Basically from Sakurai (1.2)

- **Hilbert space.**

  Hilbert space is a complex vector space in infinite dimensions.

- Property of **ket vectors.**

  Two kets can be added: $|\alpha\rangle + |\beta\rangle = |\gamma\rangle$

  Multiply $|\alpha\rangle$ with complex number c, the result is another ket: $c|\alpha\rangle = |\alpha\rangle c$

  Null ket: $0|\alpha\rangle = |\alpha\rangle \Rightarrow |\alpha\rangle$ is a null ket

- **Bra vectors** and their properties.
  - Bra space is dual to ket space.

$$|\alpha\rangle \xrightarrow{D.C.} \langle\alpha|$$

$$|\alpha\rangle + |\beta\rangle \xrightarrow{D.C.} \langle\alpha| + \langle\beta|$$

$$C_\alpha|\alpha\rangle + C_\beta|\beta\rangle \xrightarrow{D.C.} C_\alpha^* \langle\alpha| + C_\beta^* \langle\beta|$$

- **Inner product:** (Postulate two fundamental properties):

  P1 $\quad \langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^*$

  P2 $\quad \langle\alpha|\alpha\rangle \geq 0$

- **Properties of Operators.**
  - Operators are equal: $\forall\, |\alpha\rangle \in \mathcal{H}$; $X|\alpha\rangle = Y|\alpha\rangle \Rightarrow X = Y$
  - null operator: $\forall\, |\alpha\rangle \in \mathcal{H}$: $X|\alpha\rangle = 0$
  - Commutativity and associativity: $X + Y = Y + X$

    $(X+Y) + Z = X + (Y+Z)$
  - Operator Always Acts on Bra from the Right side: $(\langle\alpha|)\cdot X = \langle\alpha|X$
  - Conjugate Operator: $X|\alpha\rangle \xrightarrow{D.C} \langle\alpha|X^\dagger$ (D.C. Means Dual correspondence) $(XY)^\dagger = Y^\dagger X^\dagger$
  - Hermition Operator: $X = X^\dagger$;
  - Associative in multiplication: $X(YZ) = (XY)Z$

- Associative Axiom 结合律.

  postulate
  - Any legal multiplication Among kets, bras, operators are associative
  - One Result from this Pos: $(|\alpha\rangle\langle\beta|)^\dagger = |\beta\rangle\langle\alpha|$

    proof: $|\alpha\rangle\langle\beta|\gamma\rangle \xrightarrow{D.C.} \langle\beta|\gamma\rangle^* \langle\alpha| = \langle\gamma|\,(|\beta\rangle\langle\alpha|)$
  - Another Result from this Pos:

$$\langle\beta|X|\alpha\rangle = \langle\alpha|X^\dagger|\beta\rangle^*$$

$$X^\dagger|\alpha\rangle \xrightarrow{D.C.} \langle\alpha|(X^\dagger)^\dagger$$

$$X|\alpha\rangle \xrightarrow{D.C.} \langle\alpha|X$$

proof:

$$\langle\beta|X|\alpha\rangle = \langle\beta|\cdot(X|\alpha\rangle) = \left|(\langle\alpha|X^\dagger)\cdot|\beta\rangle\right|^* = \langle\alpha|X^\dagger|\beta\rangle^*$$

if X is a hermitian operator, then $\langle\alpha|X|\beta\rangle = \langle\beta|X|\alpha\rangle^*$

- Third result from this Pos: $\langle\beta|X|\alpha\rangle = \langle\alpha|X^\dagger|\beta\rangle^*$; $\langle\beta|(X^\dagger)^\dagger|\alpha\rangle = \langle\alpha|X^\dagger|\beta\rangle^* \rightarrow (X^\dagger)^\dagger = X$

观测量 Observable:

- An Observable acts on kets from left: $A\cdot(|\alpha\rangle) = A|\alpha\rangle$
- 物理的观测量(observable)一般是 Hermitian 的 ($X^\dagger = X$).
  - Eigenvalues of a hermitian operator A are real, the eigen kets of A corresponding to different eigenvalues are orthogonal.

    proof:

$$A|a'\rangle = a'|a'\rangle \Rightarrow \langle a''|A|a'\rangle = \langle a''|a'\rangle a'$$
$$\langle a''|A = a''^* \langle a''| \Rightarrow \langle a''|A|a'\rangle = \langle a''|a'\rangle a''^*$$
$$(a' - a''^*)\langle a''|a'\rangle = 0$$
$$\Downarrow$$
$$\begin{cases} a'' = a' \Rightarrow a' = a'^* & (a' \text{ is a real number}). \\ a'' \neq a' \Rightarrow \langle a''|a'\rangle = 0 \end{cases}$$

  - It is conventional to normalise $|a'\rangle$ so that $\{|a'\rangle\}$ form an Orthonormal set.

$$\langle a''|a'\rangle = \delta_{a''a'}$$

- Postulates: Observable A has complete eigenkets.

  Means: $|\alpha\rangle = \sum_a C_a |a\rangle \Longrightarrow C_a = \langle a|\alpha\rangle$

$$|\alpha\rangle = \sum_a \langle a|\alpha\rangle |a\rangle = \left(\sum_a |a\rangle\langle a|\right)|\alpha\rangle$$
$$\Downarrow$$
$$\sum_a |a\rangle\langle a| = \mathbb{I} \qquad \text{Completeness relation.}$$

- Matrix Representation:

$$X = \sum_{a_i}\sum_{a_j} |a_i\rangle\langle a_i|X|a_j\rangle\langle a_j|$$

  arrange a matrix:

$$\langle a_i|X|a_j\rangle$$
$$\underset{\text{row}}{\Uparrow} \qquad \underset{\text{colum}}{\Uparrow}$$

$$X \doteq \begin{bmatrix} \langle a_0|X|a_0\rangle & \langle a_0|X|a_1\rangle & \cdots \\ \langle a_1|X|a_0\rangle & \ddots & \\ \vdots & & \end{bmatrix}$$

  - Good result 1 by using this notation:

$$\langle a_i|X|a_j\rangle = \langle a_j|X^\dagger|a_i\rangle^* \qquad \text{(associative axiom ;上一页最后一行)}$$
$$\Downarrow$$
$$\langle a_i|X^\dagger|a_j\rangle = \langle a_j|X|a_i\rangle^* \qquad \text{(untary of matrix)}$$

  - Good result 2 by Matrix Representation:

$$\langle a_i|XY|a_j\rangle = \sum_{a_k} \langle a_i|X|a_k\rangle\langle a_k|Y|a_j\rangle \quad \text{(same with matrix product)}$$

  - Good result 3 by this:

$$X|\alpha\rangle = |\gamma\rangle \Rightarrow \langle \alpha_i|\gamma\rangle = \gamma_i = \langle \alpha_i|X|\alpha\rangle = \sum_j \langle \alpha_i|X|\alpha_j\rangle\langle\alpha_j|\alpha\rangle$$

  Consider : $|\alpha\rangle \doteq \begin{pmatrix} \langle \alpha_1|\alpha\rangle \\ \langle \alpha_2|\alpha\rangle \\ \vdots \end{pmatrix}$; this is a simple Matrix Product Problem.

Measurement. Uncertainty relation.

— Before the measurement of observable A, the state would be:

$$|\alpha\rangle = \sum_{a'} C_{a'} |a'\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle$$

When measurement is performed, the system is thrown into one of the eigenstates.

$$|\alpha\rangle \xrightarrow{\text{Measurement}} |a'\rangle$$

Probability for a' $= |\langle a'|\alpha\rangle|^2$

— Expectation value of A:

$$\langle A\rangle \equiv \langle\alpha|A|\alpha\rangle$$
$$= \sum_{a'}\sum_{a''} \langle\alpha|a'\rangle\langle a'|A|a''\rangle\langle a''|\alpha\rangle$$
$$= \sum_{a'} a' \, |\langle a'|\alpha\rangle|^2$$

— Uncertainty Relation:

$$\Delta A \equiv A - \langle A\rangle$$
$$\langle(\Delta A)^2\rangle = \langle (A^2 - 2A\langle A\rangle + \langle A\rangle^2)\rangle = \langle A^2\rangle - \langle A\rangle^2$$
$$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \frac{1}{4}|\langle[A,B]\rangle|^2$$

proof

proof: Schwartz identity: $\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2$

$$\left(\langle\alpha| + \lambda^*\langle\beta|\right)\left(|\alpha\rangle + \lambda|\beta\rangle\right) \geq 0 \qquad \lambda = -\frac{\langle\beta|\alpha\rangle}{\langle\beta|\beta\rangle}$$
$$\Downarrow$$
$$\langle\alpha|\alpha\rangle + \lambda^*\lambda\langle\beta|\beta\rangle + \lambda^*\langle\beta|\alpha\rangle + \lambda\langle\alpha|\beta\rangle \geq 0 \Rightarrow \langle\alpha|\alpha\rangle + \frac{\langle\alpha|\beta\rangle}{\langle\beta|\beta\rangle}\frac{\langle\beta|\alpha\rangle}{\langle\beta|\beta\rangle}\langle\beta|\beta\rangle - \frac{\langle\alpha|\beta\rangle}{\langle\beta|\beta\rangle}\langle\beta|\alpha\rangle - \frac{\langle\beta|\alpha\rangle}{\langle\beta|\beta\rangle}\langle\alpha|\beta\rangle \geq 0$$
$$\Uparrow$$
$$\langle\alpha|\alpha\rangle + \frac{|\langle\alpha|\beta\rangle|^2}{\langle\beta|\beta\rangle} - \frac{|\langle\alpha|\beta\rangle|^2}{\langle\beta|\beta\rangle} - \frac{|\langle\alpha|\beta\rangle|^2}{\langle\beta|\beta\rangle} \geq 0$$
$$\Uparrow$$
$$\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2$$

$$\Delta A^\dagger = (A - \langle A\rangle)^\dagger = A^\dagger - \langle A\rangle^* = A - \langle A\rangle = \Delta A$$ (expectation value of hermitian operator is real)

$$|\alpha\rangle = \Delta A|\rangle$$
$$|\beta\rangle = \Delta B|\rangle$$

$$\begin{cases} \langle\alpha|\alpha\rangle = \langle|(\Delta A)^2|\rangle = \langle(\Delta A)^2\rangle \\ \langle\beta|\beta\rangle = \langle(\Delta B)^2\rangle \end{cases}$$

$$\begin{cases} \langle\alpha|\beta\rangle = \langle|\Delta A\Delta B|\rangle = \langle\Delta A\Delta B\rangle \\ \langle\beta|\alpha\rangle = \langle|\Delta B\Delta A|\rangle = \langle\Delta B\Delta A\rangle \end{cases} \Rightarrow |\langle\alpha|\beta\rangle|^2 = |\langle\Delta A\Delta B\rangle|^2$$

$$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq |\langle\Delta A\Delta B\rangle|^2$$

Noticed:

$$\begin{cases} \Delta A\Delta B = \frac{1}{2}[\Delta A,\Delta B] + \frac{1}{2}\{\Delta A,\Delta B\} \; ; \; [\Delta A,\Delta B] = [A,B] \\ ([A,B])^\dagger = -[A,B] \quad \text{(anti-hermitian)} \\ (\{A,B\})^\dagger = \{A,B\} \quad \text{(hermitian)} \end{cases}$$

$$\{\Delta A,\Delta B\} = (A-\langle A\rangle)(B-\langle B\rangle) + (B-\langle B\rangle)(A-\langle A\rangle)$$
$$\Downarrow$$
$$= \{A,B\} - 2B\langle A\rangle - 2A\langle B\rangle + 2\langle A\rangle\langle B\rangle$$
$$\Downarrow$$
$$\langle\{\Delta A,\Delta B\}\rangle = \langle\{A,B\}\rangle - 2\langle A\rangle\langle B\rangle \quad \text{(real!)}$$

$$\langle\Delta A\Delta B\rangle = \frac{1}{2}\langle[\Delta A,\Delta B]\rangle + \frac{1}{2}\langle\{\Delta A,\Delta B\}\rangle$$

$\Uparrow$ imaginary $\qquad \Uparrow$ real

$$|\langle\Delta A\Delta B\rangle|^2 = \frac{1}{4}|\langle[\Delta A,\Delta B]\rangle|^2 + \frac{1}{4}|\langle\{\Delta A,\Delta B\}\rangle|^2 \leq \langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle$$
$$\Downarrow$$
$$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \frac{1}{4}|\langle[A,B]\rangle|^2$$

Transformation operator and transformation matrix.

- Theorem: Given two sets of base kets, both satisfying orthonormality and completeness, there exist an unitary operator U such that:

$$|b^{(1)}\rangle = U|a^{(1)}\rangle \quad |b^{(2)}\rangle = U|a^{(2)}\rangle \quad \dots \quad |b^{(N)}\rangle = U|a^{(N)}\rangle$$

Unitary means: $U^\dagger U = UU^\dagger = \mathbb{I}$.

proof: $U = \sum_k |b^{(k)}\rangle\langle a^{(k)}| \Rightarrow U^\dagger = \sum_k |a^{(k)}\rangle\langle b^{(k)}|$

$$\Downarrow$$
$$UU^\dagger = \mathbb{I}$$

- Matrix elements of transformation operator:

$$\langle a^{(k)}|U|a^{(l)}\rangle = \langle a^{(k)}|b^{(l)}\rangle = U_{kl}$$

It is instructive to study matrix representation of operator U in the old $\{|a'\rangle\}$ basis.

- The coefficient in new basis:

$$\langle b^{(k)}|\alpha\rangle = \sum_l \langle b^{(k)}|a^{(l)}\rangle\langle a^{(l)}|\alpha\rangle = \sum_l \langle a^{(k)}|U^\dagger|a^{(l)}\rangle \langle a^{(l)}|\alpha\rangle$$

$$(\text{new}) = U^\dagger (\text{old})$$

- Relationship between matrix elements between old and new!

$$\langle b^{(k)}|X|b^{(l)}\rangle = \sum_m\sum_n \langle b^{(k)}|a^{(m)}\rangle\langle a^{(m)}|X|a^{(n)}\rangle\langle a^{(n)}|b^{(l)}\rangle$$
$$= \sum_m\sum_n \langle a^{(k)}|U^\dagger|a^{(m)}\rangle\langle a^{(m)}|X|a^{(n)}\rangle\langle a^{(n)}|U|a^{(l)}\rangle$$
$$X' = U^\dagger X U$$

- use old basis to represent new basis

$$|b^{(i)}\rangle = U|a^{(i)}\rangle = \sum_j |a^{(j)}\rangle\langle a^{(j)}|U|a^{(i)}\rangle = \sum_j |a^{(j)}\rangle U_{ji}$$

coefficient $= \begin{pmatrix} U_{1i} \\ U_{2i} \\ \vdots \end{pmatrix}$ for $|b^{(i)}\rangle$

- trace relation:

$$\mathrm{tr}(XY) = \mathrm{tr}(YX)$$
$$\mathrm{tr}(U^\dagger X U) = \mathrm{tr}(X)$$
$$\mathrm{tr}(|a'\rangle\langle a''|) = \delta_{a'a''}$$
$$\mathrm{tr}(|b'\rangle\langle a'|) = \langle a'|b'\rangle$$

Continuous spectrum case.

- Analogue with eigenvalue equation:

$$\hat{\xi}|\xi'\rangle = \xi'|\xi'\rangle$$

$$\langle\xi'|\xi''\rangle = \delta(\xi'-\xi'') \longleftarrow \langle a'|a''\rangle = \delta_{a'a''}$$

$$\int d\xi' |\xi'\rangle\langle\xi'| = \mathbb{I} \longleftarrow \sum_{a'} |a'\rangle\langle a'| = \mathbb{I}$$

$$|\alpha\rangle = \int d\xi' |\xi'\rangle\langle\xi'|\alpha\rangle \longleftarrow |\alpha\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle$$

$$\langle\beta|\alpha\rangle = \int d\xi' \langle\beta|\xi'\rangle\langle\xi'|\alpha\rangle \longleftarrow \langle\beta|\alpha\rangle = \sum_{a'} \langle\beta|a'\rangle\langle a'|\alpha\rangle$$

$$\langle\xi''|\hat{\xi}|\xi'\rangle = \xi'\delta(\xi''-\xi') \longleftarrow \langle a''|A|a'\rangle = a'\delta_{a'',a'}$$

- Position measurement!

Knowing that a measurement in quantum mechanics is essentially a filtering process!

Consider eigenkets $|x'\rangle$ of the position operator $\hat{x}$.

$$\hat{x}|x'\rangle = x'|x'\rangle$$

For arbitrary state ket $|\alpha\rangle$:

$$|\alpha\rangle = \int_{-\infty}^{+\infty} dx' |x'\rangle\langle x'|\alpha\rangle$$

Consider a measurement, A realistic measurement clicks when a particle is located within some narrow range $(x'-\Delta/2, x'+\Delta/2)$

$$|\alpha\rangle = \int_{-\infty}^{+\infty} dx' |x'\rangle\langle x'|\alpha\rangle \xrightarrow{\text{measurement}} \int_{x'-\Delta/2}^{x'+\Delta/2} dx'' |x''\rangle\langle x''|\alpha\rangle$$

The probability for detector to click is given by:

$$|\langle x'|\alpha\rangle|^2 dx'$$

Normalization:

$$\langle\alpha|\alpha\rangle = 1 \Rightarrow \int_{-}^{+} dx' \langle\alpha|x'\rangle\langle x'|\alpha\rangle = \mathbb{I}$$

It is assumed in nonrelativistic quantum mechanics that the position eigenkets $|x'\rangle$ are complete.

$$|\alpha\rangle = \int d^3x' |\vec{x}'\rangle\langle\vec{x}'|\alpha\rangle$$

$$|\vec{x}'\rangle \equiv |x', y', z'\rangle \Longrightarrow \text{We must have: } [x_i, x_j] = 0$$

- Translation: consider a infinitely transformation done by: $\mathcal{J}(d\vec{x}')$

$$\mathcal{J}(d\vec{x}')|\vec{x}'\rangle = |\vec{x}' + d\vec{x}'\rangle$$

1rd property

Require that if ket $|\alpha\rangle$ is normalized to unity, the translated ket $\mathcal{J}(d\vec{x}')|\alpha\rangle$ also be normalised to unity:

$$\langle\alpha|\alpha\rangle = \langle\alpha|\mathcal{J}(d\vec{x}')^\dagger \mathcal{J}(d\vec{x}')|\alpha\rangle = \mathbb{I}$$

$$\Downarrow$$

$$\mathcal{J}(d\vec{x})^\dagger \mathcal{J}(d\vec{x}) = \mathbb{I} \quad \text{(the translation is unitary)}$$

2rd property

Demand that:

$$\mathcal{J}(d\vec{x}'')\,\mathcal{J}(d\vec{x}') = \mathcal{J}(d\vec{x}'' + d\vec{x}')$$

3rd property:

$$\mathcal{J}(-d\vec{x}') = \mathcal{J}^{-1}(d\vec{x}')$$

4rd

$$\lim_{d\vec{x}'\to 0} \mathcal{J}(d\vec{x}') = \mathbb{I}$$

- If we take the infinitesimal translation operator to be:

$$\mathcal{T}(d\vec{x}') = 1 - i\vec{K}\cdot d\vec{x}' \qquad K^\dagger = K$$

$$\begin{cases} \mathcal{T}^\dagger(d\vec{x}')\,\mathcal{T}(d\vec{x}') = (1 + i\vec{K}^\dagger\cdot d\vec{x}')(1 - i\vec{K}\cdot d\vec{x}') \doteq \mathbb{I} \\ \mathcal{T}(d\vec{x}'')\,\mathcal{T}(d\vec{x}') = (1 - i\vec{K}\cdot d\vec{x}'')(1 - i\vec{K}\cdot d\vec{x}') \doteq \mathcal{T}(d\vec{x}' + d\vec{x}'') \end{cases}$$

- Extremely fundamental relation between K and x

$$\hat{x}\,\mathcal{T}(dx')\,|x'\rangle = \hat{x}\,|x' + dx'\rangle = (x' + dx')\,|x' + dx'\rangle$$

$$\mathcal{T}(dx)\,\hat{x}\,|x'\rangle = x'\,\mathcal{T}(dx')|x'\rangle = x'\,|x' + dx'\rangle$$

$$[\hat{x}, \hat{\mathcal{T}}(dx')]\,|x'\rangle = dx'\,|x' + dx'\rangle \approx dx'\,|x'\rangle$$

$$[\hat{x}, \hat{\mathcal{T}}(dx')] = d\vec{x}' \quad \text{也可验证:} \; [\hat{x}_i, \hat{\mathcal{T}}(d\vec{x}')] = dx_i'$$

$$-i\,\hat{x}_i\vec{K}\cdot d\vec{x}' + i\vec{K}\cdot d\vec{x}'\,\hat{x}_i = d\vec{x}'_i$$

$$\Downarrow$$

$$[\hat{x}_i, \hat{K}_j] = i\delta_{ij}$$

- Momentum as generator of infinitesimal translation:

$$\mathcal{T}(d\vec{x}') = \mathbb{I} - i\vec{p}\cdot d\vec{x}'/\hbar$$

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

- Translation in different direction commutes leads to commutation in $\hat{p}$

$$\mathcal{T}(\Delta x'\,e_x) = \lim_{N\to+\infty}\left(1 - \frac{i\,p_x\Delta x'}{N\hbar}\right)^N = \exp\left(-\frac{i}{\hbar}p_x\Delta x'\right)$$

require that:

$$\mathcal{T}(\Delta y'\,e_y)\,\mathcal{T}(\Delta x'\,e_x) = \mathcal{T}(\Delta x'\,e_x)\,\mathcal{T}(\Delta y'\,e_y)$$

$$\left[\left(1 - \frac{i\,p_y\Delta y'}{\hbar}\cdots\right), \left(1 - i\frac{p_x}{\hbar}\Delta x'\cdots\right)\right] = 0$$

$$\Rightarrow \approx -\frac{(\Delta x')(\Delta y')[p_y, p_x]}{\hbar^2} = 0 \quad \Rightarrow [p_x, p_y] = 0$$

- $|p'\rangle$ is an eigenket of $\mathcal{T}(d\vec{x}')$:

$\vec{p}'$ 是向量, not an operator!

$$\mathcal{T}(d\vec{x}')\,|p'\rangle = \left(1 - \frac{i\,\vec{p}\cdot d\vec{x}'}{\hbar}\right)|p'\rangle = \left(1 - \frac{i\,\vec{p}'\cdot d\vec{x}'}{\hbar}\right)|p'\rangle$$

Wave function in position and momentum space.

- for a state ket $|\alpha\rangle$

$$|\alpha\rangle = \int d^3x' \, |x'\rangle\langle x'|\alpha\rangle$$

The expansion coefficient $\langle x'|\alpha\rangle$ is explained that $|\langle x'|\alpha\rangle|^2 d^3x'$ is the probability for the particle to be found in a narrow interval dx' around x'.

Denote:

$$\langle x'|\alpha\rangle = \psi_\alpha(x')$$

Then:

$$\langle\beta|\alpha\rangle = \int d^3x' \, \langle\beta|x'\rangle\langle x'|\alpha\rangle = \int d^3x' \, \psi_\beta^*(x')\psi_\alpha(x')$$

$$\langle\beta|A|\alpha\rangle = \int d^3x' \int d^3x'' \, \langle\beta|x'\rangle\langle x'|A|x''\rangle\langle x''|\alpha\rangle$$

$$= \int d^3x' \int d^3x'' \, \psi_\beta^*(x')\langle x'|A|x''\rangle\psi_\alpha(x'').$$

We know, the matrix element $\langle x'|A|x''\rangle$, in general, is a function of two variables x' and x''.

If the observable A is a function of position operator x.

$$\langle\beta|f(x)|\alpha\rangle = \iint d^3x' \, d^3x'' \, \psi_\beta^*(x')\langle x'|f(x)|x''\rangle\psi_\alpha(x'')$$ x is an operator here

$$= \iint d^3x' \, d^3x'' \, \psi_\beta^*(x') \, \delta^{(3)}(x'-x'') f(x') \cdot \psi_\alpha(x'')$$

$$= \int d^3x' \cdot \psi_\beta^*(x') f(x') \psi_\alpha(x')$$

- Momentum operator in the Position basis: (one dimensional problem)

$$\left(1 - i\frac{\hat{p}\Delta x'}{\hbar}\right)|\alpha\rangle = \int dx' \, T(\Delta x')|x'\rangle\langle x'|\alpha\rangle$$

$$= \int dx' \, |x'+\Delta x'\rangle\langle x'|\alpha\rangle$$

$$= \int dx' \, |x'\rangle\langle x'-\Delta x'|\alpha\rangle$$

$$= \int dx' \, |x'\rangle\left(\langle x'|\alpha\rangle - \Delta x'\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\right)$$

Comparsion of both sides:

$$\hat{p}|\alpha\rangle = \int dx' \, |x'\rangle\left(-i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\right)$$

$$\langle x'|\hat{p}|\alpha\rangle = -i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle$$

$$\langle x'|\hat{p}|x''\rangle = -i\hbar\frac{\partial}{\partial x'}\delta(x'-x'')$$

(1.248. J.J.Sakurai)

From this we get a very important identity:

$$\langle\beta|\hat{p}|\alpha\rangle = \int dx' \, \langle\beta|x'\rangle\langle x'|\hat{p}|\alpha\rangle$$

$$= \int dx' \, \psi_\beta^*(x') \, -i\hbar\frac{\partial}{\partial x'}\psi_\alpha(x')$$

Also:

$$\langle x'|p^n|\alpha\rangle = (-i\hbar)^n\frac{\partial^n}{\partial x'^n}\langle x'|\alpha\rangle$$

$$\langle\beta|p^n|\alpha\rangle = \int dx' \, \psi_\beta^*(x')(-i\hbar)^n\frac{\partial^n}{\partial x'^n}\psi_\alpha(x')$$

- Momentum – Space Wave function: The base eigenkets in p-basis satisfy:

$$\hat{p}|p'\rangle = p'|p'\rangle$$

$$\langle p'|p''\rangle = \delta(p'-p'') \qquad \phi_\alpha(p') = \langle p'|\alpha\rangle$$

$$|\alpha\rangle = \int dp' \, |p'\rangle\langle p'|\alpha\rangle \xrightarrow{\text{normalise } |\alpha\rangle} \int dp' \, \langle\alpha|p'\rangle\langle p'|\alpha\rangle = \int dp' \, |\phi_\alpha(p')|^2 = 1$$

- Relation between x-representation and P-representation.

$$\langle x'|P|p'\rangle = -i\hbar\frac{\partial}{\partial x'}\langle x'|p'\rangle$$ (momentum operator in the position basis) (上一页中间).

$$= p'\langle x'|p'\rangle$$

$$\Downarrow$$

$$\langle x'|p'\rangle = N\exp\left(\frac{ip'x'}{\hbar}\right)$$

This says the wave function of a momentum eigenstate is a plane wave.

$$\langle x'|x''\rangle = \int dp'\langle x'|p'\rangle\langle p'|x''\rangle = \delta(x'-x'')$$

Math problem!

$$= |N|^2\int dp'\exp\left(\frac{ip'(x'-x'')}{\hbar}\right) \Rightarrow \boxed{\int dx\, e^{ipx} = 2\pi\delta(p)}$$

$$= 2\pi\hbar|N|^2\delta(x'-x'')$$

$$\langle x'|p'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp\left(\frac{ip'x'}{\hbar}\right) \quad !!!$$

$$\psi_\alpha(x') = \langle x'|\alpha\rangle = \int dp'\langle x'|p'\rangle\langle p'|\alpha\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int dp'\cdot\exp\left(\frac{ip'x'}{\hbar}\right)\phi_\alpha(p')$$

$$\phi_\alpha(p') = \langle p'|\alpha\rangle = \int dx'\langle p'|x'\rangle\langle x'|\alpha\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int dx'\cdot\exp\left(-\frac{ip'x'}{\hbar}\right)\psi_\alpha(x')$$

same with Fourier transformation!

对于3维问题(Generalise to three dimension):

$$\langle \vec{x}'|\vec{p}'\rangle = \frac{1}{(2\pi\hbar)^{3/2}}\exp\left(\frac{i\vec{p}'\cdot\vec{x}'}{\hbar}\right) \quad !!!$$

2.3 Harmonic oscillator

$$H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2 \qquad \omega = \sqrt{\frac{k}{m}}$$

Define two non-Hermitian operator:

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right), \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right)$$

Commutation relation:

$$[a, a^\dagger] = 1$$

Define number operator:

$$N = a^\dagger a. \qquad \text{(which is hermitian)}$$

Straight to show that:

$$N = \frac{m\omega}{2\hbar}\left(x^2 + \frac{p^2}{m^2\omega^2}\right) + \frac{i}{2\hbar}[x, p] = \frac{H}{\hbar\omega} - \frac{1}{2}$$

Important relation between number operator and Hermitian operator:

$$H = \hbar\omega\left(N + \frac{1}{2}\right)$$

N can be diagonalized simultaneous with H.

Suppose: $\quad N|n\rangle = n|n\rangle$

$$H|n\rangle = \left(n + \frac{1}{2}\right)|n\rangle$$

Noticed:

$$[N, a] = [a^\dagger a, a] = a^\dagger[a, a] + [a^\dagger, a]a = -a$$

$$[N, a^\dagger] = +a^\dagger$$

$$N a^\dagger|n\rangle = (n+1)a^\dagger|n\rangle$$

$$N a|n\rangle = (n-1)a|n\rangle$$

$$\langle n|a^\dagger a|n\rangle = \langle n|n|n\rangle = n \Rightarrow \qquad a|n\rangle = \sqrt{n}\,|n-1\rangle$$

$$\langle n|a a^\dagger|n\rangle = \langle n|a^\dagger a + [a, a^\dagger]|n\rangle = \langle n|n+1|n\rangle \Rightarrow \quad a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

- positivity of norm of $a|n\rangle$ leads to $n \geq 0$!

  $\langle n|a^\dagger a|n\rangle = n\langle n|n\rangle = n \geq 0 \Rightarrow n \geq 0! \Rightarrow$ n has to be integral! (如果 n 不是 integral, $a|0.1\rangle = \sqrt{0.1}\,|-0.9\rangle$ 小于0了.)

- by recursion: $|1\rangle = \frac{1}{\sqrt{1}} a^\dagger|0\rangle \quad \cdots \quad |n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle$

- Matrix elements:

$$\langle n'|a|n\rangle = \sqrt{n}\,\delta_{n', n-1} \qquad \langle n'|a^\dagger|n\rangle = \sqrt{n+1}\cdot\delta_{n', n+1}$$

$$\begin{cases} x = \sqrt{\frac{\hbar}{2m\omega}}\,(a + a^\dagger) \\ p = i\sqrt{\frac{m\hbar\omega}{2}}\,(-a + a^\dagger) \end{cases}$$

$$\langle n'|x|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\,\delta_{n', n-1} + \sqrt{n+1}\,\delta_{n', n+1}\right)$$

$$\langle n'|p|n\rangle = i\sqrt{\frac{m\hbar\omega}{2}}\left(-\sqrt{n}\,\delta_{n', n-1} + \sqrt{n+1}\,\delta_{n', n+1}\right)$$

- use operator method to obtain energy eigenfunctions in position space!

ground space:

$$a|0\rangle = 0$$

$$\langle x'|a|0\rangle = \sqrt{\frac{m\omega}{2\hbar}}\,\langle x'|\left(x + i\frac{p}{m\omega}\right)|0\rangle = 0$$

differential equation for ground state:

$$\left(x' + x_0^2 \frac{d}{dx'}\right)\langle x'|0\rangle = 0 \qquad x_0 = \sqrt{\frac{\hbar}{m\omega}}$$

Normalized solution

$$\langle x'|0\rangle = \frac{1}{\pi^{1/4}\sqrt{x_0}} \cdot \exp\left(-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right)$$

excited states :

$$\langle x'|1\rangle = \langle x'|a^\dagger|0\rangle = \frac{1}{\sqrt{2}\,x_0}\left(x' - x_0^2\frac{d}{dx'}\right)\langle x'|0\rangle$$

$$\langle x'|2\rangle = \frac{1}{\sqrt{2}}\langle x'|(a^\dagger)^2|0\rangle = \frac{1}{\sqrt{2!}}\cdot\left(\frac{1}{\sqrt{2}\,x_0}\right)^2\left(x' - x_0^2\frac{d}{dx'}\right)^2\langle x'|0\rangle$$

$$\langle x'|n\rangle = \frac{1}{\pi^{1/4}\cdot\sqrt{2^n\cdot n!}}\cdot\left(\frac{1}{x_0^{n+1}}\right)\cdot\left(x' - x_0^2\frac{d}{dx'}\right)^n\cdot\exp\left(-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right) \qquad x_0 \equiv \sqrt{\frac{\hbar}{m\omega}}$$

▽ Instructive to Look at expectation values of x^2, p^2 for ground states!

$$x^2 = \frac{\hbar}{2m\omega}\left(a^2 + a^{\dagger 2} + a^\dagger a + a a^\dagger\right)$$

$$\langle 0|x^2|0\rangle = \frac{\hbar}{2m\omega} \qquad \langle x\rangle = 0$$

$$\langle 0|p^2|0\rangle = \frac{\hbar m\omega}{2} \qquad \langle p\rangle = 0$$

$$\langle 0|\frac{p^2}{2m}|0\rangle = \frac{1}{4}\hbar\omega = \frac{1}{2}\langle 0|H|0\rangle$$

$$\langle 0|\frac{1}{2}m\omega^2x^2|0\rangle = \frac{1}{4}\hbar\omega = \frac{1}{2}\langle 0|H|0\rangle$$

$$\langle 0|(\Delta x)^2|0\rangle = \langle 0|x^2|0\rangle = \frac{\hbar}{2m\omega}$$

$$\langle 0|(\Delta p)^2|0\rangle = \langle 0|p^2|0\rangle = \frac{\hbar m\omega}{2} \Rightarrow \langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle = \frac{\hbar^2}{4} \geq \frac{1}{4}\left|\langle[x, p]\rangle\right|^2$$

The uncertainty products for excited states :

$$\langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle = \left(n + \frac{1}{2}\right)^2\hbar^2$$

Quantum Dynamics

- Time evolution operator:

$$|\alpha, t_0, t\rangle = U(t, t_0)|\alpha, t_0\rangle \qquad \text{where } |\alpha, t_0, t\rangle|_{t=t_0} = |\alpha, t_0\rangle$$

1st feature: If the state ket is initially normalized to unity, it must remain normalized to unity at all later times.

$$\langle\alpha, t_0|\alpha, t_0\rangle = 1 \Rightarrow \langle\alpha, t_0 t|\alpha\, t_0\, t\rangle = 1 \Rightarrow U^{\dagger}(t, t_0)U(t, t_0) = 1$$

2 st feature: composition property

$$U(t_2, t_0) = U(t_2, t_1)\,U(t_1, t_0)$$

3 st feature: $\lim_{dt\to 0} U(t_0+dt, t_0) = \mathbb{I}$

- Assert All these feature are satisfied by:

$$U(t_0+dt, t_0) = 1 - i\Omega\, dt:$$

$$\Omega^{\dagger} = \Omega \qquad (\text{hermition operator})$$

- Assume Hamiltonian operator is the generator of time-Evolution operator:

$$U(t_0+dt, t) = \mathbb{I} - i\frac{H}{\hbar}dt$$

- Schrödinger equation:

$$U(t+dt, t_0) = U(t+dt, t)\,U(t, t_0) = \left(1 - i\frac{H}{\hbar}dt\right)U(t, t_0)$$

$$U(t+dt, t_0) - U(t, t_0) = -i\frac{H}{\hbar}dt\; U(t, t_0)$$

$$i\hbar\frac{\partial}{\partial t}U(t, t_0) = H\,U(t, t_0) \Rightarrow i\hbar\frac{\partial}{\partial t}U^{\dagger} = -U^{\dagger}H$$

Schrodinger equation for state ket:

$$i\hbar\frac{\partial}{\partial t}|\alpha, t_0, t\rangle = H|\alpha, t_0, t\rangle$$

- Case 1: Hamiltonian operator is independent of time.

$$U(t, t_0) = \exp\left(-i\frac{H(t-t_0)}{\hbar}\right)$$

Case 2: H is dependent on t, but H at different times commute.

$$U(t, t_0) = \exp\left(-\left(\frac{i}{\hbar}\right)\int_{t_0}^{t} dt'\, H(t')\right)$$

Case 3: Dyson series!

$$U(t, t_0) = 1 + \sum_{n=1}^{+\infty}\left(\frac{1}{i\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_1}^{t} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n\, H(t_1)\cdots H(t_n)$$

- Stationary state 定态:

Base kets are eigenkets of A such that:

$$[A, H] = 0$$

Eigen kets of A are also eigenkets of H

$$H|a'\rangle = E_{a'}|a'\rangle$$

$$\exp\left(-i\frac{H}{\hbar}t\right) = \sum_{a'}\sum_{a''}|a''\rangle\langle a''|\exp\left(-\frac{iH}{\hbar}t\right)|a'\rangle\langle a'| = \sum_{a'}|a'\rangle\exp\left(-\frac{iE_{a'}t}{\hbar}\right)\langle a'|$$

Then, if:

$$|\alpha, t_0=0\rangle = |\alpha\rangle, \quad \Rightarrow \quad |\alpha\rangle = C_{a'}|a'\rangle \qquad C_{a'} = \langle a'|\alpha\rangle$$

$$C_{a'}(t) = C_{a'}(t=0)\cdot \exp(-i\frac{E_{a'}}{\hbar}t)$$

▹ For state $|\alpha, t_0=0\rangle = |a'\rangle$

$$\langle B\rangle = \langle a'|\exp(i\frac{E_{a'}}{\hbar}t)\ B\ \exp(-i\frac{E_{a'}}{\hbar}t)|a'\rangle = \langle a'|B|a'\rangle$$

Which is stational state! (expectation value does not change for energy eigenstates)

▹ For superposition of energy eigenkets are not Stationary state

$$|\alpha, t_0=0\rangle = \sum_{a'} C_{a'}|a'\rangle$$

$$\langle B\rangle = \langle\alpha, t_0=0, t|\ B|\alpha, t_0=0, t\rangle$$

$$= \sum_{a'a''} C_{a'}^{*}\exp(i\frac{E_{a'}}{\hbar}t)\langle a'|\ B|a''\rangle\ C_{a''}\ \exp(-i\frac{E_{a''}}{\hbar}t)$$

$$= \sum_{a'a''} \langle a'|B|a''\rangle \cdot C_{a'}^{*}C_{a''}\cdot \exp(\frac{-i}{\hbar}(E_{a''}-E_{a'})t)$$

Bohr frequency condition:

$$w_{a'a''} = \frac{(E_{a''}-E_{a'})}{\hbar}$$

Heisenberg Picture (旧)

- Introduce the time evolution operator:（定义了演化算符）

$$U(t) = e^{-\frac{i}{\hbar}\hat{H}t}$$

则态可以有演化:

$$|\alpha, t\rangle = \sum_n C_n \cdot e^{-i\frac{1}{\hbar}\hat{H}t} \cdot |n, 0\rangle$$
$$= e^{-\frac{i}{\hbar}\hat{H}t} \sum_n C_n |n, 0\rangle$$
$$= U(t)|n, 0\rangle$$

- Heisenberg Picture 的性质:
  - $U(t)$ 是一个么正算符

    $U^{+}U = 1 \quad U^{+} = U^{-1} = U(-t)$
  - U^{+} 也是一个时间演化算符

    $U^{+}(t) = U(-t)$
  - $U^{+}(t)$ 可以将一个态转变为另一个表达

    $U^{+}(t)|\alpha, t\rangle = U(-t)|\alpha, t\rangle = U(-t)U(t)|\alpha, 0\rangle = |\alpha, 0\rangle$
- 在新的表达中，态可以表示为时间独立的态.

  $|\alpha, 0\rangle$
- 力学量算符的转换:

  $A \to U(-t)\hat{A}U^{+}(-t) = U^{+}(t)AU(t)$
- 在这样新的一组表达下，叫作 Heisenberg 绘景.

  $|\alpha\rangle^{H} = U(-t)|\alpha, t\rangle^{S} = U^{+}(t)|\alpha, t\rangle^{S} = |\alpha, 0\rangle^{S}$

  $A^{H} = U(-t)\hat{A}^{S}U^{+}(-t) = U^{+}(t)\hat{A}^{S}U(t)$
- Heisenberg equation of motion:

$$\frac{d}{dt}(A^{H}) = \frac{d}{dt}(U^{+}(t)AU(t)) = \frac{d}{dt}(e^{\frac{i}{\hbar}\hat{H}t}Ae^{-\frac{i}{\hbar}\hat{H}t})$$
$$= \frac{i}{\hbar}[H, U^{+}(t)AU(t)]$$
$$= \frac{i}{\hbar}[H, A^{H}]$$

S.picture 中 equation of motion 是态的方程.
H.picture 中 equation of motion 是 operator 的方程.

