat{A}^\dagger}$$

- Relations: $e^{\hat{A}} e^{\hat{B}} = \left(e^{\hat{A}+\hat{B}}\right) e^{[\hat{A},\hat{B}]/2} \neq e^{\hat{A}+\hat{B}}$ if $[\hat{A},\hat{B}] \neq 0$

$$e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + [\hat{A},\hat{B}] + \frac{1}{2!}[\hat{A},[\hat{A},\hat{B}]] + \frac{1}{3!}[\hat{A},[\hat{A},[\hat{A},\hat{B}]]] + \cdots$$

Infinitesimal and Finite Unitary Transformations

Goal : Effects of unitary transformations on $|\,\rangle$'s, $\langle\,|$'s, operators, and scalars.

$$|\psi'\rangle = \hat{U}|\psi\rangle \quad , \quad \langle\psi'| = \langle\psi|\hat{U}^\dagger$$

- let operator $\hat{A}$ s.t. $\hat{A}|\psi\rangle = |\phi\rangle$. What is $\hat{A}'|\psi'\rangle = |\phi'\rangle = ?$, under the above unitary transformation?

$$\left.\begin{aligned} \hat{A}'|\psi'\rangle &\overset{1}{=} \hat{A}'\hat{U}|\psi\rangle \\ &\overset{2}{=} |\phi'\rangle = \hat{U}|\phi\rangle \end{aligned}\right\} \Rightarrow \hat{A}'\hat{U}|\psi\rangle = \hat{U}|\phi\rangle \overset{2}{=} \hat{U}\hat{A}|\psi\rangle$$

$\hat{U}^\dagger \cdot \|$

$$\Rightarrow \hat{U}^\dagger\hat{A}'\hat{U}|\psi\rangle = \underbrace{\hat{U}^\dagger\hat{U}}_{\mathbb{1}}\hat{A}|\psi\rangle = \hat{A}|\psi\rangle$$

$$\Rightarrow \boxed{\hat{U}^\dagger\hat{A}'\hat{U} = \hat{A}} \qquad \| \hat{U} \cdot\ \cdot \hat{U}^\dagger$$

$$\Leftrightarrow \underbrace{\hat{U}\hat{U}^\dagger}_{\mathbb{1}}\hat{A}'\underbrace{\hat{U}\hat{U}^\dagger}_{\mathbb{1}} = \hat{U}\hat{A}\hat{U}^\dagger$$

$$\Rightarrow \boxed{\hat{A}' = \hat{U}\hat{A}\hat{U}^\dagger}$$

(!) extremely useful when calculating the effect of operators under a change of basis via a unitary transformation

Infinitesimal Unitary Transformations

Let a unitary transformation $\hat{U}$ depend on an infinitesimal parameter ε.

$$\hat{U}_\varepsilon(\hat{G}) = \mathbb{1} + i\varepsilon\hat{G}$$

, where $\hat{G}$ is the generator of the infinitesimal transformation $\hat{U}$

- unitary iff $\varepsilon \in \mathbb{R}$ and $\hat{G}^\dagger = \hat{G}$:

$$\hat{U}_\varepsilon\hat{U}_\varepsilon^\dagger = (\mathbb{1} + i\varepsilon\hat{G})(\mathbb{1} - i\varepsilon\hat{G}^\dagger) = \mathbb{1} + i\varepsilon(\hat{G} - \hat{G}^\dagger) + \underbrace{\cancel{\varepsilon^2\hat{G}\hat{G}^\dagger}}_{O(2)} \simeq \mathbb{1} + i\varepsilon(\hat{G} - \hat{G}^\dagger)$$

$(= \mathbb{1}$ if $\hat{G} = \hat{G}^\dagger$ and $\varepsilon \in \mathbb{R})$

(active transformation)

- Action on a vector $|\psi\rangle$:

$$|\psi'\rangle = \hat{U}_\varepsilon(\hat{G})|\psi\rangle = (\hat{1} + i\varepsilon\hat{G})|\psi\rangle = |\psi\rangle + \underbrace{i\varepsilon\hat{G}|\psi\rangle}$$

a small (infinitesimal) correction to $|\psi\rangle$ ... $= \delta|\psi\rangle$

(passive transformation)

- Transformation of an operator $\hat{A}$:

$$\hat{A}' = \hat{U}\hat{A}\hat{U}^\dagger = (\hat{1} + i\varepsilon\hat{G})\hat{A}(\hat{1} - i\varepsilon\hat{G}^\dagger)$$

$$\approx \hat{A} + i\varepsilon[\hat{G},\hat{A}] \quad (\text{neglecting } \mathcal{O}(2) \text{ in } \varepsilon \ldots)$$

↳ invariant if $[\hat{G},\hat{A}] = 0$

* A finite unitary transformation results from applying many successive infinitesimal transformations:

- Let $\hat{U}_\alpha(\hat{G})$ be a finite unitary transf. with finite "step" α;

$$\hat{U}_\alpha(\hat{G}) = \lim_{N\to\infty} \prod_{k=1}^{N} \hat{U}_\varepsilon(\hat{G}) = \lim_{N\to\infty} \prod_{k=1}^{N} (\hat{1} + i\varepsilon\hat{G})$$

$$\varepsilon = \frac{\alpha}{N}$$

$$= \lim_{N\to\infty} \prod_{k=1}^{N} \left(\hat{1} + i\frac{\alpha}{N}\hat{G}\right) = \lim_{N\to\infty}\left(\hat{1} + i\alpha\hat{G}\right)^N$$

$$= e^{i\alpha\hat{G}}$$

HW

Note: If $[\hat{G},\hat{A}] = 0$ then $\hat{A}' = e^{i\alpha\hat{G}}\hat{A}e^{-i\alpha\hat{G}^\dagger} = \hat{A}$

(show at home)

Change of Basis and Unitary Transformations

Basis change: $|\phi_n\rangle \to |\phi_n'\rangle$, $n = 1,2,3,\ldots$ $\quad |\phi_n'\rangle = \hat{U}|\phi_n\rangle$

old $\to$ new

Formulation of the problem: Knowing the components of kets and bras, and operators in the old basis $\{|\phi_n\rangle\}$, what ~~are~~ do they become in the new basis $\{|\phi_n'\rangle\}$?

Any ket, bra: $|\psi'\rangle = [?]\,|\psi\rangle$, $\langle\psi'| = \langle\psi|\,[?]$

transformation matrices

M.R. of any operator: $A'_{mn} = ?$ in terms of A_{mn} in the old basis

---

Components in new basis:

$$\langle\phi_m'|\psi\rangle = \langle\phi_m'|\,\hat{1}_{old}\,|\psi\rangle = \langle\phi_m'|\sum_n |\phi_n\rangle\langle\phi_n|\psi\rangle$$

$$= \sum_n \langle\phi_m'|\phi_n\rangle\langle\phi_n|\psi\rangle$$

$$= \sum_n U_{mn}\,\langle\phi_n|\psi\rangle$$

comp. in old basis

basis transformation matrix elements

$U_{mn} \equiv \langle\phi_m'|\phi_n\rangle$; $\boxed{\hat{U}^\dagger\hat{U} = \hat{U}\hat{U}^\dagger = \hat{1} \text{ i.e. unitary}}$

MR : $\underset{new}{|\psi'\rangle} = \hat{U}\underset{old}{|\psi\rangle}$; $\underset{new}{\langle\psi'|} = \underset{old}{\langle\psi|}\hat{U}^\dagger$ ("active transf.")

Operators:

$$A'_{mn} = \langle\phi_m'|\hat{A}|\phi_n'\rangle = \langle\phi_m'|\,\hat{1}_{old}\,|\hat{A}|\,\hat{1}_{old}\,|\phi_n'\rangle$$

$$= \langle\phi_m'|\sum_j |\phi_j\rangle\langle\phi_j|\hat{A}\sum_i |\phi_i\rangle\langle\phi_i|\phi_n'\rangle$$

$$= \sum_{j,i} \underbrace{\langle\phi_m'|\phi_j\rangle}_{U_{mj}}\underbrace{\langle\phi_j|\hat{A}|\phi_i\rangle}_{A_{ji}}\underbrace{\langle\phi_i|\phi_n'\rangle}_{U^*_{in}} = \sum_{j,i} U_{mj}A_{ji}U^*_{in}$$

$\Rightarrow$ MR is: $\hat{A}' = \hat{U}\hat{A}\hat{U}^{+}$ -> a similarity transformation ("passive transformation")

op. in new basis — op. in old basis

<u>Hilbert Space</u> "$\mathcal{H}$": A set of vectors ($|A\rangle, |B\rangle, |C\rangle \dots$) and a set of scalars ($\alpha, \beta, \gamma, \dots$) satisfying the following:

HS1: $\mathcal{H}$ is a LVS
HS2: $\mathcal{H}$ has a defined inner product
HS3: $\mathcal{H}$ is separable
HS4: $\mathcal{H}$ is complete.

<u>Commuting Operators</u>

Theorem: If two operators commute, then a complete basis of simultaneous e-vectors can always be found.

The 5 Postulates of Quantum Mechanics

P1: State of a system

The state of any physical system is fully specified, at any time t, by a state vector $|\psi(t)\rangle$ in a Hilbert space $\mathcal{H}$. Any superposition of state vectors is also a state vector.

P2: Observables and Operators

To every measurable quantity A - an "observable" or "dynamic variable" - there corresponds a linear Hermitian operator $\hat{A}$ whose eigenvectors form a complete basis.

P3 Measurements and Eigenvalues

The measurement of an observable A is represented by the action of operator $\hat{A}$ on state vector $|\psi(t)\rangle$. The only possible outcomes of the measurement are the eigenvalues $\{a_n\}$ of operator $\hat{A}$.

If the measurement outcome is e-value a_n, the state of the system immediately after the measurement is given by the projection of the ~~(initial)~~ state vector $|\psi(t)\rangle$ onto eigenvector $|a_n\rangle$ corresponding to e-value a_n, for operator $\hat{A}$, i.e.:

$$|\psi\rangle_{\substack{\text{right}\\ \text{after}\\ \text{measurement}}} = \frac{\hat{\mathbb{P}}_n\,|\psi(t)\rangle}{\sqrt{\langle\psi|\mathbb{P}_n|\psi\rangle}} = \frac{|a_n\rangle\langle a_n|\psi(t)\rangle}{\sqrt{|\langle a_n|\psi\rangle|^2}}$$

collapse

P4 Probabilistic Outcome of Measurements

(a) Discrete spectra: When measuring observable A of a system in state $|\psi\rangle$, the probability of obtaining e-value a_n (non-degenerate!) is

$$P(a_n) = \frac{|\langle a_n|\psi\rangle|^2}{\langle\psi|\psi\rangle}$$

$\rightarrow$ if $|\psi\rangle$ is normalized i.e. $\langle\psi|\psi\rangle = 1$ $\rightarrow$ $P(a_n) = |\langle a_n|\psi\rangle|^2$

For normalised $|\psi\rangle$, $\langle\psi|\psi\rangle = 1$ and $\langle a_n|\psi\rangle$ is the "probability amplitude" to find ~~the~~ the system in state $|a_n\rangle$

~~- if the state~~

- if the eigenvalue a_n is m-times degenerate, then

$$P(a_n) = \frac{\sum_{j=1}^{m} |\langle a_n^j|\psi\rangle|^2}{\langle\psi|\psi\rangle}$$

. if the system is already in an eigenstate of $\hat{A}$, say $|a_n\rangle$, then a measurement of observable A yields eigenvalue a_n with 100% certainty i.e $P(a_n) = 1$ (since $\hat{A}|a_n\rangle = a_n|a_n\rangle$)

b) Continuous spectra:

- define the probability density to ~~find~~ measure a value for A between a and $a+da$:

$$dP(a) = \frac{|\psi(a)|^2 da}{\langle\psi|\psi\rangle} = \frac{|\psi(a)|^2 da}{\int_{-\infty}^{\infty} da' |\psi(a')|^2}$$

$$\text{or} \;= |\psi(a)|^2 da \quad \text{for } \langle\psi|\psi\rangle = 1$$

P5 Time Evolution

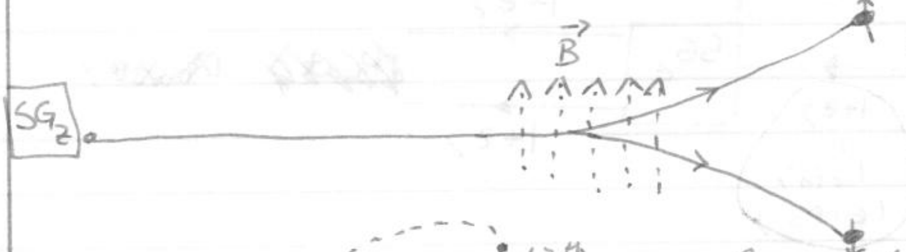
The state of a system evolves in time according to the Schrödinger equation:

$$i\hbar \frac{d|\psi(t)\rangle}{dt} = \hat{H}|\psi(t)\rangle$$

$\hat{H}$ is a linear Hermitian operator that corresponds to the total energy of the system

Stern-Gerlach Experiment. Spin-1/2 Statistics

SG (1922): Ag atoms in inhomogeneous magnetic field $\vec{B} = \vec{B}(z)$



$$\vec{F} = -\vec{\nabla} U = -\vec{\nabla}\left(-\vec{\mu}\cdot\vec{B}\right) = \vec{\nabla}\left(\vec{\mu}\cdot\vec{B}\right) \simeq \left(\mu_z \partial_z B\right)\hat{z}$$

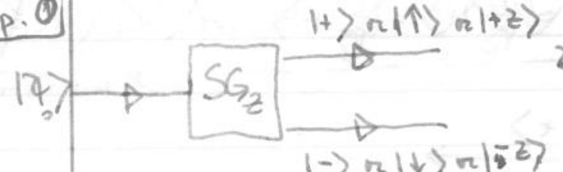
$$\left(\vec{\mu} = \frac{2e}{2m_e c}\vec{S} = \frac{-|e|}{m_e c}\vec{S}\right)$$

↳ responsible for Ag's intrinsic sp

$$|F| \simeq \mu_z \frac{e}{m_e c} S_z \frac{\partial B}{\partial z}$$

$$\left[SI: \ \vec{\mu} = \frac{-|e|}{m_e}\vec{S} \right]$$

$\boxed{Exp. ①}$



Initial state: $|\psi_0\rangle = \langle +|\psi_0\rangle |+\rangle + \langle +|\psi_0\rangle |-\rangle$

$= |+\rangle\langle +|\psi_0\rangle + |-\rangle\langle -|\psi_0\rangle$

S_z observable: $\hat{S}_z |+\rangle = \hbar/2\, |+\rangle \ ; \ \hat{S}_z |-\rangle = -\hbar/2\, |-\rangle$ $\quad \left(\hbar = 6.582 \times 10^{-16}\ \mathrm{eVs}\right)$

$\hat{S}_z^{+} = \hat{S}_z$ Hermitian op.

$|\psi_0\rangle = a_+ |+\rangle + a_- |-\rangle \ ; \ a_\pm = \langle \pm|\psi_0\rangle = 1/\sqrt{2}$ $\quad$ no phase factor by convention

$\mathcal{P}_\uparrow = |a_+|^2 \ ; \ \mathcal{P}_\downarrow = |a_-|^2 \ ; \ \mathcal{P}_{\uparrow \text{ or } \downarrow} = |a_+|^2 + |a_-|^2 \overset{!}{=} 1$ (normalization)

$\quad \overset{\shortparallel}{1/2} \qquad \overset{\shortparallel}{1/2}$

$\{|+z\rangle, |-z\rangle\}$ form an orthonormal basis:

$\langle +z|-z\rangle = \langle -z|+z\rangle^* = 0$

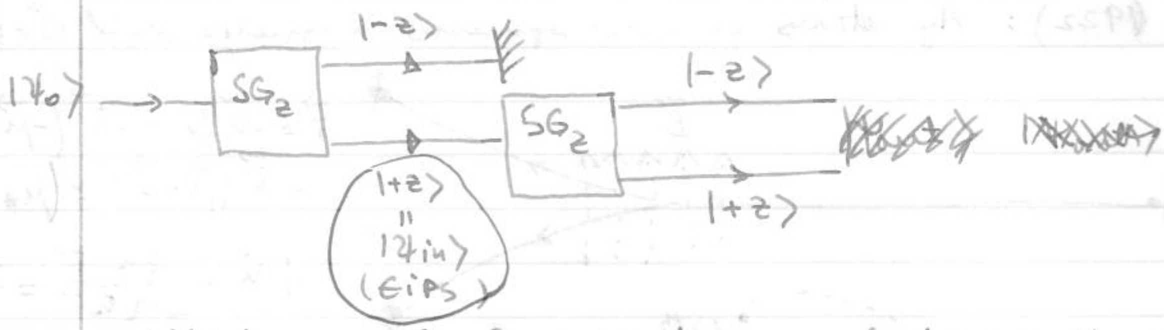
$\langle +|+\rangle = \langle -|-\rangle = 1$

$\langle \psi_0|\psi_0\rangle \overset{!}{=} 1 \Rightarrow$

$|a_+|^2 + |a_-|^2 \overset{!}{=} 1$

~~Ex~~ Sequential SG devices. Ensembles of identically prepared systems:
(EiPS)

Exp. 1



$|\psi_{in}\rangle \rightarrow$ state of identically prepared atoms (all with $S_z = +\hbar/2$)

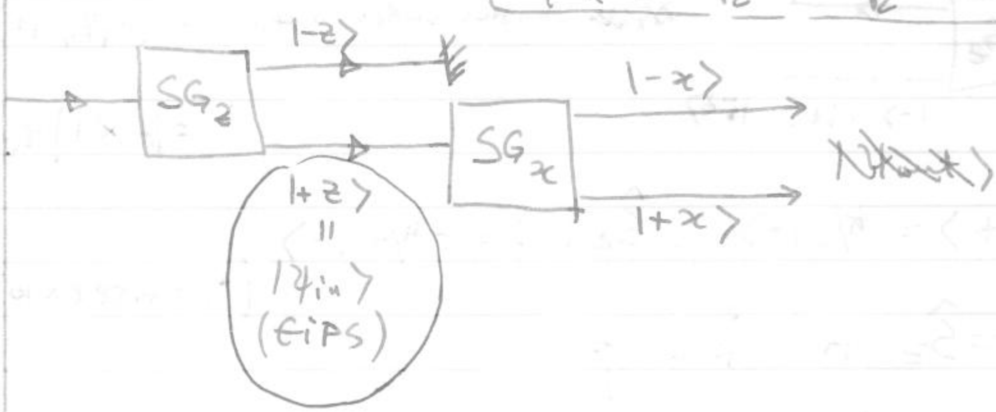
$$|\psi_{in}\rangle = |+z\rangle = |+z\rangle\langle +z|\psi_{in}\rangle + |-z\rangle\langle -z|\psi_{in}\rangle$$

$$= \underbrace{|+z\rangle\langle +z|+z\rangle}_{=1} + \underbrace{|-z\rangle\langle -z|+z\rangle}_{=0} = |+z\rangle \checkmark$$

$a_+ = 1 \; ; \; a_- = 0$ ~~$|\psi_{out}\rangle = |+\rangle\langle +|\psi_{out}\rangle + |-\rangle\langle -|\psi_{out}\rangle = \frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}}|-\rangle$ i.e. $a_+ = a_- = 1/\sqrt{2}$~~

not too important

Exp. 2



$$|\psi_{in}\rangle = |+z\rangle = |+x\rangle\langle +x|\psi_{in}\rangle + |-x\rangle\langle -x|\psi_{in}\rangle$$

$$= |+x\rangle\langle +x|+z\rangle + |-x\rangle\langle -x|+z\rangle$$

$$= \frac{1}{\sqrt{2}}|+x\rangle + \frac{1}{\sqrt{2}}|-x\rangle \quad \text{in } \{|\pm x\rangle\} \text{ basis !}$$

$= ?$ in $\{|\pm z\rangle\}$ basis ?

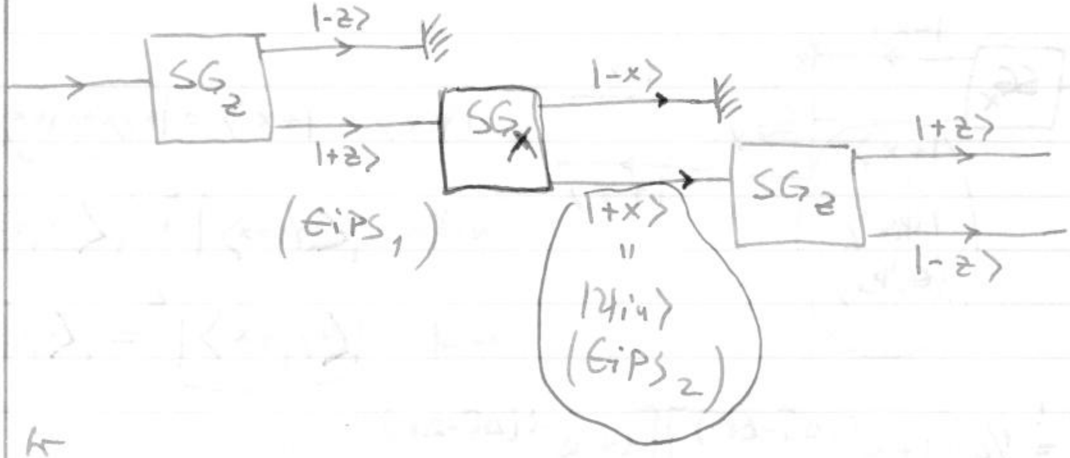
Need: $|\pm x\rangle = |+z\rangle\underbrace{\langle +z|\pm x\rangle}_{\{a, b\}_+} + |-z\rangle\underbrace{\langle -z|\pm x\rangle}_{\{a, b\}_-} = \{a, b\}_+ |+z\rangle + \{a, b\}_- |-z\rangle$, with $\{a, b\}_+ = ?$, $\{a, b\}_- = ?$

$$\text{or} \begin{bmatrix} |+x\rangle \\ |-x\rangle \end{bmatrix} = \begin{bmatrix} a_+ & a_- \\ b_+ & b_- \end{bmatrix} \begin{bmatrix} |+z\rangle \\ |-z\rangle \end{bmatrix}$$

unitary ~~rotation matrix~~

Experimentally, to obtain the unitary transformation from $|+x\rangle$ to $\{|\pm z\rangle\}$ (or $|-x\rangle$ to $\{|\pm z\rangle\}$) one needs to create another EiPS by subsequently blocking off $S_z = -\hbar/2$ (or $S_z = +\hbar/2$) and adding one more SG_z:

Exp. 3



to

$$|\psi_{in}\rangle = |+x\rangle = a_+|+z\rangle + a_-|-z\rangle \ , \quad a_\pm = ?$$

or

$$\left(|\psi_{in}\rangle = |-x\rangle = b_+|+z\rangle + b_-|-z\rangle \ , \quad b_\pm = ?\right)$$

Stat: $|a_+|^2 = |a_-|^2 = 1/2$; $|a_+|^2 + |a_-|^2 = 1$ (total prob.)

$$\Rightarrow \quad a_+ = 1/\sqrt{2}\, e^{i\delta_1} \ , \quad a_- = 1/\sqrt{2}\, e^{i\delta_2}$$

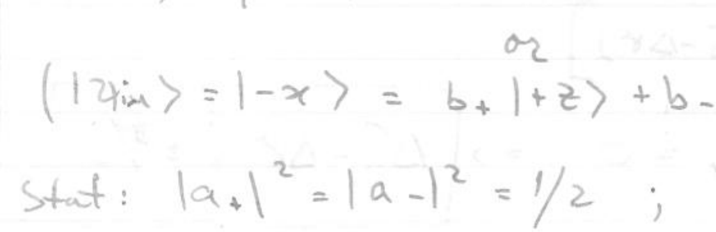
$$\Rightarrow |+x\rangle = 1/\sqrt{2}\left(e^{i\delta_1}|+z\rangle + e^{i\delta_2}|-z\rangle\right)$$

$$= 1/\sqrt{2}\, e^{i\delta_1}\left(|+z\rangle + e^{i(\delta_2-\delta_1)}|-z\rangle\right)$$

Do expectation value $\langle S_z\rangle = \langle +x|S_z|+x\rangle$ and uncertainty → p. 30(a)

Exp. 3'
(5 in book)

Now for $|+y\rangle \to \{|+z\rangle, |-z\rangle\}$ (or $|-y\rangle \to \{|+z\rangle, |-z\rangle\}$):



$$|\psi_{in}\rangle = |+y\rangle = a_+|+z\rangle + a_-|-z\rangle \quad \left(\text{or } |-y\rangle = b_+|+z\rangle + b_-|-z\rangle\right)$$

$$|a_+|^2 = |a_-|^2 = 1/2 \Rightarrow a_+ = 1/\sqrt{2}\, e^{i\gamma_1} \ , \quad a_- = 1/\sqrt{2}\, e^{i\gamma_2}$$

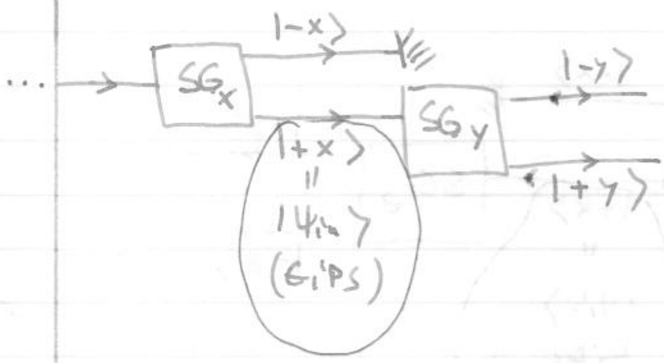
$$\Rightarrow |+y\rangle = 1/\sqrt{2}\, e^{i\gamma_1}\left(|+z\rangle + e^{i(\gamma_2-\gamma_1)}|-z\rangle\right)$$

Combine statistics for S_x, S_y i.e. GIPS for S_x (vs S_y):

Let $\Delta\delta \equiv \delta_2 - \delta_1$, $\Delta\gamma \equiv \gamma_2 - \gamma_1$, $|\pm z\rangle \equiv |\pm\rangle$!

$$|+x\rangle = \tfrac{1}{\sqrt{2}}\, e^{i\delta_1}\left(|+\rangle + e^{i\Delta\delta}|-\rangle\right)$$

$$|+y\rangle = \tfrac{1}{\sqrt{2}}\, e^{i\gamma_1}\left(|+\rangle + e^{i\Delta\gamma}|-\rangle\right) \; ; \; \langle +y| = \tfrac{1}{\sqrt{2}}\, e^{-i\gamma_1}\left(\langle +| + e^{-i\Delta\gamma}\langle -|\right)$$



$$|\psi_{in}\rangle = |+x\rangle = |+y\rangle\underbrace{\langle +y|+x\rangle} + |-y\rangle\underbrace{\langle -y|+x\rangle}$$

with $\left|\langle +y|+x\rangle\right|^2 + \left|\langle -y|+x\rangle\right|^2 = 1$

and $\underline{\left|\langle +y|+x\rangle\right|^2} = \left|\langle -y|+x\rangle\right|^2 = \underline{1/2}$

$$\Leftrightarrow \; 1/2 \overset{!}{=} 1/4\left[1 + e^{i(\Delta\delta - \Delta\gamma)}\right]\left[1 + e^{-i(\Delta\delta-\Delta\gamma)}\right] = \ldots$$

$$= 1/2\left[1 + \cos(\Delta\delta - \Delta\gamma)\right]$$

$$\Rightarrow \cos(\Delta\delta - \Delta\gamma) \overset{!}{=} 0 \quad \Rightarrow \boxed{\Delta\delta - \Delta\gamma \overset{!}{=} \pm \pi/2}$$

Arbitrary Phase: $\boxed{\text{Let } \Delta\delta = 0}$ $\Leftrightarrow \begin{cases} \delta_1 = \delta_2 \\ \Delta\gamma = \pm\pi/2 = \gamma_2 - \gamma_1 \end{cases}$

$\hookrightarrow \underline{\text{let}} \begin{cases} \delta_1 = \delta_2 = 0 \\ \underline{\gamma_1 = 0} \end{cases}$ $\Rightarrow \begin{cases} \gamma_2 = \pm\pi/2 = \Delta\gamma \\ \delta_2 = 0 = \Delta\delta \end{cases}$

$$\Rightarrow \boxed{\begin{aligned} |\pm x\rangle &= \tfrac{1}{\sqrt{2}}\left(|+z\rangle \pm |-z\rangle\right) \\ |\pm y\rangle &= \tfrac{1}{\sqrt{2}}\left(|+z\rangle + e^{\pm i\pi/2}|-z\rangle\right) \\ &= \tfrac{1}{\sqrt{2}}\left(|+z\rangle \pm i|-z\rangle\right) \end{aligned}}$$

Discuss
right } handedness
left
(Book p. 20)

5

Spin-1/2 ~~overview~~ summary:

$\hat{S}_x |\pm x\rangle = \pm \hbar/2 |\pm x\rangle$
$\hat{S}_y |\pm y\rangle = \pm \hbar/2 |\pm y\rangle$
$\hat{S}_z |\pm z\rangle = \pm \hbar/2 |\pm z\rangle$

In basis of $\hat{S}_z$ i.e. $\{|\pm z\rangle\}$ or $\{|\pm\rangle\}$:

$\hat{S}_x |\pm x\rangle = \pm \hbar/2 \; 1/\sqrt{2} \left(|+\rangle \pm |-\rangle\right)$

$\hat{S}_y |\pm y\rangle = \pm \hbar/2 \; 1/\sqrt{2} \left(|+\rangle \pm i|-\rangle\right)$

$\hat{S}_z |\pm z\rangle = \pm \hbar/2 \; |\pm\rangle$

Spectral Decomposition of an Operator

Any operator : $\hat{A} = \hat{\mathbb{1}} \hat{A} \hat{\mathbb{1}} = \sum_i |a_i\rangle\langle a_i| \hat{A} \sum_j |a_j\rangle\langle a_j|$

in e-kets of $\hat{A}$

EVP of $\hat{A}$: $\boxed{\hat{A}|a_i\rangle = a_i |a_i\rangle \quad i = 1, \dots, n}$

$= \sum_{ij} |a_i\rangle \underbrace{\langle a_i|\hat{A}|a_j\rangle}\langle a_j| =$

$= \sum_{ij} |a_i\rangle A_{ij} \langle a_j| = \sum_{ij} A_{ij} |a_i\rangle\langle a_j|$ $\Rightarrow$

but $A_{ij} = \langle a_i|\underline{\hat{A}|a_j\rangle} = \langle a_i| a_j |a_j\rangle = a_j \langle a_i|a_j\rangle = a_j \delta_{ij}$

$$\Rightarrow \boxed{\hat{A} = \sum_{ij} a_j \delta_{ij} |a_i\rangle\langle a_j| = \sum_i a_i |a_i\rangle\langle a_i|} \; //$$

So, $\hat{S}_x = +\hbar/2 |+x\rangle\langle +x| - \hbar/2 |-x\rangle\langle -x| = \hbar/2 \left(|+\rangle\langle -| + |-\rangle\langle +|\right)$ ✓

$\hat{S}_y = +\hbar/2 |+y\rangle\langle +y| - \hbar/2 |-y\rangle\langle -y| = i\hbar/2 \left(-|+\rangle\langle -| + |-\rangle\langle +|\right)$ ✓

$\hat{S}_z = +\hbar/2 |+z\rangle\langle +z| - \hbar/2 |-z\rangle\langle -z| = \hbar/2 \left(|+\rangle\langle +| - |-\rangle\langle -|\right)$ ✓

$\hat{S}_x = \hbar/2 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$; $\hat{S}_y = \hbar/2 \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$; $\hat{S}_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

(2.2.) Rotation operators

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- spin states precess about $\vec B$ fields etc...

