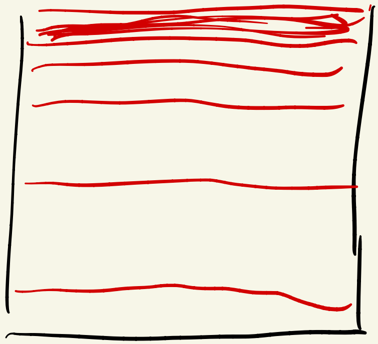
SPUM 202 Lecture 4.

– Spectrum (光谱).

$\mathcal{H}$.



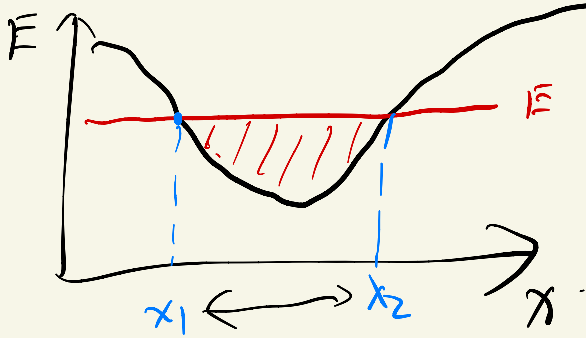

$\hat{\mathcal{H}} \Psi_{nlm_l} = E_n \Psi_{nlm_l}$

$E_n$.

The eigenfunction of an observable gives us a series of eigenvalues. The collection of all the eigenvalues is called the spectrum

* Discrete spectrum.

Def: one eigenfunction represent one wavefunction. (bond-state).




potential well.

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

$E_n = \hbar(n + \frac{1}{2})$, $n = 0 \ldots$

* Continuous spectrum.

The wave fuction is a linear combination of eigenfuctions

Ex: free particle, $\hat{H} = \frac{p^2}{2m}$

electron-gas

Task: Discrete → continuous.

$$\sum \to \int d\xi.$$

Assume we have an Hermatian operator $\hat{A}$ and its eigenfuctions: $\{|a\rangle\}$.

So, for $|a\rangle, |a'\rangle \in \{|a\rangle\}$

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

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

For discrete case.

$$\langle a'|a''\rangle = \delta_{a'a''} = \begin{cases} 0 & a' \neq a'' \\ 1 & a' = a'' \end{cases}$$

Kronecker-delta.

$\hat{B}$ represent a continuous spectrum. $\{|b\rangle\}$

$$\langle b'|b''\rangle = \delta(b'-b'').$$

Dirac' Delta fution.

- Normalization

① $$\sum_{a'} |a'\rangle\langle a'| = 1 \rightarrow$$ ② $$\int db' \, |b'\rangle\langle b'| = 1.$$

- State representation.

① $$|\alpha\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle \rightarrow$$ ② $$|\alpha\rangle = \int db' |b'\rangle\langle b'|\alpha\rangle$$

- Normalization of coefficient.

① $$\sum_{a'} |\langle a'|\alpha\rangle|^2 = 1$$ ② $$\int db' \, |\langle b'|\alpha\rangle|^2 = 1$$

- Matrix element

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

$$\langle b'' | \hat{B} | b' \rangle = \int db' \, b' \delta(b' - b'')$$

- position $\hat{x}$

$$x = (x, y, z) = (x_1, x_2, x_3).$$

$\hat{x}$ can generate a set of continuous spectrum

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

For arbitrary physical state $|\alpha\rangle$.

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

Integrate on the entire space.