- Heisenberg picture 中 equation of motion of $\hat{x}$ & $\hat{p}$ $\quad \hat{H} = \frac{\hat{p}^2}{2m} + V(x)$

$$\frac{d}{dt}\hat{x} = \frac{1}{i\hbar}[\hat{x}, H] = \frac{1}{i\hbar}[\hat{x}, \frac{\hat{p}^2}{2m} + V(x)] = \frac{1}{i\hbar}[\hat{x}, \frac{1}{2m}\hat{p}\hat{p}] = \frac{1}{m}\hat{p}$$

- Equation of motion for $\hat{p}$.

$$\frac{d}{dt}\hat{p} = \frac{1}{i\hbar}[\hat{p}, T + V(x)] = \frac{1}{i\hbar}[\hat{p}, V(x)] = -\frac{\partial}{\partial x}V(x)$$

- 由 $\hat{x}$ 和 $\hat{p}$ 的 Equation of motion 可以导致:

$$\frac{d^2}{dt^2}x = \frac{d}{dt}\frac{p}{m} = -\frac{1}{m}\frac{\partial}{\partial x}V(x)$$
$$m\frac{d^2}{dt^2}\langle x\rangle = -\langle \nabla V(x)\rangle$$

↑ PPT上讲这个方程是 Ehrenfest theorm.

考师的PPT中有一个问题:
为什么不是:

$$\dot{p} = -i[U(t)^{+}\hat{p}^{S}U(t), H]$$

问: $\frac{d\hat{p}}{dt}$ 不是0, 具体该怎么写?
$\hat{p}^{H}$ 和 H^{H} 有对易关系?

Heisenberg Picture (新) (P77 sakurai)

- Approach:

  1: $|\alpha\rangle \to U|\alpha\rangle$;

  2: $A \longrightarrow U^{\dagger} X U$

- example:

$$|\alpha\rangle \longrightarrow (1 - i\frac{p\cdot dx'}{\hbar})|\alpha\rangle$$

using approach 2:

$$|\alpha\rangle \to |\alpha\rangle$$

$$x \to (1 + i\frac{p\cdot dx'}{\hbar})\, x\, (1 - i\frac{p\cdot dx'}{\hbar})$$

$$= x + (\frac{i}{\hbar})[p\cdot dx', x]$$

$$= x + dx'$$

$\langle x\rangle \longrightarrow \langle x\rangle + dx'$ (Both approach lead to same result of expectation value of x)

- In all

$$\left.\begin{aligned} |\alpha\rangle^{H} &= |\alpha, t_0, t=t_0\rangle^{S} \\ A^{H} &= U(t,t_0)^{\dagger} A^{S} U(t,t_0) \end{aligned}\right\} \Rightarrow \text{ in variant of } \langle A\rangle \Rightarrow \langle A\rangle_H = \langle A\rangle_S$$

- Heisenberg equation of motion:

$$\frac{dA^{(H)}}{dt} = \frac{\partial U^{\dagger}}{\partial t} A^{(S)} U + U^{\dagger} A^{S} \frac{\partial U}{\partial t}$$

$$= -\frac{1}{i\hbar} U^{\dagger} H U U^{\dagger} A^{(S)} U + \frac{1}{i\hbar} U^{\dagger} A^{S} U U^{\dagger} H U$$

$$= \frac{1}{i\hbar}[A^{(H)}, U^{\dagger} H U]$$

$H^{(H)} = U^{\dagger} H U$, if $U(t,0) = \exp(-i\frac{H}{\hbar}t)$; $H^{(H)} = H$.

- Free particles. Ehrenfest's Theorem.

These two relation is useful:

$$\left\{\begin{aligned} &[x_i, F(p)] = i\hbar\frac{\partial F}{\partial p_i} \\ &[p_i, G(x)] = -i\hbar\frac{\partial G}{\partial x_i} \end{aligned}\right.$$

1° to a free particle of mass m:

$$H = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2)$$

$$\left\{\begin{aligned} &\frac{dp_i(t)}{dt} = \frac{1}{i\hbar}[p_i(t), H^{H}] = 0 \Rightarrow p_i(t) = p_i(0) \\ &\frac{dx_i(t)}{dt} = \frac{1}{i\hbar}[x_i(t), H^{H}] = \frac{1}{i\hbar}\frac{\partial}{\partial p_i}\left(\frac{p_i^2}{2m}\right)\cdot(i\hbar) = \frac{p_i}{m} \end{aligned}\right.$$

$$x_i(t) = x_i(0) + \frac{p_i(0)}{m}t \qquad ([x_i(t), p_i(t)] = i\hbar \text{ 这个被}U^{\dagger}AU\text{保证了!})$$

Noticed:

$$[x_i(t), x_i(0)] = [\frac{p_i(0)}{m}t, x_i(0)] = -\frac{i\hbar}{m}t$$

Uncertainty relation:

$$\langle(\Delta x_i)^2_t\rangle\langle(\Delta x_i)^2_0\rangle \geq \frac{\hbar^2 t^2}{4m^2}$$

2° add a potential to free particle:

$$H = \frac{p^2}{2m} + V(x)$$

$$\begin{cases} \dfrac{dp_i(t)}{dt} = \dfrac{1}{i\hbar}[p_i(t), H^H] = \dfrac{1}{i\hbar}[p_i(t), V(x(t))] = \dfrac{1}{i\hbar}(-i\hbar)\dfrac{\partial}{\partial x}V(x(t)) = -\dfrac{\partial V}{\partial x}\Big|_{x(t)} \\ \dfrac{dx_i(t)}{dt} = \dfrac{1}{i\hbar}[x_i(t), H^H] = \dfrac{1}{i\hbar}[x_i(t), \sum_i \dfrac{p_i^2}{2m}] = \dfrac{p_i(t)}{m} \end{cases}$$

这个被 $U^\dagger A U$ 保证了!

$$\left([x_i(t), p_i(t)] = i\hbar \right)$$

$$\frac{d^2 x_i(t)}{dt^2} = \frac{1}{m}\frac{dp_i(t)}{dt} = -\frac{1}{m}\frac{\partial V}{\partial x}\Big|_{x=x(t)}$$

Taking expectation values: (Ehrenfest theorem)

$$m\frac{d^2}{dt^2}\langle x\rangle = -\langle \nabla V(x)\rangle$$

Interaction picture (相互作用绘景)，(1日)

$$H = H_0 + H_\iota$$
$$U_0(t) = e^{-\frac{i}{\hbar}H_0 t} \Leftarrow$$ H_0注意.

态和力学量：

$$|\alpha\rangle^\iota = U_0(-t)\,|\alpha, t\rangle^S$$
$$A^\iota = U_0^\dagger A^S U_0$$

Equation of motion:

$$i\hbar \frac{\partial}{\partial t}|\alpha\rangle^\iota = H_\iota |\alpha\rangle^\iota$$
$$\frac{d}{dt}A^\iota = \frac{1}{i\hbar}[A^\iota, H_0]$$

Interaction 绘景，新：

Hamiltonian：$H = H_0 + H_I$

$$U_0(t)|\alpha, t_0, t\rangle^I = |\alpha, t_0, t\rangle \Rightarrow |\alpha, t_0, t\rangle^I = U_0^\dagger(t)|\alpha, t_0, t\rangle$$

$U_0(-t)$ satisfies:

$$i\hbar\frac{\partial}{\partial t}(U_0(t)) = H_0 U_0(t) \Rightarrow -i\hbar\frac{\partial}{\partial t}(U_0^\dagger(t)) = U_0^\dagger H_0$$

力学量：

$$A \rightarrow U_0^\dagger(t) A \cdot U_0(t) = A^I \rightarrow \langle\alpha|^I A^I |\alpha\rangle^I = \langle\alpha|A|\alpha\rangle$$

力学量随时间变化：

$$\frac{d}{dt}(A^I) = \frac{\partial}{\partial t}(U_0^\dagger(t))A\cdot U_0(t) + U_0^\dagger(t) A \frac{\partial}{\partial t}(U_0(t)) = -\frac{1}{i\hbar}U_0^\dagger H_0 U_0 U_0^\dagger A U_0 + \frac{1}{i\hbar}U_0^\dagger A U_0 U_0^\dagger H_0 U_0$$
$$= \frac{1}{i\hbar}[U_0^\dagger A U_0, U_0^\dagger H_0 U_0] = \frac{1}{i\hbar}[A^I, H^I]$$

态矢随时间变化：

$$\frac{\partial}{\partial t}|\alpha, t_0, t\rangle^I = \frac{\partial}{\partial t}\left(U_0^\dagger |\alpha, t_0, t\rangle\right)$$
$$= -\frac{1}{i\hbar}U_0^\dagger H_0 |\alpha, t_0, t\rangle + \frac{1}{i\hbar}U_0^\dagger (H_0 + H_I)|\alpha, t_0, t\rangle$$
$$= \frac{1}{i\hbar}U_0^\dagger H_I |\alpha, t_0, t\rangle$$
$$= \frac{1}{i\hbar}U_0^\dagger H_I U_0 U_0^\dagger |\alpha, t_0, t\rangle$$
$$= \frac{1}{i\hbar}H_I^I |\alpha, t_0, t\rangle^I$$

Schrodinger wave equation.

- Time dependent wave equation. $\Downarrow$ All in Schrodinger Picture.

$$\psi(x',t) = \langle x'|\alpha, t_0, t\rangle$$

$$H = \frac{p^2}{2m} + V(x)$$

$$\langle x''|V(x)|x'\rangle = V(x')\,\delta^{(3)}(x'-x'')$$

$$i\hbar\frac{\partial}{\partial t}\langle x'|\alpha, t_0, t\rangle = \langle x'|H|\alpha, t_0; t\rangle$$

(used fact that position eigenbras in schrodinger Pic do not change with time)

$$\langle x'|\frac{p^2}{2m}|\alpha, t_0; t\rangle = -\left(\frac{\hbar^2}{2m}\right)\nabla'^2\langle x'|\alpha, t_0; t\rangle \quad \Leftarrow \text{used (1.252) sakurai}$$

$$i\hbar\frac{\partial}{\partial t}\langle x'|\alpha, t_0; t\rangle = -\left(\frac{\hbar^2}{2m}\right)\nabla'^2\langle x'|\alpha, t_0, t\rangle + V(x')\langle x'|\alpha, t_0; t\rangle$$

$$i\hbar\frac{\partial}{\partial t}\psi(x',t) = -\frac{\hbar^2}{2m}\nabla'^2\psi(x',t) + V(x')\psi(x',t)$$

The quantum mechanics based on wave equation is know as wave mechanics.

- Time-independent Wave equation.

Focus on the partial differential equation satisfied by energy eigen functions

Showed before that the stationary state is evolute by $\exp(-i\frac{E_{a'}}{\hbar}t)$

Then:

$$\langle x'|a', t_0; t\rangle = \langle x'|a'\rangle\exp(-i\frac{E_{a'}}{\hbar}t)$$

Insert this to schrödinger equation.

$$-\left(\frac{\hbar^2}{2m}\right)\nabla'^2\langle x'|a'\rangle + V(x')\langle x'|a'\rangle = E_{a'}\langle x'|a'\rangle$$

The time-independent wave equation of E would be:

$$-\frac{\hbar^2}{2m}\nabla'^2 u_E(x') + V(x')u_E(x') = E u_E(x')$$

Some boundary condition should be imposed:

If we seek solution with: $E < \lim_{|x'|\to+\infty} V(x')$

Boundary Condition $u_E(x')\to 0$ as $|x'|\to+\infty$

- Interpretation of wave function.

use x for x' because the position operator would not appear.

Consider Schrödinger equation:

$$\begin{cases} i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\nabla^2\psi(x,t) + V(x)\psi(x,t) \\ -i\hbar\frac{\partial}{\partial t}\psi^*(x,t) = \frac{\hbar^2}{2m}\nabla^2\psi^*(x,t) - V(x)\psi^*(x,t) \end{cases}$$

$$\Downarrow$$

$$\frac{\partial}{\partial t}(\psi^*\psi) = \frac{1}{-i\hbar}\left[\frac{\hbar^2}{2m}\psi\nabla^2\psi^* - \frac{\hbar^2}{2m}\psi^*\nabla^2\psi\right]$$

$$= -i\frac{\hbar}{2m}(\psi\nabla^2\psi^* - \psi^*\nabla^2\psi)$$

$$= -i\frac{\hbar}{2m}\nabla\cdot(\psi\nabla\psi^* - \psi^*\nabla\psi)$$

$$\frac{\partial\rho}{\partial t} + \nabla\cdot j = 0$$

$$j = -\frac{i\hbar}{2m}(\psi^*\nabla\psi - \psi\nabla\psi^*) = \frac{\hbar}{m}\,\mathrm{Im}(\psi^*\nabla\psi)$$

$\langle\alpha|\beta\rangle$

$\langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^*$

The reality of potential V.

(hermiticity of V) played important role.

$$\langle P\rangle_t = \langle\alpha, t_0, t|P|\alpha, t_0, t\rangle = \int d^3x'\langle\alpha, t_0, t|x'\rangle\langle x'|P|\alpha, t_0, t\rangle = \int d^3x'\,\langle\alpha, t_0, t|P|x'\rangle\langle x'|\alpha, t_0, t\rangle$$

$$= \int d^3x'\,\psi^*(x',t)(-i\hbar\nabla')\psi(x',t) = \int d^3x'\,(-i\hbar\nabla'\psi)^*\psi$$

$$= -i\hbar\int d^3x'\,\psi^*\nabla\psi \quad = i\hbar\int d^3x'\,\psi\nabla'\psi^*$$

$$\langle p \rangle_t = \frac{1}{2}(i\hbar)\int d^3x' \left(-\psi^* \nabla \psi + \psi \nabla \psi^*\right)$$

$$\frac{\langle p \rangle_t}{m} = \frac{-i\hbar}{2m}\int d^3x' \left(-\psi^* \nabla \psi + \psi \nabla \psi^*\right) = \int d^3x' \, j(x', t)$$

let us write:

$$\psi(x, t) = \sqrt{\rho(x,t)} \cdot \exp\left(i \frac{S(x,t)}{\hbar}\right)$$

$$\psi^* \nabla \psi = \sqrt{\rho}\, \nabla(\sqrt{\rho}) + \left(\frac{i}{\hbar}\right) \sqrt{\rho}\, \nabla S$$

in this case: $j = \frac{\rho \nabla S}{m}$

Elementary solution to schrodinger wave function

— Free Particle in three dimension.

Free Particle means $V(x)=0$.

Schrödinger time independent wave function:

$$\nabla^2 U_E(x) = -\frac{2mE}{\hbar^2} U_E(x)$$

Define vector $\vec{k}$.

$$|\vec{k}|^2 = k_x^2 + k_y^2 + k_z^2 = \frac{2mE}{\hbar^2} = \frac{p^2}{\hbar^2}$$

Writing $U_E(x) = U_x(x) U_y(y) U_z(z)$

Arrive:

$$\left(\frac{1}{U_x}\frac{d^2U_x}{dx^2} + k_x^2\right) + \left(\frac{1}{U_y}\frac{d^2U_y}{dy^2} + k_y^2\right) + \left(\frac{1}{U_z}\frac{d^2U_z}{dz^2} + k_z^2\right) = 0$$

$$U_E(\vec{x}) = C e^{i\vec{k}\cdot\vec{x}}$$

Apply Box normalization:

$$U_x(x+L) = U_x(x) \qquad k_x = \frac{2\pi}{L}n_x \;;\; k_y = \frac{2\pi}{L}n_y \;;\; k_z = \frac{2\pi}{L}n_z$$

$$1 = \int dx \int dy \int dz\, U_E^*(x) U_E(x) = L^3 |C|^2 \qquad C = \frac{1}{L^{3/2}}$$

$$U_E(x) = \frac{1}{L^{3/2}} e^{i\vec{k}\cdot\vec{x}}$$

$$E = \frac{p^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2)$$

To calculate density of state, imagine a spherical shell in k space.

$$|k| = 2\pi\frac{|n|}{L} \;;\; E = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 |n|^2 = 2\pi^2 \frac{\hbar^2}{mL^2}|n|^2$$

The number of states dN with in shell $4\pi|n|^2 d|n|$:

$$\frac{dN}{dE} = \frac{1}{2\pi^2\hbar^2\frac{1}{mL^2}\,2|n|\,d|n|}\cdot 4\pi|n|^2 \cdot d|n| = \frac{4\pi\,|n|\cdot m\cdot L^2}{4\pi^2\hbar^2} = \frac{1}{\pi}\cdot\frac{mL^2}{\hbar^2}\,\frac{L}{2\pi}\,\frac{\sqrt{2mE}}{\hbar}$$

$$= \frac{m^{3/2}E^{1/2}L^3}{\sqrt{2}\,\pi^2\hbar^3} \qquad \text{DOS.}$$

— The simple Harmonic oscillator:

We solve the time-independent function for $V(x) = \frac{1}{2}m\omega^2 x^2$

Differential Equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}U_E(x) + \frac{1}{2}m\omega^2 x^2 U_E(x) = E\,U_E(x)$$

$$-\frac{\partial^2}{\partial x^2}U_E + \frac{m^2\omega^2}{\hbar^2}x^2 U_E = \frac{2mE}{\hbar^2}U_E$$

Letting: $y = x\cdot\sqrt{\frac{m\omega}{\hbar}} = \frac{x}{x_0} \qquad x_0 = \sqrt{\frac{\hbar}{m\omega}}$

$$-\frac{d^2}{dy^2}U_E + y^2 U_E = \frac{2E}{\hbar\omega}U_E$$

Denote this equation as:

$$\frac{d^2}{dy^2}U(y) + (\varepsilon - y^2)U(y) = 0 \qquad \varepsilon = \frac{2E}{\hbar\omega} \qquad y = \frac{x}{x_0} \qquad x_0 = \sqrt{\frac{\hbar}{m\omega}}$$

$y \to \pm\infty$, the solution must tend to zero

$$W''(y) - y^2 W(y) = 0$$

$W(y) \propto \exp\left(\pm\frac{y^2}{2}\right) \longrightarrow$ so we have to choose the minus sign.

Then we "remove" the asymtotic behavior of the wave function

$$U(y) = h(y)\,e^{-y^2/2}$$

$$\frac{d^2}{dy^2}h - 2y\frac{dh}{dy} + (\varepsilon - 1)h(y) = 0$$

Approach 1: a normalizable solution is only possible when series terminates.

$\Downarrow$

One Forces the termination by imposing $\varepsilon - 1 = 2n$ (Sakurai P99. do not Unders)

Approach 2: Introduce Hermite polynomials:

$$g(x,t) = e^{-t^2+2tx} = \sum_{n=0}^{+\infty} H_n(x) \frac{1}{n!} t^n$$

Some property of $H_n(x)$

1° $H_0(x) = 1$; the term $g(x,t)$ for t^0 order is 1.

2° $H_n(0) = (-1)^{n/2} \frac{n!}{(n/2)!}$

proof: when $x = 0$,

$$g(x,t) = e^{-t^2} = \sum_{n=0}^{+\infty} \frac{(-1)^{n/2}}{(n/2)!} t^n = \sum_{n=0}^{+\infty} \frac{(-1)^{n/2}}{(n/2)!} \frac{n!}{n!} \cdot t^n$$ (Restrict our result to even number)

$$H_n(0) = \frac{(-1)^{n/2}}{(n/2)!} \cdot n!$$

3° $H_n(-x) = (-1)^n H_n(x)$

This is Because $g(x,t) = \sum_n H_n(x) \frac{t^n}{n!}$

$$\begin{cases} g(x,-t) = \sum_n H_n(x) \frac{t^n}{n!} \cdot (-1)^n \\ g(-x,t) = \sum_n H_n(-x) \frac{t^n}{n!} \end{cases}$$

$g(x,t) = e^{-t^2+2tx}$

$\Downarrow$

$g(x,-t) = g(-x,t)$

$$H_n(-x) = (-1)^n H_n(x)$$

4° induction way to derive hermitian polynomials:

$$\frac{\partial g}{\partial x} = 2t\,g = \sum_n H_n(x) \frac{1}{n!} \cdot 2 \cdot t^{n+1} = \sum_n H_{n-1}(x) \frac{1}{(n-1)!} \cdot 2 \cdot t^n = \sum_{n=1} 2H_{n-1}(x) \frac{n!}{(n-1)!} \frac{1}{n!} \cdot t^n$$

$$\frac{\partial g}{\partial x} = \sum_n H_n'(x) \frac{t^n}{n!}$$

$$H_n'(x) = 2n H_{n-1}(x) \quad (n = 1, 2 \cdots)$$

Considered: $H_0(x) = 1$ $\qquad H_n(0) = \frac{(-1)^{n/2}}{(n/2)!} \cdot n!$

$H_1'(x) = 2 \qquad H_1(x) = 2x$

$H_2'(x) = 8x \qquad H_2(x) = 4x^2 - 2$

$H_3'(x) = 24x^2 - 12 \qquad H_3(x) = 8x^3 - 12x$

5° Find Relation between Hermitian function and Schrodinger Function

$$\frac{\partial g}{\partial t} = -2t\,g + 2x\,g$$

$$= -\sum_{n=0} 2H_n(x) \frac{t^{n+1}}{n!} + \sum_{n=0} 2x H_n(x) \frac{t^n}{n!}$$

$\Downarrow$ $\frac{1}{(n+1)!} \frac{(n+1)}{n!} \cdot (n+1)!$

$$= \sum_{n=1}^{+\infty} -2n H_{n-1}(x) \frac{t^n}{n!} + \sum_{n=0} 2x H_n(x) \frac{t^n}{n!}$$

$$\frac{\partial g}{\partial t} = \sum_{n=0}^{+\infty} H_n(x) \frac{n}{n!} t^{n-1} = \sum_{n=0}^{+\infty} H_{n+1}(x) \frac{t^n}{n!}$$

$$H_{n+1} = -2n H_{n-1} + 2x H_n$$

$$H_{n+1} - 2x H_n + 2n H_{n-1} = 0 \Rightarrow 2(n-1) H_{n-2} = 2x H_{n-1} - H_n$$

Noticed:

$$H_n' = 2n H_{n-1}$$

$$H_n'' = 2n H_{n-1}' = 2n \cdot 2(n-1) \cdot H_{n-2}$$

$$= 2n (2x H_{n-1} - H_n) = 2x H_n' - 2n H_n \quad (n = 2 \cdots)$$

$$H_n'' - 2x H_n' + 2n H_n = 0$$

$\begin{cases} H_1 = 2x \\ H_0 = 1 \end{cases}$ satisfies this equation

Compare: $h'' - 2y h' + (\varepsilon - 1) h = 0 \Rightarrow \varepsilon = 1 + 2n$

$E = (n+\frac{1}{2})\hbar\omega$

$u_n(x) = C_n H_n(x\sqrt{\frac{m\omega}{\hbar}})e^{-m\omega x^2 \frac{1}{2\hbar}}$ 注意 $\frac{m\omega x^2}{\hbar}$ 是无量纲的.

6. $\int_{-\infty}^{+\infty} H_n(x) H_m(x) e^{-x^2} dx = \pi^{1/2} \cdot 2^n \cdot n! \cdot \delta_{mn}$. (Sakurai Prob 2.25).

—— The Linear Potential:

The Linear Potential $V(x) = k|x|$

Schrodinger, time-independent function:

$$-\frac{\hbar^2}{2m}\frac{d^2 u_E}{dx^2} + k|x|u_E(x) = E\,u_E(x)$$

It is easiest way to deal with this value by restricting $x \geq 0$.

There are two types of solution:

$$\begin{cases} u_E(-x) = -u_E(x) \Rightarrow u_E(0) = 0 \\ u_E(-x) = u_E(x) \Rightarrow u_E'(0) = 0 \end{cases}$$ > Both need satisfy $u_E(x) \to 0$ when $|x| \to \infty$

Dimension Less length scale:

$$x_0 = \left(\frac{\hbar^2}{mk}\right)^{1/3}$$

Energy scale

$$E_0 = kx_0 = \left(\frac{\hbar^2 k^2}{m}\right)^{1/3}$$

$$y = \frac{x}{x_0} \qquad \varepsilon = \frac{E}{E_0}$$

$$\frac{d^2 u_E}{dy^2} - 2(y-\varepsilon)u_E(y) = 0$$

Noticed:

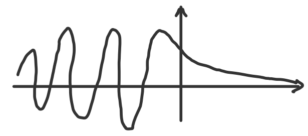
at $y = \varepsilon$, $x = x_0\varepsilon = \frac{x_0}{E_0}E = \frac{E}{k}$. $\Rightarrow$ Classical turning Point.

Translated position variable:

$$\boxed{z = 2^{1/3}(y-\varepsilon)}$$

$$\frac{d^2 u_E}{dz^2} - z\,u_E(z) = 0$$

This is the Airy Function, it has solution



$z = 2^{1/3}(y-\varepsilon) \Leftarrow$ Quantized energy

$\Downarrow$

$Ai'(z) = 0$ when $z = -1.019, -3.249 \cdots$

$Ai(z) = 0$ when $z = -2.338, -4.088 \cdots$

Ground State Energy:

$$E = \frac{1.019}{2^{1/3}}\left(\frac{\hbar^2 k^2}{m}\right)^{1/3}$$

WKB Approximation:

WKB means G. Wentzel, A. Kramers. L. Brillouin.

Consider time - independent Schrodinger eguation.

$$\frac{d^2 u_E}{dx^2} + \frac{2m}{\hbar^2}(E - V(x))u_E(x) = 0$$

Define Quantities:

$$\begin{cases} k(x) = \left(\frac{2m}{\hbar^2}(E - V(x))\right)^{1/2} & E \geq V(x) \\ k(x) = -i\left(\frac{2m}{\hbar^2}(V(x) - E)\right)^{1/2} = -i\,k(x) & E < V(x) \end{cases}$$

Schrödinger Equation Becomes:

$$\frac{d^2 u_E}{dx^2} + (k(x))^2 u_E(x) = 0.$$

If $V(x)$ were not changing with x, $k(x)$ would be a constant.

$$u(x) \propto \exp(\pm i k x)$$

Assume $V(x)$ change slowly with x.

$$u_E(x) \equiv \exp(i W(x)/\hbar)$$

Wave Function would be:

$$i\hbar \frac{d^2 W}{dx^2} - \left(\frac{dW}{dx}\right)^2 + \hbar^2 (k(x))^2 = 0$$

Consider solution to this function under condition:

$$\hbar \left|\frac{d^2 W}{dx^2}\right| \ll \left|\frac{dW}{dx}\right|^2 \Leftarrow \text{Slowly invariant Condition.}$$

For $E > V(x)$

Lowest Approximation for $W(x)$

$$W_0'(x) = \pm \hbar k(x) \Leftarrow \left(\frac{dW}{dx}\right)^2 = \hbar^2 (k(x))^2$$

Leading Order:

$$\left(\frac{dW_1}{dx}\right)^2 = \hbar^2 (k(x))^2 + i\hbar W_0''(x)$$

$$= \hbar^2 (k(x))^2 \pm i\hbar^2 k'(x)$$

Consider second term is much smaller than first term:

$$W(x) \doteq W_1(x) = \pm \hbar \int dx' \left(k^2(x') \pm i k'(x')\right)^{1/2}$$

$\Rightarrow$ Reguesting that: $k'(x') \ll k^2(x')$

$\Uparrow$ noticed this is never the case when $k(x)=0$!

$$\approx \pm \hbar \int dx'\, k(x') \left(1 \pm \frac{i}{2}\frac{k'(x')}{k^2(x')}\right)$$

$$= \pm \hbar \int dx'\, k(x') + \frac{i}{2}\hbar \ln(k(x))$$

First order approximation for wave function

$$u_E(x) = \exp(iW(x)/\hbar) = \frac{1}{[k(x)]^{1/2}} \exp\left[\pm i \int^x dx'\, k(x')\right]$$

For $E < V(x)$

$$\left(\frac{dW_1}{dx}\right)^2 = \hbar^2 (k(x))^2 + i\hbar W_0''(x)$$

$$= -\hbar^2 k^2(x) + i\hbar W_0''(x)$$

$$\left(\frac{dW_0}{dx}\right)^2 = -\hbar^2 k^2(x) \Rightarrow \frac{dW_0}{dx} = \pm i\hbar k(x)$$

$$\left(\frac{dW_1}{dx}\right)^2 = -\hbar^2 k^2(x) \mp \hbar^2 k'(x) = -\hbar^2 \left(k^2(x) \pm k'(x)\right)$$

$$\frac{dW_1}{dx} = \pm i\hbar \sqrt{k^2(x) \pm k'(x)} = \pm i\hbar k(x) + i\hbar \frac{1}{2}\frac{k'(x)}{k(x)}$$

$$W_1(x) = \pm i\hbar \int^x k(x')dx' + \frac{1}{2} i\hbar \ln(k(x))$$

$$u_E(x) = \exp\left(\frac{i}{\hbar} W(x)\right) = \frac{1}{\sqrt{k(x)}} \cdot \exp\left(\pm \int^x k(x')\,dx'\right)$$

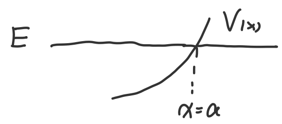
In all:

$$u_E(x) = \frac{1}{\sqrt{k(x)}} \cdot \exp\left(\pm \int^x k(x')dx'\right) \qquad E < V(x)$$

$$u_E(x) = \frac{1}{\sqrt{k(x)}} \exp\left(\pm i \int^x k(x')dx'\right) \qquad E > V(x)$$

— 因为在 $E = V(x)$ 时, $k^2(x) = 0$, 此时不能用 WKB 近似, 此时要精确求解:

认为在 $x \approx a$ 时 $V(x) - E = g(x-a)$.



则: $\frac{d^2u_E}{dx^2} + \frac{2m}{\hbar^2}(E - V(x))u_E = 0$

变量代换: $x-a = \alpha z$, z 无量纲!

$$\alpha^{-2}\frac{d^2u_E}{dz^2} - \frac{2mg}{\hbar^2}\cdot\alpha\cdot z\cdot u_E = 0$$

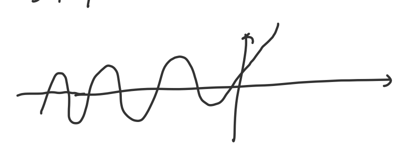
取: $\alpha = \left(\frac{2mg}{\hbar^2}\right)^{-1/3}$ 则:

$$\frac{d^2u_E}{dz^2} - z\cdot u_E = 0.$$

这是 Airy Function!

- $Ai(z) = \begin{cases} \frac{1}{2}\pi^{-1/2}\cdot z^{-1/4}\cdot e^{-\xi} & z \gg 0 \\ \pi^{-1/2}\cdot|z|^{-1/4}\cdot\cos(\xi - \frac{\pi}{4}) & z \ll 0 \end{cases}$ $\qquad \xi = \frac{2}{3}|z|^{3/2}$

- $Bi(z) = \begin{cases} \pi^{-1/2}\cdot z^{-1/4}\cdot e^{\xi} & z \gg 0 \\ -\pi^{-1/2}\cdot|z|^{-1/4}\cdot\sin(\xi - \frac{\pi}{4}) & z \ll 0 \end{cases}$



—— 考虑 WKB 近似对于方程 $-\frac{\hbar^2}{2m}\frac{d^2u_E}{dx^2} + g(x-a)u_E = 0$ 的求解:

$$k^2(x) = -\frac{2mg}{\hbar^2}(x-a)$$

$$\begin{cases} k(x) = \sqrt{\frac{2mg}{\hbar^2}(a-x)} & x<a \\ k(x) = -i\sqrt{\frac{2mg}{\hbar^2}(x-a)} = -i\,k(x) & x>a \\ \Downarrow \\ k(x) = \sqrt{\frac{2mg}{\hbar^2}(x-a)} \end{cases}$$

$$\begin{cases} z = \left(\frac{2mg}{\hbar^2}\right)^{\frac{1}{3}}(x-a) \\ z^{\frac{1}{4}} = \left(\frac{2mg}{\hbar^2}\right)^{\frac{1}{12}-\frac{1}{2}}\sqrt{\frac{2mg}{\hbar^2}}\,(x-a)^{\frac{1}{4}} \end{cases}$$

$$\int_a^x k(x')dx' = \frac{2}{3}\left(\frac{2mg}{\hbar^2}\right)^{\frac{1}{2}}(x-a)^{3/2} = \frac{2}{3}|z|^{3/2} = \xi$$

$$\int_x^a k(x')dx' = \frac{2}{3}|z|^{3/2} = \xi$$

则, 若在远点有解: $(x \gg a)$

$$u_E(x) = \frac{A}{\sqrt{k(x)}}\cdot\exp\left(-\int_a^x k(x')dx'\right) + \frac{B}{\sqrt{k(x)}}\cdot\exp\left(+\int_a^x k(x')dx'\right) \quad \text{—}\circ$$

$$= 2A\cdot\left(\frac{2mg}{\hbar^2}\right)^{\frac{1}{12}-\frac{1}{2}}\cdot\pi^{1/2}\frac{\pi^{-1/2}}{2}\frac{1}{|z|^{1/4}}\cdot\exp(-\xi) + B\cdot\left(\frac{2mg}{\hbar^2}\right)^{\frac{1}{12}-\frac{1}{2}}\cdot\pi^{1/2}\cdot\pi^{-1/2}\frac{1}{|z|^{1/4}}\cdot\exp(+\xi)$$

$$= 2A\cdot\left(\frac{2mg}{\hbar^2}\right)^{\frac{1}{12}-\frac{1}{2}}\cdot\pi^{1/2}\cdot Ai(z) + B\cdot\left(\frac{2mg}{\hbar^2}\right)^{\frac{1}{12}-\frac{1}{2}}\cdot\pi^{1/2}\cdot Bi(z)$$

于是在 $x \ll a$ 时, 解是:

$$u_E(x) = 2A\cdot\left(\frac{2mg}{\hbar^2}\right)^{\frac{1}{12}-\frac{1}{2}}\cdot\pi^{1/2}\cdot Ai(z) + B\cdot\left(\frac{2mg}{\hbar^2}\right)^{\frac{1}{12}-\frac{1}{2}}\cdot\pi^{1/2}\cdot Bi(z)$$

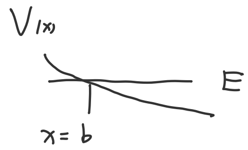
$$= 2A\left(\frac{2mg}{\hbar^2}\right)^{\frac{1}{12}-\frac{1}{2}}\cdot\pi^{1/2}\cdot\pi^{-1/2}\cdot\frac{1}{|z|^{1/4}}\cdot\cos(\xi-\frac{\pi}{4}) - B\cdot\left(\frac{2mg}{\hbar^2}\right)^{\frac{1}{12}-\frac{1}{2}}\cdot\pi^{1/2}\,\pi^{-1/2}\cdot\frac{1}{|z|^{1/4}}\sin(\xi-\frac{\pi}{4})$$

$$= 2A\frac{1}{\sqrt{k(x)}}\cdot\cos\left(\int_x^a k(x')dx' - \frac{\pi}{4}\right) - B\cdot\frac{1}{\sqrt{k(x)}}\cdot\sin\left(\int_x^a k(x')dx' - \frac{\pi}{4}\right) \quad \text{—}\circ$$

于是有所谓系数关系.

$$\begin{cases} \frac{A}{\sqrt{k(x)}}\cdot\exp\left(-\int_a^x k(x')dx'\right) + \frac{B}{\sqrt{k(x)}}\cdot\exp\left(+\int_a^x k(x')dx'\right) & (x \gg a) \\ 2A\frac{1}{\sqrt{k(x)}}\cdot\cos\left(\int_x^a k(x')dx' - \frac{\pi}{4}\right) - B\cdot\frac{1}{\sqrt{k(x)}}\cdot\sin\left(\int_x^a k(x')dx' - \frac{\pi}{4}\right) & (x \ll a) \end{cases}$$

若有:边界:



同理:

$$\left\{\begin{array}{l} \frac{A'}{\sqrt{k(x)}} \exp\left(-\int_x^b k(x')dx'\right) + \frac{B'}{\sqrt{k(x')}} \exp\left(\int_x^b k(x')dx'\right) \quad \Updownarrow \\ 2\frac{A'}{\sqrt{k(x)}} \cdot \cos\left(\int_b^x k(x')dx' - \frac{\pi}{4}\right) - \frac{B'}{\sqrt{k(x)}} \sin\left(\int_b^x k(x')dx' - \frac{\pi}{4}\right) \end{array}\right.$$

—— 用 WKB 近似得到的系数关系得到 Sommerfeld Quantization

ignore the Diffuse term in the wave Function

$$u_E(x) = A' \frac{1}{\sqrt{k(x)}} \cdot \exp\left(-\int_x^b k(x') dx'\right) \quad \text{when} \quad x \ll b$$

$$\Downarrow$$

$$u_E(x) = 2A' \frac{1}{\sqrt{k(x)}} \cdot \cos\left(\int_b^x k(x')dx' - \frac{\pi}{4}\right)$$

$$= 2A' \frac{1}{\sqrt{k(x)}} \cdot \cos\left(\int_b^a k(x') dx' - \int_x^a k(x')dx' - \frac{\pi}{4}\right) \qquad \cos(\alpha) = \sin(\alpha + \frac{\pi}{2})$$

$$= 2A' \frac{1}{\sqrt{k(x)}} \cdot \sin\left(\int_b^a k(x') dx' - \int_x^a k(x')dx' + \frac{\pi}{4}\right)$$

$$= 2A' \frac{1}{\sqrt{k(x)}} \cdot \sin\left(\int_b^a k(x')dx'\right) \cos\left(\int_x^a k(x')dx' - \frac{\pi}{4}\right)$$

$$- 2A' \frac{1}{\sqrt{k(x)}} \cos\left(\int_b^a k(x')dx'\right) \cdot \sin\left(\int_x^a k(x')dx' - \frac{\pi}{4}\right)$$

The second term is non-physical term:

$$\int_b^a k(x')dx' = (n + \tfrac{1}{2})\pi$$

$$\oint p(x')dx' = 2\int_b^a \hbar k(x')dx' = 2\pi\hbar \cdot (n + \tfrac{1}{2}) = (n + \tfrac{1}{2})h \quad \Leftarrow \text{Sommerfeld Quantization}$$

Spin-1/2 System.

- Stern-Gerlach experiment. $\longrightarrow$ Derive S_x S_y S_z Operator:

The system has bases kets: $|+\rangle$ $|-\rangle$!

Experiment: S_x+ beam subjected to $SG\hat{z}$. The Beam Split into two components with same intense!

$$|\langle + | S_x ; + \rangle| = |\langle - | S_x , + \rangle| = \frac{1}{\sqrt{2}}$$

Construct:

$$|S_x ; +\rangle = \frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}} e^{i\delta_1} |-\rangle$$

Orthogonality relation:

$$|S_x ; -\rangle = \frac{1}{\sqrt{2}}|+\rangle - \frac{1}{\sqrt{2}} e^{i\delta_1} |-\rangle$$

Operator:

$$\hat{S}_x = \frac{\hbar}{2} |S_x;+\rangle\langle S_x;+| - \frac{\hbar}{2} |S_x;-\rangle\langle S_x;-|$$

$$= \frac{\hbar}{2}\left(e^{-i\delta_1} |+\rangle\langle -| + e^{i\delta_1} |-\rangle\langle +|\right)$$

Similarity:

$$|S_y ; \pm\rangle = \frac{1}{\sqrt{2}}|+\rangle \pm \frac{1}{\sqrt{2}} e^{i\delta_2} |-\rangle$$

$$\hat{S}_y = \frac{\hbar}{2}\left(e^{-i\delta_2} |+\rangle\langle -| + e^{i\delta_2} |-\rangle\langle +|\right)$$

Experiment Shows:

$$|\langle S_y , \pm | S_x , +\rangle| = |\langle S_y , \pm | S_x - \rangle| = \frac{1}{\sqrt{2}}$$

$$\frac{1}{2} \left| 1 \pm e^{i(\delta_1 \overset{\Downarrow}{-} \delta_2)} \right| = \frac{1}{\sqrt{2}} \Rightarrow \delta_2 - \delta_1 = \frac{\pi}{2} \text{ or } -\frac{\pi}{2}$$ $\Leftarrow$ 和角动量有关！不知连系.