$\hat{R}_z(\pi/2)$: $|+x\rangle = \hat{R}_z(\pi/2)|+z\rangle$ ccw = "positive" rotations (def'd)

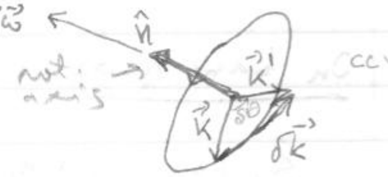
For $|\psi\rangle = a|+z\rangle + b|-z\rangle$: $\hat{R}_z(\pi/2)|\psi\rangle = \dots = a|+x\rangle + b|-x\rangle$

$\hat{R}_z^\dagger(\pi/2)$: $\langle +x| = \langle +z|\hat{R}_z^\dagger(\pi/2)$ s.t. $1 = \langle +x|+x\rangle = \dots = \langle +z|+z\rangle$

$\iff \boxed{\hat{R}^\dagger = \hat{R}^{-1}}$ unitary operator : $\hat{R}^\dagger\hat{R} = 1$ $\left(= \hat{R}\hat{R}^\dagger\right)$ -> generalize $\hat{U}$ (p.13-15)

Generators of Rotations

1) infinitesimal rotations:



$\vec{k}' = \vec{k} + \delta\vec{k} = \vec{k} + \delta\vec{\omega}\times\vec{k}$; $\delta\vec{\omega} = \delta\theta\,\hat{n}$

$\Rightarrow \delta\vec{k} = \delta\theta\,\hat{n}\times\vec{k}$ $(= \delta\theta\,\varepsilon_{ijk}\hat{x}_i n_j k_k \dots)$

Let $\hat{n} = \hat{x}_3 = \hat{z}$: $\delta\vec{\omega} = \delta\theta\,\hat{z}$ $\Rightarrow$ $\delta\vec{k} = \delta\vec{\omega}\times\vec{k} = \delta\theta(\hat{z}\times\vec{k}) = \delta\theta\left[\hat{y}k_x - \hat{x}k_y\right]$

set $\hat{R}_z(\delta\theta) \doteq \mathbb{1} - i\delta\theta\,\hat{I}_z \iff \hat{I}_z = \frac{\mathbb{1}-\hat{R}}{i\delta\theta} = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ since $\boxed{\hat{R}_z(\delta\theta) = \begin{pmatrix} 1 & -\delta\theta & 0 \\ \delta\theta & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}}$ start

$\left(e^{-i\delta\theta\hat{I}_z} = 1 - i\delta\theta\,\hat{I}_z - \frac{\delta\theta^2}{2}\hat{I}_z^2 + \dots\right)$

$\Rightarrow \boxed{\vec{k}' = \hat{R}_z(\delta\theta)\vec{k} \approx (\mathbb{1} - i\delta\theta\,\hat{I}_z)\vec{k}}$

$\hat{I}_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}$

$\hat{I}_y = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}$

$$[\hat{I}_i, \hat{I}_j] = i\varepsilon_{ijk}\hat{I}_k \quad \left(= i\sum_k \varepsilon_{ijk}\hat{I}_k\right)$$

In Hilbert (ket) space: $|\psi'\rangle = \hat{R}_z(\delta\theta)|\psi\rangle = \left(\mathbb{1} - i\frac{\delta\theta}{\hbar}\hat{J}_z\right)|\psi\rangle$ $\left(\langle\psi'| = \langle\psi|\hat{R}_z^\dagger\right)$

$\hat{I}_z = \frac{\hat{J}_z}{\hbar}$

2) Finite rotation: $\delta\theta = \lim_{N\to\infty}\theta/N$

$\hat{J}_z \equiv \hbar\hat{I}_z$

$$\boxed{\hat{R}_z(\theta) = \lim_{N\to\infty}\left[\hat{R}_z(\delta\theta)\right]^N = \lim_{N\to\infty}\left[\mathbb{1} - i\frac{\theta}{N\hbar}\hat{J}_z\right]^N = e^{-i\frac{\theta}{\hbar}\hat{J}_z}}$$

$\hat{J}_z$ - ang. momentum op. = gen. of rotations (infinitesimal)

Read: Eigenstates & eigenvalues p137-41

$\hat{J}_z|\pm z\rangle \overset{SG}{=} \left(\pm\frac{\hbar}{2}\right)|\pm z\rangle$ (EVP for $\hat{J}_z$)

show, using $\hat{R}_z(\theta)$

Read: Projection & identity ops (sec. 2.3)
Matrix Rep. of Ops (sec 2.4)
Change of Basis (sec. 2.5)

ANGULAR MOMENTUM (Ch 3 Townsend)

Read: 3.1

(3.1) Rotations do not commute (read p. 75-78)

Finite rot.: $\hat{R}_z(\phi) = e^{-i\frac{\hat{J}_z\phi}{\hbar}}$, $\hat{R}_x = \cdots$, $\hat{R}_y = \cdots$

$$\hat{R}_x\hat{R}_y = e^{-i\hat{J}_x\phi/\hbar}\, e^{-i\hat{J}_y\phi/\hbar}$$

$[\hat{R}_x(\phi), \hat{R}_y(\phi)] = \hat{R}_z(\phi) - \hat{1}$

Taylor, for small ϕ

$$\simeq \sum_n \left(\frac{-i\phi}{\hbar}\right)^n \frac{\hat{J}_x^n}{n!} \sum_m \left(\frac{-i\phi}{\hbar}\right)^m \frac{\hat{J}_y^m}{m!} \overset{!}{=} \left(\hat{1} - i\frac{\hat{J}_z\phi^2}{\hbar}\right) - \hat{1}$$

Eq (3.8)

$\mathcal{O}(2)$

To $\mathcal{O}(2)$ $\cancel{\mathcal{O}(\phi)}$ $\Rightarrow$ $\hat{J}_x\hat{J}_y - \hat{J}_y\hat{J}_x = i\hbar\hat{J}_z$

$[\hat{J}_i, \hat{J}_j] = i\hbar\,\varepsilon_{ijk}\hat{J}_k$

$$\boxed{[\hat{J}_{\substack{x\\y\\z}}, \hat{J}_{\substack{y\\z\\x}}] = i\hbar\hat{J}_{\substack{z\\x\\y}}}$$

Ang. mom. commutation relations

(3.2) Commuting operators share e-states

Let $[\hat{A},\hat{B}] = 0$. Assume $|a\rangle$ is only e-state of $\hat{A}$:

$\hat{A}|a\rangle = a|a\rangle$

$\hat{B}\hat{A}|a\rangle = \hat{B}a|a\rangle = a(\hat{B}|a\rangle)$

$\overset{?}{=} \hat{A}(\hat{B}|a\rangle)$

$\Rightarrow |Ba\rangle \equiv \hat{B}|a\rangle$ is also e-state of $\hat{A}$

But that e-state is unique by construction

$\rightarrow \hat{B}|a\rangle \propto |a\rangle$ i.e. $\hat{B}|a\rangle = b|a\rangle$

(3.3) E-values and E-states of Angular Momentum

$$\hat{J}^2 = \vec{J}\cdot\vec{J} = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2$$

Use $[\hat{A}, \hat{B}\hat{C}] = \hat{B}[\hat{A},\hat{C}] + [\hat{A},\hat{B}]\hat{C}$ to show

$[\hat{J}_z, \hat{J}^2] = 0 \Rightarrow$ share e-states $|\lambda, m\rangle$

$$\boxed{\begin{aligned} J^2|\lambda m\rangle &= \lambda\hbar^2|\lambda m\rangle \\ J_z|\lambda m\rangle &= m\hbar|\lambda m\rangle \end{aligned}}$$

$\lambda \geq 0$
(See proof p. 83)
p. 83

Read | Spin-1 p. 83-85

Special Ops: Ladder Operators;

$$\hat{J}_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} ; \quad \hat{J}_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} ; \quad \hat{J}_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

in $\hat{J}_z$ basis.

$$\hat{J}^2 = 2\hbar^2\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = 2\hbar^2 \hat{\mathbb{1}} \quad \Rightarrow [\hat{J}^2, \hat{J}_i] = 0$$

$i = x, y, z$

$\Rightarrow$ shared e-states (basis):

$$|1,1\rangle \equiv \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} ; \quad |1,0\rangle \equiv \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} ; \quad |1,-1\rangle = \begin{bmatrix} 0 \\ 0 \\ +1 \end{bmatrix}$$

$\downarrow$ $+\hbar$ $\quad$ $\downarrow$ 0 $\quad$ $\downarrow$ $-\hbar$

$$\hat{J}_z|11\rangle = \hbar|11\rangle$$
$$\hat{J}_z|1,0\rangle = 0$$
$$\hat{J}_z|1,-1\rangle = -\hbar|1,-1\rangle$$

Now, form special operators:

$$\hat{J}_x + i\hat{J}_y = \hbar\sqrt{2}\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \equiv \hat{J}_+$$

$$\hat{J}_x - i\hat{J}_y = \hbar\sqrt{2}\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \equiv \hat{J}_-$$

$$[\hat{J}_+, \hat{J}_-] = 2\hbar\hat{J}_z \quad (1)$$

$$[\hat{J}_\pm, \hat{J}_z] = \mp\hbar\hat{J}_\pm \quad (2)$$

$$\hat{J}_\pm\hat{J}_\mp = \hat{J}^2 - \hat{J}_z^2 \pm \hbar\hat{J}_z \quad (3)$$

How do they operate?

$$(\hat{J}_x + i\hat{J}_y)|1,-1\rangle = \hbar\sqrt{2}|1,0\rangle$$

$$(\hat{J}_x + i\hat{J}_y)|1,0\rangle = \hbar\sqrt{2}|1,1\rangle$$

raises e-values

$$(\hat{J}_x + i\hat{J}_y)|1,1\rangle = 0 \quad \left(= \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}\right)$$

$$(\hat{J}_x - i\hat{J}_y)|1,-1\rangle = 0$$

$$(\hat{J}_x - i\hat{J}_y)|1,0\rangle = \hbar\sqrt{2}|1,-1\rangle$$

lowers e-values

$$(\hat{J}_x - i\hat{J}_y)|1,1\rangle = \hbar\sqrt{2}|1,0\rangle$$

$$\boxed{\hat{J}_\pm \equiv \hat{J}_x \pm i\hat{J}_y \quad \text{raising/lowering operators}}$$

("ladder")

Properties $\hat{J}_\pm^{\dagger} = \hat{J}_\mp$ (not Hermitian!)

$$\boxed{[\hat{J}_z, \hat{J}_\pm] = \pm\hbar\hat{J}_\pm}$$

Explicit action of $\hat{J}_\pm$:

$$\hat{J}_z \underbrace{\hat{J}_+ |\lambda m\rangle} = \left(\hat{J}_+ \hat{J}_z + \hbar \hat{J}_+\right) |\lambda m\rangle$$

$$= \hat{J}_+ \left(m\hbar\, |\lambda m\rangle\right) + \hbar \hat{J}_+ |\lambda m\rangle$$

$$= (m+1)\hbar\ \underbrace{\hat{J}_+ |\lambda m\rangle}$$

-> "$\hat{J}_+ |\lambda m\rangle$" is e-state of $\hat{J}_z$, for e-value "$(m+1)\hbar$"

$$\hat{J}_z \underbrace{\hat{J}_- |\lambda m\rangle} = (m-1)\hbar\ \underbrace{\hat{J}_- |\lambda m\rangle}$$

-> "$\hat{J}_+ |\lambda m\rangle$" is e-state of $\hat{J}_z$, for e-value "$(m-1)\hbar$"

Also e-states of $\hat{J}^2$ (since $[\hat{J}^2, \hat{J}_\pm] = 0$) :

$$\hat{J}^2 \left(\hat{J}_\pm |\lambda m\rangle\right) = \hat{J}_\pm \hat{J}^2 |\lambda m\rangle = \lambda\hbar^2 \left(\hat{J}_\pm |\lambda m\rangle\right)$$

Find e-values (λ) on the ladder... :
e-states $|\lambda m\rangle$

$$\hat{J}^2 |jm\rangle = j(j+1)\hbar^2 |jm\rangle$$

$$\hat{J}_z |jm\rangle = m\hbar\, |jm\rangle$$

$$m = -j, \ldots, 0, \ldots +j \quad \} 2j+1$$

p. 20 black notes

(p. 90)

(3.4) MR of $\hat{J}_\pm$:

$$\hat{J}_\pm |jm\rangle = \sqrt{j(j+1) - m(m\pm 1)}\ \hbar\ |j, m\pm 1\rangle$$

$$\langle jn| \hat{J}_\pm |jm\rangle = \sqrt{j(j+1) - m(m\pm 1)}\ \hbar\ \delta_{n, m\pm 1}$$

p. 24 black notes

↳ Ex. 3.3 / 91

(3.5) Uncertainty Relations for Angular Momentum

Spin-1/2 EVP Derived from Commutation Relations

+ No shared e-states for $\{\hat{J}^2, \hat{J}_z, \hat{J}_x, \hat{J}_y\}$ $\left([\vec{J}^2, \hat{J}_i] = 0; [\vec{J}_i, \vec{J}_j] = \varepsilon_{ijk} i\hbar \hat{J}_k \neq 0\right)$

Generalize:

$$\rightarrow \| \; [\hat{J}_x, \hat{J}_y] = i\hbar \hat{J}_z \iff [\hat{A}, \hat{B}] = i\,\hat{C} \; \| \leftarrow$$

+ Schwarz Ineq ("SI"): $\boxed{\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2}$ $\quad |\vec{\alpha}||\vec{\beta}| \geq |\vec{\alpha}\cdot\vec{\beta}|^2$

$\sum_i |\alpha_i|^2 \sum_j |\beta_j|^2 \geq |\sum_i \alpha_i \beta_i^*|^2$

<u>let</u> $|\alpha\rangle = (\hat{A} - \langle A\rangle)|\psi\rangle \quad , \langle A\rangle \equiv \langle\psi|\hat{A}|\psi\rangle$

$|\beta\rangle = (\hat{B} - \langle B\rangle)|\psi\rangle \quad \langle B\rangle \equiv \langle\psi|\hat{B}|\psi\rangle$

$\hat{A}, \hat{B}$ - Hermitian

→ Then

$$\langle\alpha|\alpha\rangle = \langle\psi|(\hat{A} - \langle A\rangle)^2|\psi\rangle \equiv \langle\psi|(\Delta A)^2|\psi\rangle = \langle(\Delta A)^2\rangle$$

$$\langle\beta|\beta\rangle = \ldots \langle(\Delta B)^2\rangle$$

$$\langle\alpha|\beta\rangle = \langle\psi|(\hat{A} - \langle A\rangle)(\hat{B} - \langle B\rangle)|\psi\rangle \equiv \langle(\hat{A} - \langle A\rangle)(\hat{B} - \langle B\rangle)\rangle \equiv \langle(\Delta A)(\Delta B)\rangle$$

→ SI:

$$\Rightarrow \boxed{\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \tfrac{1}{4}|\langle[\hat{A}, \hat{B}]\rangle|^2 = \tfrac{1}{4}|\langle C\rangle|^2}$$

$$\sqrt{\;} \Rightarrow \boxed{\sqrt{\langle(\Delta A)^2\rangle}\sqrt{\langle(\Delta B)^2\rangle} \geq \tfrac{1}{2}|\langle C\rangle|}$$

or simply

$$(\Delta A)(\Delta B) \geq 1/2 |\langle C\rangle|$$

just a notation

URAM 2
S1/2 - 1

AM6

$$\boxed{\sqrt{\langle(\Delta J_x)^2\rangle\langle(\Delta J_y)^2\rangle} \geq \hbar/2\,|\langle J_z\rangle|}$$

or $(\Delta J_x)(\Delta J_y) \geq \hbar/2\,|\langle J_z\rangle| \Rightarrow$ $\boxed{\vec{J} \text{ cannot be along any axis}}$

$\boxed{s = 1/2}$: $\langle S_z\rangle = \pm\hbar/2 \neq 0 \Rightarrow$ uncertainty in S_x, S_y

$\Rightarrow \vec{S}$ does not fully align with x, y, z

(S_z basis) $\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$\hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

$\hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

NEXT: Spin-1/2 E-value Problem (Townsend 3.6) from Commutation Relations, p. 25 black notes for $\hat{S}_z$

$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$; $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$; $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

E-value Problem for $\hat{S}_x, \hat{S}_y$:

in $\hat{S}_z$ basis: $\hat{\vec{S}} = \hbar/2\,\hat{\vec{\sigma}}$, $\hat{\vec{\sigma}} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$ = Pauli matrices

Generalize: $\hat{S}_n = \hat{\vec{S}}\cdot\vec{n}$. Let $\hat{S}_n|\mu\rangle = \mu\hbar/2\,|\mu\rangle$, $\boxed{\vec{n} = \vec{x}\cos\phi + \vec{y}\sin\phi}$ (2D problem)

$\Rightarrow \hat{S}_n = \hat{S}_x\cos\phi + \hat{S}_y\sin\phi$

EVP: $\Rightarrow (\hat{S}_x\cos\phi + \hat{S}_y\sin\phi)|\mu\rangle = \mu\hbar/2\,|\mu\rangle$; (S_z) $|\mu\rangle = |+z\rangle\langle+z|\mu\rangle + |-z\rangle\langle-z|\mu\rangle$

in basis $\{|\pm z\rangle = |\pm\rangle\}$

$\Rightarrow (\hat{S}_x\cos\phi + \hat{S}_y\sin\phi)(|+\rangle\langle+|\mu\rangle + |-\rangle\langle-|\mu\rangle)$

$$= \mu\hbar/2\,(|+\rangle\langle+|\mu\rangle + |-\rangle\langle-|\mu\rangle)$$

MR:

$$\left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\cos\phi + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\sin\theta\right]\begin{pmatrix} \langle+|\mu\rangle \\ \langle-|\mu\rangle \end{pmatrix} = \mu\begin{pmatrix} \langle+|\mu\rangle \\ \langle-|\mu\rangle \end{pmatrix}$$

$$\begin{pmatrix} 0 & \cos\phi - i\sin\theta \\ \cos\phi + i\sin\phi & 0 \end{pmatrix}\begin{pmatrix} \langle+z|\mu\rangle \\ \langle-z|\mu\rangle \end{pmatrix} = \mu\begin{pmatrix} \langle+z|\mu\rangle \\ \langle-z|\mu\rangle \end{pmatrix}$$

$$\begin{pmatrix} 0 & e^{-i\phi} \\ e^{+i\phi} & 0 \end{pmatrix}\begin{pmatrix} \langle+|\mu\rangle \\ \langle-|\mu\rangle \end{pmatrix} = \mu\begin{pmatrix} \langle+|\mu\rangle \\ \langle-|\mu\rangle \end{pmatrix} \Leftrightarrow \begin{pmatrix} -\mu & e^{-i\phi} \\ e^{i\phi} & -\mu \end{pmatrix}\begin{pmatrix} \langle+|\mu\rangle \\ \langle-|\mu\rangle \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$\sigma_x = |+\rangle\langle -| + |-\rangle\langle +|$

$\sigma_y = i\,(-|+\rangle\langle -| + |-\rangle\langle +|)$

AM7

Non-trivial solutions iff

$$\begin{vmatrix} -\mu & e^{-i\phi} \\ e^{i\phi} & -\mu \end{vmatrix} = 0 \iff \mu^2 - 1 = 0 \iff \boxed{\mu = \pm 1}$$

$\hat{S}_n|\mu\rangle = \pm\hbar/2\,|\mu\rangle$

$\boxed{\mu = +1}$ Let $|\mu = +1\rangle = a_+|+z\rangle + b_+|-z\rangle$

$|\mu=+1\rangle \equiv |+n\rangle = \begin{pmatrix} a_+ \\ b_+ \end{pmatrix}$

EVP:
$$\begin{pmatrix} 0 & e^{-i\phi} \\ e^{i\phi} & 0 \end{pmatrix}\begin{pmatrix} a_+ \\ b_+ \end{pmatrix} = + \begin{pmatrix} a \\ b \end{pmatrix}$$

$$\Rightarrow \begin{cases} b e^{-i\phi} = a \\ a e^{i\phi} = b \end{cases} \Rightarrow \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} b e^{-i\phi} \\ b \end{pmatrix} = b \begin{pmatrix} e^{-i\phi} \\ 1 \end{pmatrix}$$

Normalize: $\langle\mu|\mu\rangle \overset{!}{=} 1 \Rightarrow (a^* \; b^*)\begin{pmatrix} a \\ b \end{pmatrix} \overset{!}{=} 1$

$\Rightarrow |a|^2 + |b|^2 = 1 \Rightarrow |b|^2 + |b|^2 = 1 \Rightarrow 2|b|^2 = 1$

$\Rightarrow |b| = 1/2 \Rightarrow \boxed{b = 1/\sqrt{2}}$ up to a const. phase.

$\Rightarrow \boxed{a = 1/\sqrt{2}\, e^{-i\phi}} \Rightarrow$

$$\Rightarrow \boxed{|\mu = +1\rangle = 1/\sqrt{2}\begin{pmatrix} e^{-i\phi} \\ 1 \end{pmatrix} \equiv |+n\rangle}$$ in S_z basis

$\Rightarrow |+n\rangle = 1/\sqrt{2}\left(e^{-i\phi}|+z\rangle + |-z\rangle\right)$ or $1/\sqrt{2}\left(|+z\rangle + e^{+i\phi}|-z\rangle\right)$

$\boxed{\mu = -1} \Rightarrow |-n\rangle = 1/\sqrt{2}\left(e^{-i\phi}|+z\rangle - |-z\rangle\right)$ or $1/\sqrt{2}\left(|+z\rangle - e^{+i\phi}|-z\rangle\right)$

$\phi = 0 \Rightarrow |\pm n\rangle = |\pm x\rangle = 1/\sqrt{2}\left(|+z\rangle \pm |-z\rangle\right)$

$\phi = \pi/2 \Rightarrow |\pm n\rangle = |\pm y\rangle = 1/\sqrt{2}\left(|+z\rangle \pm i|-z\rangle\right)$

Theoretical predictions match SG exp.

Do Ex 3.4 / 99

Commutator algebra

Tensor Product

AM8

$[\hat{A}]_{m\times n}$, $[\hat{B}]_{p\times q}$

$$\hat{A}\otimes\hat{B} = [a_{ij}\hat{B}] = \begin{pmatrix} a_{11}\hat{B} & \cdots & a_{1n}\hat{B} \\ \vdots & & \\ a_{n1}\hat{B} & \cdots & a_{nn}\hat{B} \end{pmatrix} \to mp\times nq$$

$$\hat{\sigma}_x\otimes\hat{\sigma}_z = \left(\begin{array}{c|c} 0 & \hat{\sigma}_z \\ \hat{\sigma}_z & 0 \end{array}\right) = \left(\begin{array}{cc|cc} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ \hline 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{array}\right)$$

$|u\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$, $|v\rangle = \begin{pmatrix} c \\ d \end{pmatrix}$

$$|u\rangle\otimes|v\rangle = \begin{pmatrix} a|v\rangle \\ b|v\rangle \end{pmatrix} = \begin{pmatrix} ac \\ ad \\ bc \\ bd \end{pmatrix} \equiv |u\rangle_1|v\rangle_2 \equiv |u_1 v_2\rangle$$

Properties

1) $(\hat{A}\otimes\hat{B})(\hat{C}\otimes\hat{D}) = (\hat{A}\hat{C})\otimes(\hat{B}\hat{D})$

$\hookrightarrow$ $(A_1\otimes B_1)(A_2\otimes B_2)(A_3\otimes B_3) = A_1A_2A_3 \otimes B_1B_2B_3 \dots$

$A\otimes(B+C) = A\otimes B + A\otimes C$

$(\hat{A}\otimes\hat{B})^\dagger = \hat{A}^\dagger\otimes\hat{B}^\dagger$, $(\hat{A}\otimes\hat{B})^{-1} = \hat{A}^{-1}\otimes\hat{B}^{-1}$

$\mathrm{tr}(A\otimes B) = (\mathrm{tr}\,A)(\mathrm{tr}\,B)$

$\det(A\otimes B) = [\det(\hat{A})]^m\,[\det(\hat{B})]^n$ if $\hat{A}\to m\times m$, $\hat{B}\to n\times n$

$|a\rangle\langle b|\otimes|c\rangle\langle d| = (|a\rangle\otimes|c\rangle)(\langle b|\otimes\langle d|)$

> Orbital Angular Momentum as the Generator of ~~Basis~~ Rotations

2D Rotations $\hat{R}(\varphi,\vec{z})$ rot. about the $\vec{z}$-axis

$\vec{r} = x\vec{x} + y\vec{y} \to \vec{r}' = x'\vec{x} + y'\vec{y}$ | $\vec{p} = p_x\vec{x} + p_y\vec{y} \to \vec{p}' = p'_x\vec{x} + p'_y\vec{y}$

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} \quad \Bigg| \quad \begin{pmatrix} p_x' \\ p_y' \end{pmatrix} = \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix}\begin{pmatrix} p_x \\ p_y \end{pmatrix}$$

Q.M. State : $|\psi\rangle \to |\psi'\rangle = \hat{R}(\varphi,\vec{z})|\psi\rangle$

- require that expectation values are rotated similarly:

$\langle x\rangle' \equiv \langle x\rangle_{\psi'}$ etc $= \langle\psi'|\hat{x}|\psi'\rangle$

$$\begin{pmatrix} \langle x\rangle' \\ \langle y\rangle' \end{pmatrix} = \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix}\begin{pmatrix} \langle x\rangle \\ \langle y\rangle \end{pmatrix}$$

$\langle x\rangle \equiv \langle x\rangle_\psi$ etc. $= \langle\psi|\hat{x}|\psi\rangle$

$$\begin{pmatrix} \langle p_x\rangle' \\ \langle p_y\rangle' \end{pmatrix} = \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix}\begin{pmatrix} \langle p_x\rangle \\ \langle p_y\rangle \end{pmatrix}$$

ORBITAL ANGULAR MOMENTUM $\vec{L} = \vec{R}\times\vec{P}$

Let $\hat{R}(\varphi\vec{z})|\vec{r}\rangle = \hat{R}(\varphi\vec{z})|x,y\rangle \overset{!}{=} |x\cos\varphi - y\sin\varphi,\ x\sin\varphi + y\cos\varphi\rangle$

$\equiv |x', y'\rangle = |\vec{r}'\rangle$

Construct $\hat{R}(\varphi\vec{z})$:

- infinitesimal rotation : $\boxed{\hat{R}(d\varphi,\vec{z}) = \hat{1} - i\frac{d\varphi}{\hbar}\hat{L}_z}$ $\boxed{\hat{L}_z = ?}$ generator of the infinit. rotations

HW

HW: $\hat{R}|\vec{r}\rangle = \hat{R}|x,y\rangle = |x - y\,d\varphi,\ x + y\,d\varphi\rangle$ to $O(1)$ in $d\varphi$

$\Rightarrow \langle x,y|\hat{R}(d\varphi,\vec{z})|\psi\rangle \overset{!}{=} \psi(x + y\,d\varphi,\ y - x\,d\varphi)$

$\Rightarrow \langle x,y|\hat{1} - \frac{i\,d\varphi}{\hbar}\hat{L}_z|\psi\rangle = \underbrace{\langle x,y|\psi\rangle}_{\psi(x,y)} - \frac{i\,d\varphi}{\hbar}\langle x,y|\hat{L}_z|\psi\rangle \overset{!}{=}{}^{O(1)}$

$\simeq \underbrace{\psi(x,y)} + \frac{\partial\psi}{\partial x}(y\,d\varphi) - \frac{\partial\psi}{\partial y}(x\,d\varphi) \to \langle x,y|\hat{L}_z|\psi\rangle \simeq \left[\frac{\partial\psi}{\partial x}(y\,d\varphi) - \frac{\partial\psi}{\partial y}(x\,d\varphi)\right]\frac{i\hbar}{d\varphi}$

$= x\left(-i\hbar\frac{\partial}{\partial y}\right) - y\left(-i\hbar\frac{\partial}{\partial x}\right)\psi(x,y)$

i.e. $\boxed{\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x}$ $= \left(\vec{\hat{r}} \times \vec{\hat{p}}\right)_x$ ✓

(in position representation)

Commutators $[\hat{x}, \hat{L}_z] = -i\hbar \hat{y} \Rightarrow [\hat{x}_i, \hat{L}_j] = -i\hbar \varepsilon_{ijk} x_k$

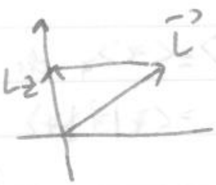
The E-value Problem of $\hat{L}$

$$\hat{L}^2 = \vec{\hat{L}} \cdot \vec{\hat{L}} = \sum_{i=1}^{3} \hat{L}_i^2$$

$[\hat{L}_z, \hat{L}^2] = 0 \rightarrow [\hat{L}_i, \hat{L}^2] = 0$, $i = 1,2,3$ $\Rightarrow$ simult. eigenkets: $|\lambda m\rangle$

$$\begin{cases} \hat{L}_z |\lambda m\rangle = m\hbar |\lambda m\rangle \\ \hat{L}^2 |\lambda m\rangle = \lambda \hbar^2 |\lambda m\rangle \end{cases}$$

- $\lambda \geq 0$ $\quad (\langle \lambda m | \hat{L}^2 | \lambda m\rangle \geq 0)$
- $\lambda \geq m^2$ (projection $|L_z| \leq L$)



~~$m_{max} \equiv \ell \Rightarrow \hat{L}_+ |\lambda \ell\rangle \stackrel{!}{=} 0$~~

Define Raising lowering ops. $\hat{L}_\pm \equiv \hat{L}_x \pm i \hat{L}_y$, $\quad \hat{L}_\pm \neq \hat{L}_\pm^\dagger$

Utility: $[\hat{L}_z, \hat{L}_\pm] = \pm \hbar \hat{L}_\pm$

$$\begin{aligned} \hat{L}_z \hat{L}_+ |\lambda m\rangle &\stackrel{!}{=} (L_+ L_z + \hbar \hat{L}_+) |\lambda m\rangle \\ &= L_+ L_z |\lambda m\rangle + \hbar \hat{L}_+ |\lambda m\rangle \\ &= (m+1)\hbar \left(\hat{L}_+ |\lambda m\rangle\right) \end{aligned}$$

$\Rightarrow$ $\boxed{\hat{L}_+ |\lambda m\rangle \text{ is an e-state of } \hat{L}_z \text{ with e-value } \text{"}(m+1)\hbar\text{"}}$

$$\hat{L}_z \hat{L}_- |\lambda m\rangle \stackrel{!}{=} (m-1)\hbar\, \hat{L}_- |\lambda m\rangle$$

