CONTINUOUS SPECTRA (ONLY)

set λ_μ solve for $|f_\mu\rangle$ for a given λ_μ

$$\checkmark \quad \hat{F}|f_\mu\rangle = \lambda_\mu |f_\mu\rangle$$

μ is a continuous variable

$\lambda_\mu \equiv \lambda(\mu)$ is a function of μ.

$f_\mu(q) \equiv f(q;\mu)$ is a function of q parameterized by μ!

$q_1, \ldots, q_f$

$\mu \longrightarrow \mu + \Delta\mu$, $\lambda_\mu \longrightarrow \lambda_{\mu+\Delta\mu}$:

$|f_{\mu+\Delta\mu}\rangle$ or $f_{\mu+\Delta\mu}(q)$

is a solution corresponding to $\lambda_{\mu+\Delta\mu}$.

Example:

$$\hat{F} = \hat{p}_x = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

$$\hat{p}_x u_k(x) = \hbar k\, u_k(x)$$

$$u_k(x) = A e^{ikx}, \quad \int_{-\infty}^{\infty} |u_k(x)|^2 dx = \infty$$

Conventional normalization does not work.

We will prove that $|f_\mu\rangle$ is orthogonal to $|f_\nu\rangle$ if $\mu \neq \nu$.

We start from the statement that all $|f_\mu\rangle$s form a complete set,

$$|\varphi\rangle = \int c_\mu |f_\mu\rangle \, d\mu \quad W$$

$$\varphi(q) = \int c_\mu f_\mu(q) \, d\mu$$

In a discrete case (assuming $\|\varphi\|=1$)

$$|c_\mu|^2 = P(F=\lambda_\mu)$$

In a continuous case

$|c_\mu|^2 d\mu$ = probability that F has a value from the interval $(\lambda_\mu, \lambda_\mu + d\lambda_\mu)$

√ $|c_\mu|^2 d\mu = P[FE(\lambda_\mu, \lambda_\mu + d\lambda_\mu)]$

Assuming that $\|\varphi\| = 1$,

$$\int \varphi^*(q)\varphi(q)\, d\tau = 1$$

$$\int \underbrace{|c_\mu|^2 d\mu}_{P[FE(\lambda_\mu, \lambda_\mu + d\lambda_\mu)]} = 1$$ √

$$1 = \langle \varphi | \varphi \rangle = \left\langle \int c_\mu f_\mu \, d\mu \middle| \varphi \right\rangle$$

$$\left.\begin{aligned} &= \int c_\mu^* \langle f_\mu | \varphi \rangle \, d\mu \\ &= \int c_\mu^* c_\mu \, d\mu \end{aligned}\right\}$$

$$\int c_\mu^* \overbrace{\left[\langle f_\mu|\varphi\rangle - c_\mu\right]}^{0} d\mu$$
$$= 0$$

$$c_\mu = \langle f_\mu|\varphi\rangle$$ (as in discrete case)

Orthogonality of $|f_\mu\rangle$s:

$$c_\mu = \langle f_\mu|\varphi\rangle$$
$$= \langle f_\mu| \int c_\nu f_\nu \, d\nu \rangle$$
$$= \int c_\nu \langle f_\mu|f_\nu\rangle d\nu$$

Compare this with

✓ $$\int f(x)\,\delta(x-y)\,dx = f(y)$$

$$c(\mu) = \int c(\nu)\, g(\mu,\nu)\, d\nu$$

$$g(\mu,\nu) = \langle f_\mu | f_\nu \rangle$$

$$g(\mu,\nu) = \delta(\mu-\nu)$$

$$\int c(\nu)\, \delta(\mu-\nu)\, d\nu = c(\mu)$$

$$\langle f_\mu | f_\nu \rangle = \delta(\mu-\nu)$$

If $\mu \neq \nu$, $\langle f_\mu | f_\nu \rangle = 0$.

$$|f_\mu\rangle \perp |f_\nu\rangle$$

(again similar to discrete case)