Let: $\delta_1 = 0$ $\delta_2 = \pi/2$

$$|S_x , \pm\rangle = \frac{1}{\sqrt{2}}|+\rangle \pm \frac{1}{\sqrt{2}}|-\rangle$$

$$|S_y , \pm\rangle = \frac{1}{\sqrt{2}}|+\rangle \pm \frac{i}{\sqrt{2}}|-\rangle$$

$$S_x = \frac{\hbar}{2}\left(|+\rangle\langle -| + |-\rangle\langle +| \right)$$

$$S_y = \frac{i\hbar}{2}\left(-|+\rangle\langle -| + |-\rangle\langle +| \right)$$

$$S_z = \frac{\hbar}{2}\left(|+\rangle\langle +| - |-\rangle\langle -| \right)$$

Pauli Two components Formalism.

$$|+\rangle \doteq \begin{pmatrix}1\\0\end{pmatrix} \equiv \chi_+ \qquad |-\rangle \doteq \begin{pmatrix}0\\1\end{pmatrix} \equiv \chi_-$$

$$\langle +| \doteq (1, 0) \equiv \chi_+^\dagger \qquad \langle -| \doteq (0, 1) \equiv \chi_-^\dagger$$

$$|\alpha\rangle = |+\rangle\langle +|\alpha\rangle + |-\rangle\langle -|\alpha\rangle = \begin{pmatrix}\langle +|\alpha\rangle\\ \langle -|\alpha\rangle\end{pmatrix}$$

$$\langle\alpha| = \langle\alpha|+\rangle\langle +| + \langle\alpha|-\rangle\langle -| = (\langle\alpha|+\rangle, \langle\alpha|-\rangle)$$

$$\chi = \begin{pmatrix}\langle +|\alpha\rangle\\ \langle -|\alpha\rangle\end{pmatrix} = \begin{pmatrix}C_+\\ C_-\end{pmatrix} = C_+\chi_+ + C_-\chi_-$$

Definition of Pauli Matrix:

$$\langle \pm|S_k|+\rangle = \frac{\hbar}{2}(\sigma_k)_{\pm,+}$$

$$\langle \pm|S_k|-\rangle = \frac{\hbar}{2}(\sigma_k)_{\pm,-}$$

于是:

$$\langle\alpha|S_k|\alpha\rangle = \sum_{a'a''}\langle\alpha|a'\rangle\langle a'|S_k|a''\rangle\langle a''|\alpha\rangle = \frac{\hbar}{2}\chi^\dagger\sigma_k\chi$$

$$\sigma_1 = \begin{pmatrix}0&1\\1&0\end{pmatrix} \quad \sigma_2 = \begin{pmatrix}0&-i\\i&0\end{pmatrix} \quad \sigma_3 = \begin{pmatrix}1&0\\0&-1\end{pmatrix}$$

Property of Pauli Matrix:

$$\begin{cases}\{\sigma_i, \sigma_j\} = 2\delta_{ij}\\ [\sigma_i, \sigma_j] = 2i\,\varepsilon_{ijk}\sigma_k\end{cases}$$

$$\begin{cases}\sigma_i = \sigma_i^\dagger & \text{Hermitian}\\ \det(\sigma_i) = 1 & \text{Special.}\\ \mathrm{Tr}(\sigma_i) = 0 & \text{traceless}\end{cases}$$

$$\sigma\cdot a = \sum_k a_k\sigma_k$$

$$= \begin{pmatrix}a_3 & a_1 + ia_2\\ a_1 - ia_2 & -a_3\end{pmatrix}$$

$$(\sigma\cdot a)(\sigma\cdot b) = a\cdot b\,\mathbb{I} + i\,\sigma\cdot(a\times b)$$

proof:

$$\sum_j\sigma_j a_j\sum_k\sigma_k b_k = \sum_{j,k}\left(\frac{1}{2}\{\sigma_j, \sigma_k\} + \frac{1}{2}[\sigma_j, \sigma_k]\right)a_j b_k$$

$$= \sum_{j,k}(\delta_{jk}\mathbb{I} + i\,\varepsilon_{jkl}\sigma_l)a_j b_k$$

$$= a\cdot b\,\mathbb{I} + i\,\sigma\cdot(a\times b)$$

If a is a real vector:

$$(\sigma\cdot a)^2 = |a|^2\,\mathbb{I}$$

Rotation and angular momentum.

The convention we follow in this book is the rotation affects the system itself. (not the axis). The coordinates remain unchanged.

$$R_z(\phi) = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$R_x(\phi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\phi & -\sin\phi \\ 0 & \sin\phi & \cos\phi \end{pmatrix}$$

$$R_y(\phi) = \begin{pmatrix} \cos\phi & 0 & \sin\phi \\ 0 & 1 & 0 \\ -\sin\phi & 0 & \cos\phi \end{pmatrix}$$

Infinitesimal small form:

$$R_z(\varepsilon) = \begin{pmatrix} 1-\frac{\varepsilon^2}{2} & -\varepsilon & 0 \\ \varepsilon & 1-\frac{\varepsilon^2}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad R_x = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1-\frac{\varepsilon^2}{2} & -\varepsilon \\ 0 & \varepsilon & 1-\frac{\varepsilon^2}{2} \end{pmatrix}$$

$$R_y = \begin{pmatrix} 1-\frac{\varepsilon^2}{2} & 0 & \varepsilon \\ 0 & 1 & 0 \\ -\varepsilon & 0 & 1-\frac{\varepsilon^2}{2} \end{pmatrix}$$

$$R_x(\varepsilon) R_y(\varepsilon) - R_y(\varepsilon) R_x(\varepsilon) = \begin{pmatrix} 0 & -\varepsilon^2 & 0 \\ \varepsilon^2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = R_z(\varepsilon^2) - \mathbb{I} = R_z(\varepsilon^2) - R_{any}(0)$$

— Given A rotation R, it induces quantum operator in ket space: $\mathcal{D}(R)$

Suppose infinitesimal Rotation Operator: $|\alpha\rangle \longrightarrow |\alpha\rangle_R = \mathcal{D}(R)|\alpha\rangle$

$$U_\varepsilon = 1 - iG\varepsilon \qquad G = \frac{J}{\hbar}$$

$$U_\varepsilon = 1 - i\frac{J}{\hbar}\varepsilon$$

For example:

$$\mathcal{D}_z(\phi) = \lim_{N\to+\infty}\left(1 - i\frac{J_z}{\hbar}\frac{\phi}{N}\right)^N = \exp\left(-i\frac{J_z\phi}{\hbar}\right) \overset{\text{Taylor expansion}}{\approx} 1 - i\frac{J_z\phi}{\hbar} - \frac{J_z^2\phi^2}{2\hbar^2}\cdots$$

$$\mathcal{D}_{\hat{n}}(\phi) = \exp\left(-i\frac{J\cdot\hat{n}}{\hbar}\phi\right)$$

Postulates $\mathcal{D}(R)$ has same group property as R!

Identity: $\mathcal{D}(R)\mathbb{I} = \mathbb{I}\mathcal{D}(R)$ $\Leftarrow R\cdot\mathbb{I} = R$

Closure: $\mathcal{D}(R_1)\mathcal{D}(R_2) = \mathcal{D}(R_3)$ $\Leftarrow R_1R_2 = R_3$

Inverse: $\mathcal{D}(R^{-1})\mathcal{D}(R) = \mathcal{D}(R)\mathcal{D}(R^{-1}) = \mathbb{I}$ $\Leftarrow RR^{-1} = R^{-1}R = \mathbb{I}$

Associativity: $\left(\mathcal{D}(R_1)\mathcal{D}(R_2)\right)\mathcal{D}(R_3) = \mathcal{D}(R_1)\left(\mathcal{D}(R_2)\mathcal{D}(R_3)\right) = \mathcal{D}(R_1)\mathcal{D}(R_2)\mathcal{D}(R_3)$ $\Leftarrow R_1(R_2R_3) = (R_1R_2)R_3 = R_1R_2R_3$

—— commutation Relation For angular momentum operator:

$$\mathcal{D}(R_x(\varepsilon))\mathcal{D}(R_y(\varepsilon)) - \mathcal{D}(R_y(\varepsilon))\mathcal{D}(R_x(\varepsilon)) = \mathcal{D}(R_z(\varepsilon^2)) - \mathbb{I}$$

$$\left(1 - i\frac{J_x\varepsilon}{\hbar} - \frac{J_x^2\varepsilon^2}{2\hbar^2}\right)\left(1 - i\frac{J_y\varepsilon}{\hbar} - \frac{J_y^2\varepsilon^2}{2\hbar^2}\right) - \left(1 - i\frac{J_y\varepsilon}{\hbar} - \frac{J_y^2\varepsilon^2}{2\hbar^2}\right)\left(1 - i\frac{J_x\varepsilon}{\hbar} - \frac{J_x^2\varepsilon^2}{2\hbar^2}\right)$$

$$= 1 - i\frac{J_z\varepsilon^2}{\hbar} - 1$$

leads to: $[J_x, J_y] = i\hbar J_z$

Repeating this argument with rotations:

$$[J_i, J_j] = i\hbar\,\varepsilon_{ijk}J_k$$

— Translation of average number of angular momentum operator:

$$\langle J_x \rangle_{R_z(\phi)} = \langle \alpha | \mathcal{D}^\dagger(R_z(\phi))\ J_x\ \mathcal{D}(R_z(\phi)) | \alpha \rangle$$

$$= \langle \alpha | \exp\left(i \frac{J_z \phi}{\hbar}\right) \cdot J_x \cdot \exp\left(-i \frac{J_z \phi}{\hbar}\right) | \alpha \rangle$$

$$= \langle \alpha | J_x + \left(\frac{i\phi}{\hbar}\right)[J_z, J_x] + \frac{1}{2!}\left(\frac{i\phi}{\hbar}\right)^2 [J_z, [J_z, J_x]] \cdots | \alpha \rangle$$

$$= \langle \alpha | J_x \left(1 - \frac{1}{2!}\phi^2 \cdots\right) - J_y \left(\phi - \frac{1}{3!}\phi^3 \cdots\right) | \alpha \rangle$$

$$= \langle \alpha | J_x \cos\phi - J_y \sin\phi | \alpha \rangle$$

$\Downarrow$ 不加证明说:

$$\langle J_k \rangle_R = \sum_l R_{kl} \langle J_l \rangle$$

Baker - Hausdroff Lemma:

$$\exp(iG\lambda) A \cdot \exp(-iG\lambda) = A + i\lambda[G, A] + \frac{(i\lambda)^2}{2!}[G, [G, A]] + \frac{(i\lambda)^n}{n!}[G, \cdots [G, A] \cdots]$$

$[J_i, J_j] = i\hbar\, \varepsilon_{ijk} J_k$
$\Updownarrow$

Rotations in two component formalism ← This is because: $[S_i, S_j] = i\hbar\, \varepsilon_{ijk} S_k$

$$\exp\left(-\frac{i S\cdot\hat{n}}{\hbar}\phi\right) \doteq \exp\left(-i\frac{\sigma\cdot\hat{n}\phi}{2}\right) \Rightarrow \chi \longmapsto \exp\left(-i\frac{\sigma\cdot\hat{n}\phi}{2}\right)\chi$$

— $(\sigma\cdot\hat{n})^n = \begin{cases} 1 & \text{for } n = \text{even number} \\ \sigma\cdot\hat{n} & \text{for } n = \text{odd number.} \end{cases}$

proved before in Dirac two component formalism. $(\sigma\cdot\hat{n})^2 = |\hat{n}|^2 \mathbb{I} = \mathbb{I}$

—
$$\exp\left(-i\frac{\sigma\cdot\hat{n}}{2}\phi\right) = \left(1 - \frac{(\sigma\cdot\hat{n})^2}{2!}\left(\frac{\phi}{2}\right)^2 + \frac{(\sigma\cdot\hat{n})^4}{4!}\left(\frac{\phi}{2}\right)^4 \cdots\right)$$
$$-i\left((\sigma\cdot\hat{n})\frac{\phi}{2} - \frac{(\sigma\cdot\hat{n})^3}{3!}\left(\frac{\phi}{2}\right)^3 + \cdots\right)$$
$$= \mathbb{I}\cdot\cos\left(\frac{\phi}{2}\right) - i(\sigma\cdot\hat{n})\sin(\phi/2)$$

Explicitly: In 2×2 form:

$$\exp\left(-i\frac{\sigma\cdot\hat{n}}{2}\phi\right) = \begin{pmatrix} \cos\left(\frac{\phi}{2}\right) - i n_z \sin\left(\frac{\phi}{2}\right) & (-i n_x - n_y)\sin\left(\frac{\phi}{2}\right) \\ (-i n_x + n_y)\sin\left(\frac{\phi}{2}\right) & \cos\left(\frac{\phi}{2}\right) + i n_z \sin\left(\frac{\phi}{2}\right) \end{pmatrix}$$

— $\chi^\dagger \sigma \chi$ obeys translation property of a vector:

$$\chi^\dagger \sigma_k \chi \longmapsto \sum_l R_{kl}\cdot \chi^\dagger \sigma_l \chi$$

— 2π problem:

$$S_x = \frac{\hbar}{2}\left(|+\rangle\langle -| + |-\rangle\langle +|\right)$$
$$S_y = i\frac{\hbar}{2}\left(-|+\rangle\langle -| + |-\rangle\langle +|\right)$$
$$S_z = \frac{\hbar}{2}\left(|+\rangle\langle +| - |-\rangle\langle -|\right)$$

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

$$\exp\left(-i\frac{S_z}{\hbar}\phi\right)|\alpha\rangle = \exp\left[-i\frac{\phi}{2}\left(|+\rangle\langle +| - |-\rangle\langle -|\right)\right]\cdot|\alpha\rangle$$
$$= \exp\left(-i\frac{\phi}{2}|+\rangle\langle +|\right)\exp\left(-i\frac{\phi}{2}|-\rangle\langle -|\right)|\alpha\rangle$$
$$= e^{-i\frac{\phi}{2}}\cdot|+\rangle\langle +|\alpha\rangle + e^{-i\frac{\phi}{2}}|-\rangle\langle -|\alpha\rangle$$
$$\Downarrow$$

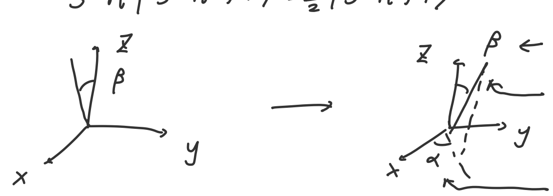
$$|\alpha\rangle_{R_z(2\pi)} = -|\alpha\rangle$$

— Construct spinor satisfying:

$$\sigma\cdot\hat{n}\,\chi = \chi$$

In orther words:

$$S\cdot\hat{n}\,|S\cdot\hat{n};+\rangle = \frac{\hbar}{2}|S\cdot\hat{n};+\rangle$$



← First rotation

After rotation, this is the direction of $\hat{n}$.

second rotation

$$\chi = \left(\cos\left(\frac{\alpha}{2}\right) - i\sigma_3\sin\left(\frac{\alpha}{2}\right)\right)\left(\cos\left(\frac{\beta}{2}\right) - i\sigma_2\sin\left(\frac{\beta}{2}\right)\right)\cdot\begin{pmatrix}1\\0\end{pmatrix}$$
$$= \begin{pmatrix} \cos\left(\frac{\beta}{2}\right)e^{-i\alpha/2} \\ \sin\left(\frac{\beta}{2}\right)e^{i\alpha/2} \end{pmatrix}$$

— Cayley klein Parameter: (for SU(2) Group)

$$U(a,b) = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix} \qquad |a|^2 + |b|^2 = 1$$

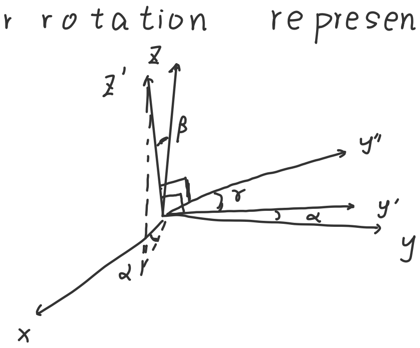
$$U(a_1,b_1)\, U(a_2,b_2) = U(a_1 a_2 - b_1 b_2^*,\ a_1 b_2 + a_2^* b_1)$$

$$U^{-1}(a,b) = U(a^*, -b)$$

$$\left.\begin{matrix} U(a,b) \\ \underbrace{U(-a,-b)} \end{matrix}\right\rangle \text{ same } 3\times 3 \text{ matrix}$$

$$= \underbrace{(-\mathbb{I})}_{\text{In } SO(3),\ \text{is } \mathbb{I}} U(a,b)$$

Euler rotation represented by



$$R(\alpha,\beta,\gamma) = R_{z'}(\gamma)\, R_{y'}(\beta)\, R_z(\alpha)$$

Consider:

$$\begin{cases} R_{y'}(\beta) = R_z(\alpha)\, R_y(\beta)\, R_z^{-1}(\alpha) \\ R_{z'}(\gamma) = R_{y'}(\beta)\, R_z(\gamma)\, R_{y'}^{-1}(\beta) \end{cases}$$

$$R(\alpha,\beta,\gamma) = R_{y'}(\beta)\, R_z(\gamma)\, R_{y'}^{-1}(\beta) \quad R_{y'}(\beta) \quad R_z(\alpha)$$

$$= R_z(\alpha)\, R_y(\beta)\, R_z^{-1}(\alpha) \quad R_z(\gamma) \quad R_z(\alpha)$$

$$= R_z(\alpha)\, R_y(\beta)\, R_z(\gamma)$$

Then:

$$\mathcal{D}(\alpha,\beta,\gamma) = \mathcal{D}_z(\alpha)\, \mathcal{D}_y(\beta)\, \mathcal{D}_z(\gamma)$$

Matrix representation of this product:

$$\exp\left(-i\frac{\sigma_z \alpha}{2}\right) \cdot \exp\left(-i\frac{\sigma_y \beta}{2}\right) \cdot \exp\left(-i\frac{\sigma_z \gamma}{2}\right)$$

$$= \begin{pmatrix} e^{-i\alpha/2} & 0 \\ 0 & e^{i\alpha/2} \end{pmatrix} \begin{pmatrix} \cos(\beta/2) & -\sin(\beta/2) \\ \sin(\beta/2) & \cos(\beta/2) \end{pmatrix} \cdot \begin{pmatrix} e^{-i\gamma/2} & 0 \\ 0 & e^{i\gamma/2} \end{pmatrix}$$

$$= \begin{pmatrix} e^{-i(\alpha+\gamma)/2} \cos(\beta/2) & -e^{-i(\alpha-\gamma)/2} \cdot \sin(\beta/2) \\ e^{i(\alpha-\gamma)/2} \cdot \sin(\beta/2) & e^{i(\alpha+\gamma)/2} \cdot \cos(\beta/2) \end{pmatrix}$$

For rotation operator $\mathcal{D}(\alpha,\beta,\gamma)$. It's matrix element:

$$\mathcal{D}^{(1/2)}_{m'm}(\alpha,\beta,\gamma) = \langle j=\tfrac{1}{2}, m' |\ \exp\left(-i\frac{J_z \alpha}{\hbar}\right) \exp\left(-i\frac{J_y \beta}{\hbar}\right) \exp\left(-i\frac{J_z \gamma}{\hbar}\right) | j=\tfrac{1}{2}, m\rangle$$

Evolution of a state in Spin 1/2 system, and its relation with rotation.

$$H = -\underbrace{\frac{e}{m_e c}}_{\text{magnetic moment}} S \cdot B = -\omega S_z \qquad \omega = \frac{|e| B}{m_e c}$$

$$U(t,0) = \exp\left(-i\frac{Ht}{\hbar}\right) = \exp\left(-i\frac{S_z \omega t}{\hbar}\right)$$

$$\begin{cases} \langle S_x \rangle_t = \langle S_x \rangle_{t=0} \cos(\omega t) - \langle S_y \rangle_{t=0} \sin \omega t \\ \langle S_y \rangle_t = \langle S_y \rangle_{t=0} \cos(\omega t) + \langle S_x \rangle_{t=0} \sin \omega t \\ \langle S_z \rangle_t = \langle S_z \rangle_{t=0} \end{cases}$$

$$|\alpha, t_0 ; t\rangle = \exp\left(-i \frac{S_z \omega t}{\hbar}\right) \cdot \underbrace{\left(|+\rangle\langle+| + |-\rangle\langle-| \right)}_{= \mathbb{I}} \cdot |\alpha\rangle$$

$$= \exp\left(-i \frac{\omega t}{2}\right) \cdot |+\rangle\langle+|\alpha\rangle + e^{i \frac{\omega t}{2}} |-\rangle\langle-|\alpha\rangle$$

← Sakurai!

3.5 Eigen lues and Eigen states of Angular Momentum:

$$J^2 = J_x J_x + J_y J_y + J_z J_z$$

$$[J^2, J_k] = 0 \quad (k = 1, 2, 3)$$

$$[J_i, J_j] = i\hbar \, \varepsilon_{ijk} J_k .$$

Proof: for $k = 3$ case:

$$[J_x J_x + J_y J_y + J_z J_z, J_z] = J_x [J_x, J_z] + [J_x, J_z] J_x + J_y [J_y, J_z] + [J_y, J_z] \cdot J_y$$

$$= J_x(-i\hbar J_y) - i\hbar J_y \cdot J_x + J_y (i\hbar J_x) + (i\hbar J_x) J_y$$

$$= 0$$

Noticed that: (上面用到了这个关系!

$$[J_x J_x, J_z] = J_x J_x J_z - J_z J_x J_x = J_x J_x J_z - J_x J_z J_x + J_x J_z J_x - J_z J_x J_x$$

$$= J_x [J_x, J_z] + [J_x, J_z] J_x$$

Looking for simultaneous eigenkets of J^2 and J_z.

$$J^2 |a, b\rangle = a |a, b\rangle$$

$$J_z |a, b\rangle = b |a, b\rangle$$

Ladder operator:

$$J_\pm = J_x \pm i J_y$$

satisfies:

$$[J_z, J_\pm] = \pm \hbar J_\pm$$

$$[J^2, J_\pm] = 0$$

- $J_z (J_\pm |a.b\rangle) = J_\pm (J_z |a.b\rangle) + [J_z, J_\pm] |a.b\rangle$
  $= (b \pm \hbar) J_\pm |a, b\rangle$

- $J^2 (J_\pm |a.b\rangle) = J_\pm (J^2 |a.b\rangle) + [J^2, J_\pm] |a.b\rangle$
  $= a \cdot J_\pm |a.b\rangle$

To summarize: $J_\pm |a.b\rangle$ are the simultaneous eigenket for J^2 and J_z. with eigenvalue a and $b \pm \hbar$.

Important property: $a^2 \geq b^2$.

proof: Noticed:

$$J^2 - J_z^2 = \frac{1}{2}(J_+ J_- + J_- J_+)$$

Consider: (Require $|a.b\rangle$ Normalized!

$$\langle a.b | J^2 - J_z^2 | a.b \rangle = a^2 - b^2$$

Noticed:

$$\langle a.b | J_+ J_- | a.b \rangle = \left(J_- |a.b\rangle \right)^{D.C.} J_- |a.b\rangle \geq 0$$

Then:

$$a^2 - b^2 \geq 0 \; !$$

Actually: $\frac{1}{2}(J_+ J_- + J_- J_+) = J_x^2 + J_y^2$

$$\frac{1}{2}(J_+ J_- + J_- J_+) = \frac{1}{2}\Big((J_x + i J_y)(J_x - i J_y) + (J_x - i J_y)(J_x + i J_y) \Big)$$

$$= \frac{1}{2}\Big(J_x J_x + J_y J_y + i (J_y J_x - J_x J_y) + J_x J_x + J_y J_y + i (J_x J_y - J_y J_x) \Big)$$

$$= J_x J_x + J_y J_y$$

Relation between a; b_{min}; b_{max}:

- Relation of b_{max}, a: $J_+ |a, b_{max}\rangle = 0$

In this case: $J_- J_+ |a, b_{max}\rangle = 0$

Which means:

$$a - b_{max}^2 - \hbar b_{max} = 0$$

$$a = b_{max}(b_{max} + \hbar)$$

$$J_- J_+ = (J_x - iJ_y)(J_x + iJ_y)$$
$$= J_x J_x + J_y J_y + i(J_x J_y - J_y J_x)$$
$$= J^2 - J_z^2 + i(i\hbar J_z)$$
$$= J^2 - J_z^2 - \hbar J_z$$

- Relation between b_{min} and a:

$$J_- |a, b_{min}\rangle = 0$$
$$J_+ J_- |a, b_{min}\rangle = 0$$
$$a - b_{min}^2 + \hbar b_{min} = 0$$
$$a = b_{min}(b_{min} - \hbar)$$

$$J_+ J_- = (J_x + iJ_y)(J_x - iJ_y)$$
$$= J_x^2 + J_y^2 - i(J_x J_y - J_y J_x)$$
$$= J^2 - J_z^2 - i[J_x, J_y]$$
$$= J^2 - J_z^2 - i(i\hbar J_z)$$
$$= J^2 - J_z^2 + \hbar J_z$$

- Relation between b_{max} and b_{min}:

$$b_{min}(b_{min} - \hbar) = b_{max}(b_{max} + \hbar)$$
$$b_{max}^2 - b_{min}^2 + \hbar(b_{max} + b_{min}) = 0$$
$$(b_{max} + b_{min})(b_{max} - b_{min} + \hbar) = 0$$

$$\begin{cases} b_{min} = -b_{max} & (\checkmark) \\ b_{min} = b_{max} + \hbar & (\times) \end{cases}$$

—— Common way to label the state:

we must be able to reach $|a, b_{max}\rangle$ by apply J_+ successively to $|a, b_{min}\rangle$

$$b_{max} = b_{min} + n\hbar$$

$b_{max} = \frac{n}{2}\hbar = j\hbar$ suppose $j = \frac{n}{2}$ (j can be integral or half integral)

$$a = b_{max}(b_{max} + \hbar) = \hbar^2 j(j+1)$$

$$\begin{cases} J^2 |j, m\rangle = j(j+1)|j, m\rangle \\ J_z |j, m\rangle = m\hbar |j, m\rangle \end{cases}$$

—— Matrix elements for angular momentum:

- Matrix elements for angular momentum J^2 and J_z. They are easy to obtain:

$$\langle j', m'| J^2 |j, m\rangle = \hbar^2 j(j+1) \quad \delta_{j'j}\,\delta_{m'm}$$

$$\langle j', m'| J_z |j, m\rangle = \hbar m \quad \delta_{j'j}\,\delta_{m'm}$$

- Matrix elements for $J_\pm$:

Coefficient for Ladder operator:

▽ for J_-: $J_+ J_- = (J_x + iJ_y)(J_x - iJ_y) = J_x^2 + J_y^2 + i(J_y J_x - J_x J_y) = J^2 - J_z^2 \underbrace{- i(i\hbar J_z)}_{+\hbar J_z}$

$$\langle j, m| J_+ J_- |j, m\rangle = \langle j, m| J^2 - J_z^2 + \hbar J_z |j, m\rangle = \hbar^2[j(j+1) - m^2 + m]$$

Suppose: $J_- |j, m\rangle = C_{j,m}^- |j, m-1\rangle$

Then: $|C_{jm}^-|^2 = \hbar^2[j(j+1) - m(m-1)] = \hbar^2[j^2 - m^2 + j + m] = \hbar^2[(j+m)(j-m) + (j+m)] = \hbar^2 (j+m)(j-m+1)$

$$C_{jm}^- = \hbar\sqrt{(j+m)(j-m+1)}$$ ⇐ Exist phase problem!

- for J_+ : $J_- J_+ = J^2 - J_z^2 - \hbar J_z$.

  $\langle j,m | J_- J_+ | j,m \rangle = \hbar^2 (j(j+1) - m^2 - m) = \hbar^2 (j^2 - m^2 + (j-m)) = \hbar^2 (j-m)(j+m+1)$

  Then: $J_+ | j,m \rangle = C_{jm}^{+} | j, m+1 \rangle$

  $C_{jm}^{+} = \hbar \sqrt{(j-m)(j+m+1)}$

  $C_{jm}^{\pm} = \hbar \sqrt{(j \mp m)(j \pm m+1)}$

- Matrix elements for $J_\pm$:

  $\langle j' m' | J_\pm | j,m \rangle = \hbar \sqrt{(j \mp m)(j \pm m+1)} \; \delta_{m' m\pm1} \, \delta_{jj'}$

  $\Downarrow$

  Can construct J_x, J_y using $J_\pm$!

3.5.4 Representation of Rotation operator:

— Matrix element of rotation operator

$$\mathcal{D}^{(j)}_{m'm}(R) = \langle j,m|\exp(-i\frac{J\cdot\hat{n}}{\hbar}\phi)|j,m\rangle$$

Matrix elements are called winger functions!

We don't need to consider matrix elements between different j-values because they all vanish trivally! ⇓ Because

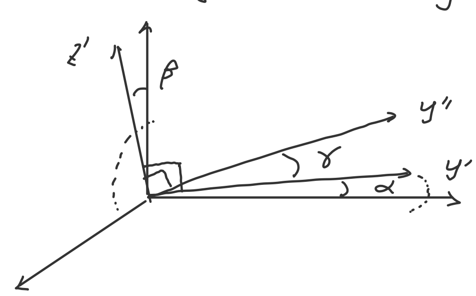
$$J^2\mathcal{D}(R)|j,m\rangle = \mathcal{D}(R)J^2|j,m\rangle = \hbar^2 j(j+1)\mathcal{D}(R)|j,m\rangle$$

- Meaning of the matrix element value:

$$\mathcal{D}(R)|j,m\rangle = \sum_{m'}|j,m'\rangle\langle j,m'|\mathcal{D}(R)|j,m\rangle$$
$$= \sum_{m'}|j,m'\rangle\mathcal{D}^{(j)}_{m'm}(R)$$

$\mathcal{D}^{(j)}_{m'm}(R)$ means the Amplitude of rotated $|j,m\rangle$ to be found at $|j,m'\rangle$

— Matrix realization of arbitrary j of Euler rotation:



$$\mathcal{D}^{(j)}_{m'm}(\alpha,\beta,\gamma) = \langle j,m'|\exp(-i\frac{J_z\alpha}{\hbar})\exp(-i\frac{J_y\beta}{\hbar})\cdot\exp(-i\frac{J_z\gamma}{\hbar})|j,m\rangle$$
$$= e^{-i(m'\alpha+m\gamma)}\cdot\langle j,m'|\exp(-i\frac{J_y\beta}{\hbar})|j,m\rangle$$
$$d^{(j)}_{m'm}(\beta) = \langle j,m'|\exp(-i\frac{J_y\beta}{\hbar})|j,m\rangle$$

- $j = 1/2$

$$d^{(1/2)}(\beta) = \begin{pmatrix} \cos(\frac{\beta}{2}) & -\sin(\beta/2) \\ \sin(\beta/2) & \cos(\beta/2) \end{pmatrix}$$

(rotation in dirac two component formalism)

- Next simplest case: $j=1$

Firstly: obtain 3×3 matrix representation of J_y,

$$J_y = \frac{1}{2i}(J_+ - J_-)$$

From:

$$\langle j',m'|J_\pm|j,m\rangle = \hbar\sqrt{(j\mp m)(j\pm m+1)}\,\delta_{jj'}\cdot\delta_{m'\,m\pm1}$$

For $j=1$; J_+:

$$\langle 1,m'|J_+|1,m\rangle = \hbar\sqrt{(1-m)(1+m+1)}\cdot\delta_{m'\,m+1}$$

$$\begin{array}{c} m'=1 \\ m'=0 \\ m'=-1 \end{array}\begin{bmatrix} 0 & \sqrt{2}\hbar & 0 \\ 0 & 0 & \sqrt{2}\hbar \\ 0 & 0 & 0 \end{bmatrix}$$

For $j=1$; J_-:

$$\langle 1,m'|J_-|1,m\rangle = \hbar\sqrt{(1+m)(1-m+1)}\,\delta_{m'\,m-1}$$

$$\begin{bmatrix} 0 & 0 & 0 \\ \sqrt{2}\hbar & 0 & 0 \\ 0 & \sqrt{2}\hbar & 0 \end{bmatrix}$$

Then :

$$J_y = \frac{1}{2i}(J_+ + J_-) = -\frac{i}{2}\hbar \begin{bmatrix} 0 & \sqrt{2} & 0 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 0 & -\sqrt{2} & 0 \end{bmatrix} = \frac{\hbar}{2}\cdot \begin{bmatrix} 0 & -\sqrt{2}i & 0 \\ \sqrt{2}i & 0 & -\sqrt{2}i \\ 0 & \sqrt{2}i & 0 \end{bmatrix}$$

Noticed :

$$\left(\frac{J_y^{(j=1)}}{\hbar}\right)^3 = \frac{J_y^{(j=1)}}{\hbar}$$

$$\left(\frac{J_y^{(j=1)}}{\hbar}\right)^2 = \left(\frac{1}{2}\cdot \begin{bmatrix} 0 & -\sqrt{2}i & 0 \\ \sqrt{2}i & 0 & -\sqrt{2}i \\ 0 & \sqrt{2}i & 0 \end{bmatrix}\cdot \frac{1}{2}\cdot \begin{bmatrix} 0 & -\sqrt{2}i & 0 \\ \sqrt{2}i & 0 & -\sqrt{2}i \\ 0 & \sqrt{2}i & 0 \end{bmatrix}\right) = \frac{1}{4}\begin{bmatrix} 2 & 0 & -2 \\ 0 & 4 & 0 \\ -2 & 0 & 2 \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & 0 & -\frac{1}{2} \\ 0 & 1 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{bmatrix}$$

$$\left(\frac{J_y^{(j=1)}}{\hbar}\right)^3 = \begin{bmatrix} \frac{1}{2} & 0 & -\frac{1}{2} \\ 0 & 1 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{bmatrix}\cdot \frac{1}{2}\cdot \begin{bmatrix} 0 & -\sqrt{2}i & 0 \\ \sqrt{2}i & 0 & -\sqrt{2}i \\ 0 & \sqrt{2}i & 0 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 0 & -\sqrt{2}i & 0 \\ \sqrt{2}i & 0 & -\sqrt{2}i \\ 0 & \sqrt{2}i & 0 \end{bmatrix} = \frac{J_y^{(j=1)}}{\hbar}$$

Consequently : For $j=1$, it is legitimate :

$$\begin{aligned} \exp\left(-i\frac{J_y\beta}{\hbar}\right) &= 1 + \left(-\frac{i}{\hbar}\right)J_y\beta \cdots \\ &= 1 + (-i)\frac{J_y}{\hbar}\beta + \frac{1}{3!}(-i)\cdot(-1)\cdot\left(\frac{J_y}{\hbar}\right)^3\beta^3 \cdots \\ &\quad + \frac{1}{2!}(-i)^2\left(\frac{J_y}{\hbar}\right)^2\beta + \frac{1}{4!}(-1)\cdot(-i)^2\cdot\left(\frac{J_y}{\hbar}\right)^4\beta^4 \cdots \\ &= 1 - i\frac{J_y}{\hbar}\left(\beta - \frac{1}{3!}\beta^3 \cdots\right) \\ &\quad + \frac{J_y^2}{\hbar^2}\left(-\frac{1}{2!}\beta^2 + \frac{1}{4!}\beta^4 \cdots\right) \\ &= 1 - i\frac{J_y}{\hbar}\sin\beta - \frac{J_y^2}{\hbar^2}(1-\cos\beta) \end{aligned}$$

So :

$$d^{(1)}(\beta) = \begin{pmatrix} \frac{1}{2}(1+\cos\beta) & -\frac{1}{\sqrt{2}}\sin\beta & \frac{1}{2}(1-\cos\beta) \\ \frac{1}{\sqrt{2}}\sin\beta & \cos\beta & -\frac{1}{\sqrt{2}}\sin\beta \\ \frac{1}{2}(1-\cos\beta) & \frac{1}{\sqrt{2}}\sin\beta & \frac{1}{2}(1+\cos\beta) \end{pmatrix}$$

3.6 Orbital Angular momentum

— When a single particle's spin-angular momentum is zero !, it's Angular momentum is equal to orbital angular momentum !

$$\hat{L} = \hat{x} \times \hat{P}$$

orbital angular momentum commutation relation :

$$[L_i, L_j] = i\hbar \, \varepsilon_{ijk} L_k$$

Next, Let:

$$\left(1 - i\frac{\delta\phi}{\hbar}L_z\right)|x', y', z'\rangle = \left(1 - i\frac{\delta\phi}{\hbar}(xP_y - yP_x)\right)|x'y'z'\rangle = \left(1 - i\frac{P_y}{\hbar}\delta\phi\, x' + i\frac{P_x}{\hbar}\delta\phi\, y'\right)|x' \; y' z'\rangle$$

$$= |x' - y'\delta\phi, \; y' + x'\delta\phi, \; z'\rangle$$

This is precisely what we expect L_z generates!