$\Rightarrow$ $\boxed{\hat{L}_- |\lambda m\rangle \text{ is an e-state of } \hat{L}_z \text{ with e-value } (m-1)\hbar}$

$[\hat{L}^2, \hat{L}_\pm] = 0 \rightarrow$ simult e-states: $\hat{L}_\pm |\lambda m\rangle$

Let $m_{max} \equiv l \Rightarrow \boxed{\hat{L}_+ |\lambda l\rangle \overset{!}{=} 0}$ (top rung of ladder)

$$\hat{L}_- \hat{L}_+ |\lambda l\rangle \overset{!}{=} (\hat{L}_x - i\hat{L}_y)(\hat{L}_x + i\hat{L}_y)|\lambda l\rangle$$

$$= (L_x^2 + L_y^2 + i[L_x, L_y])|\lambda l\rangle$$

$$= (\hat{L}_x^2 + \hat{L}_y^2 - \hbar \hat{L}_z)|\lambda l\rangle$$

$$= (L^2 - \hat{L}_z - \hbar \hat{L}_z)|\lambda l\rangle$$

$$\left.\begin{aligned} &= (\lambda - l^2 - l)\hbar^2 |\lambda l\rangle \\ &\overset{2}{=} 0 \end{aligned}\right\} \Rightarrow$$

$$\Rightarrow \boxed{\lambda = l(l+1) \equiv m_{max}(m_{max}+1)} \quad (1)$$

Let $m_{min} \equiv l' \Rightarrow \boxed{\hat{L}_- |\lambda l'\rangle \overset{!}{=} 0}$ (bottom rung)

$$\left.\begin{aligned} \hat{L}_+ \hat{L}_- |\lambda l'\rangle &\overset{1}{=} \dots (\lambda - l'^2 + l')\hbar^2 |\lambda l'\rangle \\ &\overset{2}{=} 0 \end{aligned}\right\} \Rightarrow$$

$$\Rightarrow \boxed{\lambda = l'^2 - l' = l'(l'-1) \equiv m_{min}(m_{min}-1)} \quad (2)$$

$$(1), (2) \Rightarrow l(l+1) = l'(l'-1) = \lambda \Rightarrow \begin{cases} l' = -l \\ l' = l+1 \text{ not since } l' < l \end{cases}$$

$$\Rightarrow \boxed{l' = -l \text{ or } m_{min} \overset{!}{=} -\max}$$

Let $m_{max} = n\, m_{min}$ (or $l = n l'$)

$m_{max} \equiv \ell$

$\downarrow$

$\downarrow$

$\downarrow$

$\downarrow$

$m_{min} \equiv \ell' = -\ell$

Start at the top and lower:

$\underline{2\ell \; (=2m_{max}) \text{ lowering steps}}$ $= \text{integer}$ $(= \ell - \ell' = \ell - (-\ell) = 2\ell)$

$\Rightarrow$ $\boxed{\text{allowed values for } \ell : 0, 1/2, 1, 3/2, 2, \ldots}$

(no exclusion rules yet)

$\Rightarrow$ for each ℓ: $m = \underbrace{\ell, \ell-1, \ldots 0, -1, \ldots -\ell}_{2\ell+1 \text{ states}}$

$$\Rightarrow \quad |\lambda m\rangle \equiv |\ell(\ell+1), m\rangle = |\ell m\rangle$$

$$\Rightarrow \quad \boxed{\begin{aligned} \hat{L}^2 |\ell m\rangle &= \ell(\ell+1)\hbar^2 |\ell m\rangle \\ \hat{L}_z |\ell m\rangle &= m\hbar |\ell m\rangle \end{aligned}} \quad m = \overline{-\ell, \ell}$$

Ex: $\ell = 0 \Rightarrow |00\rangle$

$\ell = 1/2 \Rightarrow |1/2, 1/2\rangle, |1/2, -1/2\rangle$

$\ell = 1 \Rightarrow |1,1\rangle, |1,-1\rangle, |1,0\rangle$

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The Uncertainty Relation

$$[\hat{L}_i, \hat{L}^2] = 0 \ , \ [\hat{L}_i, \hat{L}_j] = \varepsilon_{ijk} \hat{L}_k \, i\hbar$$

$\Rightarrow$ no simult. e-states for L^2, L_x, L_y, L_z

$\Rightarrow$ if $\langle L^2 \rangle$, $\langle L_z \rangle$ are known
then there is uncertainty w.r.t $\langle L_x \rangle, \langle L_y \rangle$:

Property: If $[\hat{A}, \hat{B}] = i\hat{C} \Rightarrow (\Delta A)(\Delta B) \geq \frac{1}{2} |\langle C \rangle|$

where dispersions are given by $\Delta A = \sqrt{\langle (A - \langle A \rangle)^2 \rangle} \dots$

$$\Rightarrow \boxed{(\Delta L_x)(\Delta L_y) \geq \frac{\hbar}{2} |\langle L_z \rangle|}$$

$\Rightarrow$ "wave-function collapse" concept

$\boxed{\text{MR of } \hat{L}_\pm}$:

$$\hat{L}_\pm |lm\rangle = c_+ \hbar |l, m\pm1\rangle \ ; \ \hat{L}_\pm^\dagger = \hat{L}_\mp$$

$$\langle lm | \hat{L}_- \hat{L}_+ | lm \rangle \overset{1}{=} \langle lm | \hat{L}_+^\dagger \hat{L}_+ | lm \rangle = |c_+|^2 \hbar^2 \langle l m{+}1 | l m{+}1 \rangle$$

$$\overset{2}{=} \langle lm | \hat{L}^2 - \hat{L}_z^2 - \hbar \hat{L}_z | lm \rangle$$

$$= (l(l+1) - m(m+1)) \hbar^2 \langle lm | lm \rangle$$

$\Rightarrow$

$\langle l m{+}1 | l m{+}1 \rangle = \langle lm | lm \rangle$ $\Rightarrow$

$$\hat{L}_+ |lm\rangle = \sqrt{l(l+1) - m(m+1)} \, \hbar \, |l, m+1\rangle$$

$$\hat{L}_- |lm\rangle = \sqrt{l(l+1) - m(m-1)} \, \hbar \, |l, m-1\rangle$$

$$\langle lm' | \hat{L}_\pm | lm \rangle = \sqrt{l(l+1) - m(m\pm1)} \, \hbar \langle lm' | l m{\pm}1 \rangle$$

$$= \sqrt{} \, \hbar \, \delta_{m' m\pm1}$$

Application — Spin-1/2 E-value Problem Revisited

$$\hat{S}^2 |sm\rangle = s(s+1)\hbar^2 |sm\rangle$$
$$\hat{S}_z |sm\rangle = m\hbar |sm\rangle \qquad s = 1/2 \Rightarrow m = \pm 1/2$$

Notation $|\pm\rangle \equiv |\pm z\rangle$

$$\hat{S}_z \doteq \begin{pmatrix} \langle + | S_z | + \rangle & \langle + | S_z | - \rangle \\ \langle - | S_z | + \rangle & \langle - | S_z | - \rangle \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar}{2}\hat{\sigma}_z$$

$$\hat{S}_x = \frac{\hat{S}_+ + \hat{S}_-}{2}, \quad \hat{S}_y = \frac{\hat{S}_+ - \hat{S}_-}{2i} \qquad \text{use M.R of } \hat{S}_\pm$$

see prev. page

$$\hat{S}_+ \doteq \begin{pmatrix} \langle + | \hat{S}_+ | + \rangle & \langle + | \hat{S}_+ | - \rangle \\ \langle - | \hat{S}_+ | + \rangle & \langle - | \hat{S}_+ | - \rangle \end{pmatrix} = \dots = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$\hat{S}_- \doteq \dots = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$\Rightarrow \hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar}{2}\hat{\sigma}_x$$

$$\hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{\hbar}{2}\hat{\sigma}_y$$

$$\hat{\vec{S}} = \frac{\hbar}{2}\hat{\vec{\sigma}} = \frac{\hbar}{2}\left(\hat{\sigma}_x \vec{x} + \hat{\sigma}_y \vec{y} + \hat{\sigma}_z \vec{z}\right)$$

Ensembles and Expectation Values

P4 defines the probability of obtaining e-value a_n of $\hat{A}$ as the outcome of measurements of observable A on a system.

↳ The statistical (probabilistic) interpretation relies on multiple measurements on an ensemble of systems identically prepared in state $|\psi\rangle$ → a "pure ensemble"

* Expectation value of $\hat{A}$ w.r.t. state $|\psi\rangle$:

$$\langle A\rangle \left(\text{or } \langle A\rangle_\psi\right) \equiv \langle\psi|\hat{A}|\psi\rangle$$

Meaning of $\langle A\rangle$:

$$\langle A\rangle = \langle\psi|\hat{1}\,\hat{A}\,\hat{1}|\psi\rangle = \langle\psi|\sum_i |a_i\rangle\langle a_i|\,\hat{A}\sum_j |a_j\rangle\langle a_j|\psi\rangle$$

$$= \sum_{ij}\langle\psi|a_i\rangle\langle a_i|\underbrace{\hat{A}|a_j\rangle}\langle a_j|\psi\rangle$$

$$= \sum_{ij}\langle\psi|a_i\rangle\langle a_i|a_j|a_j\rangle\langle a_j|\psi\rangle$$

$$= \sum_{ij}\langle\psi|a_i\rangle\, a_j\, \underbrace{\langle a_i|a_j\rangle}_{\delta_{ij}}\langle a_j|\psi\rangle$$

$$= \sum_i a_i\,\langle\psi|a_i\rangle\langle a_i|\psi\rangle =$$

$$= \sum_i a_i\,|\langle a_i|\psi\rangle|^2$$

(weighted sum of probabilities)

$$= \sum_i a_i\,\mathcal{P}(a_i) \quad = \underline{\text{average}} \text{ (on the ensemble)}$$

⇒ The expectation value of an observable is the statistical average of the possible outcomes of measuring the observable on a pure ensemble (identically prepared systems).

The Uncertainty Relation:

* Define operator $\Delta\hat{A} \equiv \hat{A} - \langle A \rangle$

* Dispersion of A: $\langle (\Delta A)^2 \rangle \equiv \langle \psi | (\Delta\hat{A})^2 | \psi \rangle$ in some state $|\psi\rangle$

$$\langle (\Delta A)^2 \rangle = \langle (A - \langle A \rangle)^2 \rangle = \langle A^2 \rangle - \langle A \rangle^2$$

$$\boxed{\langle (\Delta A)^2 \rangle \langle (\Delta B)^2 \rangle \geq \frac{1}{4} \left| \langle [\hat{A}, \hat{B}] \rangle \right|^2} \quad \text{UR}$$ (no proof → do at home)

Position, Momentum, and Translation Operators

Position: $\hat{X}(x) = x|x\rangle$ — $\psi(x) \equiv \langle x | \psi \rangle$ wavefunction in position representation

representation

- any ket $|\psi\rangle = \int_{-\infty}^{\infty} dx\, |x\rangle\langle x | \psi \rangle \equiv \int dx\, |x\rangle \psi(x)$

- A selective measurement of the position of a particle will "collapse" the state $|\psi\rangle$ of the system to within a small range of locations around the actual position x_0:

$$|\psi\rangle = \int_{-\infty}^{\infty} dx\, |x\rangle\langle x | \psi \rangle \xrightarrow{\text{meas.}} |\psi\rangle_{\text{"meas"}} = \int_{x_0 - \delta/2}^{x_0 + \delta/2} dx\, |x\rangle\langle x | \psi \rangle$$

Dirac-sense normalization: $\langle x | x' \rangle = \delta(x - x')$; $\int_{-\infty}^{\infty} dx \langle x | x' \rangle^* = 1$ $\qquad$ δ = very small

* Probability of localization at $x = x_0$:

$$d\mathcal{P}(x_0) = |\langle x_0 | \psi \rangle|^2 dx_0 = |\psi(x_0)|^2 dx_0 \quad (\text{with } \delta \equiv dx_0)$$

$\psi(x_0) = \langle x_0 | \psi \rangle$ - probability amplitude

* Normalization (assuming $\langle \psi | \psi \rangle = 1$): $\leftrightarrow \int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$

$$\int_{-\infty}^{\infty} d\mathcal{P}(x) = \int_{-\infty}^{\infty} |\langle x_0 | \psi \rangle|^2 dx_0 = 1$$

$[\hat{X}_i, \hat{X}_j] = 0$

Position operators 3D: $|\vec{r}\rangle \equiv |x, y, z\rangle$; $\hat{X}|\vec{r}\rangle = x|\vec{r}\rangle$; $\hat{Y}|\vec{r}\rangle = y|\vec{r}\rangle$; $\hat{Z}|\vec{r}\rangle = z|\vec{r}\rangle$; $|\psi\rangle = \int d^3r\, |\vec{r}\rangle\langle \vec{r} | \psi \rangle$

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Expectation values: $\langle x\rangle = \langle\psi|\hat{x}|\psi\rangle = \langle\psi|\hat{x}\int dx\,|x\rangle\langle x|\psi\rangle$ 35

$= \int dx\,x\langle\psi|x\rangle\langle x|\psi\rangle = \int dx\,|\psi(x)|^2 x$

Spatial Translation Operator

$\hat{T}(d\vec{r})|\vec{r}\rangle = |\vec{r}+d\vec{r}\rangle$ infinitesimal translation

$\hat{T}(d\vec{r})|\psi\rangle = \hat{T}(d\vec{r})\int_{\text{all space}} d\vec{r}\,|\vec{r}\rangle\langle\vec{r}|\psi\rangle = \int d\vec{r}\,\underline{\hat{T}|\vec{r}\rangle}\langle\vec{r}|\psi\rangle$

$= \int d\vec{r}\,\underline{|\vec{r}+d\vec{r}\rangle}\langle\vec{r}|\psi\rangle \underset{\vec{r}+d\vec{r}=\vec{r}'}{=} \int d\vec{r}\,|\vec{r}\rangle\langle\overline{\vec{r}-d\vec{r}}|\psi\rangle$

"backwards"

$\hat{T}(-d\vec{r})|\vec{r}\rangle = |\vec{r}-d\vec{r}\rangle \Leftrightarrow \cancel{[\hat{T}(-d\vec{r})]^\dagger}$

$\langle\vec{r}|[\hat{T}(-d\vec{r})]^\dagger = \langle\vec{r}-d\vec{r}|$

$\Rightarrow$

$\Rightarrow \hat{T}(d\vec{r})|\psi\rangle = \int d\vec{r}\,|\vec{r}\rangle\overline{\langle\vec{r}|[\hat{T}(-d\vec{r})]^\dagger}|\psi\rangle$

$\Rightarrow \hat{T}(d\vec{r})\hat{T}(+d\vec{r})|\psi\rangle = \cancel{\int d\vec{r}\,|\vec{r}\rangle\langle\vec{r}|[\hat{T}(-d\vec{r})]^\dagger|\psi\rangle}$

$= \hat{T}(-d\vec{r})\int d\vec{r}\,|\vec{r}\rangle\langle\vec{r}|[\hat{T}(-d\vec{r})]^\dagger|\psi\rangle = \int d\vec{r}\,\underline{\hat{T}(-d\vec{r})|\vec{r}\rangle}\langle\vec{r}|[\hat{T}(-d\vec{r})]^\dagger|\psi\rangle$

$= \int d\vec{r}\,|\vec{r}-d\vec{r}\rangle\underbrace{\langle\vec{r}|[\hat{T}(-d\vec{r})]^\dagger}_{\langle\vec{r}-d\vec{r}|}|\psi\rangle = \int d\vec{r}\,|\vec{r}-d\vec{r}\rangle\langle\vec{r}-d\vec{r}|\psi\rangle$

$= |\psi\rangle$

$\Rightarrow \hat{T}(-d\vec{r})\hat{T}(d\vec{r}) = \hat{T}(d\vec{r})\hat{T}(-d\vec{r}) = \mathbb{1}$

$\Rightarrow \hat{T}(-d\vec{r}) = [\hat{T}(d\vec{r})]^{-1} \overset{*}{=} [\hat{T}(d\vec{r})]^\dagger$ ⊛ below

i.e. $\boxed{\hat{T}(d\vec{r})[\hat{T}(d\vec{r})]^\dagger = [\hat{T}(d\vec{r})]^\dagger\hat{T}(d\vec{r}) = \mathbb{1}}$

to conserve probability

($\hat{T}(d\vec{r})$ is unitary to conserve probability)

⊛ $\langle r|\hat{T}^\dagger\hat{T}|r\rangle = \langle r|\hat{T}^\dagger|r+dr\rangle = \langle r+dr|\hat{T}|r\rangle^* = \langle r+dr|r+dr\rangle \overset{\text{normalization}}{=} 1 = \langle r|r\rangle \Rightarrow \boxed{\hat{T}^\dagger\hat{T} = \mathbb{1} (= \hat{T}\hat{T}^\dagger)}$

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Momentum as the generator of translations

1D: $\hat{T}_1(dx) = \hat{1} - \frac{i}{\hbar}\hat{p}_x dx$, $\hat{p}_x$ - generator of infinitesimal translations

$\hat{T}_1(dx)|x\rangle = |x+dx\rangle$

Effect on wavefunction: $\psi_{translated}(x) = \langle x|\underbrace{\psi_{transl}}\rangle = \langle x|\underbrace{\hat{T}_1(dx)|\psi_0}\rangle$

$= \cancel{\langle x|\int d\xi|\xi\rangle\langle\xi|} = \langle x|\hat{T}_1(dx)\int_{-\infty}^{\infty} d\xi|\xi\rangle\langle\xi|\psi_0\rangle$

$= \int_{-\infty}^{\infty} d\xi\,\langle x|\underbrace{\hat{T}_1(dx)|\xi}\rangle\langle\xi|\psi_0\rangle$

$= \int d\xi\,\langle x|\xi+dx\rangle\langle\xi|\psi_0\rangle = \int d\xi\,\delta(x-(\xi+dx))\,\psi_0(\xi)$

$= \int d\xi\,\delta(\xi-(x-dx))\,\psi_0(\xi) =$

$= \psi_0(x-dx)$ → propagation in the "+dx" direction

Simpler

$\hat{T}_\delta|x\rangle = |x+\delta\rangle$

$\hat{T}_\delta^\dagger|x\rangle = |x-\delta\rangle$

$\Rightarrow \langle x|\hat{T}_\delta = \langle x-\delta|$

$\langle x|\hat{T}_\delta|\psi\rangle = \langle x-\delta|\psi\rangle = \psi(x-\delta)$

Finite translation: $\hat{T}(a) = \lim_{N\to\infty}\left[\hat{1} - \frac{i}{\hbar}\hat{p}_x\left(\frac{a}{N}\right)\right]^N = e^{-i(\hat{p}_x a)/\hbar}$

$\hat{p}_x^\dagger = \hat{p}_x$ Hermitian operator (use unitarity of $\hat{T}$ to prove)

corresponds to observable "p_x".

$[\hat{x}, \hat{p}_x] = i\hbar$

$[\hat{y}, \hat{p}_y] = i\hbar$

$[\hat{z}, \hat{p}_z] = i\hbar$

~~Canonical commutation relations~~

$\cancel{[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}}$

$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$ $\quad$ $[x_i, x_j] = 0$

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The Momentum Operator in Position Representation

* Basis : $\{|x\rangle\}_{x\in(-\infty,\infty)}$: $\hat{X}|x\rangle = x|x\rangle$, $x\in(-\infty,\infty)$

* Infinitesimal translation :

$$\hat{T}_1(\delta x)|\psi\rangle = \hat{T}_1(\delta x)\,\hat{1}\,|\psi\rangle = \hat{T}_1(\delta x)\int_{-\infty}^{\infty} dx\,|x\rangle\langle x|\psi\rangle =$$

$$= \int_{-\infty}^{\infty} dx\;\hat{T}_1(\delta x)|x\rangle\langle x|\psi\rangle = \int_{-\infty}^{\infty} dx\;|x+\delta x\rangle\,\psi(x) \overset{x'=x+\delta x}{=} \int dx'\,|x'\rangle\,\psi(x'-\delta x)$$

Taylor-expand : $\psi(x'-\delta x) \simeq \psi(x') - \partial_{x'}\psi(x')\,\delta x + 1/2\,\partial^2_{x'}\psi(x')\,\delta x^2 \ldots$

$$\Rightarrow \hat{T}_1(\delta x)|\psi\rangle \underset{\mathcal{O}(1)}{\simeq} \int dx'\,|x'\rangle\left(\psi(x') - \partial_{x'}\psi(x')\,\delta x\right) =$$

$$= \int dx'\,|x'\rangle\langle x'|\psi\rangle - \int dx'\,|x'\rangle\,\partial_{x'}\langle x'|\psi\rangle\,\delta x$$

$$= \hat{1}|\psi\rangle - \int dx'\,|x'\rangle\,\partial_{x'}\langle x'|\psi\rangle\,\delta x$$

in "operatorial" form

$$\overset{1}{=} \left(\hat{1} - \int dx'\,|x'\rangle\,\delta x\,\partial_{x'}\langle x'|\right)|\psi\rangle$$

$$\overset{2}{=} \left(\hat{1} - \frac{i}{\hbar}\hat{p}_x\,\delta x\right)|\psi\rangle$$

$\Rightarrow$

$$\Rightarrow \int_{-\infty}^{\infty} dx'\,|x'\rangle\,\partial_{x'}\langle x'| = \frac{i}{\hbar}\hat{p}_x \qquad \Big|\,\frac{\hbar}{i}\,\Big|\,|\psi\rangle$$

$$\Rightarrow \boxed{\begin{aligned}\hat{p}_x|\psi\rangle &= -i\hbar\int_{-\infty}^{\infty} dx'\,|x'\rangle\,\partial_{x'}\langle x'|\psi\rangle \\ &= -i\hbar\int_{-\infty}^{\infty} dx'\,|x'\rangle\,\partial_{x'}\psi(x')\end{aligned}}$$ (1)

Action of $\hat{p}_x$ operator in the position representation

$$\Rightarrow \hat{p}_x \doteq \int_{-\infty}^{\infty} dx\,|x\rangle\left(-i\hbar\partial_x\right)\langle x|$$

Analogous to spectral decomp. differential op.

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In position space:

Hit with $\langle x|$:

$$\boxed{\begin{aligned}\langle \underline{x}|\hat{p}_x|\psi\rangle &= -i\hbar\int_{-\infty}^{\infty} dx' \langle \underline{x}|x'\rangle \partial_{x'}\psi(x') \\ &= -i\hbar\int dx'\, \delta(x'-x)\,\partial_{x'}\psi(x') \\ &= -i\hbar\,\partial_x \psi(x) = -i\hbar\,\partial_x \langle x|\psi\rangle\end{aligned}}$$ ②

Exp. value of $\hat{p}_x$ in state $|\psi\rangle$:

$$\langle p_x\rangle_\psi = \langle \underline{\psi}|\hat{p}_x|\psi\rangle \overset{①}{=} \cancel{+i\hbar\int dx'\langle\psi|x'\rangle\partial_{x'}}$$

$$= \langle\psi|\left(-i\hbar\int dx'|x'\rangle\partial_{x'}\langle x'|\psi\rangle\right) =$$

$$= -i\hbar\int dx' \langle\psi|x'\rangle\partial_{x'}\langle x'|\psi\rangle$$

$$= -i\hbar\int dx' \psi^*(x')\,\partial_{x'}\psi(x')$$

$$\equiv \langle\psi|\left(\widehat{-i\hbar\partial_x}\right)|\psi\rangle \equiv \left\langle -i\hbar\partial_x\right\rangle_\psi$$ ③

① - ③ $\Rightarrow$ $\boxed{\hat{p}_x \doteq -i\hbar\,\partial_x}$ in position representation (basis)

$$\boxed{\int_{-\infty}^{\infty} dx\, e^{i(k-k')x} = 2\pi\hbar\,\delta(k-k')}$$

Normalization for $\phi_p(x) \equiv \langle x|p\rangle$:

$$\delta(p-p') \overset{!}{=} \langle p'|p\rangle = \int_{-\infty}^{\infty} dx\, \phi^*_{p'}(x)\,\phi_p(x)$$

$$\frac{1}{2\pi\hbar}\int_{-\infty} dx\, e^{i(p-p')x/\hbar} = |N|^2 \int_{-\infty}^{\infty} dx\, e^{i(p-p')x/\hbar}$$

$$\to N = \frac{1}{\sqrt{2\pi\hbar}}$$

Momentum Representation

1D:

* Basis $\{|p\rangle\}_{p\in(-\infty,\infty)}$: $\hat{p}_x|p\rangle = p|p\rangle$
* Any state : $|\psi\rangle = \int_{-\infty}^{\infty} dp\, |p\rangle\langle p|\psi\rangle$

* Dirac-sense orthonormality : $\langle p'|p\rangle = \delta(p-p')$

$$\int_{-\infty}^{\infty} dp' \langle p'|p\rangle = \int_{-\infty}^{\infty} dp'\,\delta(p-p') = 1$$

* Any normalized state :

$$1 = \langle\psi|\psi\rangle = \langle\psi|\int_{-\infty}^{\infty} dp\,|p\rangle\langle p|\psi\rangle = \int dp\,\langle\psi|p\rangle\langle p|\psi\rangle$$

$$= \int_{-\infty}^{\infty} dp\,\psi^*(p)\,\psi(p) = \int_{-\infty}^{\infty} dp\,|\psi(p)|^2$$

$$d\mathcal{P}_{(p,\,p+dp)} = |\langle p|\psi\rangle|^2 dp = |\psi(p)|^2 dp$$

* Momentum-space wavefunction : $\underline{\psi(p) \equiv \langle p|\psi\rangle}$

* Wavefunction of momentum state in position representation:

$\langle p'|$

$$|p\rangle = \hat{\mathbb{1}}|p\rangle = \int_{-\infty}^{\infty} dx\,|x\rangle\langle x|p\rangle$$

$$\langle p'|p\rangle = \langle p'|\int_{-\infty}^{\infty} dx\,|x\rangle\langle x|p\rangle = \int_{-\infty}^{\infty} dx\,\overbrace{\langle p'|x\rangle}^{\phi^*_{p'}(x)}\overbrace{\langle x|p\rangle}^{\phi_p(x)}$$

$$\equiv \int dx\,\phi^*_{p'}(x)\,\phi_p(x) \overset{(*)}{=} \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dx\, e^{i(p-p')\frac{x}{\hbar}}$$

$$= \delta(p-p') \quad \text{as required}$$

(*) $\langle x|\hat{p}_x|p\rangle \overset{1}{=} p\langle x|p\rangle \equiv p\,\phi_p(x)$

$\overset{2}{=} -i\hbar\,\partial_x\langle x|p\rangle \equiv -i\hbar\,\partial_x\phi_p(x)$ $\Big\} \Rightarrow -i\hbar\,\partial_x\phi_p(x) = p\,\phi_p(x)$

$$\boxed{\phi_p(x) = \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}}$$

Dirac-sense Norm. Const

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or $\boxed{\phi_p(x) \equiv \langle x|p\rangle = \dfrac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}}$ Momentum-state wavefunction in position representation, normalized.

De Broglie: $\underset{\text{"pcl"}}{p} = \hbar k = \underset{\text{"WAVE"}}{h/\lambda}$ "pcl" $\longleftrightarrow$ "WAVE"

Significance of $\langle x|p\rangle$:

$\langle x|p\rangle$ "switches" between position- and momentum-representations

$$\psi(p) \equiv \langle p|\overset{1\!\!1_x}{}\psi\rangle = \int dx \underbrace{\langle p|x\rangle}_{\phi_p^*(x)}\underbrace{\langle x|\psi\rangle}_{\psi(x)} = \int dx \frac{e^{-ipx/\hbar}}{\sqrt{2\pi\hbar}}\psi(x)$$

$$= \left(1/\sqrt{2\pi\hbar}\right)\int dx\, \psi(x)\, e^{-ipx/\hbar} = FT\{\psi(x)\}$$

$$\psi(x) \equiv \langle x|\overset{1\!\!1_p}{}\psi\rangle = \int dp \underbrace{\langle x|p\rangle}_{\phi_p(x)}\underbrace{\langle p|\psi\rangle}_{\psi(p)} = \int dp \frac{e^{+ipx/\hbar}}{\sqrt{2\pi\hbar}}\psi(p)$$

$$= \left(1/\sqrt{2\pi\hbar}\right)\int dp\, \psi(p)\, e^{+ipx/\hbar} = FT^{-1}\{\psi(p)\}$$

$\psi(p)$ and $\psi(x)$ are a Fourier pair

↳ QM "knows" about FT!

~~Application~~ Heisenberg Uncertainty Principle

Since $[\hat{x}, \hat{p}_x] = i\hbar \Rightarrow \dots \Rightarrow (\Delta p)(\Delta x) \geq \hbar/2$

Application Gaussian Wave Packets (read)

Physical significance of $|\phi_p|$:

$dP_{x,x+\delta x} = dx|\phi_p(x)|^2 = \dfrac{dx}{2\pi\hbar}$. Also $\Delta p = 0$ $\left(\langle p\rangle_p^2 = \langle p^2\rangle_p = p^2\right)$

$\Rightarrow \Delta x = \infty$

Free particle → seek $\langle\psi|\psi\rangle = 1$, superposition → Wave Packet

$$\psi(x)_G = \langle x|\psi\rangle = \frac{e^{-x^2/2a^2}}{a\pi^{1/4}}, \quad \left(1 = \int dx|\psi(x)|^2\right)$$

$$\Rightarrow (\Delta x)_G = \frac{a}{\sqrt{2}},\ (\Delta p)_G = \frac{\hbar}{a\sqrt{2}} \Big\} \Rightarrow \boxed{(\Delta p)(\Delta x) \underset{\uparrow}{=} \hbar/2}$$

Ch. 4 Time Evolution (Quantum Dynamics)

- Time-evolution operator: $\hat{\mathcal{U}}(t)$ s.t. $\boxed{\hat{\mathcal{U}}(t)|\psi_0\rangle = |\psi(t)\rangle}$.

- Cons. of probability $\Leftrightarrow$ normalization: $\left(\hat{U}(t-t_0) \text{ with } t_0=0\right)$

conservation of norm $\Leftrightarrow$ unitarity

$$\left.\begin{aligned} 1 &\overset{!}{=} \langle\psi(t)|\psi(t)\rangle \overset{!}{=} \langle\psi_0|\psi_0\rangle \\ \Rightarrow\ &\langle\psi_0|\hat{\mathcal{U}}^+\hat{\mathcal{U}}|\psi_0\rangle \overset{!}{=} \langle\psi_0|\psi_0\rangle \end{aligned}\right\} \Rightarrow \boxed{\hat{\mathcal{U}}^+(t)\,\hat{\mathcal{U}}(t) \overset{!}{=} \hat{\mathbb{1}}}$$

unitary op.

- Generator of time translations: $\hat{H}$ s.t.