Closure :

$$\varphi(q) = \int \overset{\langle f_\mu | \varphi \rangle}{c_\mu} \, f_\mu(q) \, d\mu$$

$$\langle f_\mu | \varphi \rangle = \int_\Gamma f_\mu^*(q') \, \varphi(q') \, d\tau'$$

$$\varphi(q) = \int d\mu \int_\Gamma d\tau' \, f_\mu^*(q') \, \varphi(q') \, f_\mu(q)$$

$$= \int_\Gamma d\tau' \, \varphi(q') \int d\mu \, f_\mu^*(q') \, f_\mu(q)$$

$$\varphi(q) = \int_\Gamma d\tau' \, \varphi(q') \left[\int f_\mu^*(q') \, f_\mu(q) \, d\mu \right]$$

$$\varphi(q) = \int_\Gamma \varphi(q') \, \delta(q' - q) \, d\tau'$$

$$\delta(q'-q) = \prod_{l=1}^{f} \delta(q_l'-q_l)$$

$$\int f_\mu^*(q')\, f_\mu(q)\, d\mu = \delta(q'-q)$$

(in a discrete case,

$$\sum_\mu f_\mu^*(q')\, f_\mu(q) = \delta(q'-q))$$

Parseval's relation:

$$\langle\varphi|\psi\rangle = \int_\Gamma \varphi^*(q)\,\psi(q)\,d\tau$$

$$= \int_\Gamma\int_\Gamma \varphi^*(q)\,\delta(q'-q)\,\psi(q')\,d\tau\, d\tau'$$

$$= \int_{\Gamma} \int_{\Gamma} \varphi^{*}(q) \left[\int f_{\mu}^{*}(q') f_{\mu}(q) \, d\mu \right] \times \psi(q') \, d\tau' \, d\tau$$

$$= \int d\mu \left[\int_{\Gamma} \varphi^{*}(q) f_{\mu}(q) \, d\tau \right] \times \left[\int_{\Gamma} f_{\mu}^{*}(q') \psi(q') \, d\tau' \right]$$

$$= \int d\mu \, \langle \varphi | f_{\mu} \rangle \langle f_{\mu} | \psi \rangle$$

$$\langle \varphi | \psi \rangle = \int \langle \varphi | f_{\mu} \rangle \langle f_{\mu} | \psi \rangle \, d\mu$$

(in a discrete case,

$$\langle\varphi|\psi\rangle = \sum_\mu \langle\varphi|f_\mu\rangle\langle f_\mu|\psi\rangle)$$

$$\int |f_\mu\rangle\langle f_\mu| \, d\mu = \mathbb{1}$$

Expectation value:

In a discrete case

$$\sum_\mu \lambda_\mu P(F=\lambda_\mu) \quad \checkmark$$

$$= \sum_\mu \lambda_\mu |c_\mu|^2 = \ldots =$$

$$= \langle\varphi|\hat{F}|\varphi\rangle$$

Continuous case:

$$\langle \hat{F} \rangle = \int \lambda_\mu \, \underbrace{P[F \in (\lambda_\mu, \lambda_\mu + d\lambda_\mu)]}_{|c_\mu|^2 \, d\mu}$$

$$= \int \lambda_\mu |c_\mu|^2 \, d\mu$$

$$= \int \lambda_\mu \, c_\mu^* c_\mu \, d\mu$$

$$c_\mu = \langle f_\mu | \varphi \rangle$$

$$= \int \lambda_\mu \langle f_\mu | \varphi \rangle^* \langle f_\mu | \varphi \rangle \, d\mu$$

$$\overset{(a)}{=} \int \lambda_\mu \langle \varphi | f_\mu \rangle \langle f_\mu | \varphi \rangle \, d\mu$$

$$= \int \langle \varphi | \underbrace{\lambda_\mu f_\mu}_{\hat{F}|f_\mu\rangle} \rangle \langle f_\mu | \varphi \rangle \, d\mu$$

$$= \int \langle \varphi | \hat{F} f_\mu \rangle \langle f_\mu | \varphi \rangle \, d\mu$$

$$\overset{\text{TOR}}{=} \int \langle \hat{F} \varphi | f_\mu \rangle \langle f_\mu | \varphi \rangle \, d\mu$$

$$\overset{\text{closure}}{=} \langle \hat{F} \varphi | \varphi \rangle \overset{\text{TOR}}{=} \langle \varphi | \hat{F} \varphi \rangle$$