— Angular Momentum operator in position space :

- L_z operator :

$$\langle x' y' z'| \left(1 - i\frac{\delta\phi}{\hbar}L_z\right)|\alpha\rangle = \langle x' + y'\delta\phi, \; y' - x'\delta\phi, \; z'|\alpha\rangle$$

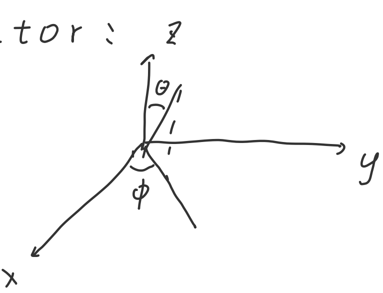
Change coordinate basis:

$$\langle r, \theta, \phi| \left(1 - i\frac{\delta\phi}{\hbar}L_z\right)|\alpha\rangle = \langle r, \theta, \phi - \delta\phi|\alpha\rangle = \langle r, \theta, \phi|\alpha\rangle - \delta\phi\frac{\partial}{\partial\phi}\langle r, \theta, \phi|\alpha\rangle$$

We can identify:

$$\langle x'|L_z|\alpha\rangle = -i\hbar\frac{\partial}{\partial\phi}\langle x'|\alpha\rangle$$

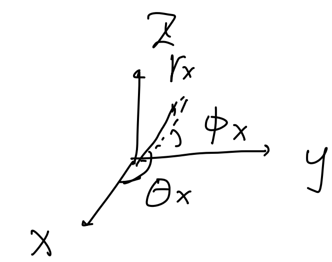
- L_x, L_y operator :



$$x = r\sin\theta\cos\phi$$

$$y = r\sin\theta\sin\phi$$

$$z = r\cos\theta$$



$$\begin{cases} r_x = r \\ \tan\phi_x = \dfrac{z}{y} = \dfrac{\cos\theta}{\sin\theta}\dfrac{1}{\sin\phi} \\ r_x \cdot \cos\theta_x = x = r\sin\theta\cos\phi \end{cases}$$

For rotation in x direction : $\delta\theta_x = 0 \quad \delta r_x = 0 \quad \delta\phi_x \neq 0$

$$d(\sin\theta\cos\phi) = 0$$

$$\cos\theta\cos\phi\, d\theta - \sin\theta\sin\phi\, d\phi = 0$$

$$\frac{1}{\cos^2\phi_x}d\phi_x = -\frac{1}{\sin^2\theta}\frac{1}{\sin\phi}d\theta - \frac{\cos\theta}{\sin\theta}\frac{\cos\phi}{\sin^2\phi}\frac{\cos\theta\cos\phi}{\sin\theta\sin\phi}d\theta$$

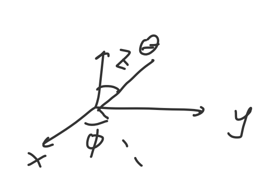
$$\left(1 + \frac{\cos^2\theta}{\sin^2\theta\sin^2\phi}\right)d\phi_x = \left(-\frac{1}{\sin^2\theta}\frac{1}{\sin\phi} - \frac{\cos^2\theta\cos^2\phi}{\sin^2\theta\sin^3\phi}\right)d\theta$$

$$= -\frac{1}{\sin^2\theta\sin\phi}\left(\frac{\cos^2\theta}{\sin^2\phi} + 1 - \cos^2\theta\right)d\theta$$

$$\Downarrow$$

$$d\theta = -\sin\phi\, d\phi_x$$

$$d\phi = -\frac{\cos\theta\cos\phi}{\sin\theta}d\phi_x$$



$$\langle x'|L_x|\alpha\rangle = -i\hbar\left(-\sin\phi\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)\langle x'|\alpha\rangle$$

$$\langle x'|L_y|\alpha\rangle = -i\hbar\left(\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)\langle x'|\alpha\rangle$$

- Ladder operator $L_\pm$:

$$\langle x'|L_\pm|\alpha\rangle = -i\hbar e^{\pm i\phi}\cdot\left(\pm i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi}\right)\cdot\langle x'|\alpha\rangle$$

- Orbital angular momentum operator L^2:

$$L^2 = L_x^2 + L_y^2 + L_z^2 = \frac{1}{2}\left(L_+L_- + L_-L_+\right) + L_z^2 \qquad (\cdots)$$

$$\langle x'|L^2|\alpha\rangle = -\hbar^2\left(\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\cdot\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right)\langle x'|\alpha\rangle$$

—— Relation Between orbital angular momentum and momentum operator:

- operator identity: $L^2 = x^2p^2 - (x\cdot p)^2 + i\hbar\, x\cdot p$

proof:

$$L^2 = \sum_{ijlmk}\cdot\varepsilon_{ijk}x_iP_j\,\varepsilon_{lmk}x_lP_m$$

$$= \sum_{ijlm}\left(\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}\right)\cdot x_iP_jx_lP_m$$

$$= \sum_{ijlm}\Big(\delta_{il}\delta_{jm}\,x_i(x_lP_j - i\hbar\delta_{jl})P_m$$
$$- \delta_{im}\delta_{jl}\,x_iP_j(P_mx_l + i\hbar\delta_{ml})\Big)$$

$$= x^2p^2 - i\hbar\, x\cdot p - \sum_{ijlm}\delta_{im}\delta_{jl}\cdot$$
$$\left[x_iP_m(x_lP_j - i\hbar\delta_{jl}) + i\hbar\,\delta_{lm}\,x_iP_j\right]$$

$$= x^2p^2 - i\hbar\, x\cdot p - (x\cdot p)^2 + 3i\hbar\, x\cdot p - i\hbar\, x\cdot p$$

$$= x^2p^2 - (x\cdot p)^2 + i\hbar\, x\cdot p$$

Noticed that:

$$\langle x'|x\cdot p|\alpha\rangle = x'\cdot(-i\hbar\nabla')\langle x'|\alpha\rangle$$
$$= -i\hbar\, r\frac{\partial}{\partial r}\langle x'|\alpha\rangle$$

$$\langle x'|(x\cdot p)^2|\alpha\rangle = -\hbar^2\, r\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\langle x'|\alpha\rangle\right)$$

$$= -\hbar^2\left(r^2\frac{\partial^2}{\partial r^2}\langle x'|\alpha\rangle + r\frac{\partial}{\partial r}\langle x'|\alpha\rangle\right)$$

Thus:

$$\langle x'|L^2|\alpha\rangle = \langle x'|\,x^2P^2 - (x\cdot P)^2 + i\hbar\, x\cdot p\,|\alpha\rangle$$
$$= r^2\langle x'|P^2|\alpha\rangle - \langle x'|(x\cdot P)^2|\alpha\rangle + i\hbar\langle x'|x\cdot p|\alpha\rangle$$
$$= r^2\langle x'|P^2|\alpha\rangle - \hbar^2\left(r^2\frac{\partial^2}{\partial r^2}\langle x'|\alpha\rangle + 2r\frac{\partial}{\partial r}\langle x'|\alpha\rangle\right)$$

Relationship between kinetic energy and orbital Angular Momentum

$$\frac{1}{2m}\langle x'|P^2|\alpha\rangle = -\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\langle x'|\alpha\rangle - \frac{1}{\hbar^2r^2}\langle x'|L^2|\alpha\rangle\right)$$

$$= -\frac{\hbar^2}{2m}\nabla'^2\langle x'|\alpha\rangle$$

$$= -\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\right]\cdot\langle x'|\alpha\rangle$$

3.6.2. Spherical Harmonics.

(省略了太多计算，以后补充吧!)

$|l,m\rangle$ span the sub-Hilbert space spanned by $|\hat{n}\rangle$

这一点还没想好如何证明.

Spherical Harmonics Y_l^m:

$$\langle \hat{n}|l,m\rangle = Y_l^m$$

satisfies:
$$\begin{cases} \langle \hat{n}|L^2|l,m\rangle = \hbar^2 l(l+1)\,\langle \hat{n}|l,m\rangle \\ \langle \hat{n}|L_z|l,m\rangle = \hbar m \quad \langle \hat{n}|l,m\rangle \end{cases}$$

leads to differential equation:
$$\begin{cases} -i\hbar\frac{\partial}{\partial\phi} Y_l^m = m\hbar\, Y_l^m & -(1) \\ \left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + l(l+1)\right]\hbar^2\, Y_l^m = 0 & -(2) \end{cases}$$

(1) means ϕ dependence of Y_l^m is $e^{im\phi}$

▽ orthogonal relation of spherical harmonics:

using the normalization relation of $|n\rangle$:
$$\int d\Omega_n\, |\hat{n}\rangle\langle\hat{n}| = 1$$

Then:
$$\langle l'm'|lm\rangle = \int d\Omega_n\, \langle l'm'|\hat{n}\rangle\langle\hat{n}|lm\rangle$$
$$= \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\cdot Y_{l'}^{m'*}\, Y_l^m = \delta_{l'l}\,\delta_{m'm}$$

▽ A way to obtain spherical harmonics (from J.J.Sakurai 3.6.2):

from $m=l$ case, $Y_l^{m=l}(\theta,\phi)$ satisfies:
$$L_+|l,l\rangle = 0$$
$$\Downarrow$$
$$\langle\hat{n}|L_+|l,l\rangle = 0$$
$$\Downarrow$$
$$-i\hbar\, e^{i\phi}\left(i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi}\right) Y_l^l = 0$$

we know the ϕ-dependence of Y_l^l is $e^{il\phi}$ $\Downarrow$ The solution:
$$Y_l^l = C_l\cdot\sin^l\theta\cdot e^{il\phi}$$

Normalisation:
$$C_l = \frac{(-1)^l}{2^l\, l!}\cdot\sqrt{\frac{(2l+1)(2l)!}{4\pi}}$$
$$\langle\hat{n}|l,m-1\rangle = \frac{1}{\hbar\sqrt{(l+m)(l-m+1)}}\,\langle\hat{n}|L_-|l,m\rangle$$
$$= \frac{1}{\sqrt{(l+m)(l-m+1)}}\cdot e^{-i\phi}\cdot\left(-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right)\cdot\langle\hat{n}|l,m\rangle$$

....

$$m\geq 0 \quad Y_l^m = \frac{(-1)^l}{2^l\cdot l!}\cdot\sqrt{\frac{(2l+1)}{4\pi}\frac{(l+m)!}{(l-m)!}}\cdot e^{im\phi}\cdot\frac{1}{\sin^m\theta}\cdot\frac{d^{l-m}}{d(\cos\theta)^{l-m}}\cdot(\sin\theta)^{2l}$$

$$m<0 \quad Y_l^{-m} = (-1)^m\,(Y_l^m)^*$$

For $m=0$
$$Y_l^m = Y_l^0(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}}\, P_l(\cos\theta)$$

▽ For $\theta=0$ $\quad Y_l^m(\theta=0, \phi=\text{not determined}) = 0$ for $m\neq 0$; Reason:
$$\langle\hat{z}|l,m\rangle = Y_l^m(\theta=0,\ldots) \Rightarrow \langle\hat{z}|L_z|l,m\rangle\frac{1}{\hbar m} = Y_l^m(\theta=0,\ldots)$$

noticed: $L_z|\hat{z}\rangle = 0 \Rightarrow$ For $m\neq 0$; $Y_l^m(\theta=0,\phi\text{ not determined}) = 0$!

▽ Why can not orbital angular momentum be half-integral: $e^{im(2\pi)}\neq 1$

3.6.3 spherical harmonics as rotation matrics.

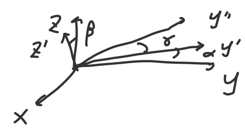
Find Proper $\mathcal{D}(R)$ to let $|\hat{n}\rangle = \mathcal{D}(R)|\hat{z}\rangle$

▿ Reason for doing so: (used the property $\langle l m' | \mathcal{D}(R) | l' m\rangle = 0 \quad (l' \neq l)$)

$$\langle l m' | \hat{n}\rangle = Y_l^{m'*}(\theta,\phi) = \sum_m \langle l m' | \mathcal{D}(R) | l, m\rangle \langle l, m | \hat{z}\rangle$$

$$= \sum_m \mathcal{D}^{(l)}(R)_{m'm} \, Y_l^{m*}(\theta=0,\ \phi=\text{not determined})$$

▿ Using the Euler rotation: ($\alpha=\phi \quad \beta=\theta \quad \gamma=0$) (可以将 $\hat{z}$ 转动到 $\hat{n}$)



$$Y_l^{m'*}(\theta,\phi) = \sum_m \mathcal{D}^{(l)}_{m'm}(\phi,\theta,0) \; \underbrace{Y_l^{m*}(0, \phi=\text{not determined})}$$

$\Downarrow$ noticed $m=0$ $\quad Y_l^m(\theta=0,\cdots)\neq 0$

$$Y_l^{m'*}(\theta,\phi) = \mathcal{D}^{(l)}_{m'0}(\phi,\theta,0)\cdot Y_l^{0*}(0,\cdots)$$

$$= \mathcal{D}^{(l)}_{m'0}(\phi,\theta,0) \sqrt{\frac{2l+1}{4\pi}} \; \underbrace{P_l(\cos\theta)\big|_{\theta=0}}_{=1}$$

$\Downarrow$

$$\mathcal{D}^{(l)}_{m0}(\alpha,\beta,\gamma=0) = \sqrt{\frac{4\pi}{2l+1}} \cdot Y_l^{m*}(\theta,\phi)\big|_{\theta=\beta,\ \phi=\alpha}$$

▿ Important property when $m=0$:

$$\mathcal{D}^{(l)}_{00}(\alpha,\beta,\gamma=0) = \langle l,0 | \mathcal{D}(R_z(\alpha))\cdot\mathcal{D}(R_y(\beta))\,\mathcal{D}(R_z(\gamma))\cdot| l,0\rangle$$

$$= \langle l,0 | \mathcal{D}(R_y(\beta)) | l,0\rangle \cdot e^{-\frac{i}{\hbar}(0\cdot\hbar)(\alpha+\gamma)}$$

$$= d^{(l)}_{00}(\beta)$$

$$d^{(l)}_{00}(\beta) = \sqrt{\frac{4\pi}{2l+1}} \; Y_l^{0*}(\theta,\phi)\big|_{\theta=\beta,\ \phi=\alpha}$$

$$d^{(l)}_{00}(\beta) = \sqrt{\frac{4\pi}{2l+1}} \cdot P_l(\cos\beta)$$

3.7 Schrodinger Equation for central potential.

Hamiltonian under consideration:

$$H = \frac{p^2}{2m} + V(r) \qquad r^2 = x^2$$

showed that:

$$[L, p^2] = [L, x^2] = 0$$

therefore: $[L, H] = [L^2, H] = 0$

3.7.1 Schrodinger equation for central potential:

The commutation relation between H and L_z, L^2 tells us we can define Eigenkets of H, L_z, L^2

$$|\alpha\rangle = |E\, l\, m\rangle$$

where:

$$\begin{cases} H|E l m\rangle = E|E l m\rangle \\ L^2|E l m\rangle = \hbar^2 l(l+1)|E l m\rangle \\ L_z|E l m\rangle = \hbar m \, |E l m\rangle \end{cases}$$

Denote: $\langle x'|E l m\rangle = R_E(r) \cdot Y_l^m(\theta, \phi) \Leftarrow \begin{cases} |E\rangle \text{ span } |r\rangle \\ |lm\rangle \text{ span } |\hat{n}\rangle \end{cases}$ $\quad \langle x'| = \langle r| \otimes \langle \theta, \phi|$

From previous: (the momentum operator can be expressed as)

$$\langle x'|\frac{p^2}{2m}|\alpha\rangle = -\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\langle x'|\alpha\rangle - \frac{1}{\hbar^2 r^2}\langle x'|L^2|\alpha\rangle\right)$$

$$= -\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\right]\langle x'|\alpha\rangle$$

Energy eigen function:

$$\left\{-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\right) + V(r)\right\}\langle x'|E l m\rangle = E\langle x'|E l m\rangle$$

$$\left\{-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{l(l+1)}{r^2}\right) + V(r)\right\} R_n(r)\, Y_l^m(\theta, \phi) = E\langle x'|E l m\rangle$$

Radical Equation:

$$\left(-\frac{\hbar^2}{2m r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{l(l+1)\hbar^2}{2m r^2} + V(r)\right) \cdot R_{El}(r) = E\, R_{El}(r)$$

$$R_{El}(r) = \frac{u_{El}(r)}{r}$$

coupled with the fact that spherical harmonics are seperately normalized, the overall normalization condition:

$$1 = \int r^2 dr\, R_{El}^*(r) R_{El}(r) = \int dr\, u_{El}^*(r) u_{El}(r)$$

$u_{El}(r)$ can be interpreted as wave function in one dimension for a particle moving in an effective potential

$$V_{eff} = V(r) + \frac{l(l+1)\hbar^2}{2m r^2}$$

- notice: exist an angular momentum barrier if $l \neq 0$. Amplitude is small for particle Locating at origin, expect for "s"$(l=0)$ state.

- solution for small $r \to 0$ when $\lim_{r\to 0} V(r) r^2 = 0$

$$\frac{d^2 u_{El}}{dr^2} = \frac{l(l+1)}{r^2} u_{El}(r)$$

the solution would be:

$$u_{El} = A r^{l+1} + \frac{B}{r^l}$$

$B=0$ under certain consideration: (Prob 3.27 sakurai, it leads to nonconservation of probability because two terms interference) ?

If $B\neq 0$: $R_{El} \sim \frac{B}{r^{l+1}}$ $\quad r\to 0$

$$\begin{cases} 1^\circ \quad l\geq 1 & \text{; the wave function is not normalizable!} \\ 2^\circ \quad l=0 & R_{El}\sim \frac{1}{r} \to \nabla^2\left(\frac{1}{r}\right) = -4\pi\delta^{(3)}(x) \Rightarrow V(r)\sim \delta^{(3)}(x) \end{cases}$$

do not know how to prove this!

consequently: $R_{El}(r)\sim r^l$ as $r\to 0$

- Bound state for $V(r)\to 0,\ r\to+\infty$

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} = Eu$$

$$\frac{d^2 u_{El}}{dr^2} = k^2 u_{El}; \qquad k^2 = -\frac{2mE}{\hbar^2} > 0 \quad r\to+\infty.$$

Solution: $\qquad u_{El}(r) \propto e^{-kr}$

- $\lim_{r\to 0} r^2 V(r)\to 0$; $\lim_{r\to+\infty} V(r)\to 0$: $\rho = kr = \frac{\sqrt{-2mE}}{\hbar}\cdot r$

$$u_{El}(\rho) = \rho^{l+1}\cdot e^{-\rho}\cdot w(\rho)$$

$$\frac{d^2w}{d\rho^2} + 2\left(\frac{l+1}{\rho} - 1\right)\frac{dw}{d\rho} + \left(\frac{V}{E} - \frac{2(l+1)}{\rho}\right)w = 0$$

3.7.2 The Free Particle and infinite spherical well

$E = \frac{\hbar^2 k^2}{2m}$ $\qquad \rho\equiv kr$

Radial Equation:

$$\left(-\frac{\hbar^2}{2mr^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{l(l+1)}{2mr^2}\hbar^2 + V(r)\right) R_{El}(r) = E R_{El}(r)$$

$$V(r) = 0$$

$$dr = \frac{1}{k}d\rho = d\rho\cdot\frac{\hbar}{\sqrt{2mE}} \qquad r = \frac{\rho}{k} = \rho\cdot\frac{\hbar}{\sqrt{2mE}}$$

$$\Downarrow$$

$$\frac{d^2R}{d\rho^2} + \frac{2}{\rho}\frac{dR}{d\rho} + \left(1 - \frac{l(l+1)}{\rho^2}\right)\cdot R = 0$$

This equation has a solution called Spherical Bessel Function!

$$j_l(\rho);\ n_l(\rho)$$

$$j_l(\rho) = (-\rho)^l\cdot\left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l\cdot\left(\frac{\sin\rho}{\rho}\right)$$

$$n_l(\rho) = -(-\rho)^l\cdot\left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l\left(\frac{\cos\rho}{\rho}\right)$$

Easy to show that (?) as $\rho\to 0$ $\begin{cases} j_l(\rho)\to\rho^l \\ n_l(\rho)\to\rho^{-(l+1)} \end{cases}$

$j_l(\rho)$ is the allowed solution here!

spherical Bessel Function are defined over the entire complex plane!

$$j_l(z) = \frac{1}{2i^l}\cdot\int_{-1}^{1} ds\cdot e^{izs}\cdot P_l(s)$$

First few Bessel Function:

$$j_0(\rho) = \frac{\sin\rho}{\rho}$$

$$j_1(\rho) = \frac{\sin\rho}{\rho^2} - \frac{\cos\rho}{\rho}$$

$$j_2(\rho) = \left(\frac{3}{\rho^3} - \frac{1}{\rho}\right)\sin\rho - \frac{3\cos\rho}{\rho^2}$$

Particle confined to an infinite spherical well:

$$\begin{cases} V(r) = 0 & r<a \\ V(r) = +\infty & r>a \end{cases}$$

Quantization condition:

$$j_l(ka) = 0$$

Requires ka equals to set of zeros of spherical Bessel Function.

$$l=0 \Rightarrow ka = \pi, 2\pi \cdots$$

$$E_{l=0} = \frac{\hbar^2}{2ma^2}[\pi^2, (2\pi)^2, \cdots]$$

$$E_{l=1} = \frac{\hbar^2}{2ma^2}[4.449^2, 7.773^2, \cdots]$$

$$E_{l=2} = \frac{\hbar^2}{2ma^2}[5.76^2, \cdots]$$

3.73 The isotropic Harmonic oscillator

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 r^2$$

Introduce dimensionless energy λ, radial coordinate ρ:

$$E = \frac{1}{2}\hbar\omega\lambda \qquad r = \left(\frac{\hbar}{m\omega}\right)^{\frac{1}{2}}\rho$$

Radial Equation of form:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u_{El} + \left(\frac{l(l+1)}{2mr^2} + V(r)\right)\cdot u_{El} = E\, u_{El}.$$

$$\frac{d^2u}{d\rho^2} - \frac{l(l+1)}{\rho^2}u(\rho) + (\lambda - \rho^2)\cdot u(\rho) = 0$$

It is worth to remove the behave of the large ρ suppose:

$$u(\rho) = \rho^{l+1}\cdot e^{-\rho^2/2}\cdot f(\rho)$$

This yields the following differential equation:

$$\rho\frac{d^2f}{d\rho^2} + 2((l+1) - \rho^2)\cdot\frac{df}{d\rho} + (\lambda - (2l+3))\cdot\rho\cdot f(\rho) = 0$$

$$f(\rho) = \sum_{n=0}^{+\infty} a_n \rho^n$$

ρ^0: $\qquad 2(l+1)a_1\rho^0 = 0 \Rightarrow a_1 = 0$

ρ^{n+1}: $\qquad \sum_{n=2}^{+\infty}\{(n+2)(n+1)a_{n+2} + 2(l+1)(n+2)a_{n+2} - 2na_n + [\lambda - (2l+3)]a_n\}\rho^{n+1} = 0$

why start from $n=2$?

Recursion:

$$\begin{cases} a_{n+2} = \dfrac{2n+2l+3-\lambda}{(n+2)(n+2l+3)}a_n \\ a_n = 0 \quad (\text{for odd } n,\ a_1 = 0) \end{cases}$$

For $n\to+\infty$, $\frac{a_{n+2}}{a_n} \longrightarrow \frac{2}{n} = \frac{1}{q}$ where $q = \frac{n}{2}$

including both odd and even integrals.

$$f(\rho) \to \text{const} \sum_q \frac{1}{q!}\cdot(\rho^2)^q \propto e^{\rho^2}$$

which means $u(\rho) \propto \exp(\rho^2/2) \to +\infty$

We need to terminates the series: $\overset{a_{n+2} = 0\, a_n}{n = 2q}$. $\quad q = 0, 1, \cdots$

$$2n + 2l + 3 - \lambda = 0$$

$$E_{ql} = \frac{1}{2}\hbar\omega(\lambda) = \hbar\omega(2q + l + \tfrac{3}{2}) \equiv (N + \tfrac{3}{2})\hbar\omega$$

Notice for even/odd values of N, only even/odd values of l are allowed.

It's natural to label the eigenstate of the hamiltonian as $|q \ell m\rangle$ or $|N \ell m\rangle$

Also

$$H = H_x + H_y + H_z$$

$$H_i = a_i^{\dagger} a_i + \frac{1}{2}$$

$$E = (n_x + n_y + n_z + \frac{3}{2})\hbar w$$

Eigenstate:

$$|n_x, n_y, n_z\rangle$$

3.7.4 The coulomb potential.

Hamiltonian:

$$V(x) = -\frac{Ze^2}{r}$$

Because $r^2 V(r) = 0,\ r \to 0$; $V(r) = 0\ r \to +\infty$, search for solution of function $w(\rho)$

$$\rho_0 = \left(\frac{2m}{-E}\right)^{\frac{1}{2}} \cdot \frac{Ze^2}{\hbar} = \left(\frac{2mc^2}{-E}\right)^{1/2} Z\alpha$$

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

$$\rho \frac{d^2 w}{d\rho^2} + 2(\ell + 1 - \rho) \cdot \frac{dw}{d\rho} + (\rho_0 - 2(\ell+1))\, w(\rho) = 0$$

kummer's equation:

$$x \frac{d^2 F}{dx^2} + (c - x)\frac{dF}{dx} - aF = 0$$

$$x = 2\rho \quad c = 2(\ell+1) \quad 2a = 2(\ell+1) - \rho_0$$

Confluent Hypergeometric Function:

$$F(a, c, x) = 1 + \frac{a}{c}\frac{x}{1!} + \frac{a(a+1)}{c(c+1)} \cdot \frac{x^2}{2!} \cdots$$

$$w(\rho) = F\left(\ell + 1 - \frac{\rho_0}{2};\ 2(\ell+1);\ 2\rho\right)$$

For large ρ:

$$w(\rho) = \sum_{\text{Large } N} \cdot \frac{a(a+1)\cdots(a+N-1)}{c(c+1)\cdots(c+N-1)} \frac{(2\rho)^N}{N!} \sim e^{\rho} \ (?)$$

For some cut-off requirement: $\underline{a + N = 0}$ $(N = 0, 1, \cdots)$

$$\rho_0 = 2(N + \ell + 1)$$

principal quantum number:

$$n = N + \ell + 1 = 1, 2, 3, \ldots \quad (N = 0, 1, 2 \ldots)$$

Energy eigenvalue:

$$\rho_0 = \left(\frac{2mc^2}{-E}\right)^{\frac{1}{2}} Z\alpha = 2n$$

$$E = -\frac{1}{2} mc^2 \frac{Z^2 \alpha^2}{n^2} = -13.6\,eV \frac{Z^2}{n^2} \ ; \ \frac{1}{k} = \frac{\sqrt{-2mE}}{\hbar} = a_0 \frac{n}{Z}$$

$$a_0 = \frac{\hbar}{mc\alpha} = \frac{\hbar^2}{me^2}$$

Degeneracy: $\sum_{\ell=0}^{n-1} (2\ell + 1) = n^2$

Wave function:

$$\psi_{n\ell m}(x) = \langle x | n \ell m\rangle = R_{n\ell}(r)\, Y_\ell^m(\theta, \phi)$$

where:

$$R_{n\ell}(r) = \frac{1}{(2\ell+1)!}\left(\frac{2Zr}{na_0}\right)^{\ell} e^{-Zr/na_0}\left[\left(\frac{2Z}{na_0}\right)^3 \frac{(n+\ell)!}{2n(n-\ell-1)!}\right]^{1/2} \cdot F\left(-n+\ell+1,\ 2\ell+2,\ 2\frac{Zr}{na_0}\right)$$

1° only $\ell = 0$, wave function are non-zero at the origin!

2° There are $n-1$ nodes for $\ell = 0$; 0 nodes for $\ell = n-1$! $(\ell = 0 \cdots n-1)$

3.8 Addition of Angular momentum

3.8.1 Simple examples of angular momentum addition.

(1) how to add orbital angular momentum and spin-angular momentum

(2) how to add spin angular momentum of two spin-1/2 particles.

(1)

- The base ket of spin-1/2 particle can be visualized as direct produt of $\{|x'\rangle\}$ and $\{|+\rangle, |-\rangle\}$
- Any operator in the space spanned by $\{|x'\rangle\}$ commutes with any operator in the space spanned by $\{|+\rangle, |-\rangle\}$.
- Rotation operator : $\exp(-i\frac{J\cdot\hat{n}}{\hbar}\phi)$

$$J = L + S$$

$$J = L\otimes\mathbb{I} + \mathbb{I}\otimes S.$$

$$\mathcal{D}(R) = \mathcal{D}^{(orb)}(R)\otimes\mathcal{D}^{(spin)}(R) = \exp(-i\frac{L\cdot\hat{n}}{\hbar}\phi)\otimes\exp(-i\frac{S\cdot\hat{n}}{\hbar}\phi)$$

- Wave function with particle with spin :

$$\langle x', \pm|\alpha\rangle = \psi_\pm(x')$$

often arranged like : $\begin{pmatrix}\psi_+(x') \\ \psi_-(x')\end{pmatrix}$.

we can use L^2, L_z, S^2, S_z to get eigen kets (their mutual eigenkets)

Also can use L^2, S^2, J^2, J_z to get eigen kets.

(2) study the two spin-1/2 particles.

total spin operator : $S = S_1 + S_2$

$$= S_1\otimes\mathbb{I} + \mathbb{I}\otimes S_2$$

$$[S_x, S_y] = i\hbar S_z$$

$$[S_i, S_j] = i\hbar\,\varepsilon_{ijk}S_k$$

Eigenvalues for various spin operators :

$$S^2 = (S_1+S_2)^2 \;:\; s(s+1)\hbar^2$$

$$S_z = S_{1z} + S_{2z} \;:\; m\hbar$$

$$S_{1z} \;:\; m_1\hbar$$

$$S_{2z} \;\;\; m_2\hbar$$

$$[S^2, S_z] = 0, \quad [S^2, S_{1z}] \neq 0$$

Base 1: $|++\rangle \quad |+-\rangle \quad |-+\rangle \quad |--\rangle$

Base 2: $\{s=1, m=0,\pm1\} \quad |s=0, m=0\rangle$

$$|s=1, m=1\rangle = |++\rangle$$

$$|s=1, m=0\rangle = \frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle)$$

$$|s=1, m=-1\rangle = |--\rangle$$

$$|s=0, m=0\rangle = \frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle) \Rightarrow \text{This is obtained by orthogonal relation.}$$

$\Leftarrow$ $S_-|s=1, m=1\rangle = (S_{1-}+S_{2-})|++\rangle$

$$\sqrt{(1+1)(1-1+1)}\,|s=1, m=0\rangle = \sqrt{(\tfrac{1}{2}+\tfrac{1}{2})(\tfrac{1}{2}-\tfrac{1}{2}+1)}\;|-+\rangle + \sqrt{(\tfrac{1}{2}+\tfrac{1}{2})(\tfrac{1}{2}-\tfrac{1}{2}+1)}\;|+-\rangle$$

3.8.2. Formal Theory for Angular momentum addition.

Infinitesimal version: (of rotation).

$$\left(1 - i\frac{J_1\cdot\hat{n}\,\delta\phi}{\hbar}\right)\otimes\left(1 - i\frac{J_2\cdot\hat{n}}{\hbar}\delta\phi\right) = 1 - \frac{i(J_1\otimes\mathbb{I} + J_2\otimes\mathbb{I})}{\hbar}\cdot\hat{n}\,\delta\phi$$

Define: $J \equiv J_1\otimes\mathbb{I} + \mathbb{I}\otimes J_2 \Rightarrow [J_i, J_j] = i\hbar\varepsilon_{ijk}J_k$

Finite Angular version:

$$\mathcal{D}_1(R)\otimes\mathcal{D}_2(R) = \exp\left(-i\frac{J_1\cdot\hat{n}}{\hbar}\delta\phi\right)\otimes\exp\left(-i\frac{J_2\cdot\hat{n}}{\hbar}\delta\phi\right)$$

Choice of basis:

1° $\quad J_1^2, J_2^2, J_{1z}, J_{2z} \qquad |j_1, j_2; m_1, m_2\rangle$

2° $\quad J_1^2, J_2^2, J^2, J_z \qquad |j_1, j_2; j, m\rangle$

this is because: $[J^2, J_1^2] = 0 \qquad [J_1^2, J_z] = 0$

$[J^2, J_2^2] = 0 \qquad [J_2^2, J_z] = 0$

$[J_1^2, J_2^2] = 0$

proof: $J^2 = (J_{1x} + J_{2x})^2 + (J_{1y} + J_{2y})^2 + (J_{1z} + J_{2z})^2$

$= J_1^2 + J_2^2 + 2J_{1x}J_{2x} + 2J_{1y}J_{2y} + 2J_{1z}J_{2z}$

$= J_1^2 + J_2^2 + 2J_{1z}J_{2z} + 2\cdot\frac{1}{2}(J_{1+} + J_{1-})\frac{1}{2}(J_{2+} + J_{2-})$

$\quad + 2\cdot\frac{1}{2i}(J_{1+} - J_{1-})\frac{1}{2i}(J_{2+} - J_{2-})$

$= \sim + \frac{1}{2}(J_{1+}J_{2+} + J_{1-}J_{2-} + J_{1+}J_{2-} + J_{1-}J_{2+})$

$\quad - \frac{1}{2}(J_{1+}J_{2-} + J_{1-}J_{2-} - J_{1+}J_{2-} - J_{1-}J_{2+})$

$= J_1^2 + J_2^2 + 2J_{1z}J_{2z} + J_{1+}J_{2-} + J_{1-}J_{2+}$

$\Downarrow$

$[J^2, J_1^2] = 0$

Base 2 satisfies:

$$J_1^2|j_1 j_2; jm\rangle = \hbar^2 j_1(j_1+1)|j_1 j_2; jm\rangle$$
$$J_2^2|j_1 j_2; jm\rangle = \hbar^2 j_2(j_2+1)|j_1 j_2; jm\rangle$$
$$J^2|j_1 j_2; jm\rangle = \hbar^2 j(j+1)|j_1 j_2; jm\rangle$$
$$J_z|j_1 j_2; jm\rangle = \hbar m|j_1 j_2; jm\rangle$$

Noticed, even though $[J^2, J_z] = 0$, $[J^2, J_{1z}] \neq 0$; $[J^2, J_{2z}] = 0$

Unitary transformation of the Basis:

$$|j_1 j_2; jm\rangle = \sum_{m_1 m_2}|j_1 j_2; m_1 m_2\rangle\langle j_1 j_2; m_1 m_2|j_1 j_2; jm\rangle$$

we call $\langle j_1 j_2; m_1 m_2|j_1 j_2; jm\rangle$ the celebsch-Gordan Coefficients
old basis $\Uparrow$ newbasis $\Uparrow$ — $\Uparrow$ which is U_{ij} for basis transformation

Property for Clebsch-Gordan coefficient:

- 1° $\quad m = m_1 + m_2$ otherwise: $\langle j_1 j_2; m_1 m_2|j_1 j_2; jm\rangle = 0$.

proof:

$$\langle j_1 j_2; m_1 m_2 | (J_z - J_{1z} - J_{2z}) | j_1 j_2; j m\rangle = 0$$

$$(m - m_1 - m_2)\langle j_1 j_2; m_1 m_2 | j_1 j_2; j m\rangle = 0$$

- 2° $|j_1 - j_2| \leq j \leq j_1 + j_2$ $\Downarrow$ in the proof, we let $j_1 > j_2$

proof ①: $N = (2j_1+1)(2j_2+1)$

$$= \sum_{j=j_1-j_2}^{j_1+j_2} (2j+1)$$

$$= \frac{1}{2}[\{2(j_1-j_2)+1\} + \{2(j_1+j_2)+1\}]\cdot(2j_2+1)$$

$$= (2j_1+1)(2j_2+1)$$

proof ②: knowing that $m = m_1 + m_2$, $m_{(max)} = j_1 + j_2$ $m_{(max)}$ is only satisfied when $m_1 = j_1$ $m_2 = j_2$ $\Downarrow$

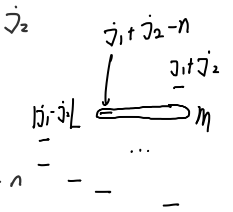
$m_{(max)} = m_1 + m_2$ $m_1 = j_1$ $m_2 = j_2 \Rightarrow j = j_1 + j_2$

A. $n \in [0, 2j_2]$
$m = (j_1 + j_2) - n$
$(j_1 - j_2) \leftarrow j_1 + j_2)$

$$\left.\begin{matrix} m_1 = j_1 - n & m_2 = j_2 \\ \vdots & \\ m_1 = j_1 & m_2 = j_2 - n \end{matrix}\right\} \longrightarrow \text{degeneracy} = n+1 \Downarrow$$

$$\left\{\begin{matrix} j = j_1 + j_2 \\ \vdots \\ j = j_1 + j_2 - n \end{matrix}\right.$$

provides this degeneracy

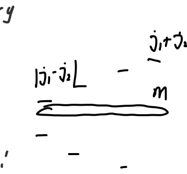


B. $n \in [2j_2, 2j_1]$
$m = (j_1 + j_2) - n$
$-(j_1 - j_2) \leftarrow (j_1 - j_2)$

$$\left.\begin{matrix} m_1 = j_1 - n & m_2 = j_2 \\ m_1 = j_1 + 2j_2 - n \ \vdots & m_2 = -j_2 \end{matrix}\right\} \longrightarrow \text{degeneracy} = 2j_2 + 1 \Downarrow$$

$$\left\{\begin{matrix} j = j_1 + j_2 \\ \vdots \\ j = j_1 - j_2 \end{matrix}\right.$$

provides this degeneracy!



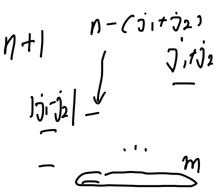
C. $n \in [2j_1, 2(j_1+j_2)]$
$-(j_1 + j_2) \leftarrow (j_1 - j_2)$

$$\left.\begin{matrix} m_1 = -j_1 & m_2 = j_2 - n + 2j_1 \\ \vdots & \\ m_1 = j_1 + 2j_2 - n & m_2 = -j_2 \end{matrix}\right\} \longrightarrow \text{degeneracy} = 2(j_1+j_2) - n + 1$$

$$\Downarrow$$

$$\left\{\begin{matrix} j = j_1 + j_2 \\ j = n - (j_1 + j_2) \end{matrix}\right.$$

provides this degeneracy.



- 3° orthogonality relation (unitary relation).

$$\sum_{jm} \langle j_1 j_2, m_1 m_2 | j_1 j_2; jm\rangle\langle j_1 j_2; jm | j_1 j_2; m_1' m_2'\rangle = \delta_{m_1 m_1'}\delta_{m_2 m_2'}$$

$$\sum_{m_1 m_2} \langle j_1 j_2; jm | j_1 j_2; m_1 m_2\rangle\langle j_1 j_2; m_1 m_2 | j_1 j_2; j' m'\rangle = \delta_{jj'}\delta_{mm'}$$

Always write as:

$$\sum_{m_1;\, m_2 = m - m_1} |\langle j_1 j_2; jm | j_1 j_2; m_1 m_2\rangle|^2 = 1$$

3.8.3 Recursion Relation for celebsch-Gordan coefficient

Fix $j_1 j_2\ j$ coefficient of different $m_1; m_2$:

$$J_\pm \quad |j_1 j_2; j m\rangle = (J_{1\pm} + J_{2\pm}) \sum_{m_1' m_2'} |j_1 j_2; m_1' m_2'\rangle\langle j_1 j_2; m_1' m_2' | j_1 j_2; jm\rangle$$

$$\sqrt{(j \mp m)(j \pm m + 1)} \quad |j_1 j_2; j\, m \pm 1\rangle = \sum_{m_1' m_2'} \Big(\sqrt{(j_1 \mp m_1')(j_1 \pm m_1' + 1)}\ |j_1, j_2; m_1' \pm 1, m_2'\rangle$$
$$+ \sqrt{(j_2 \mp m_2')(j_2 \pm m_2' + 1)}\ |j_1, j_2; m_1', m_2' \pm 1\rangle\Big)$$
$$\langle j_1 j_2; m_1' m_2' | j_1 j_2; jm\rangle$$

$$\sqrt{(j \mp m)(j \pm m + 1)} \quad |j_1 j_2; j m \pm 1\rangle = \sum_{m_1' m_2'} \Big(\sqrt{(j_1 \mp m_1')(j_1 \pm m_1' + 1)}\ |j_1, j_2; m_1' \pm 1\ m_2'\rangle$$
$$+ \sqrt{(j_2 \mp m_2')(j_2 \pm m_2' + 1)}\ |j_1 j_2, m_1'\ m_2' \pm 1\rangle\Big)\langle j_1 j_2; m_1' m_2' | j_1 j_2; jm\rangle$$

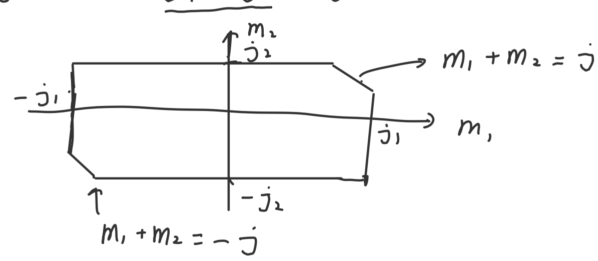
multiply $\langle j_1 j_2, m_1 m_2|$ on the right:

$$\sqrt{(j \mp m)(j \pm m + 1)}\ \langle j_1 j_2; m_1 m_2 | j_1 j_2; j\ m \pm 1\rangle = \sqrt{(j_1 \mp m_1 + 1)(j_1 \pm m_1)}\ \langle j_1 j_2; m_1 \mp 1, m_2 | j_1, j_2; jm\rangle$$
$$+ \sqrt{(j_2 \mp m_2 + 1)(j_2 \pm m_2)}\ \langle j_1 j_2; m_1\ m_2 \mp 1 | j_1 j_2; jm\rangle$$

C-G coefficient condition requires that: $m_1+m_2=m\pm1$.

(a) J_+ recursion (b) J_- recursion.