Infinitesimal

$$\hat{U}(dt) = \hat{\mathbb{1}} - \tfrac{i}{\hbar}\hat{H}\,dt \quad \to \text{infinitesimal time shift}$$

$$\frac{d\hat{\mathcal{U}}}{dt} \overset{!}{=} \frac{\hat{U}(t+dt)-\hat{\mathcal{U}}(t)}{dt} = \frac{\hat{U}(dt)\hat{U}(t) - \hat{\mathcal{U}}(t)}{dt}$$

or $\hat{U}(t)\hat{U}(\delta t)$ and use $[\hat{H},\hat{U}]=0$

$$= \frac{\left(\hat{U}(dt)-\hat{\mathbb{1}}\right)\hat{U}(t)}{dt} \overset{2}{=} -(i/\hbar)\,\hat{H}\,\hat{U}(t)$$

$U(t_1,t_2) =$ choose $= \begin{cases} U(t_2)U(t_1), & \tau>0 \\ U(t_1)U(t_2), & \tau<0 \end{cases}$

$$\Rightarrow \boxed{i\hbar\,\frac{d\hat{\mathcal{U}}(t)}{dt} = \hat{H}\,\hat{\mathcal{U}}(t)}\ \Big|\,|\psi_0\rangle \quad (\text{Apply to } |\psi_0\rangle:)$$

$$i\hbar\,{}^{d}\!/\!{}_{dt}\ \underbrace{\hat{U}(t)|\psi_0\rangle}_{|\psi(t)\rangle} = \hat{H}\,\underbrace{\hat{\mathcal{U}}(t)|\psi_0\rangle}_{|\psi(t)\rangle}$$

$$\Rightarrow \boxed{i\hbar\,{}^{d}\!/\!{}_{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle}$$

TDSE — fully describes the evolution of a system

Finite

Finite time shift $\boxed{t = N\,dt}$, $N\to\infty$:

$$\hat{U}(t) = \lim_{N\to\infty}\left[\hat{\mathcal{U}}(dt)\right]^N = \lim_{N\to\infty}\left[\hat{\mathbb{1}} - \tfrac{i}{\hbar}\hat{H}dt\right]^N = \lim_{N\to\infty}\left[\hat{\mathbb{1}} - {}^{i}\!/\!{}_{\hbar}\,\hat{H}\,\tfrac{t}{N}\right]^N \Longrightarrow$$

$$\Rightarrow \boxed{\hat{\mathcal{U}}(t) = e^{-i\hat{H}t/\hbar}} = \boxed{\sum_{n\geq 0}^{\infty}\frac{1}{n!}\left(-i\frac{\hat{H}t}{\hbar}\right)^n}$$

$$\hat{1} \stackrel{!}{=} \hat{U}^\dagger \hat{U} = e^{i\frac{\hat{H}^\dagger - \hat{H}}{\hbar}t} \quad [\hat{H}^\dagger, \hat{H}] = 0$$

$\Rightarrow$ $\boxed{\hat{H}^\dagger \stackrel{!}{=} \hat{H} \text{ Hermitian op}}$

Hamiltonian
↳ total energy of the system

Significance of $\hat{H}$:

$$\boxed{\langle H \rangle_{(t)}} = \langle \psi(t) | \hat{H} | \psi(t) \rangle \qquad [\hat{H}, \hat{U}] = 0$$

$$= \langle \psi_0 | \hat{U}^\dagger \hat{H} \hat{U} | \psi_0 \rangle = \langle \psi_0 | \underbrace{\hat{U}^\dagger \hat{U}}_{\hat{1}} \hat{H} | \psi_0 \rangle$$

$$= \langle \psi_0 | \hat{H} | \psi_0 \rangle = \boxed{\langle H \rangle_0}$$

time invariance of exp. value of $\hat{H}$

* Eigenstates of the Hamiltonian:

$$\hat{H} | E \rangle = E | E \rangle$$ - energy eigenstates

$$e^{-i\hat{H}t/\hbar} | E \rangle = \sum_{n=0}^{\infty} \frac{1}{n!} (-i\hat{H}t/\hbar)^n | E \rangle = \dots = e^{-iEt/\hbar} | E \rangle$$

only when $e^{-i\hat{H}t/\hbar}$ acts on an energy e-state!

Appl: * Initial state $|\psi_0\rangle = |E\rangle$

$$\Rightarrow |\psi(t)\rangle = \hat{U}(t) |\psi_0\rangle = \hat{U}(t) | E \rangle$$

$$= e^{-i\hat{H}t/\hbar} | E \rangle = e^{-iEt/\hbar} | E \rangle$$

just an overall phase factor $\equiv e^{-i\varphi}$

$= |\psi_0\rangle$ state properties are preserved

* $\boxed{\text{Energy e-states } (|E\rangle) \text{ are stationary states}}$

Q: So what makes things interesting? A: $|\psi_0\rangle = \sum a_i |E_i\rangle$ superposition of stationary states

Time Dependence of Expectation Values

$$\frac{d}{dt}\langle A\rangle = \frac{d}{dt}\langle\psi(t)|\hat{A}|\psi(t)\rangle =$$

$$= \left(\frac{d}{dt}\langle\psi(t)|\right)\hat{A}|\psi(t)\rangle + \langle\psi(t)|\frac{\partial\hat{A}}{\partial t}|\psi(t)\rangle + \langle\psi(t)|\hat{A}\left(\frac{d}{dt}|\psi(t)\rangle\right)$$

TDSE
$$= \left(\frac{-1}{i\hbar}\langle\psi(t)|\hat{H}\right)\hat{A}|\psi(t)\rangle + \left\langle\frac{\partial A}{\partial t}\right\rangle + \left(\frac{1}{i\hbar}\hat{H}|\psi(t)\rangle\right)$$

$$= \frac{i}{\hbar}\left\langle[\hat{H},\hat{A}]\right\rangle + \left\langle\frac{\partial A}{\partial t}\right\rangle$$

↳ explicit time dependence

Application Precession of spin-1/2 particle in a uniform magnetic field

Interaction Hamiltonian: $\hat{H} = -\hat{\vec{\mu}}\cdot\vec{B} = -\frac{gQ}{2m(c)}\hat{\vec{S}}\cdot\vec{B}$

electron

$$= \frac{-g(-e)}{2m_e(c)}\hat{S}_z B_0 \equiv \omega_0\hat{S}_z = \frac{\hbar\omega_0}{2}\hat{\sigma}_z \qquad \text{SI}: \vec{\mu} = g\frac{Q}{2m}\vec{S}$$

for electron $g=2$

$$\hat{H}|\pm z\rangle = \omega_0\hat{S}_z|\pm z\rangle = \pm\frac{\hbar\omega_0}{2}|\pm z\rangle \equiv E_\pm|\pm z\rangle$$

$|\psi(t)\rangle =$

As time goes on: $\hat{U}(t)|\psi_0\rangle = e^{-i\hat{H}t/\hbar}|\psi_0\rangle =$

$$= e^{-i\omega_0\hat{S}_z t/\hbar}|\psi_0\rangle = e^{-i\omega_0 t\hat{\sigma}_z/2}|\psi_0\rangle$$

$$= \hat{R}(\phi,\vec{z})|\psi_0\rangle \equiv \hat{R}_z(\phi)|\psi_0\rangle$$

↳ i.e. rotation (CCW) with phase angle $\boxed{\phi = +\omega_0 t} = \phi(t)$

For electron ($Q=-e<0$):

$\vec{\mu}_e \downarrow\uparrow \vec{B}_0$ —— $E_+ = +\frac{\hbar}{2}\omega_0$ ($\vec{S}\uparrow\uparrow\vec{B}_0$)

$\vec{\mu}_e \uparrow\uparrow \vec{B}_0$ —— $E_- = -\frac{\hbar}{2}\omega_0$ ($\vec{S}\downarrow\uparrow\vec{B}_0$)

$\vec{\mu}_e = -\frac{e}{m}\vec{S}$; $\hat{H} = +\frac{e}{m}B_0\hat{S}_z$

Let initial state be $\boxed{|\psi_0\rangle = |+x\rangle}$ (e.g. prepared with an SG_x device)

At later time t: $\underline{|\psi(t)\rangle = \hat{U}(t)|\psi_0\rangle} = e^{-i\hat{H}t/\hbar}|+x\rangle = e^{-i\hat{H}t/\hbar}\left(\frac{1}{\sqrt2}|+z\rangle + \frac{1}{\sqrt2}|-z\rangle\right)$

$$= \frac{1}{\sqrt2} e^{-i\hat{H}t/\hbar}|+z\rangle + \frac{1}{\sqrt2} e^{-i\hat{H}t/\hbar}|-z\rangle$$

$$\cancel{= \frac{1}{\sqrt2} e^{-i\omega_0 t/2}} = \frac{1}{\sqrt2} e^{-i\frac{\omega_0 t}{\hbar}\hat{S}_z}|+z\rangle + \frac{1}{\sqrt2} e^{-i\frac{\omega_0 t}{\hbar}\hat{S}_z}|-z\rangle$$

$$\overset{\text{Taylor}}{=} \frac{1}{\sqrt2}\sum_{n=0}^{\infty}\frac{1}{n!}\left(-i\frac{\omega_0 t}{\hbar}\right)^n \underbrace{\hat{S}_z^n|+z\rangle}_{=\left(+\frac{\hbar}{2}\right)^n|+z\rangle} + \frac{1}{\sqrt2}\sum_{n=0}^{\infty}\frac{1}{n!}\left(-i\frac{\omega_0 t}{\hbar}\right)^n \underbrace{\hat{S}_z^n|-z\rangle}_{=\left(-\frac{\hbar}{2}\right)^n|-z\rangle}$$

$$= \ldots = \frac{1}{\sqrt2} e^{-i\frac{\omega_0 t}{2}}|+z\rangle + \frac{1}{\sqrt2} e^{+i\frac{\omega_0 t}{2}}|-z\rangle$$

$$\left(= \frac{1}{\sqrt2} e^{-iE_+t/\hbar}|+z\rangle + \frac{1}{\sqrt2} e^{-iE_-t/\hbar}|-z\rangle\right)$$

$$= \frac{1}{\sqrt2} e^{-iE_+t/\hbar}\left(|+z\rangle + e^{i(E_+-E_-)t/\hbar}|-z\rangle\right)$$

$$= \frac{1}{\sqrt2} \underset{\substack{\uparrow\\ \text{overall}\\ \text{phase factor}}}{e^{-i\omega_0 t/2}}\left(|+z\rangle + e^{i\omega_0 t}|-z\rangle\right)$$

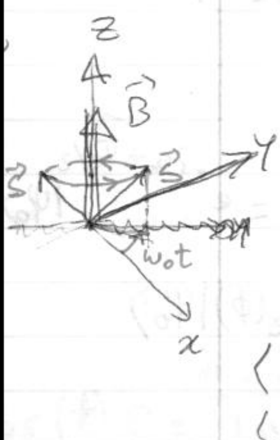
Probabilities and Expectation Values of $\hat{S}_x, \hat{S}_y, \hat{S}_z$:

$\boxed{z\text{-axis}}$ "spin-up": $P_{|+z\rangle} \equiv |\langle +z|\psi(t)\rangle|^2 = \frac{1}{2} = \text{const}$

"spin-down": $P_{|-z\rangle} \equiv |\langle -z|\psi(t)\rangle|^2 = \frac{1}{2} = \text{const}$

$\langle S_z\rangle_t = 0$

$\boxed{x\text{-}y \text{ plane}}$



$P_{|+x\rangle} = |\langle +x|\psi(t)\rangle|^2 = \ldots = \cos^2\frac{\omega_0 t}{2}$

$P_{|-x\rangle} = |\langle -x|\psi(t)\rangle|^2 = \ldots = \sin^2\frac{\omega_0 t}{2}$

$\boxed{\langle S_x\rangle_t = \langle\psi(t)|\hat{S}_x|\psi(t)\rangle = \ldots = \frac{\hbar}{2}\cos\omega_0 t}$

Precession in x-y plane

$P_{|+y\rangle} = |\langle +y|\psi(t)\rangle|^2 = \ldots = 1/2\,(1+\sin\omega_0 t)$

$P_{|-y\rangle} = |\langle -y|\psi(t)\rangle|^2 = \ldots = 1/2\,(1-\sin\omega_0 t)$

$\boxed{\langle S_y\rangle_t = \langle\psi(t)|\hat{S}_y|\psi(t)\rangle = \ldots = \frac{\hbar}{2}\sin\omega_0 t}$

$\langle S_x\rangle_t = (\hbar/2)\cos\omega_0 t \rightarrow e^{\pm i\omega_0 t}$

$\langle S_y\rangle_t = (\hbar/2)\sin\omega_0 t \rightarrow e^{\pm i(\omega_0 t + \pi/2)}$ ccw for $\omega_0 t \geq 0$

$[\hat{H},\hat{S}_z]=0$ symmetry op.

Expectation values : $\langle \dot{\ } \rangle \equiv \frac{d}{dt}\langle\ \rangle$

$$\langle \dot{S}_z \rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{S}_z]\rangle + \underbrace{\langle \partial\hat{S}_z/\partial t\rangle}_{0} = \frac{i}{\hbar}\langle[\hat{H},\hat{S}_z]\rangle =$$

$$= \frac{i}{\hbar}\langle[\omega_0\hat{S}_z,\hat{S}_z]\rangle = 0 \Rightarrow \boxed{\langle S_z\rangle = \text{constant} \checkmark \quad \text{constant of motion}} \leftrightarrow \underset{0}{[\hat{H},\hat{S}_z]}$$

$$\langle \dot{S}_x \rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{S}_x]\rangle = \frac{i}{\hbar}\langle[\omega_0\hat{S}_z,\hat{S}_x]\rangle = \frac{i}{\hbar}\omega_0\langle\underbrace{[\hat{S}_z,\hat{S}_x]}_{i\hbar\hat{S}_y}\rangle$$

$$= -\omega_0\langle \hat{S}_y\rangle \neq 0 \quad ([\hat{H},\hat{S}_x]\neq 0)$$

$$\langle \dot{S}_y \rangle = \dots = \omega_0\langle S_x\rangle \neq 0 \quad ([\hat{H},\hat{S}_y]\neq 0)$$

$$\langle \ddot{S}_x\rangle = -\omega_0\langle \dot{S}_y\rangle = -\omega_0^2\langle S_x\rangle$$

$$\langle \ddot{S}_x\rangle + \omega_0^2\langle S_x\rangle = 0 \Rightarrow \begin{cases}\langle S_x\rangle_t = A e^{-i\omega_0 t} \\ \langle S_y\rangle_t = iA e^{-i\omega_0 t} + B\end{cases}$$

Energy-Time "Uncertainty" Relation : $\boxed{(\Delta E)(\Delta t) \geq \hbar/2}$

ΔE ↑ energy uncertainty; Δt ↳ "evolutionary" time

$$\Delta E = \sqrt{\langle E^2\rangle - \langle E\rangle^2}$$

$$\langle E^2\rangle = \langle\psi(t)|\hat{H}\cdot\hat{H}|\psi(t)\rangle = \langle\psi(t)|\omega_0^2\hat{S}_z^2|\psi(t)\rangle = \omega_0^2\langle\psi(t)|\hat{S}_z^2|\psi(t)\rangle$$

$$= \frac{\omega_0^2}{2}\left[\left(\langle +z| + e^{-i\omega_0 t}\langle -z|\right)\hat{S}_z^2\left(|+z\rangle + e^{+i\omega_0 t}|-z\rangle\right)\right] =$$

$$= \frac{\omega_0^2}{2}\left[\langle +|\hat{S}_z^2|+\rangle + \langle -|\hat{S}_z^2|-\rangle\right] = \frac{\omega_0^2}{2}\left[\frac{\hbar^2}{4}+\frac{\hbar^2}{4}\right] = \frac{\omega_0^2\hbar^2}{4}$$

$$\langle E\rangle = \langle\psi(t)|\hat{H}|\psi(t)\rangle = \omega_0\langle\psi|\hat{S}_z|\psi\rangle = \frac{\omega_0}{2}\left(\frac{\hbar}{2}-\frac{\hbar}{2}\right) = 0$$

$$\Rightarrow \boxed{\Delta E = \frac{\omega_0\hbar}{2}} \Rightarrow \boxed{\Delta t \geq \frac{\cancel{\hbar}}{\cancel{2}}\Big/\left(\frac{\omega_0\cancel{\hbar}}{\cancel{2}}\right) = \frac{1}{\omega_0}} \to \text{precession period } T = \frac{2\pi}{\omega_0}$$

↳ time scale of spin dynamics.

Driving (oscillating) field $\vec{B}_1(t)$ induces a (time-dependent) magnetic dipole which generates oscillatory perturbation → absorption / emission of energy

Magnetic Resonance : Electron Spin Resonance

- for unpaired electrons

$\vec{B} = B_0 \vec{z}$ $\Rightarrow \hat{H} = -\hat{\vec{\mu}}\cdot\vec{B} = -\hat{\mu}_z B_0 = \omega_0 \hat{S}_z$, $\omega_0 = \frac{-gQ}{2mc} B_0$

$[\hat{H}, \hat{S}_z] = 0 \Rightarrow \{|\pm z\rangle\}$ are stationary states (and simultaneous e-kets) corresp. to e-values $E_\pm = \pm \hbar\omega_0/2$.

Goal: Measure precession frequency ω_0 as $\omega_0 = \frac{E_+ - E_-}{\hbar}$

Method: Induce resonant transitions between $|+z\rangle$ and $|-z\rangle$ states

typically μwave 9–10 GHz, $B_0 \sim 0.35T$ ($\approx 3500G$)

Approach: Add oscillatory B-field to B_0: $\vec{B}(t) = B_0\vec{z} + B_1 \cos\omega t\, \vec{x}$ ($B_1 \ll B_0$)

$$\Rightarrow \boxed{\hat{H} = -\hat{\vec{\mu}}\cdot\vec{B} = \omega_0 \hat{S}_z + \omega_1 \hat{S}_x \cos\omega t} \quad (1) \qquad \omega_1 = \frac{-gQ}{2m(c)} B_1$$

$\hat{H} = \hat{H}(t)$!

TDSE: $\boxed{\hat{H}|\psi(t)\rangle = i\hbar \, d/dt \, |\psi(t)\rangle}$ (2) (Work in S_z basis)

Initial cond: $|\psi_0\rangle = |+z\rangle = \begin{pmatrix}1\\0\end{pmatrix}$. Let $|\psi(t)\rangle = \begin{bmatrix}a(t)\\b(t)\end{bmatrix}$ TBD

$\hat{S}_x = \hbar/2 \begin{pmatrix}0&1\\1&0\end{pmatrix}$; $\hat{S}_z = \hbar/2 \begin{pmatrix}1&0\\0&-1\end{pmatrix}$

$$\Rightarrow (2): \boxed{\hbar/2 \begin{pmatrix}\omega_0 & \omega_1\cos\omega t\\ \omega_1\cos\omega t & -\omega_0\end{pmatrix}\begin{pmatrix}a(t)\\b(t)\end{pmatrix} = i\hbar\begin{pmatrix}\dot{a}(t)\\ \dot{b}(t)\end{pmatrix}} \quad (3)$$

$\boxed{B_1 \ll B_0 \Rightarrow \omega_1 \ll \omega_0}$

Start with $\boxed{\text{if } \omega_1 = 0}$ ($B_1 = 0$)

$$\overset{\text{TDSE}}{\Rightarrow} \hbar/2 \begin{pmatrix}\omega_0 & 0\\ 0 & -\omega_0\end{pmatrix}\begin{pmatrix}a\\b\end{pmatrix} = i\hbar\begin{pmatrix}\dot{a}\\ \dot{b}\end{pmatrix} \Rightarrow \dots \Rightarrow \begin{cases}\dot{a} + i(\omega_0/2)a = 0\\ \dot{b} - i(\omega_0/2)b = 0\end{cases}$$

$$\Rightarrow \boxed{\begin{cases}a(t) = a_0 e^{-i\omega_0 t/2}\\ b(t) = b_0 e^{+i\omega_0 t/2}\end{cases}}$$

Known: spin precession (Larmor) for $\vec{B} = B_0\vec{e}_z = $ const

Then,

$$|\psi'(t)\rangle := \hat{R}^{+}_{z}(\omega_0 t)|\psi(t)\rangle$$

* $\boxed{\text{for } \omega_1 > 0}$ try sol. of the form:

$$\begin{pmatrix} C(t) \\ D(t) \end{pmatrix} = \hat{R}^{+}_{z}(\omega_0 t)\begin{pmatrix} a(t) \\ b(t) \end{pmatrix}$$

$$\begin{cases} a(t) = C(t)\, e^{-i\omega_0 t/2} \\ b(t) = D(t)\, e^{+i\omega_0 t/2} \end{cases}$$

i.e. change to a rotating frame.

$C(t), D(t) = ?$ $\boxed{\text{Expect } C(t), D(t) \sim e^{i\omega_1 t} \quad (\omega_1 \ll \omega_0)}$

TDSE: (3): $$i\begin{pmatrix} \dot{C}(t) \\ \dot{D}(t) \end{pmatrix} = \frac{\omega_1}{2}\cos\omega t \begin{pmatrix} D(t)\, e^{i\omega_0 t} \\ C(t)\, e^{-i\omega_0 t} \end{pmatrix} = \frac{\omega_1}{4}\begin{pmatrix} D(t)\left[e^{i(\omega_0+\omega)t} + \underline{e^{i(\omega_0-\omega)t}}\right] \\ C(t)\left[\underline{e^{i(\omega-\omega_0)t}} + \underline{e^{-i(\omega_0+\omega)t}}\right] \end{pmatrix}$$

* time scale of $C(t), D(t)$: $\tau^{-1} \sim \omega_1 \; (\ll \omega_0)$ low freq.
* $\left\{ \underline{e^{i(\omega-\omega_0)t}}, \underline{e^{-i(\omega+\omega_0)t}} \right\} \times e^{\pm i\omega_1 t}$ average out to zero unless $\omega \simeq \omega_0$ (quasi resonance)

Also for $\omega \simeq \omega_0$ we have:

$\omega + \omega_0 \gg \omega - \omega_0$

$\boxed{\text{Bottomline, for } \omega \simeq \omega_0: \; \langle e^{\pm i(\omega+\omega_0)t}\rangle \ll \langle e^{\pm i(\omega-\omega_0)t}\rangle}$ $\Rightarrow e^{i(\omega+\omega_0)t}$ much faster than $e^{i(\omega-\omega_0)}$

(Rotating-wave approximation) $\Rightarrow \langle e^{i(\omega+\omega_0)t}\rangle \sim 0$

$\Rightarrow \boxed{\text{neglect } \omega+\omega_0 \text{ terms}}$

$\Rightarrow$ at $\boxed{\omega = \omega_0}$: $e^{\pm 2i\omega_0 t} \to 0$, $e^{\pm i(\omega-\omega_0)t} \to 1$

TDSE $$i\begin{pmatrix} \dot{C} \\ \dot{D} \end{pmatrix} \simeq \frac{\omega_1}{4}\begin{pmatrix} D \\ C \end{pmatrix} \Big|\, d/dt \;\to\; \begin{pmatrix} \ddot{C} \\ \ddot{D} \end{pmatrix} = -\left(\frac{\omega_1}{4}\right)^2 \begin{pmatrix} C \\ D \end{pmatrix}$$

i.c.: $C(0) = 1$, $D(0) = 0$, i.e. $|\psi_0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $\Rightarrow$ $$\boxed{\begin{aligned} C(t) &= \cos\left(\frac{\omega_1 t}{4}\right) \\ D(t) &= -i\sin\left(\frac{\omega_1 t}{4}\right) \end{aligned}}$$

Probabilities

$$P_{-z} = |\langle -z|\psi(t)\rangle|^2 = b^*(t)\,b(t) = D^*(t)\,D(t) = \sin^2\frac{\omega_1 t}{4} \quad (\text{flip})$$

$$P_{+z} = \cos^2\frac{\omega_1 t}{4}$$

$$P_{-z} + P_{+z} = 1$$

Qualitative Prelude to ESR $\boxed{ESR_b\ 1}$

Book: Slichter, Principles of Magnetic Resonance Ch.1 (p.4)

Electron Spin Resonance : Population & Energy Exchange

Resonance + Relaxation

$$\hat{H} = -\hat{\vec{\mu}}\cdot\vec{B} \overset{(SI)}{=} -\frac{gQ}{2m}\hat{\vec{S}}\cdot\vec{B} \overset{Q=-e,\ g=2}{=} \frac{e}{m_e}\hat{\vec{S}}\cdot\vec{B} = \frac{e}{m_e}\hat{\vec{S}}\cdot\left(\vec{x}B_1\cos\omega t + \vec{z}B_0\right)$$

$$\Rightarrow \hat{H} = \frac{e}{m_e}\hat{S}_x B_1\cos\omega t + \frac{e}{m_e}\hat{S}_z B_0 \equiv \omega_0\hat{S}_z + (\omega_1\cos\omega t)\hat{S}_x$$

$$\omega_0 \equiv (e/m_e)B_0 \quad , \quad \omega_1 \equiv (e/m_e)B_1$$

Adopted from Slichter, "Principles of Magnetic Resonance" (Sec: 1.3, p4) for ESR instead of NMR

let $\hat{H}_0 \equiv \omega_0\hat{S}_z$
$\hat{H}_1 \equiv \omega_1 S_x\cos\omega t$ $\Leftrightarrow$ $\boxed{\hat{H} = \hat{H}_0 + \hat{H}_1}$

EVP $\boxed{H_0}$ $\hat{H}_0|\pm z\rangle = \pm\frac{\hbar\omega_0}{2}|\pm z\rangle \equiv E_\pm|\pm z\rangle$

$\boxed{H1}$ Population dynamics under oscillating-field $\vec{B}_1$:

$$\Delta E = E_+ - E_- = \hbar\omega_0 = \frac{\hbar e}{m_e}B_0$$

$\left(\mu_B \equiv \frac{\hbar e}{2m_e}\ \text{Bohr magneton}\right)$ $\equiv \gamma B_0$
$\equiv 2\mu_B B_0$

$\vec{\mu}\uparrow\downarrow\vec{B}_0$ $(\vec{S}\uparrow\uparrow\vec{B}_0)$ E_+ ——— N_+

$\vec{\mu}\uparrow\uparrow\vec{B}_0$ $(\vec{S}\downarrow\uparrow\vec{B}_0)$ E_- ——— N_-

Rate equations:

$$\begin{cases} \dot{N}_+ = -k_{+-}N_+ + k_{-+}N_- \\ \dot{N}_- = -k_{-+}N_- + k_{+-}N_+ \end{cases}$$

$k_{\pm\mp} = \frac{\text{probabilities}}{\text{time}}$: ~~Assume~~ $\boxed{\boxed{k_{+-} = k_{-+}} \equiv k}$ ⓪ — Depends on B1

TDP: $\dot{P}_{a\to b} = \frac{2\pi}{\hbar}|\langle b|\hat{H}|a\rangle|^2\delta(\epsilon_a - \epsilon_b - \hbar\omega)$ $\dot{P}_{a\to b} = \dot{P}_{b\to a}$

~~Work on equation~~

$$\Rightarrow \begin{cases} \dot{N}_+ = -k(N_+ - N_-) & ① \\ \dot{N}_- = -k(N_- - N_+) & ② \end{cases}$$ relaxation equations

→ Work on $\dot{N}_+$ equation:

- let $\boxed{n \equiv -N_+ + N_- \ ;\ N \equiv N_+ + N_-}$ $\dot{N} = 0$ (total population is constant)

$\Rightarrow \boxed{N_\pm = (N \mp n)/2}$ $\Rightarrow$ Eq. ① becomes:

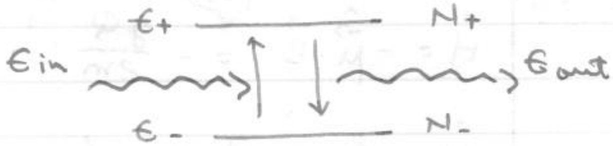
$$\left.\begin{aligned} &\tfrac{1}{2}(\dot{N} - \dot{n}) = +kn \\ &\text{but } \dot{N} = 0 \text{ (conservation of total nr of particles)} \end{aligned}\right\} \Rightarrow \boxed{\dot{n} = -2kn} \ ③$$

$$\Rightarrow \text{sol: } \boxed{n(t) = n_0 e^{-2kt}} \ ④$$

$\boxed{\lim_{t\to\infty} n(t) = 0 \Rightarrow \underline{N_+ = N_-} \text{ equilibrium due to transitions induced by } B_1(t)}$

unrealistic

Rate of energy absorption:



Energy absorbed (from the oscillating field) per unit time, by the electrons (two-level system):

absorption: $E_- \to E_+$ (by absorbing energy from the field, the electron population $N_- \to N_+$)

$$+\dot{\epsilon} = k_{-+}N_-\hbar\omega - k_{+-}N_+\hbar\omega$$

"left"

$$= +k(N_- - N_+)\hbar\omega \Rightarrow \boxed{\dot{\epsilon} = kn\hbar\omega} \quad (5)$$

$\Updownarrow$

A population difference ($n = N_- - N_+$) is needed to absorb energy

Cases ($n = N_- - N_+$):

1) $n<0 \iff N_+ > N_- \Rightarrow \dot{\epsilon} < 0$ net energy is absorbed ($\epsilon_{out} < \epsilon_{in}$)

2) $n>0 \iff N_+ < N_- \Rightarrow \dot{\epsilon} > 0$ net energy is released ($\epsilon_{out} > \epsilon_{in}$) ↳ amplifiers: (masers for nuclear spin resonance)

3) $n=0 \iff N_+ = N_- \Rightarrow \dot{\epsilon} = 0 \Rightarrow \epsilon = $ constant ↳ resonant absorption stops

4) $k=0 \iff \boxed{B_1 = 0 \; (B_0 \neq 0)} \Rightarrow \begin{cases} \dot{\epsilon} = 0 \\ n = N_- - N_+ = \text{const} \; (\dot{n}=0) \end{cases}$ see N_+ on page 1

Favored spin alignment: $\vec{S}_z \uparrow\downarrow \vec{B}_0 \Rightarrow N_- > N_+$ (since $\epsilon_+ \equiv \epsilon_{\uparrow\uparrow}$, $\epsilon_- \equiv \epsilon_{\uparrow\downarrow} \dots$)

$\boxed{E_-}$ $(\vec{\mu} \uparrow\uparrow \vec{B}_0)$ Ideal ~~magnetization~~ polarization: $N_+ = 0$ (only at $T = 0\,K$)

$\Rightarrow$ $\boxed{\text{Eqs. (3), (5) are incomplete and must be modified to account for thermal effects}}$ (spin-lattice relaxation)

Approach: The transition rates k_{+-}, k_{-+} are equal (Eq. (0)) only for an $\boxed{\text{ISOLATED}}$ system.