In practice, the best detector can do is to locate the particle within a narrow interval around $x''$. The range is $\left(x'' - \frac{\Delta}{2}, x'' + \frac{\Delta}{2}\right)$ undergoing this measurement, the state $|\alpha\rangle$ becomes

$$|\alpha\rangle = \int_{-\infty}^{+\infty} dx' \, |x'\rangle\langle x'|\alpha\rangle \to \int_{x''-\frac{\Delta}{2}}^{x''+\frac{\Delta}{2}} dx' \, |x'\rangle\langle x'|\alpha\rangle$$

$(-\infty, +\infty)$ $\xrightarrow{\text{Detect}}$ $(x''-\frac{\Delta}{2}, x''+\frac{\Delta}{2})$.

$$|x'\rangle = |x', y', z'\rangle = \underline{|x_1', x_2', x_3'\rangle}.$$

$$[x_i, x_j] = 0$$

$$x_i x_j - x_j x_i = 0$$

— Translation.

Infinitesmal translation operator. $\hat{T}(dx)$.

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

Question, $\hat{T}^{+} = \hat{T}^{-1}$ ? $(\hat{T}^{+}\hat{T} = I)$.

The answer is yes! $\hat{T}$ is unitary.

That means

$$\hat{T}^{+}(dx) = \hat{T}(-dx).$$

proof: Starting from an arbitrary state $|\alpha\rangle$.

$$\hat{T}(dx)\,|\alpha\rangle = \hat{T}(dx) \int d^3x \, |x\rangle\langle x|\alpha\rangle$$

$$= \int d^3x \ \hat{T}(dx)\,|x\rangle\langle x|\alpha\rangle.$$

$$= \int d^3x \ |x + dx\rangle\langle x|\alpha\rangle. \quad (*)$$

If we replace $x$ by $x' - dx$.

$$(*) = \int d^3(x' - dx) \ |x'\rangle\langle x' - dx|\alpha\rangle.$$

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

$$= \int d^3x \ |x\rangle\langle x - dx|\alpha\rangle$$

$$= \int d^3x \ |x\rangle\langle x| \left(T^{+}(dx)\right)^{+} |\alpha\rangle$$

But $\boxed{\hat{T}(dx)|\alpha\rangle} = \int d^3x \ |x\rangle\langle x| \boxed{\hat{T}(dx)|\alpha\rangle}$

$$\Rightarrow \langle x - dx| = \langle x|\hat{T}(dx)$$

$$= \langle x| \left(\hat{T}^{+}(dx)\right)^{+}.$$

$$= \langle x| \left(\hat{T}(-dx)\right)^{+}$$

$\Rightarrow \hat{T}^{\dagger}(dx) = \hat{T}(-dx)$.

or. $\hat{T}^{\dagger}\hat{T} = I$ . , $\hat{T}$ is unitary .

— Momentum.

Def: The quantity due to the translational symmetry of space

As we dissussed about the infinitesmal translation

$$\hat{T}^{\dagger}\hat{T} = I \quad , \quad \lim_{dx\to 0} \hat{T}(x) = 1 .$$

we could construct $\hat{T}(dx)$ as.

$$\hat{T}(dx) = \underbrace{1}_{\text{unit less}} - i \underbrace{\hat{k}}_{1/\text{length}} \cdot \underbrace{dx}_{\text{length}}$$

where $\hat{k}^{\dagger} = \hat{k}$

From the symmetry of space, $\hat{k}$ should have some relation with momentum $\hat{p}$.

$$\hat{k} = \frac{p}{\hbar} .$$

From the unit of $\hat{T}$, $\hat{k}$ should have unit $1/\text{length}$.

de Broglie. 1924.

$$\frac{2\pi}{\lambda} = \frac{p}{\hbar}$$ matter wave.

wave length. (1/length).

$$\Rightarrow \quad \hat{k} = \frac{2\pi}{\lambda} = \frac{p}{\hbar}$$

$\hbar \to$ reduced plank constant.

wavenumber.

$$\hbar = \frac{h}{2\pi}$$

$h \to$ planck...