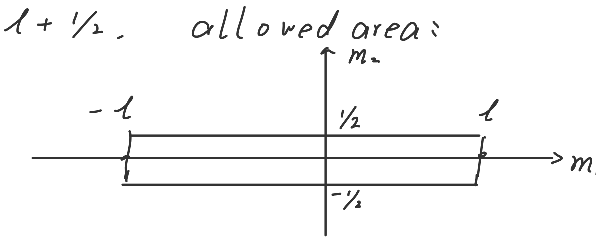
For fixed $\underline{j_1, j_2}$ j allowed plane:



Example, adding orbital and spin angular momentum of a single spin-1/2 particle

$$j_1=l \qquad m_1=m_l$$
$$j_2=1/2 \qquad m_2=m_s$$
$$j=l\pm1/2\ (l>0) \qquad j=\tfrac{1}{2}\ (l=0)$$

consider: $j=l+1/2$, allowed area:



Recursion, J_- (upper line) $\quad (m-\frac{1}{2},\frac{1}{2}) \quad (m+\frac{1}{2},\frac{1}{2})$

$$\sqrt{(l+\tfrac{1}{2}+m+1)(l+\tfrac{1}{2}-m)}\ \langle m-\tfrac{1}{2},\tfrac{1}{2}|l+\tfrac{1}{2},m\rangle=\sqrt{(l+m+\tfrac{1}{2})(l-m+\tfrac{1}{2})}\ \langle m+\tfrac{1}{2},\tfrac{1}{2}|l+\tfrac{1}{2},m+1\rangle$$

move horizontally:

$$\langle m-\tfrac{1}{2},\tfrac{1}{2}|l+\tfrac{1}{2},m\rangle=\sqrt{\frac{l+m+1/2}{l+m+3/2}}\cdot\langle m+\tfrac{1}{2},\tfrac{1}{2}|l+\tfrac{1}{2},m+1\rangle$$
$$\Downarrow$$
$$\langle m-\tfrac{1}{2},\tfrac{1}{2}|l+\tfrac{1}{2},m\rangle=\sqrt{\frac{l+m+1/2}{2l+1}}\ \langle l,\tfrac{1}{2}|l+\tfrac{1}{2},l+\tfrac{1}{2}\rangle$$

require that:

$$\langle m-\tfrac{1}{2},\tfrac{1}{2}|l+\tfrac{1}{2},l+\tfrac{1}{2}\rangle=1$$
$$\langle m-\tfrac{1}{2},\tfrac{1}{2}|l+\tfrac{1}{2},m\rangle=\sqrt{\frac{l+m+1/2}{2l+1}}$$

However, we still needs to determin:

$$|1\rangle=|j=l+\tfrac{1}{2},m\rangle=\sqrt{\frac{l+m+1/2}{2l+1}}\ |m_l=m-\tfrac{1}{2},m_s=\tfrac{1}{2}\rangle+\ ?\ |m_l=m+\tfrac{1}{2},m_s=-\tfrac{1}{2}\rangle$$
$$|2\rangle=|j=l-\tfrac{1}{2},m\rangle=\ ?\quad |m_l=m-\tfrac{1}{2},m_s=\tfrac{1}{2}\rangle+\ ?\ |m_l=m+\tfrac{1}{2},m_s=-\tfrac{1}{2}\rangle$$

using $\langle1|1\rangle=1$; $\langle1|2\rangle=0$; expect the coefficient to be:

$$\begin{pmatrix}\cos\alpha & \sin\alpha\\ -\sin\alpha & \cos\alpha\end{pmatrix}\Longrightarrow\begin{pmatrix}\sqrt{\frac{l+m+1/2}{2l+1}} & \sqrt{\frac{l-m+\frac{1}{2}}{2l+1}}\\ -\sqrt{\frac{l-m+1/2}{2l+1}} & \sqrt{\frac{l+m+1/2}{2l+1}}\end{pmatrix}$$

The eigenstate for L^2, S^2, J^2, J_z are also eigen ket for $L\cdot S$.

because:

$$L\cdot S = \frac{1}{2}(J^2 - L^2 - S^2)$$
$$\Downarrow$$
$$\frac{\hbar^2}{2}(j(j+1) - l(l+1) - s(s+1)) \quad \text{eigen value!}$$

3.8.4 Celebsch-Gordan coefficient and rotation matrix

$\mathcal{D}^{(j_1)}(R) \otimes \mathcal{D}^{(j_2)}(R)$ is reducible:

$$\begin{bmatrix} \mathcal{D}^{(j_1+j_2)} & & & \\ & \mathcal{D}^{(j_1+j_2-1)} & & \\ & & \ddots & \\ & & & \mathcal{D}^{|j_1-j_2|} \end{bmatrix}$$

In notation of group theory

$$\mathcal{D}^{(j_1)} \otimes \mathcal{D}^{(j_2)} = \mathcal{D}^{(j_1+j_2)} \oplus \mathcal{D}^{(j_1+j_2-1)} \cdots \oplus \mathcal{D}^{(|j_1-j_2|)}$$

clebsch-Gordan series:

$$\mathcal{D}^{(j_1)}_{m_1 m_1'}(R)\, \mathcal{D}^{(j_2)}_{m_2 m_2'}(R) = \sum_{j m m'} \langle j_1 j_2; m_1 m_2 | j_1 j_2; j m\rangle \langle j_1 j_2; m_1' m_2' | j_1 j_2; j m'\rangle \mathcal{D}^{(j)}_{m m'}(R)$$

proof:

$$L: \langle j_1 j_2; m_1 m_2 | \mathcal{D}(R) | j_1 j_2; m_1' m_2'\rangle = \langle j_1 m_1 | \mathcal{D}(R) | j_1 m_1'\rangle \langle j_2 m_2 | \mathcal{D}(R) | j_2 m_2'\rangle$$
$$= \mathcal{D}^{(j_1)}_{m_1 m_1'}(R)\, \mathcal{D}^{(j_2)}_{m_2 m_2'}(R)$$

$$R: \langle j_1 j_2; m_1 m_2 | \mathcal{D}(R) | j_1 j_2; m_1' m_2'\rangle = \sum_{j m j' m'} \langle j_1 j_2; m_1 m_2 | j_1 j_2; j m\rangle \langle j_1 j_2; j m | \mathcal{D}(R) | j_1 j_2; j' m'\rangle \langle j_1 j_2; j' m' | j_1 j_2\, m_1' m_2'\rangle$$

$$= \sum_{j m j' m'} \langle j_1 j_2; m_1 m_2 | j_1 j_2; j m\rangle \mathcal{D}^{(j)}_{m m'}(R)\, \delta_{j j'} \langle j_1 j_2; j' m' | j_1 j_2; m_1' m_2'\rangle$$

$$= \sum_{j m m'} \langle j_1 j_2; m_1 m_2 | j_1 j_2; j m\rangle \langle j_1 j_2; m_1' m_2' | j_1 j_2; j m'\rangle \mathcal{D}^{(j)}_{m m'}(R)$$

used the property that C-G coefficients are Real!

Application example:

using:

$$\mathcal{D}^{(l)}_{m0}(\alpha, \beta, \gamma = 0) = \sqrt{\frac{4\pi}{2l+1}}\, Y_l^{m\,*}(\theta, \phi)\Big|_{\theta=\beta,\ \phi=\alpha}$$

obtain:

$$Y_{l_1}^{m_1}(\theta,\phi)\, Y_{l_2}^{m_2}(\theta,\phi) = \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi}} \sum_{l' m'} \langle l_1 l_2; m_1 m_2 | l_1 l_2; l' m'\rangle \langle l_1 l_2; 0 0 | l_1 l_2; l' 0\rangle \sqrt{\frac{4\pi}{2l'+1}}\, Y_{l'}^{m'}(\theta,\phi)$$

multiply both side $Y_l^{m\,*}$. $\Downarrow$

$$\int d\Omega\, Y_l^{m*} Y_{l_1}^{m_1} Y_{l_2}^{m_2} = \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2l+1)}} \langle l_1 l_2 0 0 | l_1 l_2, l 0\rangle \langle l_1 l_2; m_1 m_2 | l_1 l_2; l m\rangle$$

3.9 Schwinger's oscillator model for angular Momentum

3.9.1 Angular momentum and uncoupled oscillators.

$$N_+ = a_+^\dagger a_+ \qquad N_- = a_-^\dagger a_-$$

$$[a_+, a_+^\dagger] = 1 \qquad [a_-, a_-^\dagger] = 1$$

$$[N_+, a_+] = -a_+ \qquad [N_-, a_-] = -a_-$$

$$[N_+, a_+^\dagger] = a_+^\dagger \qquad [N_-, a_-^\dagger] = +a_-^\dagger$$

$$[N, a_-^\dagger] = [a_-, a_+^\dagger] = 0$$

N_+ and N_- commute $\Rightarrow$ we build simultaneous eigenkets!

$$N_+ |n_+, n_-\rangle = n_+ |n_+, n_-\rangle$$

$$N_- |n_+, n_-\rangle = n_- |n_+, n_-\rangle$$

$$a_+^\dagger |n_+, n_-\rangle = \sqrt{n_+ + 1}\, |n_+ + 1, n_-\rangle$$

$$a_-^\dagger |n_+, n_-\rangle = \sqrt{n_- + 1}\, |n_+, n_- + 1\rangle$$

$$a_+ |n_+, n_-\rangle = \sqrt{n_+}\, |n_+ - 1, n_-\rangle$$

$$a_+ |n_+, n_-\rangle = \sqrt{n_-}\, |n_+, n_- - 1\rangle$$

$$|n_+, n_-\rangle = \frac{(a_+^\dagger)^{n_+}(a_-^\dagger)^{n_-}}{\sqrt{n_+!}\sqrt{n_-!}} |0,0\rangle$$

Define:

$$J_+ \equiv \hbar a_+^\dagger a_- \qquad J_- \equiv \hbar a_-^\dagger a_+$$

$$J_z = \frac{\hbar}{2}(a_+^\dagger a_+ - a_-^\dagger a_-) = \frac{\hbar}{2}(N_+ - N_-)$$

We can proof that:

$$[J_z, J_\pm] = \pm\hbar J_\pm$$

$$[J_+, J_-] = 2\hbar J_z.$$

proof:

$$\hbar^2 [a_+^\dagger a_-, a_-^\dagger a_+] = \hbar^2 a_+^\dagger a_- a_-^\dagger a_+ - \hbar^2 a_-^\dagger a_+ a_+^\dagger a_-$$

$$= \hbar^2 a_+^\dagger (a_-^\dagger a_- + 1) a_+ - \hbar^2 a_-^\dagger (a_+^\dagger a_+ + 1) a_-$$

$$= \hbar^2 (a_+^\dagger a_+ - a_-^\dagger a_-) = 2\hbar J_z$$

define total N:

$$N \equiv N_+ + N_- = a_+^\dagger a_+ + a_-^\dagger a_-$$

$$J^2 \equiv J_z^2 + \frac{1}{2}(J_+ J_- + J_- J_+) = \frac{\hbar^2}{2} N \left(\frac{N}{2} + 1\right)$$

can be prove!

$$J_+ |n_+, n_-\rangle = \hbar a_+^\dagger a_- |n_+, n_-\rangle$$

$$= \sqrt{n_-(n_+ + 1)}\, \hbar\, |n_+ + 1, n_- - 1\rangle$$

$$J_- |n_+, n_-\rangle = \hbar a_-^\dagger a_+ |n_+, n_-\rangle$$

$$= \sqrt{n_+(n_- + 1)}\, \hbar\, |n_+ - 1, n_+ + 1\rangle$$

$$J_z |n_+, n_-\rangle = \frac{\hbar}{2}(N_+ - N_-) |n_+, n_-\rangle$$

$$= \frac{1}{2}(n_+ - n_-)\hbar\, |n_+, n_-\rangle$$

$$J^2 |n_+, n_-\rangle = \frac{\hbar^2}{2}(n_+ + n_-)\left(\frac{n_+ + n_-}{2} + 1\right) |n_+, n_-\rangle$$

$$n_+ \to j + m \qquad n_- \to j - m \qquad j \equiv \frac{j_+ + j_-}{2} \qquad m \equiv \frac{n_+ - n_-}{2}$$

$$\sqrt{n_-(n_+ + 1)} \longrightarrow \sqrt{(j-m)(j+m+1)}$$

$$\sqrt{n_+(n_- + 1)} \longrightarrow \sqrt{(j+m)(j-m+1)}$$

$$|j,m\rangle = \frac{(a_+^\dagger)^{j+m}(a_-^\dagger)^{j-m}}{\sqrt{(j+m)!\,(j-m)!}} \cdot |0\rangle$$

$$|j,j\rangle = \frac{(a_+^\dagger)^{2j}}{\sqrt{(2j)!}} \quad |0\rangle$$

A complicated object of high j can be visualised as made up of primitive spin-1/2 particles $j+m$ of them with spin-up $j-m$ of them with spin-down!

3.9.2. Explicit formula for rotation Matrices.

focus on the

$$\mathcal{D}(R) = \mathcal{D}(\alpha,\beta,\gamma)|_{\alpha=\gamma=0} = \exp\left(-i\frac{J_y\beta}{\hbar}\right)$$

$$\mathcal{D}(R)\,|j,m\rangle = \frac{[\mathcal{D}(R)\,a_+^\dagger\,\mathcal{D}^{-1}(R)]^{j+m}\cdot[\mathcal{D}(R)\,a_-^\dagger\,\mathcal{D}^{-1}(R)]^{j-m}}{\sqrt{(j+m)!}\;\sqrt{(j-m)!}}\,\mathcal{D}(R)|0\rangle$$

$$\mathcal{D}(R)|0\rangle = |0\rangle$$

$$\mathcal{D}(R)\,a_\pm^\dagger\,\mathcal{D}^{-1}(R) = \exp\left(-i\frac{J_y\beta}{\hbar}\right) a_\pm^\dagger \exp\left(i\frac{J_y\beta}{\hbar}\right)$$

Baker–Hausdorff Lemma:

$$\exp(iG\lambda)\,A\,\exp(-iG\lambda) = A + i\lambda[G,A]\cdot + \frac{i^2\lambda^2}{2!}\cdot[G,[G,A]] \;\cdots\; + \frac{i^n\lambda^n}{n!}[G,[G,\cdots A]\cdots]$$

Let: $\quad G \longrightarrow -J_y\frac{1}{\hbar} \qquad \lambda\to\beta$

Then: $\quad \left[-\frac{J_y}{\hbar}, a_+^\dagger\right] = \frac{1}{2i}[a_-^\dagger a_+ - a_+^\dagger a_-, a_+^\dagger] = \frac{1}{2i}\,a_-^\dagger$

$$\left[-\frac{J_y}{\hbar}, \left[-\frac{J_y}{\hbar}, a_+^\dagger\right]\right] = \cdots = \frac{1}{4}a_+^\dagger$$

$$\mathcal{D}(R)\,a_+^\dagger\,\mathcal{D}^{-1}(R) = a_+^\dagger\cos\left(\tfrac{\beta}{2}\right) + a_-^\dagger\sin\left(\tfrac{\beta}{2}\right)$$

$$\mathcal{D}(R)\,a_-^\dagger\,\mathcal{D}^{-1}(R) = a_-^\dagger\cos\left(\tfrac{\beta}{2}\right) - a_+^\dagger\sin\left(\tfrac{\beta}{2}\right)$$

The basic spin-up state is supposed to transform as:

$$a_+^\dagger|0\rangle \longrightarrow \cos\left(\tfrac{\beta}{2}\right) a_+^\dagger|0\rangle + \sin\left(\tfrac{\beta}{2}\right)\cdot a_-^\dagger|0\rangle$$

Using Binomial theorem:

$$(x+y)^N = \sum_k \frac{N!}{(N-k)!\,k!}\cdot x^{N-k}\cdot y^k.$$

$$\mathcal{D}(\alpha=0,\beta,\gamma=0)\cdot|j,m\rangle = \frac{(\mathcal{D}(R)\,a_+^\dagger\mathcal{D}^{-1}(R))^{j+m}(\mathcal{D}(R)\,a_-^\dagger\mathcal{D}^{-1}(R))^{j-m}}{\sqrt{(j+m)!\,(j-m)!}}\,\mathcal{D}(R)|0\rangle$$

$$= \frac{(a_+^\dagger\cos(\frac{\beta}{2}) + a_-^\dagger\sin(\frac{\beta}{2}))^{j+m}(a_-^\dagger\cos(\frac{\beta}{2}) - a_+^\dagger\sin(\frac{\beta}{2}))^{j-m}}{\sqrt{(j+m)!\,(j-m)!}}\,\mathcal{D}(R)|0\rangle$$

$$= \sum_{kl}\frac{(j+m)!\,(j-m)!}{(j+m-k)!\,k!\,(j-m-l)!\,l!}\cdot\frac{(a_+^\dagger\cos(\frac{\beta}{2}))^{j+m-k}(a_-^\dagger\sin(\frac{\beta}{2}))^k}{\sqrt{(j+m)!\,(j-m)!}}\cdot$$

$$(-a_+^\dagger\sin(\tfrac{\beta}{2}))^{j-m-l}\cdot(a_-^\dagger\cos(\tfrac{\beta}{2}))^l\;|0\rangle$$

Compare with

$$\mathcal{D}(\alpha=0,\beta,\gamma=0)|j,m\rangle = \sum_{m'}|j,m'\rangle\,d^{(j)}_{m'm}(\beta)$$

$$= \sum_{m'} d^{(j)}_{m'm}(\beta)\,\frac{(a_+^\dagger)^{j+m'}\cdot(a_-^\dagger)^{j-m'}}{\sqrt{(j+m')!\,(j-m')!}}\cdot|0\rangle$$

compare coefficient of $a_+^\dagger$ & $a_-^\dagger$

$$\begin{cases} 2j-k-l = j-m' \\ j-m' = k+l \end{cases} \Rightarrow \quad l = j-k-m'$$

coefficient of exponents $\cos(\beta/2)$ $\sin(\beta/2)$

$$j+m-k+l = 2j-2k+m-m'$$

$$k+j-m-l = 2k-m+m'$$

$$j-m-l = k-m+m'$$

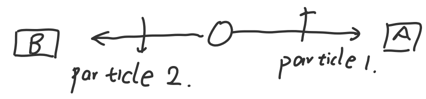
Wigner's formula for $d^{(j)}_{m'm}(\beta)$

$$d^{(j)}_{m'm}(\beta) = \sum_k (-1)^{k-m+m'} \frac{\sqrt{(j+m)!(j-m)!(j+m')!(j-m')!}}{(j+m-k)!\cdot k!\cdot(j-k-m')!(k-m+m')!} \left(\cos\left(\frac{\beta}{2}\right)\right)^{2j-2k+m-m'} \left(\sin\left(\frac{\beta}{2}\right)\right)^{2k-m+m'}$$

3.10 spin-correlation measurement and Bell's inequality.

consider two-electron system in a $\underbrace{\text{spin-singlet}}_{S=0}$ state

$$|\text{spin singlet}\rangle = \frac{1}{\sqrt{2}}\left(|\hat{z}+,\hat{z}-\rangle - |\hat{z}-,\hat{z}+\rangle\right)$$



if A measures ↑

B measures ↓

Einstein's locality principle and Bell's inequality.

tabel 3.2

	particle 1	particle 2
N_1	$(\hat{a}+,\hat{b}+,\hat{c}+)$	$(\hat{a}-,\hat{b}-,\hat{c}-)$
N_2	$(\hat{a}+,\hat{b}+,\hat{c}-)$	$(\hat{a}-,\hat{b}-,\hat{c}+)$
N_3	$(\hat{a}+,\hat{b}-,\hat{c}+)$	$(\hat{a}-,\hat{b}+,\hat{c}-)$
N_4	$(\hat{a}+,\hat{b}-,\hat{c}-)$	$(\hat{a}-,\hat{b}+,\hat{c}+)$
N_5	$(\hat{a}-,\hat{b}+,\hat{c}+)$	$(\hat{a}+,\hat{b}-,\hat{c}-)$
N_6	$(\hat{a}-,\hat{b}+,\hat{c}-)$	$(\hat{a}+,\hat{b}-,\hat{c}+)$
N_7	$(\hat{a}-,\hat{b}-,\hat{c}+)$	$(\hat{a}+,\hat{b}+,\hat{c}-)$
N_8	$(\hat{a}-,\hat{b}-,\hat{c}-)$	$(\hat{a}+,\hat{b}+,\hat{c}+)$

suppose $\begin{cases} A \text{ finds } S_1\cdot\hat{a} \text{ be } +, \\ B \text{ finds } S_2\cdot\hat{b} \text{ be } -. \end{cases}$ $\underline{N_3+N_4}$

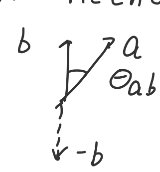
$$N_3+N_4 \le N_2+N_4+N_3+N_7$$

$$P(\hat{a}+,\hat{b}+) = \frac{N_3+N_4}{\sum_i N_i} \qquad P(\hat{a}+,\hat{c}+) = \frac{N_2+N_4}{\sum_i N_i}, \qquad P(\hat{c}+,\hat{b}+) = \frac{N_3+N_7}{\sum_i N_i}$$

Bell's Inequality:

$$P(\hat{a}+,\hat{b}+) \le P(\hat{a}+,\hat{c}+) + P(\hat{c}+,\hat{b}+)$$

3.10.3 Quantum mechanics and Bell's inequality.

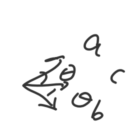


From previous section eigen state for $S\cdot\hat{n}$

$$P(\hat{a}+,\hat{b}+) = \frac{1}{2}\cos^2\left(\frac{\pi-\theta_{ab}}{2}\right) = \sin^2\left(\frac{\theta_{ab}}{2}\right)$$

Bell's inequolity:

$$\sin^2\left(\frac{\theta_{ab}}{2}\right) \le \sin^2\left(\frac{\theta_{ac}}{2}\right) + \sin^2\left(\frac{\theta_{cb}}{2}\right)$$



$\theta = \frac{\pi}{4}$ not hold!

3.11 Tensor operators

3.11.1 Vector operator.

$$\langle\alpha|V_i|\alpha\rangle \longmapsto \langle\alpha|\mathcal{D}^\dagger(R)\, V_i\, \mathcal{D}(R)|\alpha\rangle$$

The expectation value of vector operators are expect to change as:

$$\langle\alpha|V_i|\alpha\rangle \to \sum_j R_{ij}\langle\alpha|V_j|\alpha\rangle$$

$$\mathcal{D}(R)\, V_i\, \mathcal{D}^\dagger(R) = \sum_j R_{ij} V_j$$

Infinitesimal version:

$$\mathcal{D}(R) = 1 - \frac{i\varepsilon}{\hbar} J\cdot\hat{n}$$

$$V_i + \frac{\varepsilon}{i\hbar}[V_i, J\cdot\hat{n}] = \sum_j R_{ij}(\hat{n},\varepsilon) V_j.$$

In particular. $\hat{n} = \hat{z}$.

$$R(\hat{z},\varepsilon) = \begin{pmatrix} 1 & -\varepsilon & 0 \\ \varepsilon & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$i=1$: $\quad V_x + \frac{\varepsilon}{i\hbar}[V_x, J_z] = V_x - \varepsilon V_y$

$i=2$: $\quad V_y + \frac{\varepsilon}{i\hbar}[V_y, J_z] = V_y + \varepsilon V_x$

$i=3$ $\quad V_z + \frac{\varepsilon}{i\hbar}[V_z, J_z] = V_z$

In all:

$$[V_i, V_j] = i\,\varepsilon_{ijk}\hbar J_k \Longleftarrow$$ This can be viewed as definition of vector operator!

3.11.2 Cartesian Tensor Versus Irreducible tensors.

Cartesian Tensor: the number of indices is called the rank of the tensor!

$$T_{ijk\cdots} \longrightarrow \sum_{i'j'\cdots} R_{ii'}R_{jj'}\cdots T_{i'j'k'\cdots}$$

The simplest Cartesian operator is dyadic formed of two vectors U and V.

$$T_{ij} = U_i V_j$$

$$U_iU_j = \underset{\substack{\Uparrow \\ \text{trace}}}{\frac{U\cdot V}{3}\delta_{ij}} + \underset{\substack{\Uparrow \\ \text{anti-symmetric}}}{\frac{U_iV_j - U_jV_i}{2}} + \underset{\substack{\Uparrow \\ \text{symmetric and traceless}}}{\left(\frac{U_iV_j + U_jV_i}{2} - \frac{U\cdot V}{3}\delta_{ij}\right)}$$

$$3\times 3 = 1 + 3 + 5$$

In fact this is the simplest nontrivial example to illustrate the reduction of a cartesian tensor into irreducible spherical tensor.

Example of Spherical tensor of rank k:

$$T^{(k)}_q = Y^{m=q}_{l=k}(V)$$

$k=1$; $l=1$

$$Y^0_1 = \sqrt{\frac{3}{4\pi}}\cos\theta = \sqrt{\frac{3}{4\pi}}\frac{z}{r} \to T^{(1)}_0 = \sqrt{\frac{3}{4\pi}} V_z$$

$$Y^{\pm1}_1 = \mp\sqrt{\frac{3}{4\pi}}\frac{x+iy}{\sqrt{2}r} \quad \to T^{(1)}_{\pm1} = \sqrt{\frac{3}{4\pi}}\left(\mp\frac{V_x + iV_y}{\sqrt{2}}\right)$$

This can be generalized to higher k, for example

$$Y^{\pm2}_2 = \sqrt{\frac{15}{32\pi}}\cdot\frac{(x+iy)^2}{r^2} \to T^{(2)}_{\pm2} = \sqrt{\frac{15}{32\pi}}(V_x \pm iV_y)^2$$

▽ $T^{(k)}_q$ are irreducible, just as $Y^{(m)}_l$ are.

we want to see the transformation of spherical tensor constructed in this manner.

For direction eigenket $|\hat{n}\rangle$

$$|\hat{n}\rangle \longmapsto \mathcal{D}(R)\,|\hat{n}\rangle \equiv |\hat{n}'\rangle$$

we whish to exam how $Y_l^m(\hat{n}') = \langle n'|l m\rangle$ would look in terms of $Y_l^m(\hat{n})$.

This can be seen by starting with:

$$\mathcal{D}(R^{-1})\,|l,m\rangle = \sum_{m'} |l,m'\rangle\langle l,m'|\,\mathcal{D}(R^{-1})|l,m\rangle$$
$$= \sum_{m'} |l,m'\rangle\, \mathcal{D}^{(l)}_{m'm}(R^{-1})$$

Acting $\langle\hat{n}|$ on the left:

$$\langle\hat{n}|\,\mathcal{D}(R^{-1})\,|l,m\rangle = \sum_{m'} \langle\hat{n}|l,m'\rangle\, \mathcal{D}^{(l)}_{m'm}(R^{-1})$$
$$Y_l^m(n') = \sum_{m'} Y_l^{m'}(\hat{n})\, \mathcal{D}^{(l)}_{m'm}(R^{-1})$$

If there is an operator that acts like $Y_l^m(V)$, it is reasonable to expect.

$$\mathcal{D}^{\dagger}(R)\, Y_l^m(V)\, \mathcal{D}(R) = \sum_{m'} Y_l^{m'}(V)\cdot \mathcal{D}^{(l)*}_{mm'}(R)$$

| where we have used the unitarity of the rotation to rewrite $\mathcal{D}^{(l)}_{m'm}(R^{-1})$

Definition of spherical tensor operator of rank k with $2k+1$ elements.

$$\mathcal{D}^{\dagger}(R)\; T_q^{(k)}\; \mathcal{D}(R) = \sum_{q'=-k}^{k} \mathcal{D}^{(k)*}_{qq'}(R)\, T_{q'}^{(k)}$$

or equivalently

$$\mathcal{D}(R)\; T_q^{(k)}\; \mathcal{D}^{\dagger}(R) = \sum_{q'=-k}^{k} \mathcal{D}^{(k)}_{q'q}(R)\, T_{q'}^{(k)}$$

A more convenient definition of a spherical tensor is obtained by considering the infinitesimal form of above equation:

$$\left(1 - i\frac{J\cdot\hat{n}}{\hbar}\varepsilon\right) T_q^{(k)} \left(1 + i\frac{J\cdot\hat{n}}{\hbar}\varepsilon\right) = \sum_{q'=-k}^{k} T_{q'}^{(k)}\cdot\langle kq'|\left(1 - i\frac{J\cdot\hat{n}}{\hbar}\varepsilon\right)|kq\rangle$$
$$[J\cdot\hat{n},\, T_q^{(k)}] = \sum_{q'} T_{q'}^{(k)}\,\langle kq'|\,J\cdot\hat{n}\,|kq\rangle$$

Taking $\hat{n}$ to be $\hat{z}$ and $\hat{x}+i\hat{y}$ direction and using the nonvanishing matrix elements of J_z and $J_\pm$, we obtain:

$$[J_z,\, T_q^{(k)}] = \hbar q\, T_q^{(k)}$$
$$[J_\pm,\, T_q^{(k)}] = \hbar\sqrt{(k\mp q)(k\pm q+1)}\cdot T_{q\pm1}^{(k)}$$

These commutation relation can be viewed as the definition of spherical tensor operator!

3.11.3 Product of Tensors.

A simple example of spherical tensor:

$$T_0^{(0)} = -\frac{U\cdot V}{3} = \frac{U_{+1}V_{-1} + U_{-1}V_{+1} - U_0V_0}{3}$$
$$T_q^{(1)} = \frac{(U\times V)_q}{i\sqrt{2}}$$
$$T_{\pm2}^{(2)} = U_{\pm1}\,V_{\pm1}$$
$$T_{\pm1}^{(2)} = \frac{U_{\pm1}V_0 + U_0V_{\pm1}}{\sqrt{2}}$$
$$T_0^{(2)} = \frac{U_{+1}V_{-1} + 2U_0V_0 + U_{-1}V_{+1}}{\sqrt{6}}$$

In which $U_{+1} = -(U_x + iU_y)/\sqrt{2}$ $\quad U_{-1} = (U_x - iU_y)/\sqrt{2}$ $\quad U_0 = U_z$.

The preceding transformation property can be cheked by compare with Y_l^m

For instance

$$Y_2^0 = \sqrt{\frac{5}{16\pi}} \cdot \frac{3z^2 - r^2}{r^2}$$

where $3z^2 - r^2$ can be written as

$$2z^2 + 2\cdot\left(-\frac{(x+iy)}{\sqrt{2}}\frac{(x-iy)}{\sqrt{2}}\right)$$

Hence, Y_2^0 is a special case for $T_0^{(2)}$ for $U = V \sim r$.

Theorem 5: Let $X_{q_1}^{(k_1)}$ $Z_{q_2}^{(k_2)}$ be irreducible spherical tensors of rank k_1 and k_2. then

$$T_q^{(k)} = \sum_{q_1 q_2} \langle k_1 k_2\; q_1 q_2 | k_1 k_2\; k q\rangle\, X_{q_1}^{(k_1)}\, Z_{q_2}^{(k_2)}$$

is a spherical tensor of rank k.

proof: we want to show what $T_q^{(k)}$ behaves under rotation.

$$\mathcal{D}^\dagger(R)\, T_q^{(k)}\, \mathcal{D}(R) = \sum_{q_1}\sum_{q_2} \langle k_1 k_2; q_1 q_2 | k_1 k_2; k q\rangle\, \mathcal{D}^\dagger(R)\, X_{q_1}^{(k_1)}\, \mathcal{D}(R)\,\mathcal{D}^\dagger(R)\, Z_{q_2}^{(k_2)}\,\mathcal{D}(R)$$

$$= \sum_{q_1 q_2 q_1' q_2' q'' q'} \langle k_1 k_2; q_1 q_2|k_1 k_2; kq\rangle\, X_{q_1'}^{(k_1)}\, \mathcal{D}_{q_1' q_1}^{(k_1)}(R^{-1})\, Z_{q_2'}^{(k_2)}\, \mathcal{D}_{q_2' q_2}^{(k_2)}(R^{-1})$$

using the property

$$\mathcal{D}_{m_1 m_1'}^{(j_1)}(R)\,\mathcal{D}_{m_2 m_2'}^{(j_2)}(R) = \sum_{j m m'} \langle j_1 j_2; m_1 m_2|j_1 j_2; jm\rangle\langle j_1 j_2; m_1' m_2'|j_1 j_2; j m'\rangle\, \mathcal{D}_{mm'}^{(j)}(R)$$

$$= \sum_{k'' q_1 q_2 q_1' q_2' q'' q'} \langle k_1 k_2\; q_1 q_2|k_1 k_2\; kq\rangle\langle k_1 k_2\; q_1' q_2'|k_1 k_2\; k'' q'\rangle\langle k_1 k_2; q_1 q_2|k_1 k_2, k'' q''\rangle$$
$$\mathcal{D}_{q'q''}^{(k'')}(R^{-1})\, X_{q_1'}^{(k_1)}\, Z_{q_2'}^{(k_2)}$$

} used the orthogonality of C-G coefficients!

$$= \sum_{k'' q_1' q_2' q'' q'} \delta_{kk''}\,\delta_{qq''}\,\langle k_1 k_2; q_1' q_2'|k_1 k_2; k'' q'\rangle$$
$$\mathcal{D}_{q'q''}^{(k'')}(R^{-1})\, X_{q_1'}^{(k_1)}\, X_{q_2'}^{(k_2)}$$

$$= \sum_{q'}\left(\sum_{q_1' q_2'} \langle k_1 k_2; q_1' q_2'|k_1 k_2; kq'\rangle\, X_{q_1'}^{(k_1)}\, Z_{q_2'}^{(k_2)}\right)\mathcal{D}_{q'q}^{(k)}(R^{-1})$$

$$= \sum_{q'} T_{q'}^{(k)}\, \mathcal{D}_{q'q}^{(k)}(R^{-1})$$

$$= \sum_{q'} \mathcal{D}_{qq'}^{(k)*}(R)\, T_{q'}^{(k)}$$

3.11.4 Matrix elements of Tensor operators.

The Wigner-Eckart Theorem.

▽ m selection rule

$$\langle \alpha', j', m'|T_q^{(k)}|\alpha, j, m\rangle = 0 \qquad \text{unless} \qquad m' = q+m.$$

proof1: using $[J_z, T_q^{(k)}] = \hbar q\, T_q^{(k)}$

$$\langle\alpha', j', m'|\,[J_z, T_q^{(k)}] - \hbar q \cdot T_q^{(k)}\,|\alpha, j, m\rangle = 0.$$

$$\langle\alpha', j', m'|\,J_z T_q^{(k)} - T_q^{(k)} J_z - \hbar q\, T_q^{(k)}\,|\alpha, j, m\rangle = 0$$

$$((m'-m)\hbar - q\hbar)\,\langle\alpha', j', m'|\,T_q^{(k)}\,|\alpha, j, m\rangle = 0$$

end of proof!

proof 2: $T_q^{(k)}$ under rotation:

$$\mathcal{D}\, T_q^{(k)}\,|\alpha, j, m\rangle = \mathcal{D}\, T_q^{(k)}\,\mathcal{D}^\dagger\mathcal{D}\,|\alpha, j, m\rangle$$

$\mathcal{D}$ stands for rotation around $\hat{z}$ for ϕ.

$$\mathcal{D}(R)\, T_q^{(k)}\, \mathcal{D}^\dagger(R) = \sum_{q'=-k}^{k} \mathcal{D}_{q'q}^{(k)}(R)\, T_{q'}^{(k)}$$

$$\mathcal{D}_z(\phi) = \lim_{N\to+\infty} \left(1 - i\frac{J_z}{\hbar}\cdot\frac{\phi}{N}\right)^N = \exp\left(-i\frac{J_z\phi}{\hbar}\right) := 1 - i\frac{J_z\phi}{\hbar} - \frac{J_z^2\phi^2}{2\hbar^2}\cdots$$

$$\mathcal{D}\, T_q^{(k)} |\alpha, j, m\rangle = \sum_{q'=-k}^{k} \mathcal{D}_{q'q}^{(k)}(R)\, T_{q'}^{(k)}\, \exp\left(-i\frac{J_z\phi}{\hbar}\right) |\alpha, j, m\rangle$$

$$= \sum_{q'} \langle k\, q'|\exp(-iJ_z\tfrac{\phi}{\hbar})|k\, q\rangle\, T_{q'}^{(k)}\, e^{-im\phi} |\alpha, j, m\rangle$$

$$= T_q^{(k)}\, e^{-iq\phi}\, e^{-im\phi}\, |\alpha j m\rangle$$

Noticed:

$$\begin{cases} \langle\alpha', j', m'|\mathcal{D}\, T_q^{(k)}|\alpha, j, m\rangle = e^{-iq\phi}\, e^{-im\phi}\, \langle\alpha', j', m'|T_q^{(k)}|\alpha, j, m\rangle \\ \langle\alpha', j', m'|\mathcal{D}\, T_q^{(k)}|\alpha, j, m\rangle = \langle\alpha', j', m'|\mathcal{D}(\hat{z}\phi)\, T_q^{(k)}|\alpha, j, m\rangle \end{cases}$$

$$\Downarrow \qquad = e^{-im'\phi}\, \langle\alpha', j', m'|T_q^{(k)}|\alpha, j, m\rangle$$

$\langle\alpha', j', m'|T_q^{(k)}|\alpha, j, m\rangle \neq 0$ only when $m' = q + m$!

▽ **Wigner – Eckart Theorem**

the matrix elements of tensor operators with respect to angular-momentum eigenstates satisfy

$$\langle\alpha' j' m'|T_q^{(k)}|\alpha j m\rangle = \langle j k; m\, q|j, k; j' m'\rangle \cdot \frac{\overbrace{\langle\alpha j'||T^{(k)}||\alpha j\rangle}^{\text{Reduced matrix elements}}}{\sqrt{2j'+1}}$$

where the double bar means independent of m, m', q

proof : using (3.468 b. sakurai) ⇓

$$[J_\pm, T_q^{(k)}] = \hbar\sqrt{(k\mp q)(k\pm q+1)}\, T_{q\pm1}^{(k)}$$

$$\langle\alpha', j', m'|[J_\pm, T_q^{(k)}]|\alpha, j, m\rangle = \langle\alpha' j' m'|\hbar\sqrt{(k\mp q)(k\pm q+1)}\, T_{q\pm1}^{(k)}|\alpha j m\rangle$$

$$\Downarrow$$

$$\sqrt{(j'\pm m')(j'\mp m'+1)}\, \langle\alpha' j' m'\pm1|T_{q\pm1}^{(k)}|\alpha, j, m\rangle$$

$$= \sqrt{(j\mp m)(j\pm m+1)}\, \langle\alpha', j', m'|T_q^{(k)}|\alpha, j, m\pm1\rangle$$

$$+\sqrt{(k\mp q)(k\pm q+1)}\, \langle\alpha' j' m'|T_{q\pm1}^{(k)}|\alpha, j, m\rangle$$

Compare with celebsch – Gordan coefficient relation.

$$\sqrt{(j\mp m)(j\pm m+1)}\, \langle j_1 j_2; m_1 m_2|j_1 j_2; j\, m\pm1\rangle$$

$$= \sqrt{(j_1\mp m_1+1)(j_1\pm m_1)}\, \langle j_1 j_2; m_1\mp1\, m_2|j_1 j_2; j\, m\rangle$$

$$+\sqrt{(j_2\mp m_2+1)(j_2\pm m_2)}\, \langle j_1 j_2; m_1\, m_2\mp1|j_1 j_2; j\, m\rangle$$

If making substitution to tensor operator matrix recursion relation

$$j'\to j \quad m'\to m \quad j\to j_1 \quad m\to m_1 \quad k\to j_2 \quad q\to m_2$$

The recursion relation is the same!

The element $\langle j_1 j_2; m_1\, m_2\pm1|j_1 j_2; j\, m\rangle$ in clebsch – Gordan Coefficient correspond to

$$\langle\alpha' j' m'|T_{q\pm1}^{(k)}|\alpha, j, m\rangle$$

$$\langle\alpha\, j'\, m'|T_{q\pm1}^{(k)}|\alpha\, j\, m\rangle = (\text{universal proportionality constant independent of } m, q, m')\, \langle j k; m\, q\pm1|j k; j m'\rangle$$

▽ **Example of wigner – Eckart theorem!**

Example 1: Tensor of rank 0 : $T_0^{(0)} = S$. The matrix element of a scalar operator satisfies

$$\langle\alpha' j' m'|S|\alpha j m\rangle = \delta_{jj'}\delta_{mm'}\frac{\langle\alpha' j'||S||\alpha j\rangle}{\sqrt{2j'+1}}$$

Example 2 : The Projection theorem

this theorem states that (spherical components of vector operator V can be written as $V_{q=\pm1,0}$)

$$\langle \alpha', j\, m' | V_q | \alpha, j\, m\rangle = \frac{\langle \alpha'\, j\, m | J\cdot V | \alpha, j\, m\rangle}{\hbar^2\, j(j+1)} \langle j\, m' | J_q | j\, m\rangle$$

In which, we choose

$$J_{\pm1} = \mp \frac{1}{\sqrt{2}} (J_x \pm i J_y) = \mp \frac{1}{\sqrt{2}} J_\pm \qquad J_0 = J_z.$$

Proof:

$$\langle \alpha', jm | J\cdot V | \alpha, jm\rangle = \langle \alpha'\, jm | J_0 V_0 - J_{+1} V_{-1} - J_{-1} V_{+1} | \alpha, jm\rangle$$

$$= m\hbar \langle \alpha', jm | V_0 | \alpha, jm\rangle + \frac{\hbar}{\sqrt{2}} \sqrt{(j+m)(j-m+1)} \langle \alpha', j, m-1 | V_{-1} | \alpha, j, m\rangle$$
$$- \frac{\hbar}{\sqrt{2}} \sqrt{(j-m)(j+m+1)} \langle \alpha', j, m+1 | V_{+1} | \alpha, j, m\rangle$$

from Wigner - Eckart theorem:

$$\langle \alpha', j' m' | V_q^{(1)} | \alpha, j, m\rangle = \langle j, 1; m, q | j, 1; j' m'\rangle \cdot \frac{\langle \alpha'\, j' || V^{(1)} || \alpha, j\rangle}{\sqrt{2j'+1}}$$

specifically:

$$\begin{cases} \langle \alpha', j, m | V_0^{(1)} | \alpha, j, m\rangle = \langle j, 1; m\, 0 | j, 1; j\, m\rangle \dfrac{1}{\sqrt{2j+1}} \langle \alpha'\, j || V^{(1)} || \alpha, j\rangle \\ \langle \alpha', j, m-1 | V_{-1}^{(0)} | \alpha, j, m\rangle = \langle j, 1; m, -1 | j, 1; j, m-1\rangle \dfrac{1}{\sqrt{2j+1}} \langle \alpha'\, j || V^{(1)} || \alpha, j\rangle \\ \langle \alpha', j, m+1 | V_{+1}^{(0)} | \alpha, j, m\rangle = \langle j, 1; m, 1 | j, 1; j, m+1\rangle \dfrac{1}{\sqrt{2j+1}} \langle \alpha'\, j || V^{(1)} || \alpha, j\rangle \end{cases}$$

$$\to \langle \alpha', jm | J\cdot V | \alpha, jm\rangle = C_{jm} \langle \alpha'\, j || V^{(1)} || \alpha\, j\rangle$$

- Where, C_{jm} is independent of α', α, V !!!
- Furthermore, C_{jm} is independent of m because $J\cdot V$ is a scalar operator! $\longrightarrow$ we can write it as C_j!