If the system releases heat to a heat reservoir via $\epsilon_+ \to \epsilon_-$ transitions $\Rightarrow$ system NOT ISOLATED $\Rightarrow$ $\boxed{k_{+-} \neq k_{-+}}$

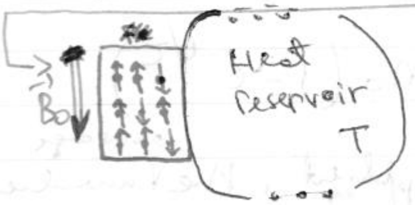
Thermal Relaxation Effects

Spins will relax due to thermal fluctuations

~~////~~ Consider a piece of iron under a static field $\vec{B}_0 = B_0 \hat{z}$

↳ Apply $\vec{B}_0 \Rightarrow$ magnetization $\Rightarrow \begin{cases} E_- \to E_+ \text{ (spin alignment)} \\ E_+ \to E_- \text{ (a number of spins anti-align i.e. } \underline{N_- \neq 0}\text{)} \end{cases}$

The system is NOT ISOLATED but must be close to a heat reservoir! ↳ $\boxed{\text{heating the sample}}$



$\boxed{\text{Heat flow continues until the final populations } N^0_\pm \text{ correspond to the temperature T of the reservoir}}$

Boltzmann

$$\frac{N^0_+}{N^0_-} = e^{-\Delta\epsilon/k_BT} = e^{-\gamma B_0/k_BT} \equiv e^{-2\mu_B B_0/k_BT}$$

Population kinetics : (Notation: $k_{+-} = k_\downarrow$, $k_{-+} = k_\uparrow$)

$$\boxed{\dot{N}_+ = N_- k_\uparrow - N_+ k_\downarrow} \quad (6)$$

→ Steady state $\boxed{\dot{N}_+ = 0} \Leftrightarrow \boxed{N^0_- k_\uparrow = N^0_+ k_\downarrow} \Rightarrow \boxed{k_\uparrow / k_\downarrow = N^0_+ / N^0_-}$ (7)

$$\Rightarrow \boxed{\frac{k_\uparrow}{k_\downarrow} = e^{-\Delta\epsilon/k_BT} = e^{-\gamma B_0/k_BT} \equiv e^{-2\mu_B B_0/k_BT}} \quad (8)$$

detailed balancing

Let: $\underbrace{n_0 \equiv N^0_- - N^0_+}_{\text{finals } (t\to\infty)}$, $n \equiv N_- - N_+$, $N \equiv N^0_+ + N^0_- = N_+ + N_- = \text{const} \ (\Rightarrow \dot{N} = 0)$ (total no. is constant)

$N_\pm =$

$N_\pm = \frac{1}{2}(N \mp n)$

→ (6) :

$$-\frac{1}{2}\dot{n} = \frac{1}{2}(N+n)k_\uparrow - \frac{1}{2}(N-n)k_\downarrow$$

← using $N_\pm = \frac{1}{2}(N \mp n)$

$$\boxed{\dot{n} = +N(k_\downarrow - k_\uparrow) - n(k_\uparrow + k_\downarrow)} \quad (9)$$

$$\dot{n} = \underbrace{(k_\uparrow + k_\downarrow)}_{\equiv 1/\tau} \left[+N \underbrace{\frac{k_\downarrow - k_\uparrow}{k_\uparrow + k_\downarrow}}_{= +n_0 \ (7)} - n \right]$$

(spin-lattice) relaxation time

$$\Rightarrow \boxed{\dot{n} = \frac{n_0 - n}{\tau}} \quad (10)$$

relaxation-type equation

Correction to (3)

~~Sol~~ Solution for (10):

$$\boxed{n(t) = n_0 + C e^{-t/\tau}} \quad (11) \quad , \quad C = \text{constant}$$

Example | Initially ~~unmagnetized~~ unpolarized sample : $n(0) = 0 \iff 0 = n_0 + C$

$$\Rightarrow C = -n_0 \quad \Rightarrow \quad n(t) = n_0\left(1 - e^{-t/\tau}\right)$$

(While the external $\vec{B}_0$ field is applied, the average number of aligned spins – ~~magnetization~~ polarization – increases exponentially until equilibrium is attained for which $n(t \to \infty) = n_0$)

$\Rightarrow$ ~~Population kinetics~~ for thermal processes:

* Population evolution due to both induced transitions and thermal effects:

$$\boxed{\dot{n} = \dot{n}\Big|_{\substack{\text{induced}\\ \text{transitions}}} + \dot{n}\Big|_{\text{thermal}} = -2Kn + \frac{n_0 - n}{\tau}} \quad (12)$$

(3) (10) cf (10)

* Absorption rate, corrected for thermal effects:

(12) $\Rightarrow$ $\dot{n} \simeq 0$ $\iff$ $\boxed{n\Big|_{corr} \simeq \frac{n_0}{1 + 2K\tau}}$ (13)

Steady state (equil. approx)

$$\Rightarrow \boxed{\dot{E}\Big|_{corr} = K\, n\Big|_{corr} \hbar\omega \simeq \frac{K}{1 + 2K\tau} n_0 \hbar\omega}$$

(Note : K is a rate in 1/sec i.e. "frequency" !)

Schrödinger's Equation in Position Representation

TDSE:

$$\langle x| \; \hat{H}|\Psi(t)\rangle = i\hbar \frac{d}{dt}|\Psi(t)\rangle$$

$$\langle x|\hat{H}|\Psi(t)\rangle = i\hbar \langle x|\frac{d}{dt}|\Psi(t)\rangle \quad (1)$$

$$\hat{H} = \frac{\hat{P}^2}{2m} + V(\hat{x}) = -\hbar^2/2m\, \partial_x^2 + V(\hat{x})$$

$\{|x\rangle\}$ in position space ($\hat{x}|x\rangle = x|x\rangle$)

$$\Rightarrow \langle x|\hat{H}|\Psi(t)\rangle = \langle x|\left(-\frac{\hbar^2}{2m}\partial_x^2 + V(x)\right)|\Psi(t)\rangle$$

$$\text{"}\hat{H}\langle x|\Psi(t)\rangle\text{"} = \left(-\frac{\hbar^2}{2m}\partial_x^2 + V(x)\right)\langle x|\Psi(t)\rangle$$

$$\hat{H}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t) \quad (2)$$

(Diff. equation: $\frac{\partial f}{\partial t} = D\nabla^2 f$)

(1) & (2) $\Rightarrow$

$$\boxed{\left[-\hbar^2/2m\, \partial_x^2 + V(x)\right]\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t)}$$

TDSE in x-space

If $|\Psi_E(t)\rangle$ is an energy e-state i.e. $|\Psi_E(t)\rangle = |E\rangle e^{-iEt/\hbar}$ such that $\hat{H}|E\rangle = E|E\rangle$, then $\Psi_E(x,t) \equiv \langle x|\Psi_E(t)\rangle = \langle x|E\rangle e^{-iEt/\hbar}$

$$\Rightarrow \text{TDSE: } \boxed{\left[-\hbar^2/2m\, \partial_x^2 + V(x)\right]\langle x|E\rangle = E\langle x|E\rangle} \text{ or}$$

$$\boxed{\left[-\hbar^2/2m\, \partial_x^2 + V(x)\right]\varphi_E(x) = E\varphi_E(x)} \text{ i.e. TISE in position space}$$

where $\varphi_E(x) \equiv \langle x|E\rangle$

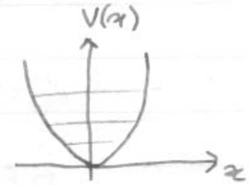
Read
6.8 Potential well
6.9 Infinite potential well

General TISE

$$\Big[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \underbrace{V(x)}_{\leftarrow \text{problem specific}}\Big]\psi(x) = \epsilon\,\psi(x) \quad , \quad \hat{H}\psi(x) = \epsilon\,\psi(x)$$

Application Ch 7

= Simple Harmonic Oscillator (SHO) =



$$V(\hat{x}) = \tfrac{1}{2} m\omega^2 \hat{x}^2 \equiv \tfrac{1}{2} m\omega^2 \hat{x}\cdot\hat{x}$$

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2 \quad , \quad [\hat{x}, \hat{p}_x] = i\hbar$$

Let $\hat{p}_x \equiv \hat{p}$

Define operators
$$\hat{a} \equiv \sqrt{\frac{m\omega}{2\hbar}}\Big(\hat{x} + \frac{i}{m\omega}\hat{p}_x\Big)$$
$$\hat{a}^+ = \sqrt{\frac{m\omega}{2\hbar}}\Big(\hat{x} - \frac{i}{m\omega}\hat{p}_x\Big)$$

$$\boxed{[\hat{a}, \hat{a}^+] = \hat{1}} \quad C_0$$

$$\Rightarrow \begin{cases} \hat{x} = (\hbar/2m\omega)^{1/2}(\hat{a} + \hat{a}^+) \\ \hat{p}_x = -i\left(\frac{m\omega\hbar}{2}\right)^{1/2}(\hat{a} - \hat{a}^+) \end{cases}$$

Motivation:
seek $\hat{H} = \hbar\omega(\hat{X}^2 + \hat{P}^2)$
$\hat{X} \equiv \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x}$, $\hat{P} \equiv \frac{1}{\sqrt{2m\hbar\omega}}\,\hat{p}$
$\hookrightarrow \hat{a} = \hat{X} + i\hat{P}$ || $\hat{a}^+ = \hat{X} - i\hat{P}$

$$\Rightarrow \hat{H} = \hbar\omega/2\,(\hat{a}^+\hat{a} + \hat{a}\hat{a}^+) = \hbar\omega(\hat{a}^+\hat{a} + 1/2) \equiv \hbar\omega(\hat{N} + 1/2)$$

$\boxed{\hat{N} \equiv \hat{a}^+\hat{a}}$ Number operator

$[\hat{H}, \hat{N}] = 0 \Rightarrow \hat{H}, \hat{N}$ share e-states $\Rightarrow$ the e-value problem for $\hat{H}$ is transferred to $\hat{N}$

Let $\boxed{\hat{N}|\eta\rangle = \eta|\eta\rangle}$

$\hookrightarrow$ stationary states (of Energy Op)

$$\langle N\rangle_\eta = \langle\eta|\hat{N}|\eta\rangle \overset{1}{=} \eta\langle\eta|\eta\rangle$$
$$\overset{2}{=} \langle\eta|\hat{a}^+\hat{a}|\eta\rangle \equiv \langle a\eta|a\eta\rangle \Big\} \Rightarrow$$

$$\Rightarrow \langle a\eta|a\eta\rangle = \eta\langle\eta|\eta\rangle \Rightarrow \boxed{\eta \geq 0}$$ positive e-values of $\hat{N}$

Commutators:
$$\boxed{\begin{aligned} [\hat{N}, \hat{a}] &= -\hat{a} = \hat{N}\hat{a} - \hat{a}\hat{N} \quad C_1 \\ [\hat{N}, \hat{a}^+] &= \hat{a}^+ = \hat{N}\hat{a}^+ - \hat{a}^+\hat{N} \quad C_2 \end{aligned}}$$

Goal: Find e-values and e-states of $\hat{H}$:

Start at $|\eta\rangle$:

$$\left.\begin{aligned}\hat{N}\hat{a}^+|\eta\rangle &\overset{C_2}{=} (\hat{a}^+\hat{N} + \hat{a}^+)|\eta\rangle \\ &= (\hat{a}^+\eta + \hat{a}^+)|\eta\rangle \\ &= (\eta+1)\hat{a}^+|\eta\rangle\end{aligned}\right\} \Rightarrow \boxed{\hat{a}^+|\eta\rangle = C_+|\eta+1\rangle}$$

'raising'
'creation' operator

$$\hat{N}\hat{a}|\eta\rangle \overset{C_1}{=} (\eta-1)\hat{a}|\eta\rangle \Rightarrow \boxed{\hat{a}|\eta\rangle = C_-|\eta-1\rangle}$$

"lowering"
"annihilation" operator

η_{min}

Bottom rung: $\hat{a}|\eta_{min}\rangle \overset{!}{=} |\phi\rangle$ null state

$$\left.\begin{aligned}\hat{a}^+(\hat{a}|\eta_{min}\rangle) &\overset{1}{=} \hat{N}|\eta_{min}\rangle = \eta_{min}|\eta_{min}\rangle \\ &\overset{2}{=} |\phi\rangle\end{aligned}\right\} \Rightarrow$$

$\eta \to n$ $\Rightarrow \boxed{\eta_{min} = 0 \ , \ |\eta_{min}\rangle = |0\rangle}$ $\Rightarrow$ label for $\boxed{\text{ground state } (\neq \text{null state})}$

Raise n times:
from GND state $|0\rangle$: $\hat{N}|n\rangle = n|n\rangle$, $n = 0, 1, 2, \ldots$

$$\Rightarrow \boxed{\hat{H}|n\rangle = \hbar\omega(\hat{N} + 1/2)|n\rangle = \hbar\omega(n+1/2)|n\rangle \equiv \epsilon_n|n\rangle}$$

$n = 0, 1, 2, \ldots$

$\epsilon_n = \hbar\omega(n+1/2)$ <u>energy levels of SHO</u>

$C_+, C_- = ?$

$$\boxed{\hat{a}^+|n\rangle = C_+|n+1\rangle \ , \ \hat{a}|n\rangle = C_-|n-1\rangle}$$

$$\left.\begin{aligned}\langle n|\hat{a}\hat{a}^+|n\rangle &\overset{1}{=} |C_+|^2\langle n+1|n+1\rangle \\ &\overset{2}{=} (n+1)\langle n|n\rangle\end{aligned}\right\} \Rightarrow |C_+|^2 = (n+1)\frac{\langle n|n\rangle}{\langle n+1|n+1\rangle} = n+1$$

C_0

Choose $\boxed{C_+ = \sqrt{n+1}}$

$$\left.\begin{aligned}\langle n|\underbrace{\hat{a}^+\hat{a}}_{\hat{N}}|n\rangle &\overset{1}{=} |C_-|^2\langle n-1|n-1\rangle \\ &\overset{2}{=} n\langle n|n\rangle\end{aligned}\right\} \Rightarrow \boxed{C_- = \sqrt{n}}$$

$$\Rightarrow \begin{cases} \hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle \\ \hat{a}^+|n\rangle = \sqrt{n+1}\,|n+1\rangle \end{cases}$$

M. R. of $\hat{a}, \hat{a}^+$ in energy basis:

$$(a^+)_{n'n} \equiv \langle n'|\hat{a}^+|n\rangle = \sqrt{n+1}\,\delta_{n',n+1}$$

$$a_{n'n} \equiv \langle n'|\hat{a}|n\rangle = \sqrt{n}\,\delta_{n',n-1}$$

→ infinite-dimension matrices
→ easy to get the M. R. of $\hat{p}, \hat{x}$.

* Any energy e-state:

$$\boxed{E_n = \hbar\omega(n+1/2)} \quad n=0,1,2,\ldots \qquad \boxed{|n\rangle = \frac{(\hat{a}^+)^n}{\sqrt{n!}}|0\rangle}$$

Here, $|0\rangle = |\eta_{min}\rangle = |\text{gnd state}\rangle$ (NOT null state)

Position-space SHO wave functions:

Start at gnd state

$$\hat{a}|0\rangle = 0 \quad (\text{bottom rung})$$

$$\hat{a} \to \sqrt{\frac{m\omega}{2\hbar}}\left(x+\frac{\hbar}{m\omega}\partial_x\right)$$

$$\left.\begin{aligned} \langle x|\hat{a}|0\rangle &\overset{1}{=} 0 \\ &\overset{2}{=} \left(\frac{m\omega}{2\hbar}\right)^{1/2}\langle x|\hat{x}+\frac{i}{m\omega}\hat{p}_x|0\rangle \end{aligned}\right\} \Rightarrow$$

$$\Rightarrow \langle x|\hat{x}+{}^{i}/_{m\omega}\,\hat{p}_x|0\rangle = 0$$

$$\langle x|\hat{x}|0\rangle + {}^{i}/_{m\omega}\langle x|\hat{p}_x|0\rangle = 0$$

$$x\langle x|0\rangle + \frac{i}{m\omega}\frac{\hbar}{i}\partial_x\langle x|0\rangle = 0$$

$$\Rightarrow \partial_x\langle x|0\rangle = -\frac{m\omega}{\hbar}x\langle x|0\rangle$$

$$\Rightarrow \langle x|0\rangle = C\,e^{-m\omega x^2/2\hbar} \equiv \psi_0(x)$$

Normalise $\displaystyle\int_{-\infty}^{\infty}\psi_0^*(x)\psi_0(x)\,dx = 1 \Rightarrow |C|^2 = \sqrt{\frac{\pi\hbar}{m\omega}} \to C = \left(\frac{\pi\hbar}{m\omega}\right)^{1/4}$

$$\Rightarrow \boxed{\psi_0(x) \equiv \langle x|0\rangle = \left(\frac{\pi\hbar}{m\omega}\right)^{1/4} e^{-m\omega x^2/2\hbar}}$$

Gnd-state wavefunction of SHO

$$\boxed{\begin{aligned}\psi_n(x) \equiv \langle x|n\rangle &= \langle x|\frac{(\hat{a}^+)^n}{\sqrt{n!}}|0\rangle = \frac{1}{\sqrt{n!}}\langle x|(\hat{a}^+)^n|0\rangle \\ &= \frac{1}{\sqrt{n!}}\underbrace{\left(\frac{m\omega}{2\hbar}\right)^{n/2}\left(x - \frac{\hbar}{m\omega}\frac{d}{dx}\right)^n}_{\hat{a}^n}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar}\end{aligned}}$$

$n = 0, 1, 2, \ldots$

* Exp. value of KE:

$$\underline{\langle KE\rangle_n} = \langle \frac{p_x^2}{2m}\rangle_n = \langle n|\frac{\hat{p}_x^2}{2m}|n\rangle = \langle n|\int_{-\infty}^{\infty} dx\,|x\rangle\langle x|\frac{\hat{p}_x^2}{2m}|n\rangle$$

$$= \int_{-\infty}^{\infty} dx\,\langle n|x\rangle \frac{1}{2m}\langle x|\hat{p}_x^2|n\rangle$$

$$= \frac{1}{2m}\int_{-\infty}^{\infty} dx\,\langle n|x\rangle\left(-\hbar^2\partial_x^2\right)\langle x|n\rangle = -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} dx\,\langle n|x\rangle\frac{d^2}{dx^2}\langle x|n\rangle$$

$$\equiv -\hbar^2/2m \int_{-\infty}^{\infty} dx\,\psi_n^*(x)\,\underbrace{\frac{d^2}{dx^2}\psi_n(x)}\quad //$$

$\hookrightarrow$ ↗ ~~w.~~ w. of nodes (zeros) of $\psi_n(x)$ = n

* Exp. value of PE:

$$\underline{\langle PE\rangle_n} = \langle \tfrac{1}{2}m\omega^2x^2\rangle_n = \tfrac{1}{2}m\omega^2\int_{-\infty}^{\infty} dx\; x^2\,|\langle x|n\rangle|^2$$

$$(= \langle V(x)\rangle_n) \qquad = \frac{m\omega^2}{2}\int_{-\infty}^{\infty} dx\; x^2\,|\psi_n(x)|^2 \quad //$$

↗ with w. of nodes of $\psi_n(x)$

Total energy:

$$\langle E\rangle_n = \langle KE\rangle_n + \langle PE\rangle_n = \cdots$$

ZPE (7.5)

$n=0 \Rightarrow \langle E\rangle_0 = \qquad E_0 = \hbar\omega/2$

QHO in the Classical Limit (Large n)

$$\cancel{E_n = \begin{cases} \hbar\omega(n+1/2), & \text{quantum} \\ \hbar\sqrt{g/L}, & \text{classical pendulum} \sim 10^{-33}\,J \end{cases}} \Rightarrow$$

$$\epsilon_n = \hbar\omega(n+1/2) \Rightarrow \Delta E = \hbar\omega \sim \begin{cases} \epsilon_n(n+1/2)^{-1}, & QHO \\ \hbar\sqrt{g/L}, & CHO\text{ (pendulum)} \sim 10^{-33}\,J \end{cases}$$

$$\Rightarrow \frac{\epsilon}{n+1/2} \sim 10^{-33}\,J \Rightarrow \boxed{n \sim \frac{\epsilon}{10^{-33}\,J} - \frac{1}{2}} \quad \epsilon \sim 1\,J \Rightarrow \boxed{n \sim 10^{33}} \to \infty$$

classically

Classically, pendulum turns at classical turning points where $E = V$:
(KE = 0)

$$\epsilon_n = \hbar\omega(n+1/2) \stackrel{!}{=} \frac{1}{2}m\omega^2 x_n^2$$

Wavefunctions $\psi_n(x)$ "clump" around CTPs as $n \nearrow$ ∴ CORRESPONDENCE PRINCIPLE

see ↳ $\boxed{\text{coherent states}}$

(7.7) Time Dependence of QHO Wavefunctions

Let $\boxed{|\psi_0\rangle = c_n|n\rangle + c_{n+1}|n+1\rangle}$, $\hat{H}$ indep of time $\Rightarrow$

$$\to |\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi_0\rangle = c_n e^{-i\epsilon_n t/\hbar}|n\rangle + c_{n+1}e^{-i\epsilon_{n+1}t/\hbar}|n+1\rangle$$

$$= c_n e^{-i\omega(n+1/2)t}|n\rangle + c_{n+1}e^{-i\omega(n+3/2)t}|n+1\rangle$$

$$= e^{-i(n+1/2)\omega t}\left[c_n|n\rangle + c_{n+1}e^{-i\omega t}|n+1\rangle\right]$$ ✓ not a stationary state for $\hat{A} = \hat{H}_{SHO}$

Expectation values:

$$\langle x\rangle_t \propto \cos(\omega t + \Gamma) \text{ or } \tilde{A}e^{-i\omega t}$$

EVP of SHO - alternate method

$[\hat{a}, \hat{a}^+] = \hat{1}$ (C_0)

$[\hat{N}, \hat{a}] = -\hat{a}$ (C_1)

$[\hat{N}, \hat{a}^+] = \hat{a}^+$ (C_2)

$$\hat{H} = (\hat{a}^+\hat{a} + 1/2)\hbar\omega = (\hat{N} + 1/2)\hbar\omega$$

$$[\hat{H}, \hat{N}] = 0 \Rightarrow \begin{cases} \hat{H}|n\rangle = \epsilon_n |n\rangle \\ \hat{N}|n\rangle = A_n |n\rangle \end{cases} \quad A_n \in \mathbb{R} \text{ b/c } \hat{N}^+ = \hat{N}$$

* $\hat{N}(\hat{a}^k|n\rangle) = ?$:

(1) $\rightarrow [\hat{N}, \hat{a}]|n\rangle \overset{C_1}{=} (\hat{N}\hat{a} - \hat{a}\hat{N})|n\rangle = -\hat{a}|n\rangle \Rightarrow$

$\rightarrow \underline{\hat{N}\hat{a}|n\rangle} = \hat{a}\hat{N}|n\rangle - \hat{a}|n\rangle = \hat{a}A_n|n\rangle - \hat{a}|n\rangle = \underline{(A_n - 1)\hat{a}|n\rangle}$;

(2) $\rightarrow [\hat{N}, \hat{a}](\hat{a}|n\rangle) = (\hat{N}\hat{a} - \hat{a}\hat{N})(\hat{a}|n\rangle) = -\hat{a}(\hat{a}|n\rangle) \Rightarrow$

$\rightarrow \underline{\hat{N}\hat{a}(\hat{a}|n\rangle)} = \hat{a}\hat{N}(\hat{a}|n\rangle) - \hat{a}(\hat{a}|n\rangle) = \hat{a}(A_n - 1)(\hat{a}|n\rangle) - \hat{a}(\hat{a}|n\rangle)$

$= \underline{(A_n - 2)\hat{a}(\hat{a}|n\rangle)}$

i.e. $\underline{\hat{N}\hat{a}^2|n\rangle = (A_n - 2)\hat{a}^2|n\rangle}$ "2"

⋮

(k) $\rightarrow$ $\boxed{\hat{N}(\hat{a}^k|n\rangle) = (A_n - k)(\hat{a}^k|n\rangle)}$ $\rightarrow$ lowering by k quanta "k"

Similarly

$\boxed{\hat{N}((\hat{a}^+)^k|n\rangle) = (A_n + k)((a^+)^k|n\rangle)}$ $\rightarrow$ raising by k quanta

* $\{A_n\}$ form a discrete spectrum :

- eigenkets of $\hat{N}$ assoc with e values $A_n, A_n - k, A_n + k$:

$$|n\rangle, \ \hat{a}^k|n\rangle, \ (\hat{a}^+)^k|n\rangle$$

$\rightarrow$ sequence of discrete numbers : $\{A_n, A_n \pm 1, A_n \pm 2, \dots\}$

* $A_n \geq 0$: $\langle N\rangle_n = \langle n|\hat{N}|n\rangle \overset{1}{=} \underline{\langle n|\hat{a}^+\hat{a}|n\rangle \geq 0}$, (norm of $\hat{a}|n\rangle \equiv |a_n\rangle$)

$\overset{2}{=} \langle n|A_n|n\rangle = A_n\langle n|n\rangle$ $\Rightarrow \underline{A_n \geq 0}$

2

* (Lowest e-value $A_0 = 0$): let $|0\rangle$ state such that be lowest

$\hat{N}|0\rangle = A_0|0\rangle$ (not null state, but ground state of SHO)

$\hat{N}(\hat{a}|0\rangle) = (A_0 - 1)(\hat{a}|0\rangle)$ impossible since A_0 was postulated as the lowest e-value $\Big\}$ (a)

$\Rightarrow$ $\boxed{\hat{a}|0\rangle \overset{!}{=} 0 \quad \text{null state}}$ $\langle 0|\hat{a}^\dagger = 0$

$$\left.\begin{aligned} \langle N\rangle_0 &\overset{1}{=} \langle 0|\hat{a}^\dagger\hat{a}|0\rangle = 0 \\ &\overset{2}{=} \langle 0|\hat{N}|0\rangle = \langle 0|A_0|0\rangle = A_0\langle 0|0\rangle \end{aligned}\right\} \Rightarrow \boxed{A_0 = 0}$$

$\Rightarrow$* (EVP for $\hat{H}$):

$$\hat{N}|n\rangle = A_n|n\rangle, \quad A_n = 0, 1, 2, \ldots$$

$\Rightarrow$ $\boxed{A_n \equiv n}$ integer! $(n = 0, 1, 2, \ldots)$. Therefore $\boxed{\hat{N}|n\rangle = n|n\rangle}$ $n = 0, 1, 2, 3 \ldots$

$$\boxed{\hat{H}|n\rangle = (\hat{N} + 1/2)\hbar\omega|n\rangle = (n + 1/2)\hbar\omega|n\rangle} \quad n = 0, 1, 2, 3 \ldots$$

$\Leftrightarrow$ $\hat{H}|n\rangle = \epsilon_n|n\rangle$, $\boxed{\epsilon_n \equiv (n + 1/2)\hbar\omega}$

$\langle x\rangle_n = 0$

$\langle p\rangle_n = 0$

-> $|0\rangle$ Gnd state of SHO

-> $1/2\,\hbar\omega$ = ZPE of SHO

-> $\{|n\rangle\}$ orthonormal basis: $\langle n|m\rangle = \delta_{nm}$

$$\hat{1} = \sum_{n=0}^{\infty} |n\rangle\langle n|$$

* Role of ZPE $= \hbar\omega/2$:

Preservation of Heisenberg U. R. $(\Delta x)(\Delta p) \geq \hbar/2$

Proof:

Assume ZPE $= 0$ $\Leftrightarrow$ $\underset{\text{Gnd state energy}}{\epsilon_0} = 0$ $\Leftrightarrow$ $\hat{H}|0\rangle = 0|0\rangle$ $\Leftrightarrow$ KE + PE $\overset{!}{=} 0$

$\Leftrightarrow$ $\{$KE $\overset{!}{=} 0$ and PE $\overset{!}{=} 0\}$ (KE $= p^2/2m \geq 0$, PE $= 1/2\, m\omega^2 x^2 \geq 0$)

$\Leftrightarrow$ $p = x \overset{!}{=} 0$ $\Leftrightarrow$ $(\Delta p) \overset{!}{=} 0 \overset{!}{=} (\Delta x)$ in contradiction with HUR!

$$\boxed{\langle\epsilon\rangle_0} = \frac{\langle p^2\rangle_0}{2m} + \frac{1}{2}m\omega^2\langle x^2\rangle_0 = (1/2m)\left[(\Delta p)_0^2 + \underset{0}{\langle p\rangle_0^2}\right] + (m\omega^2/2)\left[(\Delta x)_0^2 + \underset{0}{\langle x\rangle_0^2}\right]$$

$$\text{ZPE} = \frac{(\Delta p)_0^2}{2m} + \frac{m\omega^2}{2}(\Delta x)_0^2 = \frac{1}{2m}\frac{m\omega\hbar}{2} + \frac{m\omega^2}{2}\frac{\hbar}{2m\omega} = \frac{\omega\hbar}{4} + \frac{\omega\hbar}{4} = \boxed{\frac{\hbar\omega}{2}} \text{ ZPE} \checkmark$$

In any state $|n\rangle$: $(\Delta x)_n(\Delta p)_n = (n + 1/2)\hbar \geq \hbar/2$ ✓

* Action of Ladder Ops on $|n\rangle$

$$\begin{cases} \hat{N}\hat{a}|n\rangle \overset{C_1}{=} (\hat{a}\hat{N} - \hat{a})|n\rangle = (n-1)\,\hat{a}|n\rangle \\ \hat{N}\hat{a}^{+}|n\rangle \overset{C_2}{=} (\hat{a}^{+}\hat{N} + \hat{a}^{+})|n\rangle = (n+1)\,\hat{a}^{+}|n\rangle \end{cases} \quad \text{(see also p.1)}$$

Use property: if $[\hat{A},\hat{B}] = \lambda\hat{B}$ & $\hat{A}|\alpha\rangle = \alpha|\alpha\rangle \Rightarrow \hat{B}|\alpha\rangle \sim |\alpha+\lambda\rangle$

ket: $\Rightarrow \begin{cases} \hat{a}|n\rangle \overset{!}{=} C_-|n-1\rangle & (\hat{N}|n\rangle = n|n\rangle,\ \hat{N}|n-1\rangle = (n-1)|n-1\rangle \ldots) \\ \hat{a}^{+}|n\rangle \overset{!}{=} C_+|n+1\rangle & (\hat{N}|n+1\rangle = (n+1)|n+1\rangle,\ \hat{N}|n\rangle = n|n\rangle \ldots) \end{cases}$

bra: $\begin{cases} \langle n|\hat{a}^{+} = C_-^{*}\langle n-1| \\ \langle n|\hat{a} = C_+^{*}\langle n+1| \end{cases} \Rightarrow \begin{cases} \langle n|\overbrace{\hat{a}^{+}\hat{a}}^{\hat{N}}|n\rangle = |C_-|^2\langle n-1|n-1\rangle \\ \langle n|\underbrace{\hat{a}\hat{a}^{+}}_{\hat{N}+\hat{1}}|n\rangle = |C_+|^2\langle n+1|n+1\rangle \end{cases}$

$[\hat{a},\hat{a}^{+}] = \hat{1}$

$$\Rightarrow \begin{cases} \langle n|\hat{N}|n\rangle = n\langle n|n\rangle \overset{!}{=} |C_-|^2\langle n-1|n-1\rangle \\ \langle n|\hat{1}+\hat{N}|n\rangle \overset{C_0}{=} (n+1)\langle n|n\rangle \overset{!}{=} |C_+|^2\langle n+1|n+1\rangle \end{cases}$$

$\langle 1\rangle = \text{const}$

$$\Rightarrow \begin{cases} |C_-|^2 = n \Rightarrow \boxed{C_- = \sqrt{n}} \\ |C_+|^2 = n+1 \Rightarrow \boxed{C_+ = \sqrt{n+1}} \end{cases}$$

$$\Rightarrow \begin{cases} \underline{\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle} & \text{lowering / annihilation} \leftarrow \text{process of detection (measurement)} \\ \underline{\hat{a}^{+}|n\rangle = \sqrt{n+1}\,|n+1\rangle} & \text{raising / creation} \end{cases}$$

* Create any energy e-state $|n\rangle$ from the ground state $|0\rangle$:

$(\hat{a}^{+})^n|0\rangle = \sqrt{n!}\,|n\rangle \Rightarrow$

$$\boxed{|n\rangle = \frac{(\hat{a}^{+})^n|0\rangle}{\sqrt{n!}}} \qquad \boxed{\langle n| = \frac{\langle 0|\hat{a}^n}{\sqrt{n!}}}$$

$\boxed{E_n = (n+1/2)\hbar\omega}$ energy e-value

* Successive lowering / raising from e-state $|n\rangle$:

$$(\hat{a})^k |n\rangle = \frac{\sqrt{n!}}{\sqrt{(n-k)!}} |n-k\rangle \quad \left(= \sqrt{n(n-1)\dots(n-k+1)}\ |n-k\rangle \right)$$

$$\langle n|(\hat{a}^\dagger)^k = \sqrt{\frac{n!}{(n-k)!}} \langle n-k|$$

$$(\hat{a}^\dagger)^k |n\rangle = \sqrt{\frac{(n+k)!}{n!}} |n+k\rangle \quad \left(= \sqrt{n(n+1)\dots(n+k)}\ |n+k\rangle \right)$$

$$\langle n|(\hat{a})^k = \sqrt{\frac{(n+k)!}{n!}} \langle n+k|$$

* Matrix Representation of $\hat{a}, \hat{a}^\dagger$:

$$a_{mn} = \langle m|\hat{a}|n\rangle = \sqrt{n}\ \delta_{m,n-1}$$

$$(a^\dagger)_{mn} = \langle m|\hat{a}^\dagger|n\rangle = \sqrt{n+1}\ \delta_{m,n+1}$$

→ ∞ dimension space

Use: easily get MR of $\hat{x}, \hat{p}$.

$$\hat{a} \doteq \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{5} \dots \end{pmatrix} \qquad \hat{a}^\dagger \doteq \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ \sqrt{1} & 0 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{5} & 0 \dots \end{pmatrix}$$

(Matrices arbitrarily truncated...)