So, the translation operator becomes

$$\boxed{\hat{T}(dx) = 1 - i\frac{p}{\hbar}dx.}$$

— Commutation relation.

$$[X_i, \hat{P}_j] = ?$$

starting from $[\hat{x}, \hat{T}(dx)]$

For $\forall |x\rangle \in \mathcal{H}$.

$$\begin{cases} \hat{x}\hat{T}(dx)|x\rangle = \hat{x}|x+dx\rangle = (x+dx)|x+dx\rangle. \\ \hat{T}(dx)\hat{x}|x\rangle = \hat{T}(dx)x|x\rangle = x|x+dx\rangle. \end{cases}$$

$$\Rightarrow [x, \hat{T}(dx)] = dx \quad (*).$$

Bring $\hat{T}(dx) = 1 - i\frac{p}{\hbar}\cdot dx$ in (*)

(*) $= [\hat{x}, 1 - i\frac{p}{\hbar}\cdot dx] = [\hat{x}, 1] - [\hat{x}, \frac{ip}{\hbar}\cdot dx]$

$= -\frac{i}{\hbar}[\hat{x}, p\cdot dx] = dx.$

$\Leftrightarrow \boxed{[\hat{x}, p\cdot dx] = i\hbar\, dx}.$

As. $dx = (dx_1, dx_2, dx_3).$

$RHS = i\hbar(dx_1, dx_2, dx_3).$

$LHS = \hat{x}(p\cdot dx) - (p\cdot dx)\hat{x}$

$= \left(x_1 \sum_l p_l dx_l - \sum_l p_l dx_l\, x_1, \ \cdots\cdots \right).$

LHS = RHS. using Rank2 tensor form.

$$\begin{bmatrix} [x_1, p_1]dx_1 & [x_1, p_2]dx_2 & [x_1, p_3]dx_3 \\ [x_2, p_1]dx_1 & [x_2, p_2]dx_2 & [x_2, p_3]dx_3 \\ [x_3, p_1]dx_1 & [x_3, p_2]dx_2 & [x_3, p_3]dx_3 \end{bmatrix}$$

$$= i\hbar \begin{bmatrix} dx_1 & 0 & 0 \\ 0 & dx_2 & 0 \\ 0 & 0 & dx_3 \end{bmatrix}$$

$$\Rightarrow \boxed{[x_i, p_j] = i\hbar\,\delta_{ij}}$$

$$[p_i, p_j] = 0, \quad [x_i, x_j] = 0$$

— General translation:

$$\hat{T}(x) = \exp\left(-\frac{i p \cdot x}{\hbar}\right)$$

$$= 1 - \frac{i}{\hbar} p \cdot x + o((p \cdot x)^2)$$

if $x = dx$.

$$\hat{T}(dx) = 1 - \frac{i}{\hbar} \vec{p} \cdot d\vec{x}$$

Remarks: $[\hat{p}, \hat{T}] = 0$.

proof: $[p, 1] = 0$, $[p, p] = 0$

— Canonical commutation relation.

$q, p$ . $\{\ ,\ \}$ possion bracket.

Def: $[x_i, x_j] = 0 = [p_i, p_j]$,

$$[x_i, p_j] = i\hbar\delta_{ij}$$

Remem from classical mechanics, the possion bracket,

$$\{A, B\} = \sum_i \left( \frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i} \right)$$

let $A = x_i$, $B = p_j$, we get

$$\{x_i, p_j\} = \delta_{ij} = \frac{1}{i\hbar}[x_i, p_j]$$

classical — quantum

Dirac's rule.

Remarks.

(1) $[A, A] = 0$

(2) $[A, B] = -[B, A]$

(3) $[A, C] = 0$. C is a number.

(4) $[A+B, D] = [A, D] + [B, D]$.

(5) $[A, BD] = [A, B]D + B[A, D]$

(6) (Jacobi identity).

$$[A, [B, D]] + [B, [D, A]] + [D, [A, B]] = 0.$$

$\Leftrightarrow$

$$[x_i, [x_j, x_k]] = 0$$