A special example for this: $V \to J$, $\alpha' \to \alpha$.

$$\langle \alpha, j\, m | J^2 | \alpha, j\, m\rangle = C_j \langle \alpha\, j || J || \alpha\, j\rangle$$

For Wigner - Eckart theorem applied to V_q and J_q, we have

$$\frac{\langle \alpha'\, j\, m' | V_q | \alpha, j\, m\rangle}{\langle \alpha\, j\, m' | J_q | \alpha\, j\, m\rangle} = \frac{\langle \alpha'\, j || V || \alpha\, j\rangle}{\langle \alpha\, j || J || \alpha\, j\rangle}$$

However:

$$\frac{\langle \alpha'\, j || V || \alpha\, j\rangle}{\langle \alpha\, j || J || \alpha\, j\rangle} = \frac{\langle \alpha', j, m | J\cdot V | \alpha, j, m\rangle}{\langle \alpha, j, m | J^2 | \alpha, j, m\rangle}$$

Then:

$$\langle \alpha' j\, m' | V_q | \alpha\, j\, m\rangle = \langle \alpha\, j\, m' | J_q | \alpha\, j\, m\rangle \cdot \frac{\langle \alpha', j, m | J\cdot V | \alpha, j, m\rangle}{\langle \alpha, j, m | J^2 | \alpha, j, m\rangle}$$

$$= \frac{\langle \alpha', j, m | J\cdot V | \alpha, j, m\rangle}{\hbar^2\, j(j+1)} \cdot \langle j\, m' | J_q | j\, m\rangle$$

Example 3 : For vector, which is the rank 1 spherical tensor, the spherical components of V can be written as $V_{q=\pm1,0}$. we have the selection rule $\Delta m \equiv m' - m = \pm1, 0$ $\quad \Delta j \equiv j' - j = \begin{cases} \pm1 \\ 0 \end{cases}$

Density operator and Pure versus mixed ensembles.

—— Mixed ensemble: a mixed ensemble contains member with relative population w_1 is characterized by $|a^{(1)}\rangle$, some other fraction with relative population w_2 characterized by $|a^{(2)}\rangle \ldots$,

Normalise:

$$\sum_i w_i = 1$$

Ensemble average of operator: (average per constituent)

$$[A] = \sum_i w_i \langle \alpha^{(i)} | A | \alpha^{(i)} \rangle$$

$$= \sum_i \sum_{a'} w_i |\langle a' | \alpha^{(i)} \rangle|^2 a'$$

—— Define: Density operator:

$$\rho = \sum_i w_i |\alpha^{(i)}\rangle\langle\alpha^{(i)}| \quad \Rightarrow \quad \langle b'' | \rho | b' \rangle = \sum_i w_i \langle b'' | \alpha^{(i)} \rangle \langle \alpha^{(i)} | b' \rangle$$

- 1st property:

$$[A] = \sum_{b'} \sum_{b''} \langle b'' | \rho | b' \rangle \langle b' | A | b'' \rangle$$

$$= tr(\rho A).$$ ⇐ the trace is independent with representation!

- 2st: Hermitian property:

$$\rho^{\dagger} = \sum_i w_i^* |\alpha^{(i)}\rangle\langle\alpha^{(i)}| = \sum_i w_i |\alpha^{(i)}\rangle\langle\alpha^{(i)}|$$

- 3st: normalisation:

$$tr(\rho) = \sum_i \sum_{b'} w_i \langle b' | \alpha^{(i)} \rangle \langle \alpha^{(i)} | b' \rangle$$

$$= \sum_i w_i \langle \alpha^{(i)} | \alpha^{(i)} \rangle = 1$$

—— free variable in density operator:

For example: For $\frac{1}{2} \times \frac{1}{2}$ system, and ρ is 2×2 matrix. By using condition $tr(\rho)=1$ and $\rho^{\dagger}=\rho$.

$\rho = \begin{bmatrix} a & c \\ c^* & b \end{bmatrix}$; a, b are real numbers. / $a+b=1$; ⇒ There are only 3 independent real parameter.

We can show that ρ can be determined by: $[S_x]$ $[S_y]$ $[S_z]$.

A mixed ensemble can be decomposed to pure ensembles in many different ways.

—— Pure state:

$$\rho = |\alpha^{(n)}\rangle\langle\alpha^{(n)}| \quad \Rightarrow \text{idempotent } \rho^2 = \rho.$$

$$\rho(\rho - 1) = 0.$$

$$tr(\rho^2) = tr(\rho) = 1.$$

- $tr(\rho^2)$ is maximal when ensemble is pure. for mixed ensemble: $tr(\rho^2) < 1$.
- The eigen values of the density operator for a pure ensemble are zero or one.

—— Evolution of Ensemble:

Suppose: $\rho(t_0) = \sum_i w_i |\alpha^{(i)}\rangle\langle\alpha^{(i)}|$

Evolution: $|\alpha^{(i)}\rangle \longrightarrow |\alpha^{(i)}, t_0; t\rangle$

$$i\hbar\frac{\partial\rho}{\partial t} = \sum_i w_i\left(H|\alpha^{(i)},t_0;t\rangle\langle\alpha^{(i)},t_0;t| - |\alpha^{(i)},t_0;t\rangle\langle\alpha^{(i)},t_0;t|H\right)$$
$$= -[H,\rho]$$

—— Continum Generation:

$$[A] = \int d^3x' \int d^3x'' \langle x''|\rho|x'\rangle\langle x'|A|x''\rangle$$

$$\langle x''|\rho|x'\rangle = \langle x''| \sum_i w_i |\alpha^{(i)}\rangle\langle\alpha^{(i)}| \, |x'\rangle$$
$$= \sum_i w_i \;\psi_i(x'')\;\psi_i^*(x')$$

—— Density matrix for completely random ensemble:

$$\rho = \frac{1}{N}\begin{pmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{pmatrix} \qquad \rho = \sum_k \frac{1}{N}|k\rangle\langle k|$$

define:

$$\sigma = -\operatorname{tr}(\rho\ln\rho)$$

$\Downarrow$ If we use basis that ρ is diagonal.

$$\sigma = -\sum_k \rho_{kk}^{(diag)}\ln\left(\rho_{kk}^{(diag)}\right)$$

Becaus $\rho_{kk}^{(diag)}$ is a real number between $0-1$; σ is positive.

$$\begin{cases} \sigma = -\sum_{k=1}^{N}\frac{1}{N}\ln\left(\frac{1}{N}\right) = \ln N & \Leftarrow \text{completely random} \\ \sigma = 0 & \Leftarrow \text{Pure state.} \end{cases}$$

—— Entropy in quantum Mechanics:

$$S = k\sigma$$

Nature tends to maximize σ subject to constraint average of hamiltonian has certain value.

$$\rho = \sum_k \rho_{kk}\,|k\rangle\langle k|$$
$$\sigma = -\sum_k \rho_{kk}^{(diag)}\ln\left(\rho_{kk}^{(diag)}\right)$$

stable condition:

$$\frac{\partial\rho}{\partial t} = 0 = -[\rho,H] \Leftarrow \rho \text{ and } H \text{ can be simultaneously diagonalized.}$$

$$\delta\sigma = 0$$
$$[H] = \operatorname{tr}(\rho H) = U$$
$$W_k = \rho_{kk}$$

$$\begin{cases} \delta H = \delta\left(\sum_k \rho_{kk}E_k\right) = 0 \\ \delta(\operatorname{tr}\rho) = \sum_k \delta\rho_{kk} = 0 \\ \delta\sigma = \delta\left(\sum_k \rho_{kk}\ln(\rho_{kk})\right) = 0 \end{cases}$$

(Find max σ under constrain)

$$\Downarrow$$
$$\sum_k \delta\rho_{kk}\left[(1+\ln\rho_{kk}) + \beta E_k + \alpha\right] = 0$$

(Lagrange 乘子法)

$$\rho_{kk} = \exp(-\beta E_k - \alpha)$$

normalise: $\Downarrow$

$$\rho_{kk} = \frac{\exp(-\beta E_k)}{\sum_{l=1}^{N}\exp(-\beta E_l)}$$

—— Partition Function:

$$Z = \sum_{k=1}^{N}\exp(-\beta E_k) \qquad Z = \operatorname{tr}(e^{-\beta H}) \qquad \rho = \frac{e^{-\beta H}}{Z}$$

$$[A] = \frac{tr(e^{-\beta H} A)}{Z} = \frac{[\sum_{k=1}^{N} \langle A \rangle_k \exp(-\beta E_k)]}{\sum_k \exp(-\beta E_k)}$$

$$[H] = \frac{(\sum_{k=1}^{N} E_k \exp(-\beta E_k))}{\sum_{k=1}^{N} \exp(-\beta E_k)} = -\frac{\partial}{\partial \beta}(\ln Z)$$

— β related to temperature: $\beta = \frac{1}{kT}$

— Spin-$\frac{1}{2}$ System:

$$H = -\frac{e}{m_e c} S \cdot B = \omega S_z \qquad \omega = \frac{|e| B}{m_e c}$$

$$\begin{cases} E_+ = \frac{\hbar}{2}\omega \\ E_- = -\frac{\hbar}{2}\omega \end{cases}$$

$$H = \begin{pmatrix} \frac{\hbar}{2}\omega & \\ & -\frac{\hbar}{2}\omega \end{pmatrix} \Rightarrow \rho = \frac{\begin{pmatrix} e^{-\beta\frac{\hbar\omega}{2}} & 0 \\ 0 & e^{\beta\frac{\hbar\omega}{2}} \end{pmatrix}}{Z} \qquad Z = e^{-\beta\hbar\omega/2} + e^{\beta\hbar\omega/2}$$

$$[S_x] = [S_y] = 0 \qquad [S_z] = -\frac{\hbar}{2} \cdot \tanh\left(\frac{\beta\hbar\omega}{2}\right).$$

paramagnetic susceptibility χ: (顺磁化率)

$$\frac{e}{m_e c} \cdot [S_z] = \chi B$$

Brillioun's Formula:

$$\chi = \frac{|e|\hbar}{2 m_e c B} \tan\left(\frac{\beta\hbar\omega}{2}\right)$$

Chapter 4 Symmetry in Quantum Mechanics.

4.1 Symmetry, Conservation Laws and Degeneracies

4.1.1 Symmetries in Classical Physics.

If L is unchanged under displacement $q_i \to q_i + \delta q_i$

$$\frac{\partial L}{\partial q_i} = 0 \Rightarrow \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0 \Rightarrow \frac{dP_i}{dt} = 0$$

Likewise. $\frac{dP_i}{dt} = 0$ whenever $\frac{\partial H}{\partial q_i} = 0$

4.1.2 symmetry in quantum mechanics.

Definition of Symmetry operator.

In Quantum Mechanics, we associate a Unitary operator, say $\mathscr{S}$ with an operator Like translation or rotation, It has become customary to call $\mathscr{S}$ a Symmetry operator!

$$\mathscr{S} = 1 - \frac{i\epsilon}{\hbar} G$$

where G is the Hermitian generator of the symmetry operator!

suppose H is invariant under $\mathscr{S}$, we have:

$$\mathscr{S}^{\dagger} H \mathscr{S} = H$$

equivalent to:

$$[H, G] = 0 \qquad [H, \mathscr{S}] = 0$$

By virtue of Heisenberg equation of motion.

$$\frac{dG}{dt} = 0$$

Hence G is a constant of the motion!

For instant: If H is invariant under translation, the momentum is a constant of the motion.
If H is invariant under rotation, the angular momentum is a constant of motion.

If G commutes with H, then G commutes with U. (time evolution operator!) suppose at t_0 the system is in an eigenket of G, Then the ket at Later time is also an eigenket of G with same eigen value g'!

$$G\, U(t,t_0)\,|g'\rangle = U(t,t_0)\, G\,|g'\rangle = g'\, U(t,t_0)\,|g'\rangle$$

4.1.3. Degeneracies

Reason of degenercy.

suppose

$$[H, \mathscr{S}] = 0$$

for some symmetric operator, and $|n\rangle$ is an eigenket with Eigenvalue E_n. Then $\mathscr{S}|n\rangle$ is also an energy eigenket with same energy, because

$$H(\mathscr{S}|n\rangle) = \mathscr{S} H |n\rangle = E_n(\mathscr{S}|n\rangle)$$

$\mathscr{S}|n\rangle$ and $|n\rangle$ are two states with same energy (they are degenerate)

Specific example of degenercy leads by rotation.

suppose Hamiltonian is rotationally invariant, so

$$[\mathscr{D}(R), H] = 0 \quad \xrightarrow{\text{which necessarily implies that}} \quad [J, H] = 0, \quad [J^2, H] = 0$$

We can then form simultaneous eigenkets of H, J^2 and J_z. denoted by $|n, j, m\rangle$

$$\mathcal{D}(R)\,|n; j, m\rangle = \sum_{m'} |n; j\, m'\rangle\, \mathcal{D}^{(j)}_{m'm}(R)$$

The degenercy here is $2j+1$ – fold!

As an example, consider an atomic electron whose potential is written as $V(r) + V_{LS}(r) L\cdot S$

Because r and $L\cdot S$ are both rotationally invariant, we expect an $(2j+1)$ – fold degeneracy for each atomic level! (在章节 "addition of angular momentum" 中有讨论!)

4.1.4 SO(4) Symmetry in the Coulomb Potential!

Runge – Lenz vector. for $\frac{1}{r}$ potential, define Runge– Lenz vector

$$M = \frac{p\times L}{m} - \frac{Ze^2}{r}x$$

Firstly, we want to construct a Hermitian operator. Noticed. for Hermitian vector operators A and B.

$$(A\times B)^{\dagger} = -B\times A$$

Therefore, the Hermitian version of Lenz vector

$$M = \frac{1}{2m}(p\times L - L\times p) - \frac{Ze^2}{r}x$$

It can be shown that M commutes with the Hamiltonian

$$H = \frac{p^2}{2m} - \frac{Ze^2}{r}$$

$$[M, H] = 0$$

Q: How to determin the commutation relation of $\frac{1}{r}$ with others.

Other useful relations can be proven!

$$L\cdot M = 0 = M\cdot L$$

$$M^2 = \frac{2}{m}H(L^2+\hbar^2) + Z^2e^4$$

One can show that

$$[M_i, L_j] = i\hbar\, \varepsilon_{ijk} M_k$$

$$[M_i, M_j] = -i\hbar\, \varepsilon_{ijk} \frac{2}{m} H L_k$$

$$[L_i, L_j] = i\hbar\, \varepsilon_{ijk} L_k$$

The algebra is not closed due to the exist of H, In this case, we consider the eigenstates of H. Then we can replace H with E ($E<0$)

Replace M with the scaled vector operator

$$N = \left(-\frac{m}{2E}\right)^{1/2} M.$$

Closed algebra

$$[L_i, L_j] = i\hbar\, \varepsilon_{ijk} L_k$$

$$[N_i, L_j] = i\hbar\, \varepsilon_{ijk} N_k$$

$$[N_i, N_j] = i\hbar\, \varepsilon_{ijk} L_k$$

▽ What is rotation: think rotation as an operation which mixes two orthogonal axes. the number of generators for rotations in n spatial dimensions should be $C_n^2 = \frac{n!}{2!(n-2)!} = \frac{n(n-1)}{2}$ four-dimensional rotations require six generators.

- See that this algebra is the appropriate algebra for 4-dimensional rotation denote (x_1, x_2, x_3) and (P_1, P_2, P_3). generators $L_3 = \tilde{L}_{12} = x_1 P_2 - x_2 P_1$ $L_1 = \tilde{L}_{23}$ $L_2 = \tilde{L}_{31}$. If we invent a new spatial dimension x_4 and its conjugate momentum P_4, define

with usual commutation Relation.

$$\tilde{L}_{14} = x_1 P_4 - x_4 P_1 \equiv N_1$$
$$\tilde{L}_{24} = x_2 P_4 - x_4 P_2 \equiv N_2$$
$$\tilde{L}_{34} = x_3 P_4 - x_4 P_3 \equiv N_3$$

These operators obey the algebra! for example.

$$[N_1, L_2] = [x_1 P_4 - x_4 P_1, x_3 P_1 - x_1 P_3]$$
$$= P_4 [x_1, P_1] x_3 + x_4 [P_1, x_1] P_3$$
$$= i\hbar (x_3 P_4 - x_4 P_3) = i\hbar N_3$$

Define operator

$$I \equiv (L + N)/2$$
$$K \equiv (L - N)/2$$

these operators satisfies algebra

$$[I_i, I_j] = i\hbar \varepsilon_{ijk} I_k$$
$$[K_i, K_j] = i\hbar \varepsilon_{ijk} K_k$$
$$[I_i, K_j] = 0$$

It is evident that $[I, H] = 0$ $[K, H] = 0$. These operators satisfies angular momentum Algebras! we denote the eigenvalues of I^2 and K^2 by $i(i+1)\hbar^2$ and $k(k+1)\hbar^2$. with $i, k = 0, \frac{1}{2}, \frac{3}{2}, \cdots$.

Noticed $L \cdot M = M \cdot L = 0$

$$I^2 - K^2 = L \cdot N = 0$$

we must have $i = k$. on the other hand.

$$I^2 + K^2 = \frac{1}{2}(L^2 + N^2) = \frac{1}{2}\left(L^2 - \frac{m}{2E} M^2\right)$$

with (4.24) $\Leftarrow$ $M^2 = \frac{2}{m} H (L^2 + \hbar^2) + Z^2 e^4$

to the numerical relation

$$2k(k+1)\hbar^2 = \frac{1}{2}\left(-\hbar^2 - \frac{m}{2E} Z^2 e^4\right)$$

solving E. we find

$$E = -\frac{m Z^2 e^4}{2\hbar^2} \frac{1}{(2k+1)^2}$$

The degree of degenercy, in fact, is $(2i+1)(2k+1) = (2k+1)^2 = n^2$!

Carry a little further to show how one formally carries out rotations in n sphatial dimensions. $SO(n)$

Also, we have seen that the algebra for $SO(4)$ can be also thought of as two independent groups $SU(2)$, that is $SU(2) \times SU(2)$

For group of $n \times n$ orthogonal matrix R. Parameterize as

$$R = \exp(i \sum_{q=1}^{n(n-1)/2} \phi^q \tau^q)$$

where τ^q are purely imaginary, anti-symmetric matrices. $(\tau^q)^T = -\tau^q$

This anti-symmetric relation ensures R is orthogonal!

The over-all factor of i implies that the imaginary matrices τ^q are also Hermitian.

τ^q are obviously related to the generators of rotation operator!

compare the action q and action P with the rotation carried out in reverse order, then

$$(1 + i\phi^p \tau^q)(1 + i\phi^q \tau^p) - (1 + i\phi^q \tau^q)(1 + i\phi^p \tau^p)$$
$$= -\phi^p \phi^q [\tau^p, \tau^q]$$
$$= 1 - (1 + i\phi^p \phi^q \sum_r f_r^{pq} \tau^r)$$

similar with

$R_x(\varepsilon) R_y(\varepsilon) - R_y(\varepsilon) R_x(\varepsilon)$
$= R_z(\varepsilon^2) - 1$

The last line recognize the result must be a second-order rotation about two axes with some linear combinition of generators! f_r^{pq} are called structure constant for group rotations.

$$[\tau^p, \tau^q] = i \sum_r f_r^{pq} \tau^r$$

4.2 Discrete Symmetries. Parity. Space Inversion.

Parity.

Given a state $|\alpha\rangle$, we consider a space-inverted state. obtained by applying unitary operator π know as parity operator.

$$|\alpha\rangle \longrightarrow \pi|\alpha\rangle$$

Require the expectation value of x with respect to space-inverted state to be opposite sign. (A very good requirement!)

$$\langle\alpha|\pi^{\dagger}x\pi|\alpha\rangle = -\langle\alpha|x|\alpha\rangle$$

accomplished if

$$\pi^{\dagger}x\pi = -x$$

$$x\pi = -\pi x \qquad \text{(Have used the fact that } \pi \text{ is unitary)}$$

which means π and x are anti-commute!

▽ For eigen-ket of position operator, it transforms as

$$\pi|x'\rangle = e^{i\delta}|-x'\rangle$$

proof: $\quad x\pi|x'\rangle = -\pi x|x'\rangle = -\pi x'|x'\rangle = (-x')\pi|x'\rangle$

$$\pi|x'\rangle = e^{i\delta}|-x'\rangle$$

It is customary to take $e^{i\delta}=1$. $\Longrightarrow \pi^2|x'\rangle = |x'\rangle$

▽ π is not only unitary, but also Hermitian!

$$\pi^2 = 1 \;;\; \pi^{\dagger}\pi = 1$$

$\pi^{-1} = \pi^{\dagger} = \pi \longrightarrow$ eigenvalue can only be 1 or -1. $\quad \pi|\alpha\rangle = \lambda|\alpha\rangle$, $\pi^2|\alpha\rangle = \lambda^2|\alpha\rangle = |\alpha\rangle \Rightarrow \lambda = \pm 1$!

▽ For momentum,

Translation followed by parity is equivalent to parity followed by translation in the opposite direction!

$$\pi\,\mathcal{T}(dx') = \mathcal{T}(-dx')\,\pi.$$

$$\pi\left(1 - i\frac{p}{\hbar}\cdot dx'\right) = \left(1 + i\frac{p}{\hbar}\cdot dx'\right)\pi$$

$$\{\pi, p\} = 0 \quad \text{or} \quad \pi^{\dagger}p\pi = -p$$

▽ For angular momentum J.

- Orbital angular momentum.

$$[\pi, L] = 0$$

because $L = x \times p$, and both x and p are odd under Parity.

- For angular momentum J:

reconsider the orthogonal, Suppose: $R^{(parity)} = \begin{pmatrix} -1 & & \\ & -1 & \\ & & -1 \end{pmatrix}$ $\quad$ $SO(3)$, $R^{(P)}SO(3)$

we have the property:

$$R^{(parity)}R^{(rotation)} = R^{(rotation)}R^{(parity)}$$

Quantum mechanically, it is natural to postulate this relation for unitary operators.

$$\pi\,\mathcal{D}(R) = \mathcal{D}(R)\,\pi.$$

where $\mathcal{D}(R) = 1 - iJ\cdot\hat{n}\frac{\varepsilon}{\hbar}$ $\Downarrow$

$$[\pi, J] = 0 \qquad \pi^{\dagger}J\pi = J \qquad \text{together with } [\pi, L] = 0 \Rightarrow [\pi, S] = 0.$$

Under rotations, x and J transform in the same way, they are both vectors/spherical tensors.
Under parity, x is odd, J is even,
$\Downarrow$ called polar vectors; $\Downarrow$ called axial vectors/ pseudovectors

4.2.1

Wave function under Parity.

consider ψ to be wave function of spinless particle whose state ket is $|\alpha\rangle$.

$$\psi(x') = \langle x'|\alpha\rangle$$

Wave function for space-inverted state

$$\langle x'|\pi|\alpha\rangle = \langle -x'|\alpha\rangle = \psi(-x')$$

- Eigen ket of parity.

Having seen that the eigenvalue of parity must be ± 1.

$$\begin{cases} \pi|\alpha\rangle = \pm|\alpha\rangle \\ \langle x'|\pi|\alpha\rangle = \langle -x'|\alpha\rangle = \pm\langle x'|\alpha\rangle \end{cases}$$

$\Downarrow$

$$\psi(-x') = \pm\psi(x') \begin{cases} \text{even parity} \\ \text{odd parity.} \end{cases}$$

- Example — Eigenket of orbital angular momentum. Because L and π commute. (it is expected to be parity eigenket)

$$\langle x'|\alpha l m\rangle = R_\alpha(r) Y_l^m(\theta,\phi)$$

$x' \to -x'$ by

$$\begin{cases} r \to r \\ \theta \to \pi-\theta & (\cos\theta \to -\cos\theta) \\ \phi \to \phi+\pi & (e^{im\phi} \to (-1)^m e^{im\phi}) \end{cases}$$

$$Y_l^m(\theta,\phi) = (-1)^m \sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}\, P_l^m(\cos\theta)\cdot e^{im\phi}$$

For positive m:

$$P_l^{|m|}(\cos\theta) = \frac{(-1)^{m+l}}{2^l\cdot l!}\frac{(l+|m|)!}{(l-|m|)!}\sin^{-|m|}\theta\left(\frac{d}{d(\cos\theta)}\right)^{l-|m|}\sin^{2l}\theta$$

$$Y_l^m(\pi-\theta,\phi+\pi) = (-1)^l\, Y_l^m(\theta,\phi)$$

conclude that

$$\pi|\alpha l m\rangle = (-1)^l|\alpha l m\rangle$$

Easier way: work with $m=0$, note that $L_\pm^r|l, m=0\rangle$ $(r=0\ldots l)$ have the same parity because π and $(L_\pm)^r$ commute!

Theorem — Eigenket of non-degenerate Hamiltonian H. which commutes with Hamiltonian $[H,\pi]=0$.

then $|n\rangle$ is also parity eigenkets!

consider state $|\alpha\rangle$,

$$|\alpha\rangle \equiv \frac{1}{2}(1\pm\pi)|n\rangle$$

$$\pi|\alpha\rangle = \frac{1}{2}\pi(1\pm\pi)|n\rangle = \frac{1}{2}(\pi\pm1)|n\rangle = \pm\frac{1}{2}(1\pm\pi)|n\rangle = \pm|\alpha\rangle$$

$|\alpha\rangle$ is an eigenstate of π

$$H|\alpha\rangle = \frac{1}{2}(1\pm\pi)H|n\rangle = E_n\frac{1}{2}(1\pm\pi)|n\rangle$$

Because H is non-degenerate $\Rightarrow$ $|n\rangle$ and $|\alpha\rangle$ must be the same to within a multiplicative constant. $\Longrightarrow$ $|n\rangle$ must be parity eigenket! $\pi|n\rangle = \pm|n\rangle$.

$|\alpha\rangle = 0$ if we choose the "wrong" sign!

For Simple Harmonic oscillator! $|0\rangle$ is even parity because its wave function being Gaussian!

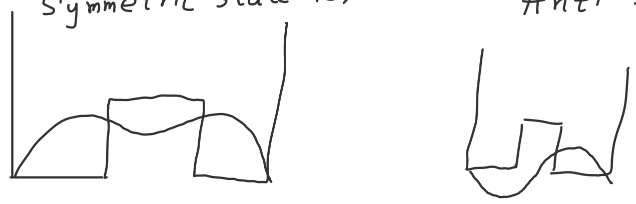
$$|1\rangle = a^\dagger|0\rangle$$

is odd parity, because $\{\pi, x\} = \{\pi, p\} = 0$; $a^\dagger$ is linear in x, p.

for n th excited state, parity is given by $(-1)^n$.

4.2.2. Symmetrical Double-Well potential ; (the exact solution need to be discussed ...)

Symmetric state $|S\rangle$ Anti-symmetric state $|A\rangle$



⇈ These are the two lowest lying states! Calculation shows $E_A > E_S$

We can form

$$|R\rangle = \frac{1}{\sqrt{2}}(|S\rangle + |A\rangle) \quad a \quad \text{concentrate in the Left}$$

$$|L\rangle = \frac{1}{\sqrt{2}}(|S\rangle - |A\rangle) \quad b \quad \text{concentrate in the Right}$$

They satisfy (they are not parity eigenstates)

$$\pi|R\rangle = |L\rangle$$

$$\pi|L\rangle = |R\rangle$$

The evolution of $|R\rangle$ state

$$|R, t_0=0; t\rangle = \frac{1}{\sqrt{2}}\left(e^{-iE_S t/\hbar}|S\rangle + e^{-iE_A t/\hbar}|A\rangle\right)$$

$$= \frac{1}{\sqrt{2}} e^{-iE_S t/\hbar}\left(|S\rangle + e^{i(E_S - E_A)t/\hbar}|A\rangle\right)$$

The system has oscillation with angular momentum

$$\omega = \frac{(E_A - E_S)}{\hbar}$$

4.2.3 Parity - Selection Rule.

Suppose $|\alpha\rangle$ and $|\beta\rangle$ are parity eigenstates

$$\pi|\alpha\rangle = \varepsilon_\alpha|\alpha\rangle$$

$$\pi|\beta\rangle = \varepsilon_\beta|\beta\rangle \qquad \text{where } \varepsilon_\alpha, \varepsilon_\beta \text{ are parity eigenvalues} (\pm 1)$$

we can show that (parity-odd operator x connects states of opposite parity)

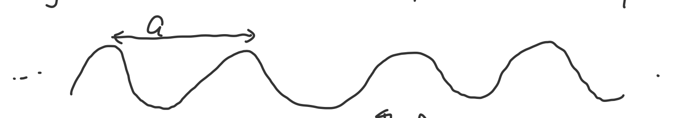
$$\langle\beta|x|\alpha\rangle = 0 \qquad \text{unless } \varepsilon_\alpha = -\varepsilon_\beta.$$

proof $\langle\beta|x|\alpha\rangle = \langle\beta|\pi^{-1}\pi\, x\, \pi^{-1}\pi|\alpha\rangle = \varepsilon_\alpha\varepsilon_\beta\langle\beta|\pi x \pi^{-1}|\alpha\rangle = -\varepsilon_\alpha\varepsilon_\beta\langle\beta|x|\alpha\rangle$

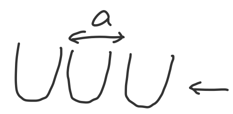
$$\int \psi_\beta^* x \psi_\alpha \, d\tau = 0 \quad \text{if } \psi_\beta \text{ and } \psi_\alpha \text{ have the same parity!}$$

4.3. Lattice Translation as a Discrete Symmetry

This part is mainly focus on the periodic potential Well!



↑ finite potential well



← Infinite potential well!

For translation operator $\tau(l)$.

$$\tau^{\dagger}(l)\, x\, \tau(l) = x + l \qquad \tau(l)\,|x'\rangle = |x'+l\rangle$$

$$\Downarrow$$

$$\tau^{\dagger}(a)\, V(x)\, \tau(a) = V(x+a) = V(x)$$

Thus, the Intire Hamiltonian satisfies

$$[H, \tau(a)] = 0.$$

1° For infinite potential well:

Consider solution $|n\rangle$ means single partical solution!

$$H\,|n\rangle = E_0\,|n\rangle \quad \longleftarrow \text{These are degenerate states.}$$

$$\tau(a)|n\rangle = |n+1\rangle$$

We want to find eigenstate of H and $\tau(a)$ simultaneously!

$$|\theta\rangle = \sum_{n=-\infty}^{+\infty} e^{in\theta}|n\rangle$$

$$\tau(a)\,|\theta\rangle = \sum_{n=-}^{\pm} e^{in\theta}\,\tau(a)|n\rangle = \sum_n e^{i(n+1)\theta} \cdot e^{-i\theta}\,|n+1\rangle$$

$$= e^{-i\theta}\,|\theta\rangle$$

$|\theta\rangle$ is a simultaneous eigenstate of H & $\tau(a)$

2° For finite barrier

$|n\rangle$ has some leakage possible into neighboring Lattice! $\langle n'|n\rangle = \delta_{nn'}$

$$\langle n|H|n\rangle = E_0$$

Tight-Binding approximation

$$\langle n\pm1|H|n\rangle = -\Delta \quad ; \quad \langle n'|H|n\rangle \neq 0 \text{ only if } n'=n \text{ or } n'=n\pm1$$

To the extend that $|n\rangle$ and $|n'\rangle$ are orthogonal when $n \neq n'$, we obtain

$$H\,|n\rangle = E_0|n\rangle - \Delta|n+1\rangle - \Delta|n-1\rangle$$

Want to use symmetry of H under $\tau(a)$ to find Energ eigen function!

$$|\theta\rangle = \sum_{n=-\infty}^{+\infty} e^{in\theta}|n\rangle$$

$$H|\theta\rangle = H\sum e^{in\theta}|n\rangle = E_0\sum e^{in\theta}|n\rangle - \Delta\sum e^{in\theta}|n+1\rangle - \Delta\sum e^{in\theta}|n-1\rangle$$

$$= E_0\sum e^{in\theta}|n\rangle - \Delta\sum\left(e^{in\theta-i\theta} + e^{in\theta+i\theta}\right)|n\rangle$$

$$= (E_0 - 2\Delta\cos\theta)\sum e^{in\theta}|n\rangle$$

$$= (E_0 - 2\Delta\cos\theta)\,|\theta\rangle$$

Bloch's theorem

Noticing that

Bloch's Theorem states, we assume.

$$\langle x'|\tau(a)|\theta\rangle = \langle x'-a|\theta\rangle \quad \Longrightarrow \quad \langle x'|\theta\rangle = e^{ikx'} u_k(x')$$

$$\langle x'|\tau(a)|\theta\rangle = e^{-i\theta}\langle x'|\theta\rangle \qquad k = \frac{\theta}{a}$$

where $u_k(x')$ is a periodic function with period a!

$$e^{ik(x'-a)} u_k(x'-a) = e^{-i\theta} \cdot e^{ikx'} u_k(x')$$

4.4. The Time-Reversal Discrete Symmetry.

—— Inspiration from Schrödinger Equation

$$i\hbar \frac{\partial \psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi$$

$$-i\hbar \frac{\partial \psi^*}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi^*$$

means $\psi^*(x,-t)$ satisfies relation: $i\hbar \frac{\partial}{\partial t}\psi^*(x,-t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi^*(x,-t)$. $\psi^*(x,-t)$ is another solution to schrodinger wave function!

—— Anti-unitary operator Θ

For states $|\alpha\rangle$; $|\beta\rangle$. after transformation $|\tilde{\alpha}\rangle = \Theta|\alpha\rangle$ $|\tilde{\beta}\rangle = \Theta|\beta\rangle$

This transformation is called anti-unitary if

$$\langle\tilde{\alpha}|\tilde{\beta}\rangle = \langle\beta|\alpha\rangle^*$$

$$\Theta(c_1|\alpha\rangle + c_2|\beta\rangle) = c_1^*\Theta|\alpha\rangle + c_2^*\Theta|\beta\rangle \longrightarrow \text{This relation alone defines antilinear operator!}$$

Anti Linear operator can be written as $\Theta = UK$. U is unitary, K is complex conjugate

K operator property

$$K c|\alpha\rangle = c^* K|\alpha\rangle$$

$$K|\alpha\rangle = K\sum_{a'}|a'\rangle\langle a'|\alpha\rangle = \sum_{a'}\langle a'|\alpha\rangle^*|a'\rangle = \sum_{a'}\langle\alpha|a'\rangle|a'\rangle.$$

The effect of K changes with basis! As a result, the form of U also depends on particular representation.

Then we check if $\Theta = UK$ satisfies requirement for Θ:

$$\Theta(c_1|\alpha\rangle + c_2|\beta\rangle) = UK(c_1|\alpha\rangle + c_2|\beta\rangle) = c_1^*UK|\alpha\rangle + c_2^*UK|\beta\rangle = c_1^*\Theta|\alpha\rangle + c_2^*\Theta|\beta\rangle$$

$$|\alpha\rangle \longrightarrow \Theta|\alpha\rangle = UK|\alpha\rangle = \sum_{a'}\langle a'|\alpha\rangle^*|a'\rangle$$

$$|\beta\rangle \longrightarrow \sum_{a''}\langle a''|\beta\rangle^*|a''\rangle$$

$$\langle\tilde{\beta}|\tilde{\alpha}\rangle = \sum_{a''a'}\langle a''|\beta\rangle\langle a''|a'\rangle\cdot\langle\alpha|a'\rangle$$

$$= \sum_{a'}\langle\alpha|a'\rangle\langle a'|\beta\rangle$$

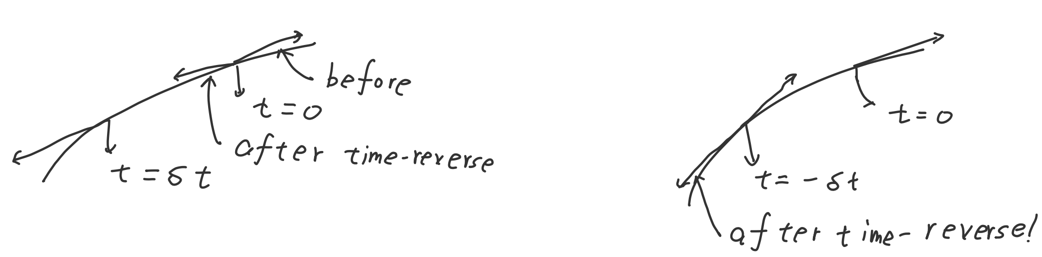
$$= \langle\beta|\alpha\rangle^*$$

—— Define Time-Reversal operator Θ

$$|\alpha\rangle \longrightarrow \Theta|\alpha\rangle$$

Requirement 1:

$$\left(1 - i\frac{H}{\hbar}\delta t\right)\Theta|\alpha\rangle = \Theta\left(1 - i\frac{H}{\hbar}(-\delta t)\right)|\alpha\rangle$$



We have

$$-iH\Theta = \Theta iH \longrightarrow H\Theta = \Theta H$$

—— Fundamental property of Hamiltonian under time-reversal.

An Important identity

$$\langle\beta|X|\alpha\rangle = \langle\tilde{\alpha}|\Theta X^{\dagger}\Theta^{-1}|\tilde{\beta}\rangle$$

where X is a linear operator

proof :

$$|\gamma\rangle \equiv X^{\dagger}|\beta\rangle$$

$$|\gamma\rangle \xleftrightarrow{D.C.} \langle\beta|X = \langle\gamma|$$

$$\langle\beta|X|\alpha\rangle = \langle\gamma|\alpha\rangle = \langle\tilde{\alpha}|\tilde{\gamma}\rangle$$

$$= \langle\tilde{\alpha}|\Theta X^{\dagger}|\beta\rangle = \langle\tilde{\alpha}|\Theta X^{\dagger}\Theta^{-1}\Theta|\beta\rangle$$

$$= \langle\tilde{\alpha}|\Theta X^{\dagger}\Theta^{-1}|\tilde{\beta}\rangle$$

For Hermitian observables A, we get.

$$\langle\beta|A|\alpha\rangle = \langle\tilde{\alpha}|\Theta A\Theta^{-1}|\tilde{\beta}\rangle$$

Define observables are even or odd under Time-reversal according to whether we have upper or Lower sign in

$$\Theta A\Theta^{-1} = \pm A.$$

which leads to

$$\langle\beta|A|\alpha\rangle = \langle\tilde{\alpha}|\pm A|\tilde{\beta}\rangle = \pm\langle\tilde{\alpha}|A|\tilde{\beta}\rangle$$

$$= \pm\langle\tilde{\beta}|A|\tilde{\alpha}\rangle^{*}$$

If $|\beta\rangle = |\alpha\rangle$

$$\langle\alpha|A|\alpha\rangle = \pm\langle\tilde{\alpha}|A|\tilde{\alpha}\rangle$$

Observables under Time-Reversal

Momentum P

we expect expectation of P behave

$$\langle\alpha|P|\alpha\rangle = -\langle\tilde{\alpha}|P|\tilde{\alpha}\rangle$$

so we take

$$\Theta P\Theta^{-1} = -P$$

Implies

$$\Theta P|p'\rangle = -\Theta P|p'\rangle = (-p')\Theta|p'\rangle$$

It is agree with assertion $\Theta|p'\rangle$ is momentum eigenket with eigenvalue $-p'$, usually $\Theta|p'\rangle = |-p'\rangle$

Position

Require

$$\langle\alpha|x|\alpha\rangle = \langle\tilde{\alpha}|x|\tilde{\alpha}\rangle$$

$$\Theta x\Theta^{-1} = x$$

$$\Theta|x'\rangle = |x'\rangle \quad \text{up to a phase} \quad (\text{usually} = 1)$$

Check the commutation relation $[x_i, P_j]|\rangle = i\hbar\delta_{ij}|\rangle$

Apply Θ to both sides

$$\Theta[x_i, P_j]\Theta^{-1}\Theta|\rangle = \Theta i\hbar\delta_{ij}|\rangle$$

$$[x_i, -P_j]\Theta|\rangle = -i\hbar\delta_{ij}\Theta|\rangle \Longrightarrow [x_i, P_j] = i\hbar\delta_{ij}$$ still satisfies the requirement!