G + tr (regular) page 52 → position-space wavefunctions

Coherent States of QHO

$\xrightarrow{\quad}$ large n

-> Used to describe "classical" behavior of QHOs; EM field quantization, classical EM field

-> e-kets of lowering op:

$|\alpha\rangle$ s.t. $\hat{a}|\alpha\rangle \overset{!}{=} \alpha|\alpha\rangle$, $\hat{a}^\dagger \neq \hat{a} \Rightarrow \underline{\alpha \in \mathbb{C}}$

$|\alpha\rangle = ?$

Let $|\alpha\rangle = \sum_{n=0}^{\infty} c_n |n\rangle$, $\hat{H}|n\rangle = E_n|n\rangle$, $E_n = \hbar\omega(n+1/2)$

$$\left.\begin{aligned} \hat{a}|\alpha\rangle &\overset{1}{=} \sum_{n=0}^{\infty} c_n \hat{a}|n\rangle = \sum_{n=0}^{\infty} c_n \sqrt{n}\,|n-1\rangle = \sum_{n=1}^{\infty} c_n \sqrt{n}\,|n-1\rangle \\ &\overset{2}{=} \alpha|\alpha\rangle = \alpha \sum_{n=0} c_n|n\rangle \end{aligned}\right\} \Rightarrow$$

$$\Rightarrow \alpha \sum_{n=0}^{\infty} c_n|n\rangle = \sum_{n=1}^{\infty} c_n\sqrt{n}\,|n-1\rangle = \sum_{n=0}^{\infty} c_{n+1}\sqrt{n+1}\,|n\rangle \Rightarrow$$

$$\Rightarrow \alpha c_n = \sqrt{n+1}\, c_{n+1} \Rightarrow \dots \Rightarrow \boxed{c_n = \frac{\alpha^n}{\sqrt{n!}} c_0}$$

$$\Rightarrow \boxed{\begin{aligned} |\alpha\rangle &= c_0 \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \\ \langle\alpha| &= c_0^* \sum_{n=0}^{\infty} \frac{(\alpha^*)^n}{\sqrt{n!}} \langle n| \end{aligned}}$$

$$\langle\alpha|\alpha\rangle = |c_0|^2 e^{|\alpha|^2} \overset{!}{=} 1 \Rightarrow c_0 = e^{-|\alpha|^2/2}$$

$$\Rightarrow \left\| \begin{aligned} |\alpha\rangle &= e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \\ \langle\alpha| &= e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{(\alpha^*)^n}{\sqrt{n!}} \langle n| \end{aligned} \right\|$$

* Scalar product: $\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$, $\hat{a}|\beta\rangle = \beta|\beta\rangle$

$$\cancel{\langle\beta|\alpha\rangle = e^{-|\alpha-\beta|^2/2}} \qquad \langle\beta|\alpha\rangle = e^{\beta^*\alpha}\, e^{-(1/2)(|\alpha|^2+|\beta|^2)}$$

$$|\langle\beta|\alpha\rangle|^2 = e^{-|\alpha-\beta|^2}$$

* Completeness (closure) relation:

$$\hat{1}_\alpha = \frac{1}{\pi}\int_{-\infty}^{\infty} d\,\mathrm{Re}(\alpha)\int_{-\infty}^{\infty} d\,\mathrm{Im}(\alpha)\; |\alpha\rangle\langle\alpha|$$

(Proof in Rousseau-Blaise p. 172 ↓ 'Quantum Oscillators' book)

* Energy fluctuations in a coherent state:

$$\langle H\rangle_\alpha = \langle\alpha|\hat{H}|\alpha\rangle = \hbar\omega\langle\alpha|\hat{a}^+\hat{a}+1/2|\alpha\rangle$$

$$= \hbar\omega\,\underbrace{\langle\alpha|\hat{a}^+\hat{a}|\alpha\rangle}_{\langle\alpha|\alpha^*\alpha|\alpha\rangle} + \frac{1}{2}\underbrace{\langle\alpha|\alpha\rangle}_{1} = \hbar\omega\left(|\alpha|^2+1/2\right)$$

$$\langle H^2\rangle_\alpha = \langle\alpha|\hat{H}^2|\alpha\rangle = (\hbar\omega)^2\langle\alpha|\left(\hat{a}^+\hat{a}+1/2\right)^2|\alpha\rangle$$

$$= (\hbar\omega)^2\langle\alpha|(\hat{a}^+\hat{a})(\hat{a}^+\hat{a}) + \hat{a}^+\hat{a} + 1/4|\alpha\rangle = \dots = (\hbar\omega)^2\left(|\alpha|^4+2|\alpha|^2+\frac{1}{4}\right)$$

Energy fluctuation:

$$\boxed{\Delta E_\alpha \equiv \Delta H_\alpha = \sqrt{\langle H^2\rangle_\alpha - \langle H\rangle_\alpha^2}} =$$

$$= \omega\hbar\sqrt{\left(|\alpha|^4+2|\alpha|^2+\frac{1}{4}\right)-\left(|\alpha|^4+|\alpha|^2+\frac{1}{4}\right)} = \boxed{\hbar\omega|\alpha|} \neq 0$$

$|\alpha\rangle$ not e-ket of $\hat{H}$

Relative fluctuation:

$$\boxed{\varepsilon_\alpha \equiv \frac{\Delta H_\alpha}{\langle H\rangle_\alpha} = \frac{|\alpha|}{|\alpha|^2+\frac{1}{2}} \to 0 \text{ for } |\alpha|\to\infty}$$

↑ "Classical" behavior ⇕ $n\to\infty$

* Coherent States are Minimum-Uncertainty States:

$$\langle x\rangle_\alpha = \langle\alpha|\hat{x}|\alpha\rangle = \sqrt{\frac{\hbar}{2m\omega}}\,\langle\alpha|\hat{a}^\dagger+\hat{a}|\alpha\rangle$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left(\alpha^* + \alpha\right)$$

$$\langle p\rangle_\alpha = \langle\alpha|\hat{p}|\alpha\rangle = i\sqrt{\frac{m\hbar\omega}{2}}\,\langle\alpha|\hat{a}^\dagger-\hat{a}|\alpha\rangle$$

$$= i\sqrt{\frac{m\hbar\omega}{2}}\left(\alpha^* - \alpha\right)$$

$$\langle x^2\rangle_\alpha = \langle\alpha|\hat{x}^2|\alpha\rangle = \cdots = \frac{\hbar}{2m\omega}\left[(\alpha+\alpha^*)^2+1\right]$$

$$\langle p^2\rangle_\alpha = \langle\alpha|\hat{p}^2|\alpha\rangle = \cdots = -\frac{m\hbar\omega}{2}\left[(\alpha^*-\alpha)^2-1\right]$$

$$\boxed{(\Delta x)_\alpha(\Delta p)_\alpha = \frac{\hbar}{2}}$$

Dynamics (Time Evolution) of Coherent States

$$|\alpha\rangle \to |\alpha(t)\rangle \quad : \qquad |\alpha(t)\rangle = e^{-i\hat{H}t/\hbar}|\alpha\rangle$$

$$|\alpha(t)\rangle = e^{-i\hat{H}t/\hbar}\left(e^{-|\alpha|^2/2}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle\right)$$

$$= e^{-|\alpha|^2/2}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}e^{-i(n+1/2)\omega t}|n\rangle = e^{-i\omega t/2}\,\underbrace{e^{-|\alpha|^2/2}\sum_{n=0}^{\infty}\frac{(\alpha e^{-i\omega t})^n}{\sqrt{n!}}|n\rangle}_{\equiv|\alpha e^{-i\omega t}\rangle}$$

$$\equiv e^{-i\omega t/2}\,|\alpha e^{-i\omega t}\rangle$$

↳ in time $|\alpha(t)\rangle$ ~~becomes~~ acquires a phase, becoming complex

* Time-dep. of position and momentum expectation values

$$\langle x\rangle_t = \langle\alpha(t)|\hat{x}|\alpha(t)\rangle = \sqrt{\frac{\hbar}{2m\omega}}\,\langle\alpha(t)|\hat{a}+\hat{a}^+|\alpha(t)\rangle$$

$$= \cdots = \sqrt{\frac{\hbar}{2m\omega}}\left(\alpha e^{-i\omega t} + \alpha^* e^{i\omega t}\right)$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\, 2|\alpha| \cos(\omega t + \delta)$$

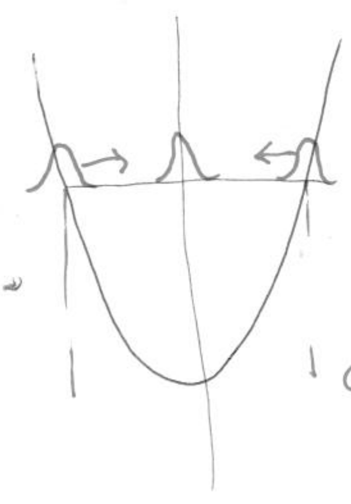
$$\langle p\rangle_t = \langle\alpha(t)|\hat{p}|\alpha(t)\rangle = \ldots -i\sqrt{\frac{m\omega\hbar}{2}}\,\langle\alpha(t)|\hat{a}-\hat{a}^+|\alpha(t)\rangle$$

$$= \cdots = -i\sqrt{\frac{m\omega\hbar}{2}}\left(\alpha e^{-i\omega t} - \alpha^* e^{i\omega t}\right)$$

$$= -\sqrt{\frac{m\omega\hbar}{2}}\, 2|\alpha| \sin(\omega t + \delta)$$

$$\boxed{\langle x\rangle_t \langle p\rangle_t = \frac{\hbar}{2}}$$

Still a minimum-uncertainty state (unlike Gaussian Wave Packet)



Class. turning pts

Application of SHO

55

Charged SHO in an Electric Field.
Electrical Susceptibility of an Elastically Bound Electron

electric perturbation

$$\hat{H}' = \hat{P}^2/2m + 1/2\, m\omega^2 \hat{x}^2 - q\mathcal{E}\hat{x} = \hat{H}_{SHO} - q\mathcal{E}\hat{x}$$

$\begin{pmatrix} q = e \\ Q_e = -1 \end{pmatrix}$

Let $|\varphi_\epsilon'\rangle$ s.t. $\hat{H}'|\varphi_\epsilon'\rangle = \epsilon'|\varphi_\epsilon'\rangle$

$\left(V = -\hat{\vec{\mu}}_e\cdot\vec{\mathcal{E}} = -q\hat{\vec{x}}\cdot\vec{\mathcal{E}} = -q\mathcal{E}\hat{x} \text{ for } \vec{\mathcal{E}} = \mathcal{E}\hat{\vec{x}} \right)$

$$\langle x| \quad \left(-\hbar^2/2m\, \partial_x^2 + 1/2\, m\omega^2 x^2 - q\mathcal{E}x\right)\varphi_\epsilon'(x) = \epsilon'\varphi_\epsilon'(x)$$

Complete the square:

$$\left[-\hbar^2/2m\, \partial^2_x + 1/2\, m\omega^2\left(x - \frac{q\mathcal{E}}{m\omega^2}\right)^2 - \frac{q^2\mathcal{E}^2}{2m\omega^2}\right]\varphi_\epsilon'(x) = \epsilon'\varphi_\epsilon'(x) \quad (1)$$

complete the square

Let $\boxed{u \equiv x - q\mathcal{E}/m\omega^2}$ (2)

$$\Rightarrow \left[-\hbar^2/2m\, \partial_u^2 + 1/2\, m\omega^2 u^2\right]\varphi_\epsilon'(u) = \epsilon''\varphi_\epsilon'(u) \quad (3) \leftarrow \text{SHO}$$

with $\underbrace{\epsilon'' = \epsilon' + q^2\mathcal{E}^2/2m\omega^2}$ (4)

Sol. of (3) is SHO: $\boxed{\epsilon_n'' = (n+1/2)\hbar\omega}$ (5) $(n = 0, 1, 2, \ldots)$

Eigenvalues: $\epsilon_n' = ?$ (4) + (5) $\Rightarrow$

$$\boxed{\epsilon_n' = \hbar\omega(n+1/2) - q^2\mathcal{E}^2/2m\omega^2} = \epsilon_n(\mathcal{E}) \quad (6)$$

↳ energies of SHO with $\mathcal{E}$-field present

correction due to $\mathcal{E}$-field (spectrum shift)

Eigenfunctions: $\varphi_n'(x) = ?$

(2) $\Rightarrow$

$$u = x - q\mathcal{E}/m\omega^2$$

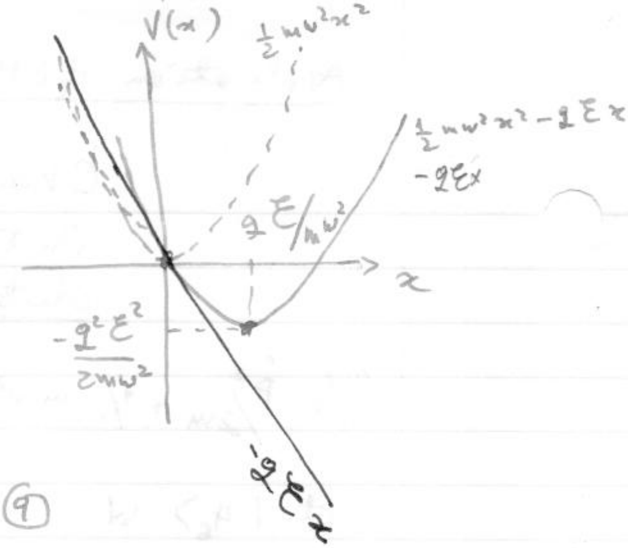
$$\Updownarrow$$

$$\boxed{\varphi_n'(x) = \varphi_n(x - q\mathcal{E}/m\omega^2) \quad (7)}$$

with $\mathcal{E}$ — without $\mathcal{E}$ → shifted e-fns

(due to the force from the $\mathcal{E}$-field on the particle)

(56)



electric dipole moment of atom : $\underset{\mu_e}{\underline{D = q\,x}}$ (8)

Polarization

$\mathcal{E} = 0$: $\langle D \rangle = q \langle \psi_n | \hat{x} | \psi_n \rangle = 0$ (9)

$\mathcal{E} \neq 0$ (slowly incr.) $|\psi_n\rangle \xrightarrow[\text{slowly}]{} |\psi_n'\rangle$

$$\Rightarrow \quad \langle D \rangle' = q \langle \psi_n' | \hat{x} | \psi_n' \rangle = q \int^{\infty} dx\, x\, |\psi_n'(x)|^2 \quad (10)$$

$$(2) + (7) \Rightarrow \boxed{\langle D \rangle' = q \underbrace{\int_{-\infty}^{\infty} u\, |\psi_n(u)|^2 du}_{=0 \text{ by symmetry}} + \frac{q^2 \mathcal{E}}{m\omega^2} \int_{-\infty}^{\infty} du\, |\psi_n(u)|^2}$$

$$= \boxed{q^2 \mathcal{E}/m\omega^2} \quad (11)$$

electrical susceptibility of atomic electron (elastically bound)

$$\chi \equiv \frac{\langle D \rangle'}{\mathcal{E}} = q^2/m\omega^2 \quad (12)$$

Interpretation of (11), (12):

$\mathcal{E}$ shifts the classical equilibrium position of the electron

i.e. $\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ in QM

$\Downarrow$

induced dipole moment

$\chi(\omega) \sim 1/\omega^2 \quad \Rightarrow \chi \nearrow$ if restoring force $\searrow$

$\chi \searrow$ if restoring force $\nearrow$

Position-Representation of Orbital Angular Momentum. (Townsend 9.9)

Eigenfunctions of $\hat{L}^2$, $\hat{L}_z$

$\hat{\vec{r}}|\vec{r}\rangle = \vec{r}|\vec{r}\rangle$, $|\vec{r}\rangle = |x,y,z\rangle = |r,\theta,\varphi\rangle = |\rho,\varphi,z\rangle$ etc.

$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}}$

$$\begin{cases} \hat{L}_x = -i\hbar\,(y\partial_z - z\partial_y) \\ \hat{L}_y = -i\hbar\,(z\partial_x - x\partial_z) \\ L_z = -i\hbar\,(x\partial_y - y\partial_x) \end{cases} \qquad \text{or } L_\alpha = -i\hbar\,\varepsilon_{\alpha\beta\gamma}\, x_\beta \partial_\gamma$$

* Spherical coord.: $x = r\sin\theta\cos\varphi$, $y = r\sin\theta\sin\varphi$, $z = r\cos\theta$, $r \geq 0$, $\theta \in [0,\pi]$, $\varphi \in [0,2\pi]$

$dV = d^3r = r^2\,dr\,d\Omega = r^2\,dr\,\sin\theta\,d\theta\,d\varphi$

$$\Rightarrow \begin{cases} \hat{L}_x = i\hbar\left(\sin\varphi\,\partial_\theta + \dfrac{\cos\varphi}{\tan\theta}\,\partial_\varphi\right) \\ \hat{L}_y = i\hbar\left(-\cos\varphi\,\partial_\theta + \dfrac{\sin\varphi}{\tan\theta}\,\partial_\varphi\right) \\ \hat{L}_z = -i\hbar\,\partial_\varphi \end{cases}$$

$$\Rightarrow \begin{cases} \hat{L}^2 = -\hbar^2\left(\partial_\theta^2 + \dfrac{1}{\tan\theta}\,\partial_\theta + \dfrac{1}{\sin^2\theta}\,\partial_\varphi^2\right) \\ \hat{L}_+ = \hbar e^{i\varphi}\left(\partial_\theta + i\cot\theta\,\partial_\varphi\right) \\ \hat{L}_- = \hbar e^{-i\varphi}\left(-\partial_\theta + i\cot\theta\,\partial_\varphi\right) \end{cases}$$

no dependence on the radial coordinate, r

* E-value problem:

No spin

$$\langle\vec{r}|\ \Big\| \begin{array}{l} \hat{L}^2\,|lm\rangle = \hbar^2 l(l+1)\,|lm\rangle \\ \hat{L}_z\,|lm\rangle = \hbar m\,|lm\rangle \end{array} \quad , m = -l,\dots,+l$$

$$\begin{cases} \langle\vec{r}|\,\hat{L}^2\,|lm\rangle = \hbar^2 l(l+1)\,\langle\vec{r}|lm\rangle \\ \langle\vec{r}|\,\hat{L}_z\,|lm\rangle = \hbar m\,\langle\vec{r}|lm\rangle \end{cases} \qquad (1)$$

$\hat{L}^2, \hat{L}_z$ only depend on θ, φ => separable

$$\langle \vec{r} | lm \rangle = \langle r, \theta, \varphi | lm \rangle = \Phi_{lm}(r,\theta,\varphi) = R(r)\, Y_{lm}(\theta,\varphi)$$

=> (1) =>
$$\begin{cases} -\left(\partial_\theta^2 + \dfrac{1}{\tan\theta}\partial_\theta + \dfrac{1}{\sin^2\theta}\partial_\varphi^2\right) Y_{lm}(\theta,\varphi) = l(l+1)\, Y_{lm}(\theta,\varphi) \\ -i\,\partial_\varphi Y_{lm}(\theta,\varphi) = m\, Y_{lm}(\theta,\varphi) \end{cases}$$

or
$$\boxed{\begin{aligned} \hat{L}^2 Y_{lm}(\theta,\varphi) &= \hbar^2 l(l+1)\, Y_{lm}(\theta,\varphi) \\ \hat{L}_z Y_{lm}(\theta,\varphi) &= m\hbar\, Y_{lm}(\theta,\varphi) \end{aligned}}$$

$$\hat{L}_\pm Y_{lm}(\theta,\varphi) = \hbar\sqrt{l(l+1) - m(m\pm1)}\; Y_{l,m\pm1}(\theta,\varphi)$$

Spherical harmonics

$$Y_{lm}(\theta,\varphi) = (-1)^m \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}\; P_{lm}(\cos\theta)\, e^{im\varphi} \quad (m \geq 0)$$

$$= \frac{(-1)^l}{2^l\, l!}\sqrt{\quad}\; e^{im\varphi}\frac{1}{\sin^m\theta}\frac{d^{l-m}}{d(\cos\theta)^{l-m}}(\sin\theta)^{2l}$$

$P_{lm}(\cos\theta)$ - Associated Legendre ~~polynomials~~ functions:

$$P_{lm}(x) = (1-x^2)^{\frac{|m|}{2}}\frac{d^{|m|}}{dx^{|m|}}P_l(x), \quad P_{l,-m}(x) = P_{lm}(x)$$

$P_l(x)$ - Legendre polynomials:

$P_0(x) = 1$
$P_1(x) = x$
$P_2(x) = (3x^2-1)/2$ etc.

Also, $Y^*_{lm}(\theta,\varphi) = (-1)^m Y_{l,-m}(\theta,\varphi)$

3

* Normalization of angular eigenfunctions:

$$\langle l^* m^* | \underbrace{\ }_{\hat{1}_r} l m \rangle = 1 \quad \Rightarrow$$

$$1 \overset{!}{=} \langle lm | \int d^3r\, |\vec{r}\rangle\langle\vec{r}|\, lm\rangle = \int d^3r\, \langle lm|\vec{r}\rangle\langle\vec{r}|lm\rangle$$

$$= \int d^3r\, \Phi^*_{lm}(\vec{r})\, \Phi_{lm}(\vec{r}) = \int d^3r\, |\Phi_{lm}(\vec{r})|^2$$

$$= \underbrace{\int_0^\infty r^2 dr\, |R(r)|^2}_{\overset{!}{=} 1} \underbrace{\int_0^\pi\int_0^{2\pi} \sin\theta\, d\theta\, d\varphi\, |Y_{lm}(\theta\varphi)|^2}_{\overset{!}{=} 1}$$

separate normalization of the radial and angular parts.

* Orthonormality and closure of Y_{lm}:

$\int_0^{4\pi} d\Omega \equiv \int_0^\pi\int_0^{2\pi} \sin\theta\, d\theta\, d\varphi \Rightarrow$

$$\int_0^{4\pi} d\Omega\, Y^*_{l'm'}(\theta,\varphi)\, Y_{lm}(\theta,\varphi) = \delta_{ll'}\,\delta_{mm'} \quad \text{(orthonormality)}$$

- Any $f(\theta\varphi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} c_{lm}\, Y_{lm}(\theta\varphi)$ (closure)

$$\text{with } c_{lm} = \int_0^{2\pi} d\varphi \int_0^\pi \sin\theta\, d\theta\, Y^*_{lm}(\theta\varphi)\, f(\theta\varphi)$$

* Orthonormal basis of $\{Y_{lm}(\theta\varphi)\}$:

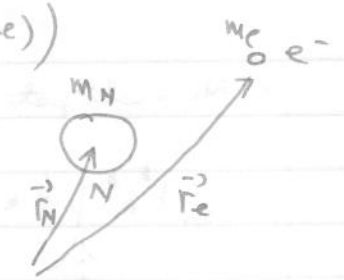
$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y^*_{lm}(\theta'\varphi')\, Y_{lm}(\theta\varphi) = \delta(\cos\theta - \cos\theta')\,\delta(\varphi - \varphi')$$

$$= \frac{1}{\sin\theta}\,\delta(\theta-\theta')\,\delta(\varphi-\varphi')$$

(completeness)

Rotationally invariant problems

<u>The Hydrogenic Atom</u> (nucleus (Ze), electron $(-e)$)



CGS units

Reduced mass: $\mu = \dfrac{m_N m_e}{m_N + m_e}$

$$\hat{H} = \frac{\hat{p}^2}{2\mu} + V(\hat{r})$$

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(r) \right] \psi(\vec{r}) = \epsilon\, \psi(\vec{r})$$

$$\nabla^2 = \frac{1}{r}\partial_r^2 r + \frac{1}{r^2}\left(\partial_\theta^2 + \frac{1}{\tan\theta}\partial_\theta + \frac{1}{\sin^2\theta}\partial_\varphi^2 \right)$$

$\Rightarrow$ ~~H =~~

$$\left[-\hbar^2/2\mu \; 1/r\, \partial_r^2 r + \hat{L}^2/2\mu r^2 + V(r) \right] \psi(r,\theta,\varphi) = \epsilon\, \psi(r,\theta,\varphi)$$

Conservation of Linear and Angular Momentum.
Translational and Rotational Invariance

* Two-body Hamiltonian : (<u>Townsend 9.2</u>)

$$\hat{H} = \hat{p}_1^2/2m_1 + \hat{p}_2^2/2m_2 + V(|\hat{\vec{r}}_2 - \hat{\vec{r}}_1|)$$

$$\hat{p}_i^2 = \sum_{\alpha=1}^{3} \hat{p}_{i\alpha}^2 \quad , \alpha = 1,2,3 \text{ or } x,y,z \quad i = 1,2$$

* Neglect spin DOF : $|\vec{r}_1, \vec{r}_2\rangle = |\vec{r}_1\rangle_1 \otimes |\vec{r}_2\rangle_2$ ($\otimes$ Direct or Tensor prod) ("Joining" of Hilbert spaces)

* Translations :

$$\hat{T}_1(\vec{a})|\vec{r}_1, \vec{r}_2\rangle = e^{-i\hat{\vec{p}}_1\cdot\vec{a}/\hbar}|\vec{r}_1\vec{r}_2\rangle = |\vec{r}_1 + \vec{a}, \vec{r}_2\rangle$$

$$\hat{T}_2(\vec{a})|\vec{r}_1\vec{r}_2\rangle = e^{-i\hat{\vec{p}}_2\cdot\vec{a}/\hbar}|\vec{r}_1\vec{r}_2\rangle = |\vec{r}_1, \vec{r}_2 + \vec{a}\rangle$$

$$\Rightarrow \begin{cases} [\hat{p}_1, \hat{p}_2] = 0 \\ \hat{T}_1(\vec{a})\hat{T}_2(\vec{a})|\vec{r}_1\vec{r}_2\rangle = \left(\hat{T}_1(\vec{a})|\vec{r}_1\rangle_1\right)\otimes\left(\hat{T}_2(\vec{a})|\vec{r}_2\rangle_2\right) = \end{cases}$$

$$= e^{-i\hat{\vec{p}}_1\cdot\vec{a}/\hbar}|\vec{r}_1\rangle_1 \otimes e^{-i\hat{\vec{p}}_2\cdot\vec{a}/\hbar}|\vec{r}_2\rangle_2$$

$$= e^{-i(\hat{\vec{p}}_1+\hat{\vec{p}}_2)\cdot\vec{a}/\hbar}|\vec{r}_1\rangle_1 \otimes |\vec{r}_2\rangle_2$$

$\boxed{\hat{\vec{P}} \text{ is the generator of simultaneous translation of both pcls.}}$

$$= e^{-i\hat{\vec{P}}\cdot\vec{a}/\hbar}|\vec{r}_1\vec{r}_2\rangle$$

where $\hat{P} \equiv \hat{p}_1 + \hat{p}_2$

inter-pcl. distance not affected

$\Downarrow$

$$[\hat{H}, \hat{T}_1(\vec{a})\cdot\hat{T}_2(\vec{a})] \Rightarrow [\hat{H}, \hat{\vec{P}}] = 0 \quad \text{transl. invariance of } \hat{H}$$

$$\Rightarrow 0 = \langle[\hat{H}, \hat{\vec{P}}]\rangle i/\hbar = \frac{d\langle\vec{P}\rangle}{dt} \Rightarrow \boxed{\langle\vec{P}\rangle = \text{const. of motion}}$$

Generator of infinitesimal spatial rotations : Orbital angular momentum $\hat{\vec{L}}$

$$\hat R_z(d\varphi) = \hat{1} - \frac{i \hat L_z d\varphi}{\hbar} \qquad \left(\hat L_{\substack{z\\x\\y}} = \hat x_{\substack{\\y\\z}} \hat p_{\substack{y\\z\\x}} - \hat y_{\substack{\\z\\x}} \hat p_{\substack{x\\y\\x}} \dots \right)$$