▽ Angular momentum

Similarly, to preserve

$$[J_i, J_j] = i\hbar \varepsilon_{ijk} J_k$$

Require

$$\Theta J \Theta^{-1} = -J$$ do not use $\Theta|m\rangle = |-m\rangle$!!!

Check:

$$\Theta [J_i, J_j] \Theta^{-1} \Theta |\rangle = \Theta \, i\hbar \varepsilon_{ijk} J_k |\rangle$$

$$[J_i, J_j] \Theta |\rangle = -i\hbar \varepsilon_{ijk} \Theta J_k \Theta^{-1} \Theta |\rangle$$

$$= i\hbar \varepsilon_{ijk} J_k \Theta |\rangle$$

—— Wave function and Time-Reversal

▽ Wave function of spinless particle change to its Complex Conjugate after Time-Reversal.

proof:

$$|\alpha\rangle = \int d^3x' \, |x'\rangle\langle x'|\alpha\rangle$$

$$\Theta|\alpha\rangle = \int d^3x' \, \Theta |x'\rangle \langle x'|\alpha\rangle$$

$$= \int d^3x' \, \langle x'|\alpha\rangle^* \, \Theta|x'\rangle = \int d^3x' |x'\rangle \langle x'|\alpha\rangle^*$$

$$\psi(x') \to \psi^*(x').$$

For instance:

$$Y_l^m \longrightarrow Y_l^{m*} = (-1)^m Y_l^{-m} (\theta, \phi).$$

$$\Theta|l,m\rangle \to (-1)^m |l,-m\rangle$$

▽ Wave function for spinless particle in momentum eigenkets

$$\Theta|\alpha\rangle = \int d^3p' \, \Theta |p'\rangle\langle p'|\alpha\rangle = \int d^3p' \, |-p'\rangle\langle p'|\alpha\rangle^* = \int d^3p' \, |p'\rangle \underset{\sim}{\langle -p'|\alpha\rangle^*}$$

$$\phi(p) \longrightarrow \phi^*(-p)$$

▽ If Hamiltonian is Invariant under Time-Reversal and energy eigenket $|n\rangle$ is non-degenerate. Then the corresponding energy eigenfunction is real

Proof:

$$H\Theta|n\rangle = \Theta H|n\rangle = E_n \Theta|n\rangle$$

So $|n\rangle$ and $\Theta|n\rangle$ have the same energy!

recall wave function for $\Theta|n\rangle$ are $\psi^*(x)$.

then:

$$\psi^*(x) = \psi(x)$$ up to a phase factor independent of x

$$\langle x'|n\rangle = \langle x'|n\rangle^*$$

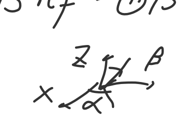
—— Spin and Time-Reversal.

▽ $\Theta^2 = -1$ for $\frac{1}{2}$ system. $|\hat{n};+\rangle = e^{-iS_z\alpha/\hbar} e^{-iS_y\beta/\hbar} |+\rangle$ ↓ because $\Theta(-iS_z)\Theta^{-1} = i\Theta S_z \Theta^{-1} = -iS_z$

$$\Theta|\hat{n};+\rangle = e^{-iS_z\alpha/\hbar} e^{-iS_y\beta/\hbar} \Theta|+\rangle$$ ↓ because $\Theta(S\cdot\hat{n}) \neq -\Theta(S\cdot\hat{n})$

$$= \eta|\hat{n},-\rangle$$

$$|\hat{n};-\rangle = e^{-iS_z\alpha/\hbar} e^{-iS_y(\beta+\pi)/\hbar} |+\rangle$$



Let $\Theta = UK$,

$$e^{-iS_z\alpha/\hbar}\, e^{-iS_y\beta/\hbar}\cdot UK|+\rangle = \eta\cdot e^{-iS_z\alpha/\hbar}\cdot e^{-iS_y(\beta+\pi)/\hbar}\cdot|+\rangle$$

Using the relation $K|+\rangle = |+\rangle$

$$U = e^{-iS_y\pi/\hbar}\cdot\eta$$

$$\Theta = e^{-iS_y\pi/\hbar}\eta\cdot K$$

$$= -i\frac{2S_y}{\hbar}K$$

$(, ') (i^{-i}) ('_{-1})$

6, 2 3

Noticed

$$e^{-i\pi S_y/\hbar}|+\rangle = +|-\rangle$$

$$e^{-i\pi S_y/\hbar}|-\rangle = -|+\rangle$$

$$\Theta(C_+|+\rangle + C_-|-\rangle) = +\eta C_+^*|-\rangle - \eta C_-^*|+\rangle$$

$$\Theta^2(C_+|+\rangle + C_-|-\rangle) = -|\eta|^2 C_+|+\rangle - |\eta|^2 C_-|-\rangle$$

$$= -(C_+|+\rangle + C_-|-\rangle)$$

$$\Theta^2 = -1$$

$\Theta^2|j = \text{half integral}\rangle = -|j = \text{half integral}\rangle$

$\Theta^2|j = \text{integral}\rangle = +|j = \text{integral}\rangle$

Proof:

$$\Theta = \eta\, e^{-i\pi J_y/\hbar}\cdot K \qquad \star$$

$|\alpha\rangle$ expanded in terms of $|j,m\rangle$ base kets.

$$\Theta(\Theta\sum|j,m\rangle\langle j,m|\alpha\rangle) = \Theta(\eta\sum e^{-i\pi J_y/\hbar}\cdot|jm\rangle\langle jm|\alpha\rangle)$$

$$= |\eta|^2\cdot e^{-2i\pi J_y/\hbar}\sum|jm\rangle\langle jm|\alpha\rangle$$

$$e^{-2i\pi J_y/\hbar}|jm\rangle = (-1)^{2j}|j,m\rangle$$

$$\Theta^2 = (-1)^{2j}\ !$$

as is evident from angular momentum eigenstate under rotation by 2π.

Some generalise $\Theta|l,m\rangle = (-1)^m|l,-m\rangle$ to $\Theta|j,m\rangle = (i)^{2m}|j,-m\rangle$.

Expectations under Time-Reverse operation.

$$\Theta T_{q=0}^{(k)}\Theta^{-1} = \pm T_{q=0}^{(k)}$$

$\Uparrow$ $T^{(k)}$ is assumed to be even or odd under Time Reversal.

Because of Wigner-Eckart Theorem. it is sufficient to exam $q=0$ component.

$$\langle\alpha,j,m|T_0^{(k)}|\alpha,j,m\rangle = \pm\langle\alpha,j,-m|T_0^{(k)}|\alpha,j,-m\rangle$$

$$|\alpha,j,-m\rangle = \mathcal{D}(0,\pi,0)\cdot|\alpha,j,m\rangle \longrightarrow$$ proved by noticing

$\langle n'|\alpha,j,-m\rangle$

$= \langle n'|\mathcal{D}(0,\pi,0)|\alpha,j,m\rangle$

(?) (3.255 – 3.258).

For $T_0^{(k)}$ (Because $\mathcal{D}^\dagger(R)T_0^{(k)}\mathcal{D}(R) = \sum_{q'=-k}^{k}\mathcal{D}_{0q'}^{(k)*}(R)T_{q'}^{(k)}$.)

$$\mathcal{D}^\dagger(0,\pi,0)\,T_0^{(k)}\mathcal{D}(0,\pi,0) =$$

$$(-1)^k\cdot T_0^{(k)} + (q\neq 0 \text{ components})$$

$\mathcal{D}_{00}^{(k)*}(0,\pi,0)$

$= P_{(k)}(-1) = (-1)^k \leftarrow$ (3.262).

$q\neq 0$ components give vanishing when standing between $\langle\alpha,j,m|$ and $|\alpha,j,m\rangle$

Result: $\langle \alpha, j, m | T_0^{(k)} | \alpha, j, m \rangle = \pm(-1)^k \cdot \langle \alpha, j, m | T_0^{(k)} | \alpha, j, m \rangle$

非简并微扰论

问题来源：设系统有 Hamiltonian：$\hat{H}=\hat{H}_0+\hat{H}'$　$\hat{H}$ 中不含有时间 t，（ψ 中是否含有 t 不影响结果）。

（其中 $\hat{H}_0$ 的解已知，为 ψ_n^0。且各个解的本征值也已知为 E_n^0
要求 $\hat{H}$ 对应的解

（但在实际计算时，用 ψ 不含 t 会好一些）

- $\hat{H}=\hat{H}_0+\lambda\hat{H}'$

最终的实际问题是 $\lambda=1$

- 假设对应的有级数解

$$\psi_n=\psi_n^0+\lambda\cdot\psi_n^1+\lambda^2\cdot\psi_n^2\cdots$$

$$E_n=E_n^0+\lambda\cdot E_n^1+\lambda^2\cdot E_n^2$$

- 代入 Hamiltonian 方程：

$$(\hat{H}_0+\lambda\hat{H}')(\psi_n^0+\lambda\psi_n^1+\lambda^2\psi_n^2\cdots)=(E_n^0+\lambda E_n^1+\lambda^2E_n^2\cdots)(\psi_n^0+\lambda\psi_n^1+\lambda^2\psi_n^2\cdots)$$

- 将 Schrodinger 方程按照 λ 的幂次展开为 0 次，1 次，2 次方程：

$$\hat{H}_0\psi_n^0=E_n^0\psi_n^0 \quad —(1)$$

$$\hat{H}'\psi_n^0+\hat{H}_0\psi_n^1=E_n^0\psi_n^1+E_n^1\psi_n^0 \quad —(2)$$

$$\hat{H}_0\psi_n^2+\hat{H}'\psi_n^1=E_n^0\psi_n^2+E_n^1\psi_n^1+E_n^2\psi_n^0 \quad —(3)$$

(1)：此方程总是成立的.

(2)：$\hat{H}'\psi_n^0-E_n^1\psi_n^0=(E_n^0-\hat{H}_0)\psi_n^1$ $\Longrightarrow$ 设：$\psi_n^1=\sum_m C_m\psi_m^0$

用 $\hat{\psi}_n^0$ 左乘以此方程：

$$\langle\psi_n^0|(\hat{H}'-E_n^1)|\psi_n^0\rangle=\langle\psi_n^0|(E_n^0-\hat{H}_0)|\psi_n^1\rangle=0$$

则：

$$E_n^1=\langle\psi_n^0|\hat{H}'|\psi_n^0\rangle$$

$$(\hat{H}'-E_n^1)\psi_n^0=\sum_m(E_n^0-\hat{H}_0)C_m\psi_m^0$$

$$\langle\psi_m^0|\hat{H}'|\psi_n^0\rangle-E_n^1\langle\psi_m^0|\psi_n^0\rangle$$

$$=\sum_k C_k\left[\langle\psi_m^0|E_n^0|\psi_k^0\rangle-\langle\psi_m^0|\hat{H}_0|\psi_k^0\rangle\right]$$

1° 当 $m\neq n$ 时：

$$H'_{mn}=C_m(E_n^0-E_m^0)$$

$$C_m^{(n)}=-\frac{H'_{mn}}{E_m^0-E_n^0}$$

2° 当：$m=n$ 时，由于 $(\psi_n^1)'=\psi_n^1+\alpha\psi_n^0$ 时，

ψ_n^1 对应的方程不改变. 则：可以说 $C_n^{(n)}$ 可以是任何值.

$$C_n^{(n)}=0$$

(3)：$\langle\psi_n^0|\hat{H}_0|\psi_n^2\rangle+\langle\psi_n^0|\hat{H}'|\psi_n^1\rangle=E_n^0\langle\psi_n^0|\psi_n^2\rangle+E_n^1\langle\psi_n^0|\psi_n^1\rangle+E_n^2\langle\psi_n^0|\psi_n^0\rangle$

$$\cancel{E_n^0\langle\psi_n^0|\psi_n^2\rangle}+\sum_m C_m^{(n)}\cdot\langle\psi_n^0|\hat{H}'|\psi_m^0\rangle=\cancel{E_n^0\langle\psi_n^0|\psi_n^2\rangle}+E_n^1\langle\psi_n^0|\psi_n^1\rangle+E_n^2$$

$$\sum_m-\frac{H'_{mn}}{E_m^0-E_n^0}\cdot H'_{nm}=E_n^2$$

$$E_n^2=\sum_m-\frac{|H'_{mn}|^2}{E_m^0-E_n^0}$$

问题：为什么：$H'_{mn}=H'^{*}_{nm}$

因为是 Unitary Matrix！

它是幺正的！

简并微扰论

- 问题的提出背景：

  能级 E_n^0；Schrodinger方程对应的解为 $\psi_{n,i}^0$，其中，i 表示着简并：

  （H 不含时间 t，ψ 也不含时间 t）。

- $$\begin{cases} H = H^0 + \lambda H' & (\lambda=1\text{代表实际情况}) \\ \psi_n = \psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 \cdots \\ E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 \cdots \end{cases}$$

  Schrodinger方程：

  $$(H^0 + \lambda H')(\psi_n^0 + \lambda \psi_n^1) = (E_n^0 + \lambda E_n^1)\cdot(\psi_n^0 + \lambda \psi_n^1)$$

  λ 的1阶对应的方程：

  $$H'|\psi_n^0\rangle + H^0|\psi_n^1\rangle = E_n^0|\psi_n^1\rangle + E_n^1|\psi_n^0\rangle$$

  用 ψ_{ni}^0 左乘以结果：

  $$\langle\psi_{ni}^0|H'|\psi_n^0\rangle + \langle\psi_{ni}^0|H^0|\psi_n^1\rangle = \langle\psi_{ni}^0|E_n^0|\psi_n^1\rangle + \langle\psi_{ni}^0|E_n^1|\psi_n^0\rangle$$

  设：$\psi_n^0 = \sum_j \alpha_j \psi_{nj}^0$（简并被解除）

  则：

  $$\sum_j \alpha_j H'_{ij} = \alpha_i \cdot E_n^1$$

  则：

  $$(H' - E_n^1)\begin{pmatrix}\alpha_1 \\ \vdots\end{pmatrix} = 0$$

  相应的，用 $\det(H' - E_n^1) = 0$ 可得 E_n^1 的具体值。

变分法（Variational Principle）

- 此方法可以解决的问题：（找到基态能量 E_{gs}）
- 找到一个归一化的波函数 $|\psi\rangle$，则有不等关系： $\langle\psi|H|\psi\rangle \geq E_{gs}$

从含时微扰论到跃迁概率.

- 体系的Hamilton算符:

$$\hat{H} = \hat{H}_0 + \hat{H}'(t)$$ ⟵ $\hat{H}$作用在x上,是t和x的函数.

$$\Psi_n(x,t) = e^{-i\frac{E_n}{\hbar}t}\cdot\psi_n(x)$$ 是H_0的本征Function

$$\Psi = \sum_m a_m(t)\Psi_m(x,t)$$ 是假设的Hamilton本征方程的解.

$$(\hat{H}_0 + \hat{H}'(t))\sum_m a_m(t)\Psi_m(x,t) = i\hbar\frac{\partial}{\partial t}\left[\sum_m a_m(t)\Psi_m(x,t)\right]$$

$$\cancel{\sum_m a_m(t)\hat{H}_0\Psi_m(t)} + \sum_m a_m(t)\hat{H}'(t)\Psi_m(x,t) = \sum_m i\hbar\frac{da_m}{dt}\cdot\Psi_m(x,t) + \cancel{\sum_m i\hbar a_m(t)\frac{d\Psi_m(x,t)}{dt}}$$

同时用$\Psi_n^*(x,t)$左乘方程两边,并对空间积分:

$$\sum_m a_m(t)\cdot exp(i(E_n-E_m)t/\hbar)\cdot H'_{nm} = i\hbar\frac{da_n}{dt}.$$

$$H'_{nm} = \langle\psi_n|H'|\psi_m\rangle$$

若替换:$H' \to \lambda H'$ $a \to a^{(0)} + \lambda a^{(1)}$ (在实际情况中$\lambda=1$)

$$\sum_m(a_m^{(0)}(t) + \lambda a_m^{(1)}(t) + \lambda^2 a_m^{(2)}(t)\cdots)\cdot exp(i\omega_{nm}t)\lambda H'_{nm} = i\hbar\frac{d}{dt}(a_n^{(0)} + \lambda a_n^{(1)} + \lambda^2 a_n^{(2)}).$$

若初态:$a_n^{(0)} = \delta_{nk}$ (仅当n=k时,才有非0的振幅) $a_n^{(0)}(t) = a_n^{(0)}(0) = \delta_{nk}$

则:

$$i\hbar\frac{d}{dt}(a_n^{(1)}(t)) = \sum_m a_m^{(0)}(t)\cdot exp(i\omega_{nm}t)\cdot H'_{nm} = exp(i\omega_{nk}t)\cdot H'_{nk}(t)$$

$$\frac{d}{dt}(a_n^{(1)}(t)) = \frac{1}{i\hbar}\cdot exp(i\omega_{nk}t)\cdot H'_{nk}(t)$$

在t时刻:从k跃迁到n的几率:

$$W_{k\to n} = |a_n^{(1)}(t)|^2$$

In which:

$$a_n^{(1)}(t) = \int_0^t\frac{1}{i\hbar}\ exp(i\omega_{nk}t)\cdot H'_{nk}(t)\,dt$$

- Fermi golden rule:

$H'_{nk}(t)$不含时间 ⟹ 那他还配叫含时微扰论…吗?(这个微扰论求的目标可不是本征值与本征态!!!

$$a_n^{(1)}(t) = \frac{1}{i\hbar}\cdot\frac{1}{i\omega_{nk}}\cdot(exp(i\omega_{nk}t)-1)\cdot H'_{nk}$$

$$|a_n^{(1)}(t)|^2 = \frac{1}{\hbar^2\omega_{nk}^2}|H'_{nk}|^2\cdot(2-2\cos(\omega_{nk}t))$$

$$= \frac{4}{\hbar^2\omega_{nk}^2}\cdot|H'_{nk}|^2\cdot\sin^2\left(\frac{1}{2}\omega_{nk}t\right)$$

跃迁的概率:

$$W = \int|a_n^{(1)}(t)|^2\cdot\rho(E_n)\,dE_n = \int_{-\infty}^{+\infty}\frac{4}{\hbar^2\omega_{nk}^2}\cdot|H'_{nk}|^2\cdot\sin^2\left(\frac{1}{2}\omega_{nk}t\right)\cdot\rho(n)\cdot\hbar\,d\omega_n$$

$$= \int_{-\infty}^{+\infty}\frac{4}{\hbar}|H'_{nk}|^2\cdot\frac{\sin^2(\frac{1}{2}\omega_{nk}t)}{\omega_{nk}^2}\cdot\rho(n)\,d\omega_{nk}$$

我们注意到Delta函数:

$$\lim_{t\to+\infty}\frac{\sin^2(xt)}{\pi t x^2}=\delta(x)$$

proof:

先证明对 x 的积分结果为1:

$$\int_{-\infty}^{+\infty}\frac{\sin^2(xt)}{\pi t x^2}dx=\int_{-\infty}^{+\infty}\frac{1}{\pi}\cdot\left(\frac{\sin^2(u)}{u^2}\right)\cdot du=1$$

Q: $\int_{-\infty}^{+\infty}\frac{\sin^2 u}{u^2}du$ 的积分该怎么算.

则前面的跃迁概率可以写为:

$$W=\int\frac{4}{\hbar}\cdot|H'_{nk}|^2\cdot\frac{\sin^2(\frac{1}{2}W_{nk}t)}{W_{nk}^2}\cdot dW_{nk}\cdot\rho(n)$$

$$=\int\frac{2\pi}{\hbar}t\cdot|H'_{nk}|^2\cdot\delta(W_{nk})\cdot dW_{nk}\cdot\rho(n)$$

$$=\frac{2\pi}{\hbar}t|H'_{kk}|^2\rho(k)$$

$$w=\frac{W}{t}=\frac{2\pi}{\hbar}|H'_{kk}|^2\rho(k)$$

ⅱ上面的这个式子叫Fermi Golden rule

∘周期性的微扰条件

周期性的微扰条件: $\hat{H}'=\hat{F}(e^{i\omega t}+e^{-i\omega t})$

$$a_n^{(1)}(t)=\int_0^t\frac{1}{i\hbar}\exp(iW_{nk}t)\cdot H'_{nk}(t)\cdot dt$$

改写: $H'_{nk}(t)=\langle\psi_n|\hat{F}(e^{i\omega t}+e^{-i\omega t})|\psi_k\rangle=F_{nk}\cdot(e^{i\omega t}+e^{-i\omega t})$

$$a_n^{(1)}(t)=\int_0^t\frac{1}{i\hbar}\cdot\exp(iW_{nk}t)\cdot F_{nk}\cdot(e^{i\omega t}+e^{-i\omega t})dt$$

$$=\frac{-1}{\hbar}\cdot F_{nk}\left(\frac{e^{i(W_{nk}+\omega)t}-1}{(W_{nk}+\omega)}+\frac{e^{i(W_{nk}-\omega)t}-1}{W_{nk}-\omega}\right)$$

当:共振发生时: $W_{n'k}=\mp\omega$

$$a_{n'}^{(1)}(t)=-\frac{1}{\hbar}\cdot F_{nk}\cdot\frac{e^{i(W_{n'k}\pm\omega)t}-1}{W_{n'k}\pm\omega}$$

$$|a_{n'}^{(1)}(t)|^2=\frac{1}{\hbar^2}|F_{nk}|^2\cdot\frac{2-2\cos(W_{n'k}\pm\omega)t}{(W_{n'k}\pm\omega)^2}$$

$$=\frac{4}{\hbar^2}|F_{nk}|^2\frac{\sin^2(\frac{1}{2}(W_{n'k}\pm\omega)t)}{(W_{n'k}\pm\omega)^2}$$

即: $W_{k\to n'}=\frac{4}{\hbar^2}|F_{nk}|^2\frac{\sin^2(\frac{1}{2}t(W_{n'k}\pm\omega))}{(W_{n'k}\pm\omega)^2}\approx\frac{4}{\hbar^2}\cdot|F_{nk}|^2\cdot\frac{1}{2}t\cdot\pi\,\delta(\underline{W_{n'k}\pm\omega})$

总的跃迁概率可以写为: $W=\int W_{k\to n'}\rho(\varepsilon_{n'})\cdot\hbar\cdot dW_{n'}=\frac{4}{\hbar^2}|F_{nk}|^2\frac{1}{2}t\pi\cdot\hbar\cdot\Big|_{\underline{W_{n'}=W_k\mp\omega}}$

WKB近似

。

对于Schrodinger方程，我们考虑解可以表示为：

$$\psi(x) = A(x)\, e^{\pm i \phi(x)}$$

$$A' \quad \boxed{i e^{i\phi} \cdot \phi'}$$

Schrodinger方程：

$$\nabla^2 \psi(x) = \frac{d^2}{dx^2}\psi(x) = A'' + A \cdot e^{i\phi(x)} \cdot [-(\phi')^2 + i\phi''] + i \cdot 2A'\phi' e^{i\phi}$$

$$\nabla^2 \psi(x) + \frac{2m}{\hbar^2}(E - V(x))\psi = 0$$

则：

$$A'' + A(-(\phi')^2 + i\phi'') + i \cdot 2A' \cdot \phi' + \frac{2m}{\hbar^2}(E - V(x)) \cdot \psi(x) = 0$$

$$\Downarrow$$

$$\begin{cases} A'' - A(\phi')^2 + \frac{2m}{\hbar^2} \cdot (E - V(x)) \cdot \psi(x) = 0 \\ A\phi'' + 2A'\phi' = 0 \end{cases}$$

由于：当A缓慢变化时，$A'' \to 0$，则：

$$\phi' = \pm \frac{\sqrt{2m(E - V(x))}}{\hbar}$$

$$\Downarrow$$

$$\phi_{\pm} = \pm \int \frac{\sqrt{2m(E - V(x))}}{\hbar} \cdot dx = \pm \int \frac{p(x)}{\hbar} \cdot dx$$

$$A \cdot \phi'' + 2A'\phi' = 0$$

$$\Downarrow$$

$$\frac{d}{dx}(A^2 \cdot \phi') = 0$$

$$\Downarrow$$

$$A = \frac{C}{\sqrt{\phi'(x)}} = \frac{C}{\sqrt{p(x)}} = \frac{C}{\sqrt{(2m(E - V(x)))^{1/2}}}$$

综上，当有条件：$A'' = 0$（V缓慢变化时）：

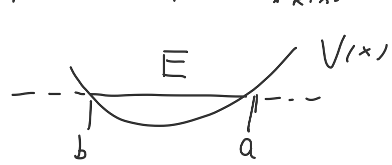
$$\psi(x) = \frac{C}{\sqrt{p(x)}} \cdot e^{\pm i \frac{1}{\hbar}\int p(x) \cdot dx} \qquad p(x) = \sqrt{2m(E - V(x))}$$

For the Results Previously.（第二章就讲到了WKB近似）

$$\begin{cases} k(x) = \left(\frac{2m}{\hbar^2}(E - V(x))\right)^{1/2} & E \geq V(x) & u_E(x) = \exp(iW(x)/\hbar) = \frac{1}{[k(x)]^{1/2}} \exp\left[\pm i \int^x dx' k(x')\right] \\ k(x) = -i\left(\frac{2m}{\hbar^2}(V(x) - E)\right)^{1/2} = -i\kappa(x) & E < V(x) & u_E(x) = \exp\left(\frac{i}{\hbar} W(x)\right) = \frac{1}{\sqrt{\kappa(x)}} \cdot \exp\left(\pm \int^x \kappa(x') dx'\right) \end{cases}$$

$$\begin{cases} \frac{A}{\sqrt{\kappa(x)}} \cdot \exp\left(-\int_a^x \kappa(x') dx'\right) + \frac{B}{\sqrt{\kappa(x)}} \cdot \exp\left(+\int_a^x \kappa(x') dx'\right) & (x \gg a) \\ 2A \frac{1}{\sqrt{k(x)}} \cdot \cos\left(\int_x^a k(x') dx' - \frac{\pi}{4}\right) - B \cdot \frac{1}{\sqrt{k(x)}} \cdot \sin\left(\int_x^a k(x') dx' - \frac{\pi}{4}\right) & (x \ll a) \end{cases}$$

$$\begin{cases} \frac{A'}{\sqrt{\kappa(x)}} \exp\left(-\int_x^b \kappa(x') dx'\right) + \frac{B'}{\sqrt{\kappa(x')}} \cdot \exp\left(\int_x^b \kappa(x') dx'\right) & x \ll b \\ \Updownarrow & \\ 2\frac{A'}{\sqrt{k(x)}} \cdot \cos\left(\int_b^x k(x') dx' - \frac{\pi}{4}\right) - \frac{B'}{\sqrt{k(x)}} \cdot \sin\left(\int_b^x k(x') dx' - \frac{\pi}{4}\right) & x \gg b \end{cases}$$



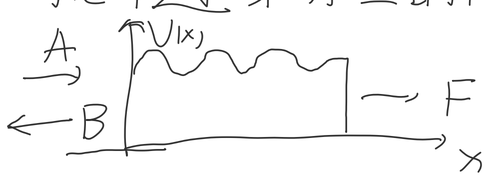
隧穿:(tunneling). Lead By WKB.

- 考察的区域:(经典不允许区: $E<V$)

$$\psi(x) = \frac{C}{\sqrt{p(x)}} \cdot e^{\pm\int \frac{1}{\hbar} p(x)\, dx} \qquad p(x) = \sqrt{2m(V(x)-E)}$$

- 考察的具体问题:(实际上也用到了近似: $V(x) >> E$)

考虑隧穿势垒的问题:



$x<0$时:

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \qquad k = \frac{1}{\hbar}\sqrt{2mE}$$

$x>a$时:

$$\psi(x) = Fe^{ikx}$$

透射系数定义为:

$$T = (|F|/|A|)^2$$

在 $x\in(0,a)$ 区间中: 用WKB近似:

$$\psi(x) = \frac{C}{\sqrt{p(x)}} \cdot e^{\frac{1}{\hbar}\int p(x)\, dx} + \frac{D}{\sqrt{p(x)}}\, e^{-\frac{1}{\hbar}\int p(x)\, dx}$$

当: $V(x) >> E$时 ($C\to 0$ 才不会发散)

$$\psi(x) = \frac{D}{\sqrt{p(x)}} \cdot e^{-\frac{1}{\hbar}\int p(x)\, dx}$$

利用边界条件: $\psi(0+) = \psi(0-)$; $\psi(a+) = \psi(a-)$, 则:

$$\begin{cases} \frac{|F|}{|A|} = e^{-\frac{1}{\hbar}\int p(x)\, dx} = e^{-\gamma} \\ T = e^{-2\gamma} \qquad \left(\gamma = \int \frac{p(x)}{\hbar}\, dx = \int \frac{1}{\hbar}\sqrt{2m(E-V(x))}\, dx\right) \end{cases}$$

Scattering Theory 散射理论.

Transition Amplitude (use Time - Dependent Perturbation Theory)

$H = H_0 + V(x)$ $\quad H_0 = \frac{p^2}{2m}$ stands for kinetic-energy operator.

$E_k = \frac{\hbar^2 k^2}{2m}$

For Interaction Picture

$|\alpha, t_0; t\rangle_I = U_I(t, t_0)\, |\alpha, t_0; t_0\rangle_I \qquad |\alpha, t_0, t\rangle_I = \exp(iH_0 t/\hbar)\, |\alpha, t_0, t\rangle_S$

$$\begin{cases} i\hbar \frac{\partial}{\partial t} U_I(t,t_0) = V_I(t)\, U_I(t, t_0) \\ V_I(t) = \exp(iH_0 t \frac{1}{\hbar}) \cdot V(t) \cdot \exp(-iH_0 t/\hbar) \end{cases}$$

one solution for U_I

$$U_I(t,t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^{t} V_I(t')\, U_I(t', t_0)\, dt'$$

Define Transition Amplitude.

$$\langle n | U_I(t, t_0) | i\rangle = \delta_{ni} - \frac{i}{\hbar} \sum_m \langle n | V | m\rangle \int_{t_0}^{t} e^{i\omega_{nm} t'} \langle m | U_I(t', t_0) | i\rangle\, dt'$$

$$\begin{cases} \langle n | i\rangle = \delta_{ni}, \quad \hbar\omega_{nm} = E_n - E_m \\ \langle x | k\rangle = \frac{1}{L^{3/2}} \cdot e^{ik\cdot x}; \quad k = \frac{2\pi}{L}(n_x, n_y, n_z) \end{cases}$$

(Box Normalization)

▽ Scatter from past to future $t_0 \to -\infty$, $t \to +\infty$

Assumption: $\langle m | U_I(t', t_0) | i\rangle = \delta_{mi}$

$$\langle n | U_I(t, t_0) | i\rangle = \delta_{ni} - \frac{i}{\hbar} V_{ni} \cdot \int_{t_0}^{t} e^{i\omega_{ni} t'}\, dt'$$

(6.9). 不理解为什么假设到底是不是对的.

Define $\langle n | U_I(t, t_0) | i\rangle = \delta_{ni} - \frac{i}{\hbar} T_{ni} \int_{t_0}^{t} e^{i\omega_{ni} t' + \varepsilon t'}\, dt'$ 这个定义好奇怪?

We work $\underbrace{t_0 \to -\infty, \ \varepsilon \to 0;\ t \to +\infty,\ \varepsilon t \ll 1}_{\text{是取极限的顺序!}}$ $\quad \begin{cases} \varepsilon t \to 1 \\ \varepsilon t_0 \to -\infty \end{cases}$

▽ Scattering from future to past!

$$U_I(t, t_0) = 1 + \frac{i}{\hbar} \int_{t}^{t_0} V_I(t')\, U_I(t', t_0)\, dt'$$

$$\langle n | U_I(t, t_0) | i\rangle = \delta_{ni} + \sum_m \frac{i}{\hbar} \int_{t}^{t_0} \langle n | V | m\rangle\, e^{i\omega_{nm} t'} \cdot \langle m | U_I(t', t_0) | i\rangle\, dt'$$

Define $\langle n | U_I(t, t_0) | i\rangle = \delta_{ni} + \frac{i}{\hbar} T_{ni} \int_{t}^{t_0} e^{i\omega_{ni} t' - \varepsilon t'}\, dt'$ 这个定义也好怪...

$\underbrace{t_0 \to +\infty \quad \varepsilon \to 0 \quad t \to -\infty}_{\text{取极限的顺序.}}$ $\quad \begin{cases} \varepsilon t \to 1 \\ \varepsilon t_0 \to -\infty \end{cases}$

Solve T matrix (6.1.2 Sakurai)

$$\langle n | U_I(t, -\infty) | i\rangle = \delta_{ni} + \frac{1}{\hbar} T_{ni} \cdot \frac{e^{i\omega_{ni} t + \varepsilon t}}{-\omega_{ni} + i\varepsilon} \qquad \text{(From Previous)}$$

$$\langle n | U_I(t, -\infty) | i\rangle = \delta_{ni} - \frac{i}{\hbar} \sum_m V_{nm} \int_{-\infty}^{t} e^{i\omega_{nm} t'} \langle m | U_I(t', -\infty) | i\rangle\, dt'$$

Insert First To second

$$\langle n | U_I(t, -\infty) | i\rangle = \delta_{ni} - \frac{i}{\hbar} \sum_m V_{nm} \int_{-\infty}^{t} e^{i\omega_{nm} t'} \left(\delta_{mi} + \frac{1}{\hbar} T_{mi} \frac{e^{i\omega_{mi} t' + \varepsilon t'}}{-\omega_{mi} + i\varepsilon}\right) dt'$$

$$= \delta_{ni} - \frac{i}{\hbar} V_{ni} \int_{-\infty}^{t} e^{i\omega_{nm} t'}\, dt' - \frac{i}{\hbar}\frac{1}{\hbar} \sum_m \int_{-\infty}^{t} V_{nm} T_{mi} \cdot \frac{e^{i(\omega_{nm} + \omega_{mi}) t' + \varepsilon t'}}{-\omega_{mi} + i\varepsilon}\, dt'$$

$$= \delta_{ni} - \frac{i}{\hbar} V_{ni} \int_{-\infty}^{t} e^{i\omega_{nm} t' + \varepsilon t'}\, dt' - \frac{i}{\hbar}\frac{1}{\hbar} \sum_m V_{nm} \frac{T_{mi}}{-\omega_{mi} + i\varepsilon} \int_{-\infty}^{t} e^{i(\omega_{nm} + \omega_{mi}) t' + \varepsilon t'}\, dt'$$

↑ 这步ε是怎么来的?

$$= \delta_{ni} - \frac{i}{\hbar} V_{ni} \int_{-\infty}^{t} e^{i\omega_{nm} t' + \varepsilon t'}\, dt' - \frac{i}{\hbar}\frac{1}{\hbar} \sum_m V_{nm} \frac{T_{mi}}{-\omega_{mi} + i\varepsilon} \int_{-\infty}^{t} e^{i\omega_{ni} t' + \varepsilon t'}\, dt'$$

$$= \delta_{ni} + \frac{1}{\hbar} T_{ni} \cdot \frac{e^{i\omega_{ni}t + \varepsilon t}}{-\omega_{ni} + \varepsilon}$$

$$T_{ni} = V_{ni} + \frac{1}{\hbar}\sum_m V_{nm} \frac{T_{mi}}{-\omega_{mi} + i\varepsilon}$$

$$= V_{ni} + \sum_m V_{nm} \frac{T_{mi}}{E_i - E_m + i\hbar\varepsilon}$$

▽ Define vector $|\psi^{(+)}\rangle$, Use this definition to derive Lippmann-Schwinger Equation.

(Sakurai 6.27)

$$\begin{cases} T_{ni} = \sum_j \langle n|V|j\rangle\langle j|\psi^{(+)}\rangle = \langle n|V|\psi^{(+)}\rangle \\ T_{ni} = V_{ni} + \frac{1}{\hbar}\sum_m V_{nm} \frac{T_{mi}}{-\omega_{mi} + i\varepsilon} \\ \quad = V_{ni} + \sum_m V_{nm} \frac{T_{mi}}{E_i - E_m + i\hbar\varepsilon} \end{cases}$$

$$\Downarrow$$

$$\langle n|V|\psi^{(+)}\rangle = \langle n|V|i\rangle + \sum_m \langle n|V|m\rangle \frac{\langle m|V|\psi^{(+)}\rangle}{E_i - E_m + i\hbar\varepsilon}$$

$$|\psi^{(+)}\rangle = |i\rangle + \sum_m \frac{1}{E_i - H_0 + i\hbar\varepsilon} |m\rangle\langle m|V|\psi^{(+)}\rangle$$

$$|\psi^{(+)}\rangle = |i\rangle + \frac{1}{E_i - H_0 + i\hbar\varepsilon} \cdot V|\psi^{(+)}\rangle \qquad \text{(Lippmann - Schwinger Equation)}$$

▽ Order - By - Order approximation Scheme for operator T:

apply V on the Left of G - L Function

$$V|\psi^{(+)}\rangle = V|i\rangle + V\frac{1}{E_i - H_0 + i\hbar\varepsilon} \cdot V|\psi^{(+)}\rangle$$

Cause: $\langle n|T|i\rangle = \langle n|V|\psi^{(+)}\rangle \Rightarrow V|\psi^{(+)}\rangle = T|i\rangle$

$$T = V + V\frac{1}{E_i - H_0 + i\hbar\varepsilon} T$$

Solution (V is weak)

$$T = V + V\frac{1}{E_i - H_0 + i\hbar\varepsilon} \cdot V + V\frac{1}{E_i - H_0 + i\hbar\varepsilon} \cdot V \cdot \frac{1}{E_i - H_0 + i\hbar\varepsilon} \cdot V + \cdots$$

Transition Rate and Cross section

Transition Rate

$$W(i\to n) = \frac{d}{dt}|\langle n|U_I(t,-\infty)|i\rangle|^2$$

$$\langle n|U_I(t,-\infty)|i\rangle = -\frac{i}{\hbar} T_{ni} \int_{-\infty}^{t} e^{i\omega_{ni}t' + \varepsilon t'} dt' = -\frac{i}{\hbar} T_{ni} \frac{e^{i\omega_{ni}t + \varepsilon t}}{i\omega_{ni} + \varepsilon} \qquad (|i\rangle \neq |n\rangle)$$

$$W(i\to n) = \frac{d}{dt}\left(\frac{1}{\hbar^2}|T_{ni}|^2 \cdot \frac{e^{2\varepsilon t}}{\omega_{ni}^2 + \varepsilon^2}\right) = \frac{1}{\hbar^2} \cdot |T_{ni}|^2 \cdot \frac{2\varepsilon \cdot e^{2\varepsilon t}}{\omega_{ni}^2 + \varepsilon^2}$$

Noticed

$$\int_{-\infty}^{+\infty} \frac{1}{\omega^2 + \varepsilon^2} d\omega = \frac{\pi}{\varepsilon} \Rightarrow \varepsilon \int_{-}^{+} \frac{1}{\omega^2 + \varepsilon^2} d\omega = \pi$$

$$\Downarrow$$

$$\lim_{\varepsilon\to 0} \frac{\varepsilon}{\omega^2 + \varepsilon^2} = \pi\,\delta(\omega)$$

$$W(i\to n) = \frac{1}{\hbar^2}|T_{ni}|^2 \cdot 2 \cdot e^{2\varepsilon t} \cdot \pi \cdot \delta(\omega_{ni})$$

$$= \frac{2\pi}{\hbar} \cdot |T_{ni}|^2 \cdot \delta(E_n - E_i) \cdot \qquad (\text{for } \varepsilon \to 0)$$

Which is independent of time, so time limit $t \to +\infty$ is trivial!