* Rotations:

$$\hat{\mathbb{R}}(d\varphi, \vec z)\,|\vec r\rangle \doteq |x - y\,d\varphi,\ y + x\,d\varphi,\ z\rangle$$

$$= \left(\hat 1 - \frac{i}{\hbar}\hat L_z\, d\varphi\right)|\vec r\rangle$$

$\hat L_z = \hat x \hat p_y - \hat y \hat p_x$ a.s.o. $\quad = \left(\hat 1 - \frac{i}{\hbar}\hat L_z\, d\varphi\right)|x, y, z\rangle$

$$[\hat L_z, \hat x] = i\hbar \hat y \ ; \ [\hat L_z, \hat y] = -i\hbar \hat x \ ; \ [\hat L_z, \hat z] = 0$$

$$\Rightarrow \quad [\hat L_z, \hat x^2 + \hat y^2 + \hat z^2] = 0 = [\hat L_z, \hat r^2]$$

$$\Rightarrow \boxed{[\hat L_z, V(\hat r)] = 0}$$

OR

$$|\vec r\rangle = |r, \theta, \varphi\rangle \ , \ \hat{\mathbb{R}}(d\varphi, \vec z)|r, \theta, \varphi\rangle = |r, \theta, \varphi + d\varphi\rangle$$

$$\hat{\mathbb{R}}(d\varphi, \vec z)\underbrace{V(\hat r)|r, \theta, \varphi\rangle} = \hat{\mathbb{R}}(d\varphi, \vec z)\underbrace{V(r)|r\theta\varphi\rangle}$$

$$= V(r)\underbrace{\hat{\mathbb{R}}(d\varphi, \vec z)|r\theta\varphi\rangle} = \underbrace{V(r)\,|r}\theta, \varphi + d\varphi\rangle$$

$$= V(\hat r)|r\theta\varphi + d\varphi\rangle = V(\hat r)\hat{\mathbb{R}}(d\varphi, \vec z)|r\theta\varphi\rangle$$

$$\Rightarrow \hat{\mathbb{R}} V(\hat r) = V(\hat r)\hat{\mathbb{R}} \quad \Rightarrow [\hat{\mathbb{R}}(d\varphi, \vec z), V(\hat r)] = 0$$

$$\Rightarrow \boxed{[\hat L_z, V(\hat r)] = 0}$$

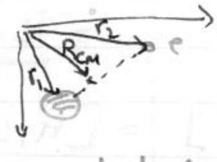
Also $\boxed{[\hat H, \hat L_x] = [\hat H, \hat L_y] = [\hat H, \hat L_z] = 0}$

Rotational invariance of $\hat H$

(Townsend 9.2)

Two-body Hamiltonian. Relative and CM coordinates

$$\hat{H} = \hat{p}_1^2/2m_1 + \hat{p}_2^2/2m_2 + V(|\vec{r}_2 - \vec{r}_1|)$$



$\vec{r} = \vec{r}_1 - \vec{r}_2$, $\vec{R}_{CM} = \dfrac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1+m_2}$, $\vec{P}_{CM} = \vec{p}_1 + \vec{p}_2$ ← total momentum

$[\hat{x}_i, \hat{P}_j] = 0$; $[\hat{X}_i, \hat{P}_j] = i\hbar\,\delta_{ij}$

relative mom: $\hat{\vec{p}} \equiv \dfrac{m_2\vec{p}_1 - m_1\vec{p}_2}{m_1+m_2}$ $\left(\vec{p} = \dfrac{m_1 m_2}{m_1+m_2}\underbrace{(\vec{v}_1 - \vec{v}_2)}_{\vec{v}_{rel}} = \dfrac{m_2\vec{p}_1 - m_1\vec{p}_2}{m_1+m_2} \right)$

$[\hat{x}_i, \hat{p}_j] = i\hbar\,\delta_{ij}$, $[\hat{X}_i, \hat{p}_j] = 0$

$\boxed{|\vec{r}_1\vec{r}_2\rangle \to |\vec{r}\,\vec{R}\rangle}$ ← relative coordinates

$$\boxed{\hat{H} = \hat{P}_{CM}^2/2M + \hat{p}^2/2\mu + V(|\vec{r}|)}$$

$M \equiv m_1 + m_2$

$\mu \equiv \dfrac{m_1 m_2}{m_1+m_2}$

$$\underbrace{\hat{P}_{CM}^2/2M}_{\hat{H}_{CM}} \qquad \underbrace{\hat{p}^2/2\mu + V(|\vec{r}|)}_{\hat{H}_{rel}}$$

$[\hat{H}_{CM}, \hat{H}_{rel}] = 0 \Rightarrow |\epsilon_{cm}, \epsilon_{rel}\rangle$:

$$\hat{H}|\epsilon_{cm}, \epsilon_{rel}\rangle = (\hat{H}_{cm} + \hat{H}_{rel})|\epsilon_{cm}, \epsilon_{rel}\rangle$$
$$= (\epsilon_{cm} + \epsilon_{rel})|\epsilon_{cm}, \epsilon_{rel}\rangle$$

e-functions of $\hat{H}_{cm}$: $\varphi_{\vec{P}_{cm}}(\vec{R}_{CM}) = \langle \vec{R}_{cm}|\vec{P}_{cm}\rangle = \dfrac{e^{i\vec{P}_{cm}\cdot\vec{R}_{cm}/\hbar}}{(2\pi\hbar)^{3/2}}$

Approach: $\boxed{\text{Analyze dynamics in the CM frame}}$

↳ $\vec{P}_{CM} = 0$, $\epsilon = \epsilon_{rel}$

↳ $\boxed{\hat{H} = \hat{p}^2/2\mu + V(\hat{r})}$

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(3D TISE in Position Space) 4

Complete Set of Commuting Operators (CSCO)

~~Bound States in Central Potentials~~ (Townsend 9.6)

+ Bound States in Central Potentials (Townsend 10.1)

$[\hat{H}, \hat{L}^2] = [\hat{H}, \hat{L}_z] = 0 \Rightarrow |E\, l\, m\rangle$:

$$\left.\begin{aligned} \hat{H}|E l m\rangle &= E|E l m\rangle \\ \hat{L}^2|E l m\rangle &= \hbar^2 l(l+1)|E l m\rangle \\ \hat{L}_z|E l m\rangle &= \hbar m|E l m\rangle \end{aligned}\right\} \text{CSCO}$$

$$\hat{H} = \hat{p}^2/2\mu + V(\hat{r})$$

TISE in $\vec{r}$-space:

$$\langle \vec{r}|\hat{H}|\psi\rangle = 1/2\mu \langle \vec{r}|\hat{p}^2|\psi\rangle + \langle \vec{r}|V(\hat{r})|\psi\rangle \stackrel{!}{=} E\langle \vec{r}|\psi\rangle$$

$$\Rightarrow \left[\cancel{1/2}\mu\left(-\hbar^2\nabla^2\right) + V(r)\right]\langle \vec{r}|\psi\rangle = E\langle \vec{r}|\psi\rangle$$

$-\hat{L}^2/\hbar^2$ in $\vec{r}$-space

$\langle \vec{r}|\psi\rangle = \psi_{Elm}(\vec{r})$

$$\Rightarrow \left[-\hbar^2/2\mu\left\{\partial_r^2 + \frac{2}{r}\partial_r + \frac{1}{r^2}\underbrace{\left[\frac{1}{\sin\theta}\partial_\theta(\sin\theta\,\partial_\theta) + \frac{1}{\sin^2\theta}\partial_\varphi^2\right]}_{=\langle \vec{r}|-\hat{L}^2/\hbar^2|\psi\rangle}\right\} + V(r)\right]\psi_{Elm}(r,\theta,\varphi) = E\,\psi_{Elm}(r,\theta,\varphi)$$

$$-\frac{\hbar^2}{2\mu}\left(\partial_r^2 + \frac{2}{r}\partial_r\right) + \frac{\hat{L}^2}{2\mu r^2}$$

$\hat{L}^2(\psi_{Elm}(r,\theta,\varphi)) = \hbar^2 l(l+1)\psi_{Elm}(r,\theta,\varphi)$

$$\Rightarrow \left[-\frac{\hbar^2}{2\mu}\left(\partial_r^2 + \frac{2}{r}\partial_r\right) + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r)\right]\psi_{Elm}(r\theta\varphi) = E\,\psi_{Elm}(r,\theta,\varphi)$$

Separate $\psi_{Elm}(r,\theta,\varphi) = R_E(r)Y_{lm}(\theta,\varphi)$:

$$\boxed{\left[-\frac{\hbar^2}{2\mu}\left(d_r^2 + \frac{2}{r}d_r\right) + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r)\right]R(r) = E R(r)}$$

Radial S.E.

Let $\boxed{u(r) = r R(r)}$

TISE

$$\Rightarrow \boxed{\left[\underbrace{-\frac{\hbar^2}{2\mu}d_r^2}_{KE} + \underbrace{\frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r)}_{V_{eff}(r)}\right]u(r) = E\,R(r)}$$

$\to$ centrifugal barrier

The problem is re-cast to a simpler 1D problem of solving for the dynamics of a particle in the effective potential

$$V_{eff}(r) \equiv \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} + V(r) \quad \left(= \frac{L^2}{2I} + V(r) \right)$$

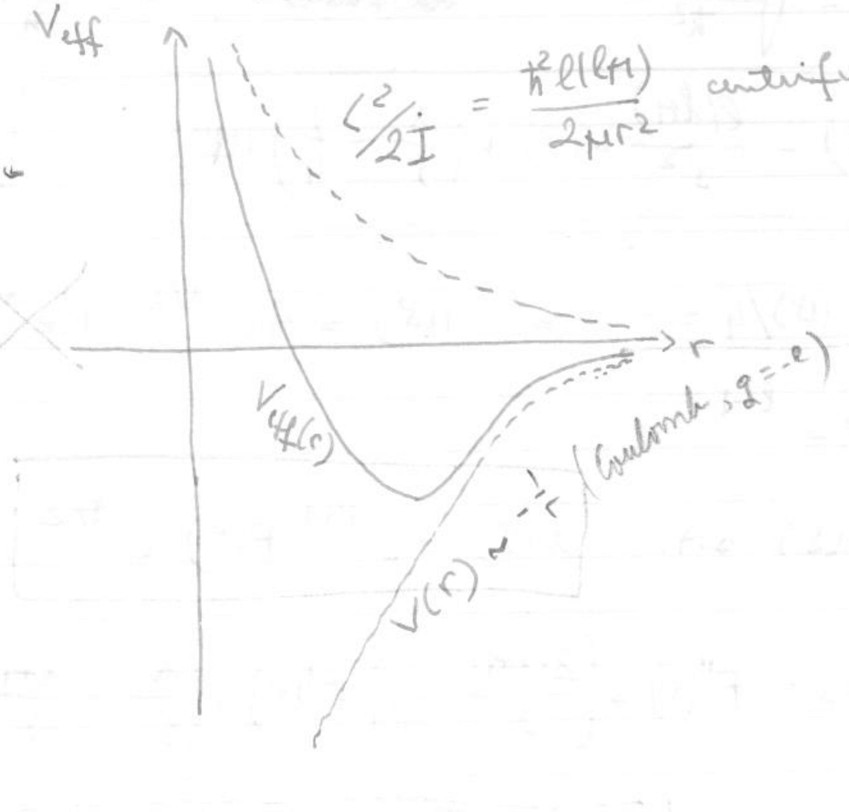
* Note:

No "m" dependence in the radial TISE $\Leftrightarrow$ $\Leftrightarrow$ rotational invariance of $\hat{H}$.

This, however, is not the real ~~...~~ state of the hydrogenic atoms $\to$ need spin DOF such that $|E \ell m s\rangle$ e^- p^+

These are the states that form a complete set and can be used as an efficient basis.

TISE: $\left[\frac{-\hbar^2}{2\mu} \frac{d^2}{dr^2} + V_{eff}(r) \right] u(r) = \epsilon\, u(r)$



(Townsend 10.1) ~~Bound States in Central Potentials~~

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TISE on p. 64

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* Transfer of normalization from $R(r)$ to $u(r)$:

$$\int_0^\infty dr\, |R(r)|^2 r^2 = 1 = \int_0^\infty dr\, |u(r)|^2$$

see Townsend p. 275-276 for details

$$u(r) \xrightarrow[r\to 0]{} r^{l+1} \quad \left(R(r) \xrightarrow[r\to 0]{} r^l\right)$$

"Boundary" Conditions:

(BC1) $\lim_{r\to 0} r^2 V(r) = 0$ i.e. $V(r) \sim \frac{1}{r^k}$, $k \le 2$ $\Rightarrow \begin{cases} u(r) \xrightarrow[r\to 0]{} r^{l+1} \\ R(r) \xrightarrow[r\to 0]{} r^l \end{cases}$

(BC2) $\lim_{r\to\infty} R(r) = \lim_{r\to\infty} u(r) = 0$ ~~+ ...~~ $\Rightarrow u(r) \xrightarrow[r\to\infty]{} e^{-ar}$

Hydrogenic Atoms. The Coulomb Potential

$$V(r) = \frac{(Ze)(-e)}{r} = -\frac{Ze^2}{r} \quad \left(\text{SI}: e \to e/4\pi\varepsilon_0 \right)$$

TISE: $\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} - \frac{Ze^2}{r} \right] u(r) = E\, u(r)$

Bound states $E = -|E| < 0$

Set $\rho \equiv \sqrt{\frac{8\mu|E|}{\hbar^2}}\, r$ ~~...~~ ; $\lambda \equiv \frac{Ze^2}{\hbar}\sqrt{\frac{\mu}{2|E|}}$

$$\boxed{u''(\rho) - \frac{l(l+1)}{\rho^2}u(\rho) + \left(\frac{\lambda}{\rho} - \frac{1}{4}\right)u(\rho) = 0} \quad (1)$$

$\rho \to \infty$: $\quad u''(\rho) - u(\rho)/4 = 0 \Rightarrow u(\rho) = Ae^{-\rho/2} + \cancel{Be^{\rho/2}}$ (BC2)

$\rho \to 0$: $\quad u(\rho) \sim \rho^{l+1}$

$\Rightarrow$ seek $F(\rho)$ s.t. $\boxed{u(\rho) = \rho^{l+1} F(\rho)\, e^{-\rho/2}}$

$\Rightarrow$ (1) becomes: $F''(\rho) + \left[\frac{2(l+1)}{\rho} - 1\right]F'(\rho) + \left(\frac{\lambda}{\rho} - \frac{l+1}{\rho}\right)F(\rho) = 0$ (2)

* Seek solution: $\boxed{F(\rho) = \sum_{k=0}^\infty c_k \rho^k, \quad c_0 \ne 0}$ (3)

(2) becomes a recurrence relation:

$$\sum_{k=2}^{\infty} k(k-1) c_k \rho^{k-2} + \sum_{k=1}^{\infty} 2(l+1)k c_k \rho^{k-2} + \sum_{k=0}^{\infty} \left[-k+\lambda-(l+1)\right] c_k \rho^{k-1} = 0$$

chg. var: $k' = k-1 \Rightarrow$

$$\sum_{k=0}^{\infty} \left\{ \left[k(k+1) + 2(l+1)(k+1)\right] c_{k+1} + \left[-k+\lambda-(l+1)\right] c_k \right\} \rho^{k-1} = 0$$

$$\Rightarrow \frac{c_{k+1}}{c_k} = \frac{k+l+1-\lambda}{(k+1)(k+2l+2)} \xrightarrow[k\to\infty]{} \frac{1}{k} \quad \text{same as } e^{\rho}$$

$\Rightarrow$ series for $F(\rho)$ (3) must terminate to avoid exponential growth to ∞.

$\Downarrow$

set $\boxed{\lambda = 1 + l + n_r}$, $n_r = 0, 1, 2, 3 \ldots$

to determine $\underline{\underline{k}}$ at which series must be truncated.

$\Rightarrow$ <u>$F(\rho)$ is a n_r-degree polynomial</u>. $\Rightarrow$ <u>Assoc. Laguerre Poly</u>

$\Rightarrow$ Quantized energies:

$$E = -\frac{\mu Z^2 e^4}{2\hbar^2 \lambda^2} = -\frac{\mu Z^2 e^4}{2\hbar^2 \underbrace{(1+l+n_r)^2}_{n}}$$

$\boxed{n \equiv 1 + l + n_r}$ Principal Quantum Number.

$(R_y)_{SI} = \frac{\mu e^4}{8 h^2 \varepsilon_0} = 2.179 \times 10^{-18}\,J = 13.6\,eV$

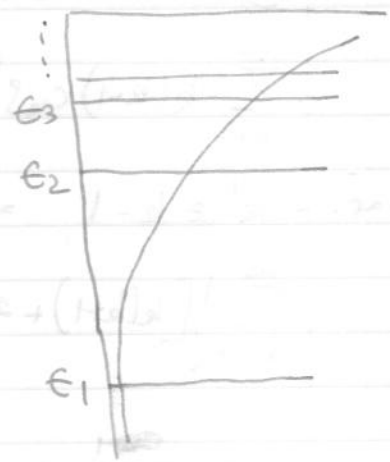
$(R_y)_{CGS} = \frac{\mu e^4}{2\hbar^2}$

$$\boxed{\epsilon_n = -\frac{\mu Z^2 e^4}{2\hbar^2 n^2}} \quad , n = 1, 2, 3, \ldots$$

$$\epsilon_n = -Z^2 \frac{R_y}{n^2} = -\frac{\mu c^2 Z^2}{2n^2} \alpha^2 \quad , \alpha = \frac{e^2}{\hbar c} = \frac{1}{137}$$

Hydrogen : $Z = 1$

$$\Rightarrow \boxed{E_n = -\frac{13.6\,\text{eV}}{n^2}}$$



Transition $\quad \hbar\omega = \epsilon_{n_i} - \epsilon_{n_f} = \frac{\mu c^2 \alpha^2}{2}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$

$$\frac{1}{\lambda} = \underbrace{\frac{\mu c \alpha^2}{2h}}_{R_H}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

Eigenfunctions of the hydrogen atom:

$$\psi_{n\ell m}(r,\theta,\varphi) = R_{n\ell}(r)\, Y_{\ell m}(\theta,\varphi) \quad ; \quad 1 = \int_0^\infty dr\, |R(r)|^2 r^2 = \int_0^\infty dr\, |u(r)|^2$$

$$1 = \int d\Omega\, |Y_{\ell m}(\theta,\varphi)|^2$$

Radial e-fcns :

The Parity Operator: Spatial Inversion Symmetry

$$\hat{\Pi}|x\rangle = |-x\rangle$$

- E-value problem: $\hat{\Pi}|\lambda\rangle = \lambda|\lambda\rangle$; $\left.\begin{array}{l}\hat{\Pi}^2|\lambda\rangle \overset{1}{=} \lambda^2|\lambda\rangle \\ \quad\quad\;\; \overset{2}{=} |\lambda\rangle\end{array}\right\} \Rightarrow$

$\boxed{\lambda = \pm 1}$ e-values of the parity operator.

- Arbitrary state in position representation: $\left\{\begin{array}{l}\langle x|\psi\rangle = \psi(x) \\ \langle -x|\psi\rangle = \psi(-x)\end{array}\right.$

$$\underline{\langle x|\hat{\Pi}}|\psi\rangle = \langle -x|\psi\rangle = \psi(-x)$$

- Parity e-states: $\left.\begin{array}{l}\underbrace{\langle x|\hat{\Pi}}_{1}\underbrace{\hat{\Pi}|\psi_\lambda\rangle}_{2} \overset{1}{=} \langle -x|\psi_\lambda\rangle = \psi_\lambda(-x) \\ \quad\quad\quad\quad\;\; \overset{2}{=} \langle x|\lambda|\psi_\lambda\rangle = \lambda\langle x|\psi_\lambda\rangle = \lambda\psi_\lambda(x)\end{array}\right\}$

$$\Rightarrow \boxed{\psi_\lambda(-x) = \lambda\psi_\lambda(x) \quad \text{with } \lambda = \pm 1}$$

$$\text{i.e.} \left\{\begin{array}{ll}\psi_+(-x) = \psi_+(x) & \text{even parity} \\ \psi_-(-x) = -\psi_-(x) & \text{odd parity}\end{array}\right.$$

- $\langle x|\hat{\Pi}\hat{H}|\psi\rangle = \underline{\langle x|\hat{\Pi}}\left(\frac{\hat{p}^2}{2m} + V(\hat{x})\right)|\psi\rangle =$

$$= \langle -x|\hat{p}^2/2m + V(\hat{x})|\psi\rangle = \left[-\partial_x^2/2m + V(-x)\right]\psi(-x)$$

$$= \left\{\begin{array}{ll}\left[-\partial_x^2/2m + \underline{V(x)}\right]\psi(-x) = \underline{\langle x|\hat{H}\hat{\Pi}|\psi\rangle} & \text{if } V(-x) = V(x) \text{ i.e. SHO} \sim x^2 \\ \Rightarrow [\hat{H},\hat{\Pi}] = 0 & \\ \left[-\partial_x^2/2m - V(x)\right]\psi(-x) \neq \langle x|\hat{H}\hat{\Pi}|\psi\rangle & \text{if } V(-x) = -V(x) \text{ i.e. Coulomb } 1/r\end{array}\right.$$

Usage: Observing behavior of $\hat{H}$ under inversion simplifies calculation of expectation values, matrix elements etc without solving the e-value problem.

In 3D: inversion in spherical coordinates $= \begin{cases} r \to r \\ \theta \to \pi-\theta \\ \varphi \to \varphi+\pi \end{cases}$

$$\hat{\Pi}\, Y_{lm}(\theta\varphi) = (-1)^l\, Y_{lm}(\theta,\varphi)$$

$$\Big(Y_{lm}(\pi-\theta, \varphi+\pi) \Big) \quad \begin{cases} \cos\theta \to \cos(\pi-\theta) = -\cos\theta \\ \sin\theta \to \sin(\pi-\theta) = \sin\theta \\ e^{im\varphi} \to e^{im(\varphi+\pi)} = (-1)^m e^{im\varphi} \end{cases}$$

$$\Rightarrow Y_{lm}(\theta\varphi) \to Y_{lm}(\theta,\varphi)(-1)^m(-1)^{l-m} = (-1)^l Y_{lm}(\theta\varphi)$$

TIP 1

Time-Independent Perturbations

1) Non-degenerate theory

$$\hat{H} = \hat{H}_0 + \hat{H}_1 \lambda \qquad \left(\hat{H}_1 \text{"}\ll\text{"} \hat{H}_0\right)$$

Known: Known: $\hat{H}_0 |\varphi_n^0\rangle = \epsilon_n^0 |\varphi_n^0\rangle$, $|\varphi_n^0\rangle \equiv |E_n^0\rangle$ (1)

GOAL

Unknown: Unknown: $\hat{H}|\psi_n\rangle = \epsilon_n |\psi_n\rangle$, $\epsilon_n, |\psi_n\rangle = ?$ (2)

λ - perturbative parameter $\lambda = 0 \Rightarrow \hat{H} = \hat{H}_0$; $\lambda \to 1 \Rightarrow \hat{H} \to \hat{H}_0 + \hat{H}_1$

Seek
$$\begin{cases} |\psi_n\rangle = |\varphi_n^0\rangle + \lambda|\varphi_n^1\rangle + \lambda^2|\varphi_n^2\rangle + \dots = \sum_{\alpha=0}^{\infty} \lambda^\alpha |\varphi_n^\alpha\rangle & (3) \\ \epsilon_n = \epsilon_n^0 + \lambda \epsilon_n^1 + \lambda \epsilon_n^2 + \dots = \sum_{\alpha=0}^{\infty} \lambda^\alpha \epsilon_n^\alpha & (4) \end{cases}$$

$$\hat{H}|\psi_n\rangle = \left(\hat{H}_0 + \lambda \hat{H}_1\right) \sum_{\alpha=0}^{\infty} \lambda^\alpha |\varphi_n^\alpha\rangle \overset{!}{=} \left(\sum_{\alpha=0}^{\infty} \lambda^\alpha \epsilon_n^\alpha\right)\left(\sum_\beta \lambda^\beta |\varphi_n^\beta\rangle\right)$$

$\Rightarrow$ power-wise identification (coeffs λ^α):

λ^0: $\hat{H}_0|\varphi_n^0\rangle = \epsilon_n^0|\varphi_n^0\rangle$

λ^1: $\hat{H}_0|\varphi_n^1\rangle + \hat{H}_1|\varphi_n^0\rangle = \epsilon_n^0|\varphi_n^1\rangle + \epsilon_n^1|\varphi_n^0\rangle$

λ^2: $\hat{H}_0|\varphi_n^2\rangle + \hat{H}_1|\varphi_n^1\rangle = \epsilon_n^0|\varphi_n^2\rangle + \epsilon_n^1|\varphi_n^1\rangle + \epsilon_n^2|\varphi_n^0\rangle$

λ^k: $\hat{H}_0|\varphi_n^k\rangle + \hat{H}_1|\varphi_n^{k-1}\rangle = \sum_{l=0}^{k} \epsilon_n^l |\varphi_n^{k-l}\rangle$ $\quad \epsilon_n = ?$

a) First-order energy e-value correction: do $\langle \varphi_n^0|$ "λ^1-term":

$$\langle \varphi_n^0|\hat{H}_0|\varphi_n^1\rangle + \langle \varphi_n^0|\hat{H}_1|\varphi_n^0\rangle = \epsilon_n^0 \langle \varphi_n^0|\varphi_n^1\rangle + \epsilon_n^1 \underbrace{\langle \varphi_n^0|\varphi_n^0\rangle}_{=1}$$

$$\epsilon_n^0 \cancel{\langle \varphi_n^0|\varphi_n^1\rangle}^{=0} + \langle \varphi_n^0|\hat{H}_1|\varphi_n^0\rangle = \epsilon_n^0 \cancel{\langle \varphi_n^0|\varphi_n^1\rangle}^{=0} + \epsilon_n^1$$

$$\Rightarrow \boxed{\epsilon_n^1 = \langle \varphi_n^0|\hat{H}_1|\varphi_n^0\rangle} \quad (5)$$

TIP 2

$|\psi_n\rangle = ?$

b) First-order e-ket correction: do $\langle \varphi_k^0|$ "λ^1-term":

previous page Eq (5)

$$\langle \varphi_k^0|\hat{H}_0|\varphi_n^1\rangle + \langle \varphi_k^0|\hat{H}_1|\varphi_n^0\rangle = \epsilon_n^0 \langle \varphi_k^0|\varphi_n^1\rangle + \epsilon_n^1 \underbrace{\langle \varphi_k^0|\varphi_n^0\rangle}_{\delta_{kn}}$$

$$\epsilon_k^0 \langle \varphi_k^0|\varphi_n^1\rangle + \langle \varphi_k^0|\hat{H}_1|\varphi_n^0\rangle = \epsilon_n^0 \langle \varphi_k^0|\varphi_n^1\rangle + \langle \varphi_n^0|\hat{H}_1|\varphi_n^0\rangle \delta_{kn}$$

$$\langle \varphi_k^0|\varphi_n^1\rangle (\epsilon_n^0 - \epsilon_k^0) = \langle \varphi_k^0|\hat{H}_1|\varphi_n^0\rangle - \underbrace{\langle \varphi_n^0|\hat{H}_1|\varphi_n^0\rangle \delta_{kn}}_{=0,\ \text{for } k\neq n}$$

$\boxed{k \neq n}$ => $\delta_{kn} = 0$

$$\boxed{\langle \varphi_k^0|\varphi_n^1\rangle = \frac{\langle \varphi_k^0|\hat{H}_1|\varphi_n^0\rangle}{\epsilon_n^0 - \epsilon_k^0}} \quad \boxed{k\neq n}$$

-> superposition coefficients (6)

in $\{|\varphi_k^0\rangle\}$ basis: unperturbed basis

$$|\varphi_n^1\rangle = \sum_k |\varphi_k^0\rangle\langle \varphi_k^0|\varphi_n^1\rangle = \sum_{k\neq n} |\varphi_k^0\rangle \frac{\langle \varphi_k^0|\hat{H}_1|\varphi_n^0\rangle}{\epsilon_n^0 - \epsilon_k^0} + |\varphi_n^0\rangle\langle \varphi_n^0|\varphi_n^1\rangle$$

⚠

$$= |\varphi_n^0\rangle\langle \varphi_n^0|\varphi_n^1\rangle + \sum_{k\neq n} |\varphi_k^0\rangle\langle \varphi_k^0|\varphi_n^1\rangle \quad (7)$$

$\langle \varphi_n^0|\varphi_n^1\rangle = ?$

$$1 \stackrel{!}{=} \langle \psi_n|\psi_n\rangle = \left(\sum_{\alpha=0}^{\infty} \lambda^\alpha \langle \varphi_n^\alpha|\right)\left(\sum_{\beta=0}^{\infty} \lambda^\beta |\varphi_n^\beta\rangle\right) =$$

$$= \sum_\alpha \sum_\beta \lambda^\alpha \lambda^\beta \langle \varphi_n^\alpha|\varphi_n^\beta\rangle$$

$$= \underbrace{\langle \varphi_n^0|\varphi_n^0\rangle}_{=1} + \lambda \underbrace{\langle \varphi_n^0|\varphi_n^1\rangle}_{\stackrel{!}{=} iA} + \lambda \underbrace{\langle \varphi_n^1|\varphi_n^0\rangle}_{=-iA} + \mathcal{O}(\lambda^2)$$

to keep $\langle \psi_n|\psi_n\rangle = 1$ → iA (A real) i.e. purely imaginary

=>

$$|\psi_n\rangle = |\varphi_n^0\rangle + \lambda|\varphi_n^1\rangle + \lambda^2|\varphi_n^2\rangle + \dots$$

$$\stackrel{(7)}{=} |\varphi_n^0\rangle + iA\lambda|\varphi_n^0\rangle + \lambda \sum_{k\neq n} |\varphi_k^0\rangle\langle \varphi_k^0|\varphi_n^1\rangle + \mathcal{O}(\lambda^2)$$

$$\approx e^{iA\lambda}|\varphi_n^0\rangle + \lambda \sum_{k\neq n} |\varphi_k^0\rangle\langle \varphi_k^0|\varphi_n^1\rangle + \dots \mathcal{O}(\lambda^2) \quad (8)$$

Phase of $|\psi_n\rangle$ ($A\lambda$) is arbitrary -> can choose $A=0$ s.t. $\boxed{\langle \varphi_n^0|\varphi_n^1\rangle \stackrel{!}{=} 0}$ (9)

=> Phase of $|\psi_n\rangle$ = Phase of $|\varphi_n^0\rangle$ to $\mathcal{O}(\lambda^1)$

Condition (9) i.e. $\boxed{\langle \varphi_n^0 | \varphi_n^1 \rangle \overset{!}{\simeq} 0}$ (to $\overset{\mathcal{O}(\lambda)}{\text{1st order in } \lambda}$)
implies the orthogonality of the 1st correction kets to the "main" kets

$$\Leftrightarrow |\psi_n\rangle = |\varphi_n^0\rangle + \lambda |\varphi_n^1\rangle + \dots = |\varphi_n^0\rangle + \lambda \underbrace{\sum_{k \neq n} |\varphi_k^0\rangle\langle \varphi_k^0 | \varphi_n^1\rangle}_{\text{small correction to } |\varphi_n^0\rangle} + \dots$$

(both in magnitude and direction)

$$\overset{(6)}{\Rightarrow} \boxed{|\psi_n\rangle = |\varphi_n^0\rangle + \lambda \sum_{k \neq n} |\varphi_k^0\rangle \frac{\langle \varphi_k^0 | \hat{H}_1 | \varphi_n^0\rangle}{\epsilon_n^0 - \epsilon_k^0} + \mathcal{O}(\lambda^2)} \quad (10)$$

Second-order energy correction: do $\langle \varphi_n^0 |$ "λ^2-term":

$$\underbrace{\langle \varphi_n^0 | \hat{H}_0}_{} | \varphi_n^2\rangle + \langle \varphi_n^0 | \hat{H}_1 | \varphi_n^1\rangle = \epsilon_n^0 \langle \varphi_n^0 | \varphi_n^2\rangle + \epsilon_n^1 \underbrace{\langle \varphi_n^0 | \varphi_n^1\rangle}_{\simeq 0 \ (\text{Eq } 9)} + \epsilon_n^2 \underbrace{\langle \varphi_n^0 | \varphi_n^0\rangle}_{=1}$$

$$\cancel{\epsilon_n^0 \langle \varphi_n^0 | \varphi_n^2\rangle} + \langle \varphi_n^0 | \hat{H}_1 | \varphi_n^1\rangle = \cancel{\epsilon_n^0 \langle \varphi_n^0 | \varphi_n^2\rangle} + \cancel{\epsilon_n^1 \langle \varphi_n^0 | \varphi_n^1\rangle} + \epsilon_n^2$$

$$\Rightarrow \epsilon_n^2 = \langle \varphi_n^0 | \hat{H}_1 \underset{\mathbb{1}}{|} \varphi_n^1\rangle = \langle \varphi_n^0 | \hat{H}_1 \sum_k |\varphi_k^0\rangle\langle \varphi_k^0 | \varphi_n^1\rangle$$

$$\overset{(7)}{=} \langle \varphi_n^0 | \hat{H}_1 | \varphi_n^0\rangle \underbrace{\langle \varphi_n^0 | \varphi_n^1\rangle}_{\simeq 0 \ (9)} + \langle \varphi_n^0 | \hat{H}_1 \sum_{k \neq n} |\varphi_k^0\rangle \underbrace{\langle \varphi_k^0 | \varphi_n^1\rangle}_{\text{use } (6)}$$

$$= \langle \varphi_n^0 | \hat{H}_1 \sum_{k \neq n} |\varphi_k^0\rangle \frac{\langle \varphi_k^0 | \hat{H}_1 | \varphi_n^0\rangle}{\epsilon_n^0 - \epsilon_k^0}$$

$$\Rightarrow \boxed{\epsilon_n^2 = \sum_{k \neq n} \frac{\langle \varphi_n^0 | \hat{H}_1 | \varphi_k^0\rangle\langle \varphi_k^0 | \hat{H}_1 | \varphi_n^0\rangle}{\epsilon_n^0 - \epsilon_k^0} = \sum_{k \neq n} \frac{\left| \langle \varphi_k^0 | \hat{H}_1 | \varphi_n^0\rangle \right|^2}{\epsilon_n^0 - \epsilon_k^0}} \quad (11)$$

Time-indep. Perturbation Theory with Degeneracy

Degeneracy: more states $\{|\varphi^0_{n,i}\rangle\}_{i=1,2,..N}$ where energy ϵ^0_n

=> divergence of ~~first~~ 2nd-order correction E^2_n term $\frac{\langle \varphi^0_k|\hat{H}_1|\varphi^0_n\rangle}{\epsilon^0_n - \epsilon^0_k}$

* Without degeneracy: $|\varphi^0_n\rangle \xrightarrow{\lambda\nearrow} |\psi_n\rangle$

* With degeneracy: $\underbrace{\sum_{i=1}^{N} a_i |\varphi^0_{n,i}\rangle}$ $\xrightarrow{\lambda\nearrow} |\psi_n\rangle$

any L.C. of degenerate states can become the exact state
unperturbed perturbed

Question: which L.C. is the one that becomes $|\psi_n\rangle$ as $\lambda_0 \nearrow 1$?