Wanna to integrate over the final states! ⟶ 不理解为什么要对 Final state 积分.

$$k = \frac{2\pi}{L}(n_x, n_y, n_z) \qquad \Delta N = d\Omega \cdot |n|^2 d|n|$$

$$|n| = \frac{L}{2\pi}|k|$$

$$E = \frac{\hbar^2}{2m} \cdot \left(\frac{2\pi}{L}\right)^2 |n|^2 \qquad \Delta E = \frac{\hbar^2}{m} \left(\frac{2\pi}{L}\right)^2 \cdot |n| \cdot d|n|$$

$$\rho(E) = \frac{\Delta N}{\Delta E} = \frac{|n| \cdot d\Omega}{\frac{\hbar^2}{m}\left(\frac{2\pi}{L}\right)^2} = \frac{m}{\hbar^2} \cdot \left(\frac{L}{2\pi}\right)^2 \cdot |n| \cdot d\Omega = \frac{m}{\hbar^2} \cdot \left(\frac{L}{2\pi}\right)^3 |k| \, d\Omega$$

$$\int_{-\infty}^{+\infty} W(i \to n) \, \rho(E_n) \cdot dE_n = \frac{2\pi}{\hbar} |T_{ni}|^2 \cdot \frac{m}{\hbar^2} \left(\frac{L}{2\pi}\right)^3 \cdot |k| \qquad (E_n = E_i)$$

$$W(i \to n) = \frac{m|k|L^3}{(2\pi)^2 \hbar^3} \cdot |T_{ni}|^2 \cdot d\Omega$$

Schrodinger Equation Probability Flux for $\langle x | k \rangle = \frac{1}{L^{3/2}} e^{ik \cdot x}$

$$j(x, t) = \frac{\hbar}{m} \frac{k}{L^3}$$

cross section.

$$\frac{d\sigma}{d\Omega} = \frac{d\left(\frac{W}{|j|}\right)}{d\Omega} = \left(\frac{m L^3}{2\pi \hbar^2}\right)^2 |T_{ni}|^2$$

Scattering Amplitude $f(k',k)$

from $\langle x|\psi^{(\pm)}\rangle$ to $f(k',k)$

$$|\psi^{(\pm)}\rangle = |i\rangle + \frac{1}{E_i - H_0 \pm i\hbar\varepsilon} V|\psi^{(\pm)}\rangle$$

$$\langle x|\psi^{(\pm)}\rangle = \langle x|i\rangle + \int d^3x' \langle x|\frac{1}{E_i - H_0 \pm i\hbar\varepsilon}|x'\rangle\langle x'|V|\psi^{(\pm)}\rangle$$

Define

$$G_\pm(x,x') = \frac{\hbar^2}{2m}\langle x|\frac{1}{E - H_0 \pm i\varepsilon}|x'\rangle$$

$$\langle x|\psi^{(\pm)}\rangle = \langle x|i\rangle - \frac{2m}{\hbar^2}\int d^3x' \frac{e^{\pm ik|x-x'|}}{4\pi|x-x'|}\langle x'|V|\psi^{(\pm)}\rangle \Leftarrow$$

Locality of V

$$\langle x'|V|x''\rangle = V(x')\,\delta^{(3)}(x'-x'')$$

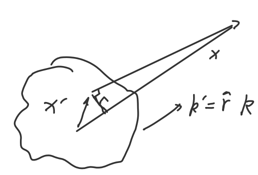
$$\langle x'|V|\psi^{(\pm)}\rangle = \int d^3x'' \langle x'|V|x''\rangle\langle x''|\psi^{(\pm)}\rangle$$

$$= V(x')\,\langle x'|\psi^{(\pm)}\rangle$$

$$\langle x|\psi^{(\pm)}\rangle = \langle x|i\rangle - \frac{2m}{\hbar^2}\int d^3x' \frac{e^{\pm ik|x-x'|}}{4\pi|x-x'|}V(x') \cdot \langle x'|\psi^{(\pm)}\rangle$$

Far away approx

$$|x| >> |x'|$$



$$|x-x'| \approx r - \hat{r}\cdot x'$$

$$\hat{r} = \frac{x}{|x|}$$

$$e^{\pm ik|x-x'|} = e^{\pm ikr}\cdot e^{\mp ik'\cdot x'} \qquad k' = \hat{r}k$$

For $i = k$. $|i\rangle = |k\rangle$

$$\langle x|\psi^{(+)}\rangle = \langle x|k\rangle - \frac{1}{4\pi}\frac{2m}{\hbar^2}\frac{e^{ikr}}{r}\int d^3x' e^{-ik'\cdot x'} V(x')\langle x'|\psi^{(+)}\rangle$$

$$= \frac{1}{L^{3/2}}\left(e^{ik\cdot x} + \frac{e^{ikr}}{r} f(k',k)\right)$$

$$f(k',k) = -\frac{1}{4\pi}\frac{2m}{\hbar^2} L^3 \int d^3x' \frac{e^{-ik'\cdot x'}}{L^{3/2}} V(x')\langle x'|\psi^{(+)}\rangle$$

$$= -\frac{mL^3}{2\pi\hbar^2}\langle k'|V|\psi^{(+)}\rangle$$

For $\langle x|\psi^{(-)}\rangle$

$$\frac{1}{L^{3/2}}\left(e^{ik\cdot x} + \frac{e^{-ikr}}{r}\left(-\frac{mL^3}{2\pi\hbar^2}\right)\cdot\langle -k'|V|\psi^{(-)}\rangle\right)$$

By comparsio with (6.30)

$$\frac{d\sigma}{d\Omega} = \left(\frac{mL^3}{2\pi\hbar^2}\right)^2 |\langle n|V|\psi^{(+)}\rangle|^2$$

$$= |f(k',k)|^2$$

$$G_\pm(x,x') = \frac{\hbar^2}{2m}\sum_{k'}\sum_{k''}\langle x|k'\rangle\langle k'|\frac{1}{E - H_0 \pm i\varepsilon}|k''\rangle\langle k''|x'\rangle$$

$$\langle k'|\frac{1}{E - \frac{\hbar^2 k'^2}{2m} \pm i\varepsilon}|k''\rangle = \frac{\delta_{k'k''}}{E - \frac{\hbar^2 k'^2}{2m} \pm i\varepsilon}$$

$$\langle x|k'\rangle = \frac{1}{L^{3/2}} e^{ik'\cdot x}$$

$$\langle k''|x'\rangle = \frac{1}{L^{3/2}} e^{-ik''\cdot x'}$$

$$E_i = E = \frac{\hbar^2}{2m}k^2$$

(这里把 i 和 k 连系起来) (而且只和入射强度有关,和方向无关!)

$$G_\pm(x,x') = \frac{1}{L^3}\sum_{k'}\frac{e^{ik'\cdot(x-x')}}{k^2 - k'^2 \pm i\varepsilon}$$

$$k' = \frac{2\pi}{L}(n_x', n_y', n_z')$$

$$\sum_{k'} \to \iiint \left(\frac{L}{2\pi}\right)^3 dk_x' dk_y' dk_z'$$

$$G_\pm(x,x') = \frac{1}{(2\pi)^3}\int d^3k' \frac{e^{ik'\cdot(x-x')}}{k^2 - k'^2 \pm i\varepsilon}$$

Using Radial Integration. $d^3k' = \int k'^2 dk' d\phi_k \cdot \sin\theta_k d\theta_k$

$$G_\pm(x,x') = \frac{1}{(2\pi)^2}\int_0^{+\infty} k'^2 dk' \int_{-1}^{1} d\mu \frac{e^{ik'\cdot|x-x'|\mu}}{k^2 - k'^2 \pm i\varepsilon}$$

(这里的 k' 是标量)

$$= \frac{1}{8\pi^2}\frac{1}{i|x-x'|}\int_{-\infty}^{+\infty} k'dk' \frac{e^{ik'|x-x'|} - e^{-ik'|x-x'|}}{k^2 - k'^2 \pm i\varepsilon} \quad \text{(even for } k'\text{)}$$

$$k^2 - k'^2 \pm i\varepsilon = -(k'-k_0)(k'+k_0) \qquad k_0 \equiv k \pm i\varepsilon'$$

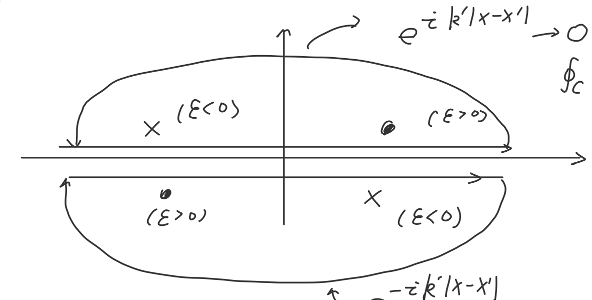
$$= k_0^2 - k'^2$$

$$= k^2 - k'^2 \pm i2k\varepsilon' \qquad \varepsilon' = \frac{1}{2k}\cdot\varepsilon$$

和 ε 的正负相同!

$$G_\pm(x,x') = \frac{1}{8\pi^2}\frac{1}{i|x-x'|}\int_{-\infty}^{+\infty} k'dk' \frac{e^{ik'|x-x'|} - e^{-ik'|x-x'|}}{-(k'-k_0)(k'+k_0)}$$

$e^{ik'|x-x'|} \to 0$. $\oint_C \frac{f(z)}{z - z_0}dz = 2\pi i f(z_0)$



$e^{-ik'|x-x'|} \to 0$

First term

$$= \frac{1}{8\pi^2}\frac{2\pi i}{i|x-x'|}(\pm k)\frac{e^{\pm ik|x-x'|}}{(-1)(\pm)(2k)} = \frac{1}{8\pi^2}\frac{1}{i|x-x'|}(-\pi i)e^{\pm ik|x-x'|}$$

$$G_\pm(x,x') = -\frac{1}{4\pi}\frac{e^{\pm ik|x-x'|}}{|x-x'|}$$

The Optical Theorem.

Want to prove $\operatorname{Im} f(k,k) = \frac{k}{4\pi}\sigma_{tot}$ $\sigma_{tot} \equiv \int d\Omega \left(\frac{d\sigma}{d\Omega}\right)$

For Lippmann-Schwinger Equation. $|i\rangle = |k\rangle$

$$|k\rangle = |\psi^{(+)}\rangle - \frac{1}{E_i - H_0 + i\hbar\varepsilon}\cdot V|\psi^{(+)}\rangle$$

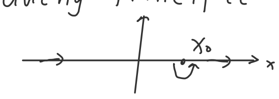
$$\langle k| = \langle\psi^{(+)}| - \langle\psi^{(+)}| V \frac{1}{E_i - H_0 - i\hbar\varepsilon}$$

$$\langle k|V|\psi^{(+)}\rangle = \langle\psi^{(+)}|V|\psi^{(+)}\rangle - \langle\psi^{(+)}|V\frac{1}{E_i - H_0 - i\hbar\varepsilon}\cdot V|\psi^{(+)}\rangle$$

$$\lim_{\varepsilon\to 0}\frac{1}{E - H_0 - i\varepsilon} = \lim_{\varepsilon\to 0}\int_{-\infty}^{+\infty}\delta(E-E')\frac{1}{E' - H_0 - i\varepsilon}\cdot dE' \Longleftarrow$$

$$= i\pi\cdot\delta(E - H_0)$$

Cauchy Principle Value.



$$\int_{-\infty}^{+\infty}\frac{f(x)}{x-x_0}dx = \int_{-\infty}^{x_0-\delta}\frac{f(x)dx}{x-x_0} + \int_{x_0+\delta}^{+\infty}\frac{f(x)}{x-x_0} + \int_C\frac{f(z)}{z-z_0}dz$$

$$= \mathcal{P}\int_{-\infty}^{+\infty}\frac{f(x)}{x-x_0}dx + \int_{-\pi}^{\pi}\frac{f(x_0)}{\delta e^{i\phi}}\cdot\delta\cdot i\cdot e^{i\phi}\cdot d\phi$$

$$= \mathcal{P}\int_{-\infty}^{+\infty}\frac{f(x)}{x-x_0}dx + i\pi f(x_0)$$

$$\mathcal{P}\int_{-\infty}^{+\infty}\frac{f(x)}{x-x_0}dx = \lim_{\delta\to 0}\left(\int_{-\infty}^{x_0-\delta}\frac{f(x)}{x-x_0}dx + \int_{x_0+\delta}^{+\infty}\frac{f(x)}{x-x_0}dx\right)$$

$$\operatorname{Im}\langle k|V|\psi^{(+)}\rangle = -\operatorname{Im}\langle\psi^{(+)}|V i\pi\delta(E-H_0)\cdot V|\psi^{(+)}\rangle$$

$$= -\langle\psi^{(+)}|V\cdot\pi\cdot\delta(E-H_0)\cdot V|\psi^{(+)}\rangle$$

$$= -\pi\cdot\langle k|T^\dagger\cdot\delta(E-H_0)\cdot T|k\rangle$$

this is the definition of $|\psi^{(+)}\rangle$

$$T|i\rangle = V|\psi^{(+)}\rangle \Longrightarrow T|k\rangle = V|\psi^{(+)}\rangle$$

Using Definition of $f(k',k)$.

$$\operatorname{Im} f(k,k) = -\frac{mL^3}{2\pi\hbar^2}\operatorname{Im}\langle k|V|\psi^{(+)}\rangle$$

$$= \frac{mL^3}{2\hbar^2}\cdot\langle k|T^\dagger\delta(E-H_0)T|k\rangle$$

$$= \frac{mL^3}{2\hbar^2}\cdot\sum_{k'}\langle k|T^\dagger\delta(E-H_0)|k'\rangle\langle k'|T|k\rangle$$

$$= \frac{mL^3}{2\hbar^2}\sum_{k'}|\langle k'|T|k\rangle|^2\delta\left(E - \frac{\hbar^2k'^2}{2m}\right)$$

$$\left\{\begin{array}{l} f(k',k) = -\frac{mL^3}{2\pi\hbar^2}\cdot\langle k'|V|\psi^{(+)}\rangle \\ \langle k'|V|\psi^{(+)}\rangle = \langle k'|T|k\rangle \end{array}\right.$$

$$\operatorname{Im} f(k,k) = \frac{mL^3}{2\hbar^2}\cdot\left(\frac{2\pi\hbar^2}{mL^3}\right)^2\sum_{k'}|f(k',k)|^2\delta\left(E - \frac{\hbar^2k'^2}{2m}\right)$$

$$n_i = \frac{L}{2\pi}k_i$$

$$\sum_{k'} \longrightarrow \int\left(\frac{L}{2\pi}\right)^3 d^3k'$$

$$d^3k' \longrightarrow \int_0^{2\pi}d\phi\int_0^{\pi}d\theta\sin\theta\cdot\int_0^{+\infty}|k'|^2\cdot d|k'|$$

$$d|k'| \longrightarrow \frac{1}{2\cdot\frac{\hbar^2}{2m}|k'|}d\left(\frac{\hbar^2k'^2}{2m}\right)$$

$$\frac{d\sigma}{d\Omega} = |f(k',k)|^2$$

$$= \frac{2\pi^2\hbar^2}{m(2\pi)^3}\cdot\int d^3k'\cdot|f(k',k)|^2\delta\left(E - \frac{\hbar^2|k|^2}{2m}\right)$$

$$= \frac{\hbar^2}{4\pi m}\cdot\frac{1}{\hbar^2\cdot|k|/m}\cdot|k|^2\int d\Omega_{k'}\frac{d\sigma}{d\Omega}$$

$$= \frac{|k|}{4\pi}\cdot\sigma_{tot}.$$

The Born Approximation

Order - By - Order approximation of T:

Replace $\hbar\varepsilon$ by ε

$$T = V + V\frac{1}{E - H_0 + i\varepsilon}V + V\frac{1}{E-H_0+i\varepsilon}V\frac{1}{E-H_0+i\varepsilon}V + \cdots + \cdots$$

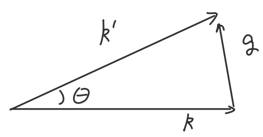
$$f(k',k) = -\frac{mL^3}{2\pi\hbar^2}\langle k'|V|\psi^{(+)}\rangle$$

First Order approx

$$T = V \qquad T|k\rangle = V|k\rangle = V|\psi^{(+)}\rangle \rightarrow |\psi^{(+)}\rangle = |k\rangle$$

$$f^{(1)}(k',k) = -\frac{m}{2\pi\hbar^2}\cdot\int d^3x'\ e^{i(k-k')\cdot x'}\ V(x')$$

For V is spherically Symmetric



$$q \equiv k - k' \qquad |q| = |k-k'| = 2|k|\sin\frac{\theta}{2} \qquad |k'| = |k| \text{ by energy conservation.}$$

$$f^{(1)}(\theta) = -\frac{m}{2\pi\hbar^2}\int_0^{2\pi}d\phi\int_0^{\pi}\sin\theta' d\theta'\cdot\int_0^{+\infty}r^2dr\cdot e^{iqr\cos\theta'}\cdot V(r)$$

$$= -\frac{2m}{\hbar^2}\frac{1}{q}\int_0^{+\infty}dr\ r\ V(r)\sin(qr)$$

1° Finite square Well.

$$V(r) = \begin{cases} V_0 & r \le a \\ 0 & r > a \end{cases}$$

$$f^{(1)}(\theta) = -\frac{2m}{\hbar^2}\frac{V_0 a^3}{(qa)^2}\left(\frac{\sin(qa)}{qa} - \cos qa\right)$$

2° Yukawa Potential

$$f^{(1)}(\theta) = -\frac{2mV_0}{\mu\hbar^2}\frac{1}{q^2+\mu^2} \qquad V(r) = \frac{V_0}{\mu r}e^{-\mu r}$$

Used $\sin qr = \mathrm{Im}(e^{iqr})$

$$\mathrm{Im}\left(\int_0^{+\infty}e^{-\mu r}e^{iqr}dr\right) = -\mathrm{Im}\left(\frac{1}{-\mu+i\varepsilon}\right) = \frac{q}{\mu^2+q^2}$$

First order approx valid condition

(6.52)

$$\langle x|\psi^{(\pm)}\rangle = \langle x|i\rangle - \frac{2m}{\hbar^2}\cdot\int d^3x'\frac{e^{\pm ik|x-x'|}}{4\pi|x-x'|}V(x')\cdot\langle x'|\psi^{(\pm)}\rangle$$

$T \approx V \qquad |i\rangle = |k\rangle \qquad |\psi^{(+)}\rangle \approx |k\rangle$ Second is much smaller than first.

$$\left|\frac{2m}{\hbar^2}\left(\frac{4\pi}{3}a^3\right)\frac{e^{ikr'}}{4\pi a}V_0\frac{e^{ik\cdot x'}}{L^{3/2}}\right| \ll \left|\frac{e^{ik\cdot x}}{L^{3/2}}\right| \qquad r' = |x-x'| \qquad V \sim V_0$$

A. Low energy $ka \ll 1$

$$\frac{m|V_0|a^2}{\hbar^2} \ll 1$$

B. High energy

$$\frac{2m}{\hbar^2}\cdot\frac{|V_0|a}{k}\ln(ka) \gg 1$$

Higher order Born Approx

$$f^{(1)}(k',k) = -\frac{m}{2\pi\hbar^2}\int d^3x'\cdot e^{i(k-k')\cdot x'}V(x')$$

$$\langle x|\psi^{(+)}\rangle = \langle x|i\rangle + \int d^3x'\ G_+(x,x')\langle x'|V|\psi^{(+)}\rangle$$

$$f(k',k) = -\frac{mL^3}{2\pi\hbar^2}\langle k'|V|\psi^{(+)}\rangle$$

$$f^{(2)} = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int d^3x'\int d^3x''\cdot e^{-ik'\cdot x'}V(x')\cdot\frac{2m}{\hbar^2}\cdot G_+(x',x'')\cdot V(x'')\cdot e^{ik\cdot x''}$$

Spherical Wave State

$H_0 = \frac{p^2}{2m}$

Noticed $[H_0, L^2] = [H_0, L_z] = 0$.

Define Spherical Wave State. $|E, l, m\rangle$

$$\langle E' l' m' | E, l, m\rangle = \delta_{ll'} \delta_{mm'} \delta(E - E')$$

In analogy with position wave function. Guess.

$$\langle k | E l m\rangle = g_{lE}(|k|) \cdot Y_l^m(\hat{k})$$

Noticed $L_z |k\hat{z}\rangle = (x p_y - y p_x) |k_x = 0\ k_y = 0\ k_z = k\rangle = 0$

$$\langle E' l' m' | k\hat{z}\rangle = 0 \quad \text{for } m' \neq 0$$

$$|k\hat{z}\rangle = \sum_{l'} \int dE' \, |E' l' m' = 0\rangle \langle E', l', m' = 0 | k\hat{z}\rangle$$

Define k. specified by θ, ϕ.

$$|k\rangle = \mathcal{D}(\alpha = \phi, \beta = \theta, \gamma = 0) \cdot |k\hat{z}\rangle$$

$$\langle E l m | k\rangle = \sum_{l'} \int dE' \cdot \langle E, l m | \mathcal{D}(\alpha = \phi, \beta = \theta, \gamma = 0) \cdot |E', l', m' = 0\rangle \langle E', l', m' = 0 | k\hat{z}\rangle$$

$$= \sum_{l'} \int dE' \, \mathcal{D}^{(l')}_{m0}(\alpha = \phi, \beta = \theta, \gamma = 0) \, \delta_{ll'} \, \delta(E - E') \cdot \langle E' l', m' = 0 | k\hat{z}\rangle$$

$$= \mathcal{D}^{(l)}_{m0}(\alpha = \phi, \beta = \theta, \gamma = 0) \cdot \langle E, l, m = 0 | k\hat{z}\rangle$$

Call $\langle E, l, m = 0 | k\hat{z}\rangle$ as

$$\sqrt{\frac{2l+1}{4\pi}} \cdot g^*_{lE}(|k|) \qquad \text{independent of orientation of } k.$$

From (3.2.60).

$$Y_l^{m'*}(\theta, \phi) = \sqrt{\frac{(2l+1)}{4\pi}} \cdot \mathcal{D}^{(l)}_{m'0}(\alpha = \phi, \beta = \theta, \gamma = 0)$$

$$\langle k | E, l, m\rangle = g_{lE}(k) \, Y_l^m(\hat{k})$$

Noticed:
$$\begin{cases} (H_0 - E) |E, l, m\rangle = 0 \\ \langle k | (H_0 - E) = \left(\frac{\hbar^2 k^2}{2m} - E\right) \langle k | \end{cases} \Rightarrow \left(\frac{\hbar^2 k^2}{2m} - E\right) \langle k | E, l, m\rangle = 0.$$

$$\Downarrow$$

$$g_{lE}(k) = N \cdot \delta\left(\frac{\hbar^2 k^2}{2m} - E\right)$$

Use normalisation condition to define N:

$$\langle E' l' m' | E l m\rangle = \int d^3k'' \, \langle E' l' m' | k''\rangle \langle k'' | E, l, m\rangle$$

$$= \int k''^2 dk'' \cdot \int d\Omega_{k''} \cdot |N|^2 \cdot \delta\left(\frac{\hbar^2 k''^2}{2m} - E'\right) \cdot \delta\left(\frac{\hbar^2 k''^2}{2m} - E\right) \cdot Y_{l'}^{m'*}(\hat{k}'') \, Y_l^m(\hat{k}'')$$

$$= \int \frac{k''^2 dE''}{dE''/dk''} \cdot \int d\Omega_{k''} \, |N|^2 \cdot \delta\left(\frac{\hbar^2 k''^2}{2m} - E'\right) \delta\left(\frac{\hbar^2 k''^2}{2m} - E\right) \cdot Y_{l'}^{m'*}(\hat{k}'') \, Y_l^m(\hat{k}'')$$

$$= |N|^2 \frac{m k'}{\hbar^2} \cdot \delta(E - E') \cdot \delta_{ll'} \delta_{mm'} \qquad E'' = \frac{\hbar^2 k''^2}{2m}$$

$$N = \frac{\hbar}{\sqrt{mk}}$$

$$g_{lE}(k) = \frac{\hbar}{\sqrt{mk}} \, \delta\left(\frac{\hbar^2 k^2}{2m} - E\right)$$

$$\langle k | E, l, m\rangle = \frac{\hbar}{\sqrt{mk}} \, \delta\left(\frac{\hbar^2 k^2}{2m} - E\right) Y_l^m(\hat{k})$$

Plane Wave can be expressed as superposition of free spherical wave states with all possible l values

$$|k\rangle = \sum_l \sum_m \int dE \, |E, l, m\rangle \langle E, l, m | k\rangle$$

$$= \sum_{l=0}^{+\infty} \sum_{m=-l}^{l} |E, l, m\rangle \Big|_{E=\hbar^2k^2/2m} \left(\frac{\hbar}{\sqrt{mk}} Y_l^{m*}(\hat{k})\right)$$

Spherical Wave state represented by position eigen kets

$$\langle x | E, l, m\rangle = C_l\, j_l(kr)\, Y_l^m(\hat{r})$$

Determin C_l

$$\langle x | k\rangle = \frac{e^{ik\cdot x}}{(2\pi)^{3/2}} = \sum_l \sum_m \int dE \cdot \langle x | E l m\rangle\langle E l m | k\rangle$$

$$= \sum_l \sum_m \int dE \cdot C_l\, j_l(kr)\, Y_l^m(\hat{r}) \frac{\hbar}{\sqrt{mk}} \delta\left(E - \frac{\hbar^2 k^2}{2m}\right) \cdot Y_l^{m*}(\hat{k})$$

$$= \sum_l \frac{(2l+1)}{4\pi} \cdot P_l(\hat{k}\cdot\hat{r}) \cdot \frac{\hbar}{\sqrt{mk}} C_l\, j_l(kr)$$

$$\sum_m Y_l^m(\hat{r}) Y_l^{m*}(\hat{r}) = \frac{2l+1}{4\pi} \cdot P_l(\hat{k}\cdot\hat{r})$$

$$\frac{e^{ik\cdot x}}{(2\pi)^{3/2}} = \sum_l \frac{1}{(2\pi)^{3/2}} \cdot \sum_l (2l+1) i^l \cdot j_l(kr) \cdot P_l(\hat{k}\cdot\hat{r})$$

(proved using $j_l(kr) = \frac{1}{2i^l} \cdot \int_{-1}^{+1} e^{ikr} P_l(\cos\theta)\, d(\cos\theta)$)

$$C_l = \frac{i^l}{\hbar} \sqrt{\frac{2mk}{\pi}}$$

In all

$$\langle k | E l m\rangle = \frac{\hbar}{\sqrt{mk}} \delta\left(E - \frac{\hbar^2 k^2}{2m}\right) Y_l^m(\hat{k})$$

$$\langle x | E l m\rangle = \frac{i^l}{\hbar} \sqrt{\frac{2mk}{\pi}}\; j_l(kr) \cdot Y_l^m(\hat{r})$$

Partial Wave Expansion.

If V is spherically symmetry, according to

$$T = V + V \frac{1}{E - H_0 + i\varepsilon} V + V \frac{1}{E - H_0 + i\varepsilon} V \frac{1}{E - H_0 + i\varepsilon} V \cdots$$

T commutes with L^2, L

T is a scalar operator (invarint under rotation)

(3.481) Wigner - Eckart Theorem

$$\langle \alpha' j' m' | S | \alpha j m\rangle = \delta_{jj'} \delta_{mm'} \frac{\langle \alpha' j' \| S \| \alpha j\rangle}{\sqrt{2j'+1}}$$

$$\langle E' l' m' | T | E, l, m\rangle = T_l(E)\, \delta_{ll'} \delta_{mm'}$$

Scattering Amplitude

(6.58)

$$f(k', k) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} L^3 \langle k' | T | k\rangle$$

$$\to -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \cdot \sum_l \sum_m \sum_{l'} \sum_{m'} \int dE \int dE' \langle k' | E' l' m'\rangle \langle E' l' m' | T | E l m\rangle \langle E l m | k\rangle$$

$$= -\frac{1}{4\pi} \frac{2m}{\hbar^2} \cdot (2\pi)^3 \frac{\hbar^2}{mk} \sum_{l,m} T_l(E) \Big|_{E=\hbar^2k^2/2m} \cdot Y_l^m(\hat{k}') Y_l^m(\hat{k})$$

($|k'|^2 = |k|^2$!!!)

Choose a coordinate that k is the positive z-direction.

$$\begin{cases} Y_l^m(\hat{k}) = \sqrt{\frac{2l+1}{4\pi}}\, \delta_{m,0} & \leftarrow P_l(1) = 1 \\ Y_l^0(\hat{k}') = \sqrt{\frac{2l+1}{4\pi}} \cdot P_l(\cos\theta) & \leftarrow \theta \text{ to be angle between } \hat{k} \text{ and } \hat{k}'. \end{cases}$$

Define Partial Wave amplitude

$$f_l(k) \equiv -\pi T_l(E)/k.$$

$$f(k', k) = f(\theta) = \sum_{l=0}^{+\infty} (2l+1) f_l(k) P_l(\cos\theta). \qquad (6.1.5)$$

Recall (6.57).

$$\langle x|\psi^{(+)}\rangle = \frac{1}{L^{3/2}}\left(e^{ik\cdot x} + \frac{e^{ikr}}{r} f(k',k)\right)$$

(6.104)

$$\left\{\begin{array}{l} \dfrac{e^{ik\cdot x}}{(2\pi)^{3/2}} = \dfrac{1}{(2\pi)^{3/2}}\cdot\sum_l (2l+1)\cdot i^l\cdot j_l(kr)\cdot P_l(\hat{k}\cdot\hat{r}) \\ j_l(kr) \xrightarrow{\text{large } r} \dfrac{e^{i(kr-\frac{l\pi}{2})} - e^{-i(kr-\frac{l\pi}{2})}}{2ikr} \\ i^l = e^{i\frac{\pi}{2}l} \end{array}\right.$$

$$\langle x|\psi^{(+)}\rangle \xrightarrow{\text{Larger}} \frac{1}{(2\pi)^{3/2}}\left(e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\right)$$

$$= \frac{1}{(2\pi)^{3/2}}\left(\sum_l (2l+1) P_l(\cos\theta)\cdot\left(\frac{e^{ikr} - e^{-i(kr-l\pi)}}{2ikr}\right) + \sum_l (2l+1)\cdot f_l(k)\cdot P_l(\cos\theta)\cdot\frac{e^{ikr}}{r}\right)$$

$$= \frac{1}{(2\pi)^{3/2}}\sum_l (2l+1)\frac{P_l(\cos\theta)}{2i|k|}\left([1+2ikf_l(k)]\frac{e^{ikr}}{r} - \frac{e^{-i(kr-l\pi)}}{r}\right)$$

Unitary and Phase shifts

(6.119) (6.120). There is no source or sink of particles. The outgoing flux must equal to incoming flux.

$$S_l(k) \equiv 1 + 2ikf_l(k)$$

Unitary relation

$$S_l(k) = e^{i2\delta_l} \Rightarrow f_l(k) = \frac{1}{k\cot\delta_l - ik} \qquad (6.125)$$

$$f(\theta) = \sum_{l=0} (2l+1)\cdot\left(\frac{e^{2i\delta_l}-1}{2ik}\right)\cdot P_l(\cos\theta)$$

$$= \frac{1}{k}\sum_{l=0} (2l+1)\, e^{i\delta_l}\sin\delta_l\, P_l(\cos\theta)$$

Total Cross section

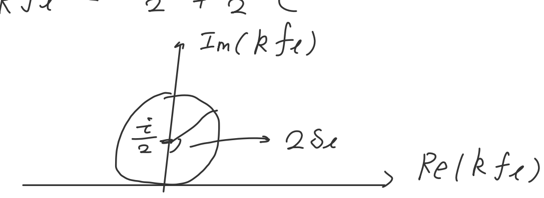
$$\sigma_{tot} = \int |f(\theta)|^2 d\Omega$$

$$= \frac{1}{k^2}\cdot\int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta)\cdot\sum_l\sum_{l'} (2l+1)(2l'+1)\, e^{i\delta_l}\sin\delta_l\, e^{-i\delta_{l'}}\sin\delta_{l'}\, P_l P_{l'}$$

$$= \frac{4\pi}{k^2}\sum_l (2l+1)\sin^2\delta_l$$

(6.125)

$$kf_l = \frac{i}{2} + \frac{1}{2}e^{-i\frac{\pi}{2}+2i\delta_l}$$



Determination of Phase Shifts.

Assume V vanishes outside of $r > R$.

suppose

$$\left\{\begin{array}{l} \langle x|\psi^{(+)}\rangle = \dfrac{1}{(2\pi)^{3/2}}\sum_l i^l (2l+1) A_l(r) P_l(\cos\theta). \qquad (r>R) \\ A_l = C_l^{(1)} h_l^{(1)}(kr) + C_l^{(2)} h_l^{(2)}(kr) \\ h_l^{(1)}(kr) = j_l(kr) + i n_l(kr) \quad h_l^{(2)}(kr) = j_l(kr) - i n_l(kr) \end{array}\right.$$

$$h_l^{(1)} \xrightarrow{r\ \text{large}} \frac{e^{i(kr - l\pi/2)}}{ikr}$$
$$h_l^{(2)} \xrightarrow{r\ \text{large}} -\frac{e^{-i(kr - l\pi/2)}}{ikr}$$

For large r (compare with (6.117))

$$\frac{1}{(2\pi)^{3/2}} \sum_l (2l+1) P_l(\cos\theta) \left(\frac{e^{2i\delta_l} e^{ikr}}{2ikr} - \frac{e^{-i(kr - l\pi)}}{2ikr} \right)$$

Must have $\begin{cases} C_l^{(1)} = \frac{1}{2} e^{2i\delta_l} \\ C_l^{(2)} = \frac{1}{2} \end{cases}$

So the radial Wave function for $r > R$

$$A_l(r) = e^{i\delta_l}[\cos\delta_l\, j_l(kr) - \sin\delta_l\, n_l(kr)]$$

To define the Phase shift, define

$$\beta_l \equiv \left(\frac{r}{A_l} \frac{dA_l}{dr} \right)\Big|_{r=R}$$
$$= kR \left(\frac{j_l'(kR)\cos\delta_l - n_l'(kR)\sin\delta_l}{j_l(kR)\cos\delta_l - n_l(kR)\sin\delta_l} \right)$$

$$\tan\delta_l = \frac{kR\, j_l'(kR) - \beta_l\, j_l(kR)}{kR\, n_l'(kR) - \beta_l\, n_l(kR)}$$

Schrodinger Equation inside the potential $r<R$. Equivalent to looking one-dimensional equation

$$\frac{d^2 u_l}{dr^2} + \left(k^2 - \frac{2m}{\hbar^2} V - \frac{l(l+1)}{r^2}\right) u_l = 0$$

$$u_l = r A_l(r)$$

$$u_l(r=0) = 0 \qquad \text{(boundary condition)}$$

$$\beta_l\big|_{\text{inside}} = \beta_l\big|_{\text{outside}} \qquad (6.144)$$

——— Hard - Sphere Scattering.

$$V = \begin{cases} \infty & r<R \\ 0 & r>R \end{cases}$$

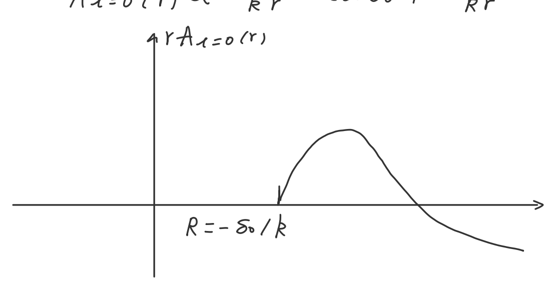
$$A_l(r)\big|_{r=R} = 0$$

$$j_l(kR)\cos\delta_l - n_l(kR)\sin\delta_l = 0$$

$$\tan\delta_l = \frac{j_l(kR)}{n_l(kR)}$$

$$\tan\delta_0 = \frac{\sin kR/kR}{-\cos kR/kR} \longrightarrow \delta_0 = -kR$$

$$A_{l=0}(r) \propto \frac{\sin kr}{kr}\cos\delta_0 + \frac{\cos kr}{kr}\sin\delta_0 = \frac{1}{kr}\sin(kr+\delta_0)$$



▽ Low energy $\quad kR$ small.

$$j_l(kr) \doteq \frac{(kr)^l}{(2l+1)!!}$$

$$n_l(kr) \doteq -\frac{(2l-1)!!}{(kr)^{l+1}}$$

$$\tan\delta_l = \frac{-(kR)^{2l+1}}{\{(2l+1)[(2l-1)!!]^2\}}$$

$$\frac{d\sigma}{d\Omega} = \frac{\sin^2\delta_0}{k^2} \simeq R^2 \quad \text{for } kR \ll 1 \qquad \sigma_{tot} = \int \frac{d\sigma}{d\Omega} d\Omega = 4\pi R^2$$

Gamow's theory of Alpha decay

(这里讲到的是Alpha衰变的理论;

量子跃迁.

Introduction to Quantum Mechanics中的十章. scattering理论.

量子散射理论: (incident plan wave):

$\psi(z) = A \cdot e^{ik\cdot z}$

$\psi(r,\theta) = A\left\{ e^{ik\cdot z} + \underbrace{f(\theta)\cdot\frac{e^{ikr}}{r}}_{\psi_{scatter}} \right\}$

generic form of solution:
wave number k is related to the incident energy. ($k = \sqrt{2mE}/\hbar$)

The probability of incident particle, traveling at speed v. pass through the infinitesimal area $d\sigma$ in time dt is:

$dP = |\psi_{incident}|^2 \cdot dV = A^2 \cdot \underline{\boxed{(v\cdot dt)}\boxed{d\sigma}}$ (射入) ? 例

This is equal to the probability that the particle scatters into the corresponding solid angle $d\Omega$.

$dP = |\psi_{scattered}|^2 \cdot dV = \frac{|A|^2 \cdot f^2}{r^2} \cdot (v\cdot dt) \cdot r^2 \cdot d\Omega$ (射出)?

入射面积

$|f(\theta)|^2 \cdot d\Omega = \boxed{d\sigma}$

$D(\theta) = d\sigma/d\Omega = |f(\theta)|^2$

Formalism (形式理论? 不确定是不是这样翻译的)

$\psi(r,\theta,\phi) = R(r)\cdot Y_l^m(\theta,\phi)$

$u(r) = r\cdot R(r)$ satisfies the radial Equation:

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V(r) + \frac{\hbar^2}{2m}\cdot\frac{l(l+1)}{r^2}\right]\cdot u = E\cdot u.$$

(radiation zone)

At very large r. The contribution of potential and centrifugal goes to 0.

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} = Eu$$

$$u = C\cdot e^{ikr} + D\cdot e^{-ikr} \Rightarrow u = C\cdot e^{ik\cdot r} \qquad R(r) = \frac{u(r)}{r} = \frac{1}{r}C\cdot e^{ik\cdot r}$$

outgoing incoming one

In the intermedium zone, the potential can be ignored while the centrifugal can not:

$$\frac{d^2u}{dr^2} - \frac{l(l+1)}{r^2}\cdot u = -k^2\cdot u$$

$u(r) = A\cdot r\cdot j_l(kr) + B\cdot r\cdot n_l(k\cdot r)$ (linear combination of Bessel Fun)

We need a linear combination analogous to e^{ikr} and e^{-ikr}:

$$h_l^{(1)}(x) = j_l(x) + i n_l(x) \qquad h_l^{(2)}(x) = j_l(x) - i n_l(x)$$

We need $R(r) \sim h_l^{(1)}(x)$

$$\psi(r,\theta,\varphi) = A\left[e^{ik\cdot z} + \sum_{l,m} C_{l,m}\cdot h_l^{(1)}(k\cdot r)\cdot Y_l^m(\theta,\varphi)\right]$$

We don't want the wave function to depend on φ:

$m = 0$

$$Y_l^0(\theta) = \sqrt{\frac{2l+1}{4\pi}}\cdot P_l(\cos\theta).$$

$$C_{l,0} = i^{l+1}\cdot k\cdot\sqrt{4\pi(2l+1)}\cdot a_l$$

$$\psi(r,\theta) = A\cdot\left\{e^{ikz} + k\cdot\sum_{l=0}^{+\infty} i^{l+1}\cdot(2l+1)a_l\cdot h_l^{(1)}(kr)\cdot P_l(\cos\theta).\right\}$$

$$D(\theta) = |f(\theta)|^2 = \sum_l\sum_{l'}(2l+1)(2l'+1)\cdot P_l(\cos\theta)\,P_{l'}(\cos\theta)$$

Phase shift:

$$\psi_i(x) = Ae^{ikx} \qquad \psi_r = Be^{-ikx} \quad (|B| = |A|).$$

$$\psi(x) = A(e^{ik\cdot x} - e^{-ik\cdot x})$$