Seek

$$\boxed{|\psi_n\rangle = \sum_{i=1}^{N} c_i |\varphi^0_{n,i}\rangle + \lambda |\varphi^1_n\rangle + \dots} \quad (12) \quad \boxed{\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle}$$

λ^1:

$$\hat{H}_0|\varphi^1_n\rangle + \hat{H}_1 \sum_{i=1}^{N} c_i|\varphi^0_{n,i}\rangle = \epsilon^0_n|\varphi^1_n\rangle + \epsilon^1_n \sum_{i=1}^{N} c_i |\varphi^0_{n,i}\rangle \quad (13)$$

identify term

$\langle \varphi^0_{n,j}|$ =>

$$\underbrace{\langle \varphi^0_{n,j}|\hat{H}_0|\varphi^1_n\rangle}_{=\epsilon^0_n\langle\varphi^0_{n,j}|\varphi^1_n\rangle} + \sum_i c_i \langle \varphi^0_{n,j}|\hat{H}_1|\varphi^0_{n,i}\rangle = \cancel{\epsilon^0_n\langle \varphi^0_{n,j}|\varphi^1_n\rangle} + \epsilon^1_n \sum_i c_i \langle\varphi^0_{n,j}|\varphi^0_{n,i}\rangle$$

$$\Rightarrow \sum_{i=1}^{N} c_i \underbrace{\langle \varphi^0_{n,j}|\hat{H}_1|\varphi^0_{n,i}\rangle}_{=(H_1)_{ji}} = \epsilon^1_n \sum_{i=1}^{N} c_i \underbrace{\langle \varphi^0_{n,j}|\varphi^0_{n,i}\rangle}_{\delta_{ij}} = \epsilon^1_n \sum_{i=1}^{N} \delta_{ij} c_i$$

$$\boxed{\sum_{i=1}^{N} c_i (H_1)_{ji} = \epsilon^1_n \sum_{i=1}^{N} c_i \delta_{ij}} \quad (14) \Rightarrow \underline{\epsilon^1_n = \dots}$$

(e-value problem for 1st order)

Ex: N = 2 =>

$$\begin{bmatrix} (H_1)_{11} & (H_1)_{12} \\ (H_1)_{21} & (H_1)_{22} \end{bmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \epsilon^{(1)}_n \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \quad (14')$$

-> solve to get e-values $\epsilon^{(1)}_n$ (1st order correction)

In the subspace of the degenerate states $\{|\varphi^0_{n,i}\rangle\}_{i=\overline{1,N}}$ (here, belonging to the unperturbed Hamiltonian $\hat{H}_0$), eq. (14) involves a diagonal perturbing Hamiltonian ($\hat{H}_1$):

$$\sum_i c_i (H_1)_{ji} = \epsilon_n^{(1)} \sum_i c_i \delta_{ij} \iff \boxed{(H_1)_{jj} = \epsilon_n^{(1)} \quad , j = 1, 2, \ldots, N} \quad (15)$$

i.e. $\hat{H}_1 \doteq \begin{pmatrix} \epsilon_n^{(1)} & & 0 \\ & \epsilon_n^{(1)} & \\ 0 & & \ddots \; \epsilon_n^{(1)} \end{pmatrix}$ so that ~~[illegible]~~:

$$\begin{pmatrix} \epsilon_n^{(1)} & \cdots & 0 \\ 0 & \cdots & \epsilon_n^{(1)} \end{pmatrix} \begin{pmatrix} c_1 \\ \vdots \\ c_N \end{pmatrix} = \epsilon_n^{(1)} \begin{pmatrix} c_1 \\ \vdots \\ c_N \end{pmatrix}$$

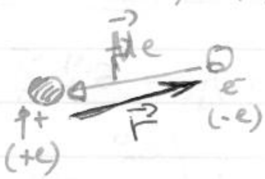
where $\begin{pmatrix} c_1 \\ \vdots \\ c_N \end{pmatrix} \doteq \sum_{i=1}^{N} c_i |\varphi^0_{n,i}\rangle$ is the ~~right~~ appropriate L.C. to be used to form the exact e-state $|\psi_n\rangle$ (eq. (12)) of the perturbed Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_1$

TIP6

Application The Stark Effect in Hydrogen : H-atom in uniform $\vec{\mathcal{E}}$-field

- unperturbed: $\hat{H}_0 = \hat{p}^2/2\mu - e^2/\hat{r}$ (in S.I. $e \to e/4\pi\varepsilon_0$) , $\mu = \frac{m_e m_p}{m_e + m_p}$

- perturbation: (dipole interaction) $\hat{H}_1 = -\vec{\mu}_e \cdot \vec{\mathcal{E}} = e\vec{r}\cdot\vec{\mathcal{E}}$



$\vec{\mu}_e = e(-\vec{r}) = -e\vec{r}$

$\hat{H}_0 |nlm\rangle = \epsilon_n^{(0)} |nlm\rangle$; $|\varphi^{(0)}_{nlm}\rangle \equiv |nlm^{(0)}\rangle$ unperturbed states

~~Det $\vec{\mu}_e = \mu_e \vec{z} \Rightarrow \hat{H}_1 = \hat{\mu}_e \vec{z}\cdot\vec{\mathcal{E}} = q$~~

Let $\vec{\mathcal{E}} = \mathcal{E}\vec{z} \Rightarrow \hat{H}_1 = -\vec{\mu}_e \cdot \mathcal{E}\vec{z} = e\mathcal{E}\hat{z}$ (16)

Ground state: $n=1$ $|\varphi^{(0)}_{100}\rangle = |100^{(0)}\rangle$, non-degenerate ; ϵ_1

1st order: $\epsilon_1^{(1)} = \langle \varphi^{(0)}_{100} | \hat{H}_1 | \varphi^{(0)}_{100}\rangle = \langle 100 | e\mathcal{E}\hat{z} | 100\rangle$

$$= e\mathcal{E}\langle 100^{\circ} | \hat{z} | 100^{\circ}\rangle = e\mathcal{E}\int d^3r \langle 100^{\circ}|\vec{r}\rangle\langle\vec{r}|\hat{z}|100^{\circ}\rangle$$

$$= e\mathcal{E}\int d^3r \langle 100^{\circ}|\vec{r}\rangle\langle\vec{r}|z|100^{\circ}\rangle = e\mathcal{E}\int d^3r\, z\, \underbrace{\langle 100^{\circ}|\vec{r}\rangle}_{\equiv\varphi^{(0)*}_{100}(\vec{r})}\underbrace{\langle\vec{r}|100^{\circ}\rangle}_{\equiv\varphi^{(0)}_{100}(\vec{r})}$$

$$= e\mathcal{E}\int d^3r\, z\, |\varphi^{(0)}_{100}(\vec{r})|^2$$

$z = r\cos\theta$

$$= e\mathcal{E}\int_0^\infty dr\, r^2 \int_0^\pi \sin\theta\, d\theta \int_0^{2\pi} d\varphi\, (\underbrace{r\cos\theta}_{z})\, |R_{10}(r)|^2\, |Y_{00}(\theta,\varphi)|^2$$

$Y_{00}(\theta,\varphi) = \frac{1}{\sqrt{4\pi}}$

$R_{10}(r) = \frac{2}{a_0^{3/2}} e^{-r/a_0}$

$$= e\mathcal{E}\int_0^\infty dr\, r^3 e^{-2r/a_0}\left(4/a_0^3\right)\cdot\left(1/4\pi\right)\int_0^\pi d\theta \sin\theta \cos\theta \cdot 2\pi = 0 \quad (17)$$

Also because $z|\varphi^{\circ}_{100}(\vec{r})|^2$ is odd under reflection

$\epsilon_1^{(1)} = 0 \iff$ no dipole moment in the ground state $(n=1)$

permanent (intrinsic)

technically this should be written $\epsilon^{(1)}_{100}$

Gen: no permanent dipole in non-degenerate states

$\boxed{2^{nd} \text{ order:}}$ ($n=1$, gnd state)

$$\epsilon_1^{(2)} = \sum_{\substack{n\ell m \\ (n \neq 1)}} \frac{\left| \langle \varphi_{n\ell m}^{(0)} | e \mathcal{E} \hat{z} | \varphi_{100}^{(0)} \rangle \right|^2}{\epsilon_1^{(0)} - \epsilon_n^{(0)}} =$$

(11) pg. TIP3

induced dipole, which interacts, in turn, with the external field $\vec{\mathcal{E}}$: $= \vec{\mu}_{induced} \cdot \vec{\mathcal{E}} \sim \vec{\mathcal{E}} \cdot \vec{\mathcal{E}} = \mathcal{E}^2$

$$= e^2 \mathcal{E}^2 \sum_{\substack{n\ell m \\ (n \neq 1)}} \frac{\left| \langle \overset{(0)}{n\ell m} | \hat{z} | 100^{(0)} \rangle \right|^2}{\epsilon_1^{(0)} - \epsilon_n^{(0)}} \neq 0 \quad \text{(*) (18)} \quad \left(\begin{aligned} \epsilon_n^{(0)} &= -\frac{13.6\ \text{eV}}{n^2} \\ \epsilon_1^{(0)} &= -13.6\ \text{eV} \end{aligned} \right)$$

$$\Updownarrow \hat{1}_r$$

$$\langle \overset{(0)}{n\ell m} | \hat{z} | 100 \rangle = \int d^3r \langle n\ell m | \vec{r} \rangle \langle \vec{r} | \hat{z} | 100 \rangle = \int d^3 r\, z \langle n\ell m | \vec{r} \rangle \langle \vec{r} | 100 \rangle$$

$$= \int d^3 r\, \underbrace{z}_{r\cos\theta}\, \varphi_{n\ell m}^{(0)*}(\vec{r})\, \varphi_{100}^{(0)}(\vec{r}) = \int_0^\infty \int_0^\pi \int_0^{2\pi} dr\, d\theta\, d\varphi\; r^3 \sin\theta \cos\theta\, R_{n\ell}^*(r) R_{10}(r) \cdot Y_{\ell m}^*(\theta\varphi)\, Y_{00}(\theta\varphi)$$

$$R_{n\ell}(r) = \frac{u_{n\ell}(r)}{r} = \frac{1}{r} \left(\frac{8\mu |\epsilon_n^{(0)}|}{\hbar^2} \right)^{\frac{\ell+1}{2}} r^{\ell+1}\, e^{-\left(\frac{8\mu|\epsilon_n^{(0)}|}{\hbar^2}\right)^{1/2}/2} F(r)$$

where μ is the electron-proton reduced mass

and $F(r) = \sum_{k=0}^{n_r} c_k r^k \left(\frac{8\mu|\epsilon_n^{(0)}|}{\hbar^2} \right)^{k/2}$ a.s.o. ...

(*) More elegant solution for (18) (Gasiorowicz p.181): (actually an upper bound, not an exact solution)

$$\epsilon_n^{(0)} - \epsilon_1^{(0)} = \left(\epsilon_n^{(0)} - \epsilon_2^{(0)} \right) + \left(\epsilon_2^{(0)} - \epsilon_1^{(0)} \right) \geq \epsilon_2^{(0)} - \epsilon_1^{(0)}$$

$$\Rightarrow \left[\epsilon_n^{(0)} - \epsilon_1^{(0)} \right]^{-1} \leq \left[\epsilon_2^{(0)} - \epsilon_1^{(0)} \right]^{-1}$$

$$\Rightarrow \left| \epsilon_1^{(0)} - \epsilon_n^{(0)} \right|^{-1} \leq \left| \epsilon_1^{(0)} - \epsilon_2^{(0)} \right|^{-1} \quad (\epsilon_n < 0 \text{ for } \underline{\text{bound}} \text{ states})$$

$$\Rightarrow \boxed{\left| \epsilon_1^{(2)} \right| \leq e^2 \mathcal{E}^2 \sum_{n \neq 1} \frac{\left| \langle \overset{(0)}{n\ell m} | \hat{z} | 100^{(0)} \rangle \right|^2}{\epsilon_2^{(0)} - \epsilon_1^{(0)}}} =$$

$$= \frac{e^2 \mathcal{E}^2}{\epsilon_2^{(0)} - \epsilon_1^{(0)}} \sum_{n \neq 1} \left| \langle \overset{(0)}{n\ell m} | \hat{z} | 100^{(0)} \rangle \right|^2 =$$

$$= \frac{e^2 \mathcal{E}^2}{\epsilon_2^{(0)} - \epsilon_1^{(0)}} \sum_{n \neq 1} \langle \overset{(0)}{100} | \hat{z} | \underline{n\ell m^{(0)} \rangle \langle \overset{(0)}{n\ell m}} | \hat{z} | 100^{(0)} \rangle = \langle \overset{(0)}{100} | \hat{z}\, \underline{\hat{1}}\, \hat{z} | 100^{(0)} \rangle \frac{e^2 \mathcal{E}^2}{\epsilon_2^{(0)} - \epsilon_1^{(0)}}$$

$$= \frac{e^2 \mathcal{E}^2}{\epsilon_2^{(0)} - \epsilon_1^{(0)}} \underbrace{\langle \overset{(0)}{100} | \hat{z}^2 | 100^{(0)} \rangle}_{a_0^2 \ (a_0 = \text{Bohr Radius})} = \boxed{\frac{e^2 \mathcal{E}^2 a_0^2}{\epsilon_2^{(0)} - \epsilon_1^{(0)}}}$$

upper bound for $\epsilon_1^{(2)}$, (Gasiorowicz p.181: beside the discrete spectrum, one must add the continuous spectrum (not bound

TIP 8

$$\epsilon_2^{(0)} - \epsilon_1^{(0)} = -\tfrac{1}{2} mc^2 \alpha^2 \left(\tfrac{1}{4} - 1\right) = \frac{8}{3} mc^2 \alpha^4 \quad (\alpha = 1/137)$$

$$\Rightarrow |\epsilon_1^{(2)}| \le \frac{8 e^2 \mathcal{E}^2 a_0^2}{3 mc^2 \alpha^2} = \frac{8}{3} \underbrace{\boxed{(4\pi\epsilon_0) \mathcal{E}^2 a_0^3}}_{\text{energy (volume)}} \quad \Rightarrow \boxed{|\epsilon_1^{(2)}| = \underset{9/4 \text{ (exact sol) Gasiorow}}{\text{const}} \, (4\pi\epsilon_0) \mathcal{E}^2 a_0^3}$$

$\boxed{\text{First excited state } (n=2)}$

Degeneracy is 4-fold : $D = n^2 = 2^2 = 4$:

(19)
$$\begin{cases} |2,0,0\rangle \equiv |\varphi^0_{200}\rangle \equiv |\varphi^0_{2,1}\rangle \\ |2,1,0\rangle \equiv |\varphi^0_{210}\rangle \equiv |\varphi^0_{2,2}\rangle \\ |2,1,1\rangle \equiv |\varphi^0_{211}\rangle \equiv |\varphi^0_{2,3}\rangle \\ |2,1,-1\rangle \equiv |\varphi^0_{21-1}\rangle \equiv |\varphi^0_{2,4}\rangle \end{cases} ; \quad \epsilon_2^{(0)} = -\frac{13.6\,\text{eV}}{4}$$

- Form matrix (14) for $\hat{H}_1$:

$$\hat{H}_1 \doteq \begin{pmatrix} \langle \varphi^0_{2,1}|\hat{H}_1|\varphi^0_{2,1}\rangle & \langle \varphi^0_{2,1}|\hat{H}_1|\varphi^0_{2,2}\rangle & \langle \varphi^0_{21}|\hat{H}_1|\varphi^0_{23}\rangle & \langle \varphi^0_{21}|\hat{H}_1|\varphi^0_{24}\rangle \\ \langle \varphi^0_{2,2}|H_1|\varphi^0_{2,1}\rangle & \langle \varphi^0_{22}|H_1|\varphi^0_{22}\rangle & \langle \varphi^0_{22}|H_1|\varphi^0_{23}\rangle & \langle \varphi^0_{22}|H_1|\varphi^0_{24}\rangle \\ \langle \varphi^0_{2,3}|H_1|\varphi^0_{2,1}\rangle & \langle \varphi^0_{23}|H_1|\varphi^0_{22}\rangle & \langle \varphi^0_{23}|H_1|\varphi^0_{23}\rangle & \langle \varphi^0_{23}|H_1|\varphi^0_{24}\rangle \\ \langle \varphi^0_{24}|H_1|\varphi^0_{2,1}\rangle & \langle \varphi^0_{24}|H_1|\varphi^0_{22}\rangle & \langle \varphi^0_{24}|H_1|\varphi^0_{23}\rangle & \langle \varphi^0_{24}|H_1|\varphi^0_{24}\rangle \end{pmatrix} \quad (20)$$

- Symmetry arguments make life easier :

(Parity) (S1) Under coordinate inversion $(r \to r,\ \theta \to \pi - \theta,\ \varphi = \varphi + \pi)$, (21)

$$\boxed{Y_{lm}(\theta,\varphi) \longrightarrow \overbrace{(-1)^l Y_{lm}(\theta,\varphi)}^{= Y_{lm}(\pi-\theta,\varphi+\pi)}} \quad \text{(Prob. 9.15 Townsend)}$$

Simpler:
$|i\rangle \equiv |2i\rangle$
$\equiv |n l_i m_i\rangle$
$= |2 l_i m_i\rangle$

$$\boxed{(H_1)_{ij}} \equiv \langle \varphi^0_{2,i}|\hat{H}_1|\varphi^0_{2,j}\rangle = e\mathcal{E} \langle \underline{\varphi^0_{2,i}}|\hat{z}|\underline{\underline{\varphi^0_{2,j}}}\rangle$$

$$\equiv e\mathcal{E} \langle \underline{\varphi^0_{2 l_i m_i}}|\hat{z}|\underline{\underline{\varphi^0_{2 l_j m_j}}}\rangle = e\mathcal{E} \langle 2 l_i m_i|\hat{z}|2 l_j m_j\rangle$$

$$= e\mathcal{E} \int d^3r \langle 2 l_i m_i|\vec{r}\rangle\langle\vec{r}|\hat{z}|2 l_j m_j\rangle = e\mathcal{E} \int d^3r \; z \underbrace{\langle 2 l_i m_i|\vec{r}\rangle}_{\varphi^{(0)*}_{2 l_i m_i}(\vec{r})} \underbrace{\langle\vec{r}|2 l_j m_j\rangle}_{\varphi^{(0)}_{2 l_j m_j}(\vec{r})}$$

$(z = r\cos\theta)$

$$= e\mathcal{E} \int_0^\infty dr \int_0^\pi d\theta \int_0^{2\pi} d\varphi \; r^3 \sin\theta\cos\theta \, R^*_{2l_i}(r) R_{2l_j}(r) Y^*_{l_i m_i}(\theta,\varphi) Y_{l_j m_j}(\theta,\varphi)$$

$$\boxed{= e\mathcal{E} \int_0^\infty dr\, r^3 R_{2l_i}(r) R_{2l_j}(r) \int d\Omega \overset{\cos\theta}{\hat{r}}\, Y^*_{l_i m_i}(\theta,\varphi) Y_{l_j m_j}(\theta,\varphi)} \quad (22)$$

(S1) $\Rightarrow (H_1)_{ij} = 0$ for $i = j$ i.e. $\boxed{(H_1)_{ii} = 0}$ (diagonals are zero)

(S2) Also, wavefcn parity (evenness/oddness) only depends on $\underline{\underline{l}}$ $\Rightarrow \boxed{(H_1)_{ij} = 0 \text{ for } l_i = l_j}$

$\Rightarrow$ so far:

so far:

$$\hat{H}_1 \doteq \begin{pmatrix} 0 & (H_1)_{12} & (H_1)_{13} & (H_1)_{14} \\ (H_1)_{21} & 0 & 0 & 0 \\ (H_1)_{31} & 0 & 0 & 0 \\ (H_1)_{41} & 0 & 0 & 0 \end{pmatrix}$$

(52) $\vec{\mathcal{E}} = \mathcal{E}\vec{z} \Rightarrow$ $\boxed{\hat{H}_1 \text{ is invariant under rotations about the z-axis i.e. } [\hat{H}_1, \hat{L}_z] = 0}$

$$\Rightarrow \boxed{\langle 2 l_i m_i | [\hat{H}_1, \hat{L}_z] | 2 l_j m_j \rangle = 0 \quad (i \neq j)}$$

$$\Rightarrow \langle 2 l_i m_i | \hat{H}_1 \hat{L}_z | 2 l_j m_j \rangle = \langle 2 l_i m_i | \hat{L}_z \hat{H}_1 | 2 l_j m_j \rangle \quad (\hat{H}_1 = e\mathcal{E}\hat{z})$$

$$\langle 2 l_i m_i | \hat{z} \hat{L}_z | 2 l_j m_j \rangle = \langle 2 l_i m_i | \hat{L}_z \hat{z} | 2 l_j m_j \rangle$$

$$\hbar m_j \langle 2 l_i m_i | \hat{z} | 2 l_j m_j \rangle = \hbar m_i \langle 2 l_i m_i | \hat{z} | 2 l_j m_j \rangle$$

$$\Rightarrow \boxed{\langle 2 l_i m_i | \hat{z} | 2 l_j m_j \rangle = 0 \text{ if } m_i \neq m_j}$$

i.e. $\boxed{(H_1)_{ij} = 0 \text{ if } m_i \neq m_j}$

Therefore,

$\neq 0$ for $l_i \neq l_j$, $m_i = m_j$

$$\hat{H}_1 \doteq \begin{pmatrix} 0 & (H_1)_{12} & 0 & 0 \\ (H_1)_{21} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (23)$$

Using (22) and the hydrogen wavefunctions,

$$(H_1)_{12} = (H_1)_{21} = -3e\mathcal{E}a_0 \quad (a_0 = \text{Bohr radius})$$

TIP 10

Therefore the e-value problem for the Stark effect in hydrogen becomes (using (14) or (14')):

$\hat{H}_1|\psi_2\rangle = \epsilon_2|\psi_2\rangle$

$$\begin{pmatrix} 0 & -3e\mathcal{E}a_0 & 0 & 0 \\ -3e\mathcal{E}a_0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = \epsilon_2^{(1)}\begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix}$$

Characteristic equation: ~~det(H_x)~~ $\det\left(\hat{H}_1 - \epsilon_2^{(1)}\hat{1}\right) \overset{!}{=} 0$

$\alpha \equiv \epsilon_2^{(1)}$
e-value TBD

$$\Leftrightarrow \begin{vmatrix} -\alpha & -3e\mathcal{E}a_0 & 0 & 0 \\ -3e\mathcal{E}a_0 & -\alpha & 0 & 0 \\ 0 & 0 & -\alpha & 0 \\ 0 & 0 & 0 & -\alpha \end{vmatrix} = 0$$

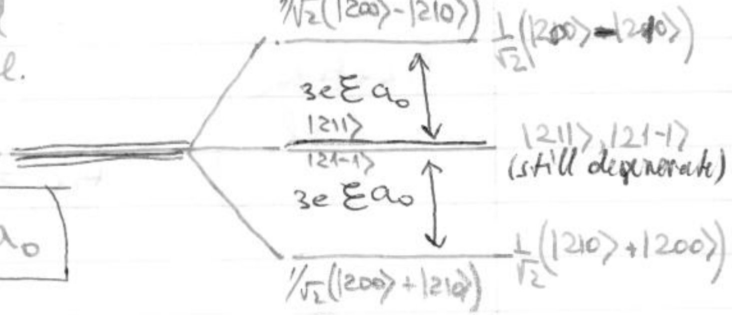
$$\Rightarrow \alpha\left(\equiv \epsilon_2^{(1)}\right) = \{\underbrace{0, 0}_{\text{still degenerate}}, \underbrace{+3e\mathcal{E}a_0, -3e\mathcal{E}a_0}_{\text{degeneracy is removed by } \mathcal{E}\text{-field}}\}$$

(12)

$$\Rightarrow |\psi_2\rangle = \left\{|211\rangle, |21-1\rangle, \frac{1}{\sqrt{2}}\left(|200\rangle - |210\rangle\right), \frac{1}{\sqrt{2}}\left(|200\rangle + |210\rangle\right)\right\}$$

→ these states diagonalize $\hat{H}_1$ in (23)

The uniform external electric field (partially) removes the degeneracy of the $n=2$ level.



$$\boxed{\epsilon_2 = \epsilon_2^{(0)} + \epsilon_2^{(1)} = \epsilon_2^{(0)} \pm 3e\mathcal{E}a_0}$$

non-zero expectation (permanent) value of ~~the~~ dipole moment which, in turn, interacts with the external field $\vec{\mathcal{E}}$,
(This interaction would be "visible" in the second-order correction $\epsilon_2^{(2)}$ via a $\mathcal{E}^2$ term)

Application: Symmetric rotator $\hat{H}_0 = \hat{L}^2/2\hat{I}$ under perturbation (Gasiorowicz 11.2) given by $\hat{H}_1 = \epsilon_1 \cos\theta$. Calculate energy shifts for states with $l=1$.

1st order

$$\epsilon^{(1)} = \langle 1, m^0 | \epsilon \cos\theta | 1, m^0 \rangle = \epsilon_1 \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta \cos\theta \, |Y_{1m}(\theta,\varphi)|^2$$

$l=1 \Rightarrow m = \{-1, 0, 1\}$ degeneracy

$$Y_{10}(\theta,\varphi) = 1/2 \sqrt{3/\pi} \cos\theta$$

$$Y_{1,\mp 1}(\theta,\varphi) = \pm 1/2 \sqrt{3/2\pi}\, e^{\mp i\varphi} \sin\theta$$

$$\Rightarrow \epsilon^{(1)} = \begin{cases} 2\pi \epsilon_1 \int_0^{\pi} d\theta \sin\theta \cos\theta \left(\frac{3}{8\pi}\right) \sin^2\theta = \frac{3\epsilon}{4} \int_{-1}^{1} du\, u(1-u^2) = 0 & (m = \pm 1) \\ 2\pi \epsilon_1 \int_0^{\pi} d\theta \sin\theta \cos\theta \left(1/2 \sqrt{3/\pi}\right)^2 \cos\theta = 0 & (m=0) \end{cases}$$

After all $\begin{cases} [\hat{\Pi}, \hat{L}^2] = 0 \Rightarrow \hat{L}, \hat{\Pi} \text{ share e-states } Y_{lm}(\theta\varphi) \\ \cos\theta = \underline{\underline{\text{odd}}} \text{ under inversion } (\vec{r} \to -\vec{r}) \end{cases}$

$\boxed{\epsilon^{(1)} = 0}$ → symmetric rotators do not have a permanent dipole moment

2nd order

$$\epsilon^{(2)} = \epsilon_1^2 \sum_{\substack{l', m' \\ (l' \neq 1)}} \frac{|\langle l m^0 | \cos\theta | l' m'^0 \rangle|^2}{\epsilon_l - \epsilon_{l'}}, \quad \text{where } \boxed{\epsilon_{l'} = \frac{\hbar^2 l'(l'+1)}{2I}}$$

$\boxed{\text{Non-zero elements only for } l' = \{0, 2\}}$ ($l'=1$ see above; for $l' \geq 3$, $\cos\theta\, Y_{1,\pm1}(\theta,\varphi) \sim Y_{2,\pm1}$ and $\cos\theta\, Y_{1,0} \sim a Y_{20} + b Y_{00} \Rightarrow$
$\Rightarrow$ using orthogonality of $Y_{l'm'} \Rightarrow \langle lm | \cos\theta | l'm' \rangle = 0$)

TiP12

Because of $\int_0^{2\pi} d\varphi$, for $m=\pm 1$ only $\{l'=2, m'=\pm 1\}$ term contributes; for $m=0$ only $\{l'=0\}$ and $\{l'=2, m'=0\}$ terms contribute.

$$\Rightarrow \begin{cases} \epsilon^{(2)}_{m=\pm 1} = -\dfrac{2I\epsilon_1^2}{\hbar^2}\dfrac{1}{15} \\ \epsilon^{(2)}_{m=0} = -\dfrac{2I\epsilon_1^2}{\hbar^2}\dfrac{1}{60} \end{cases}$$