$$\langle \hat{F} \rangle = \langle \varphi | \hat{F} | \varphi \rangle$$

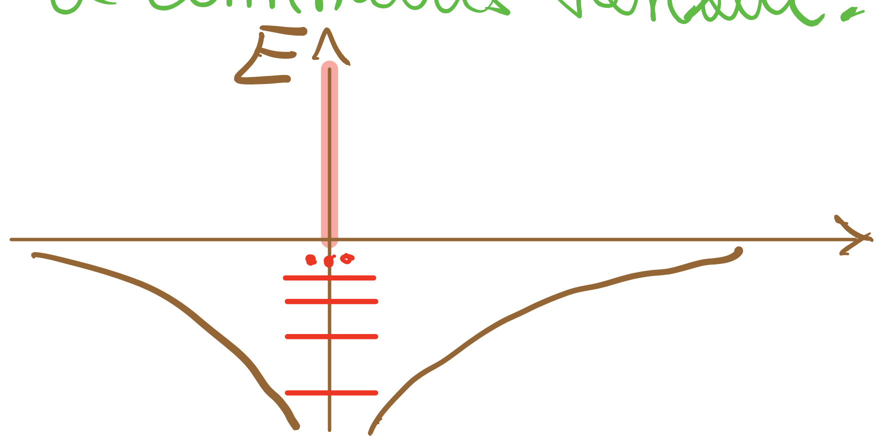
$$(\|\varphi\| = 1)$$

GENERAL CASE (DISCRETE & CONTINUOUS SPECTRA)

$$\hat{F}|f_\mu\rangle = \lambda_\mu |f_\mu\rangle$$

In a discrete case, μ has discrete values, λ_μs are eigenvalues.

In a continuous case, μ is a continuous variable.



$\{|f_\mu\rangle\}$ is complete:

$$|\varphi\rangle = \sum_\mu c_\mu |f_\mu\rangle$$ ← sum over μ

(discrete part)

$$+ \int c_\mu |f_\mu\rangle \, d\mu$$ ← integrate over μ

(continuous part)

$$c_\mu = \langle f_\mu | \varphi \rangle .$$

New symbol

$\mathop{S}_\mu$ → $\sum_\mu$ in a discrete case

$\mathop{S}_\mu$ → $\int d\mu$ in a continuous case

$$|\varphi\rangle = S_\mu\, c_\mu |f_\mu\rangle$$

$$\sum_\mu |c_\mu|^2 + \int |c_\mu|^2 d\mu$$

$$= 1 \text{ if } \|\varphi\| = 1$$

$$S_\mu |c_\mu|^2 = 1 .$$

Closure:

$$\sum_\mu f_\mu^*(q') f_\mu(q)$$

$$+ \int f_\mu^*(q') f_\mu(q)\, d\mu$$

$$= \int_\mu f_\mu^*(q') f_\mu(q)$$

$$= \delta(q'-q).$$

In a discrete part of the spectrum,

$$\langle f_\mu | f_\nu \rangle = \delta_{\mu\nu}.$$

In a continuous part,

$$\langle f_\mu | f_\nu \rangle = \delta(\mu-\nu).$$

Resolution of identity,

$$\sum_\mu |f_\mu\rangle\langle f_\mu| + \int |f_\mu\rangle\langle f_\mu| d\mu$$

$$= \mathbb{1} = \mathcal{S}_\mu |f_\mu\rangle\langle f_\mu|$$

Spectral theorem:

$$\hat{F} = \sum_\mu \lambda_\mu |f_\mu\rangle\langle f_\mu| \checkmark$$

$$+ \int \lambda_\mu \checkmark |f_\mu\rangle\langle f_\mu| \, d\mu$$

$$= \mathcal{S}_\mu \lambda_\mu |f_\mu\rangle\langle f_\mu|$$

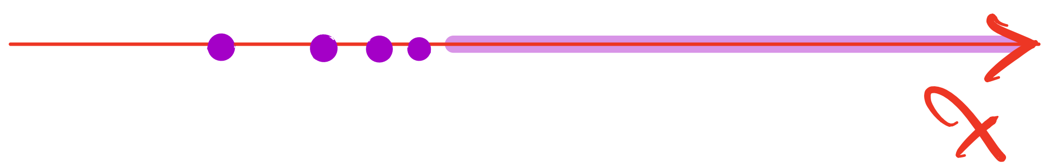
$$\hat{F} = \mathcal{S}_\mu \lambda_\mu P_{\langle f_\mu \rangle}$$

Expectation value: discrete

$$\langle \hat{F} \rangle = \sum_{\mu} \lambda_{\mu} |c_{\mu}|^2 \qquad (\|\varphi\|=1)$$

$$+ \int \lambda_{\mu} |c_{\mu}|^2 \, d\mu$$

continuous



$$\langle \hat{F} \rangle = \langle \varphi | \hat{F} | \varphi \rangle .$$

Example of a continuous spectrum: momentum operator in 3D

$$\hat{\vec{p}} = (\hat{p}_x, \hat{p}_y, \hat{p}_z)$$

$$\hat{p}_x = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

$$\hat{p}_y = \frac{\hbar}{i}\frac{\partial}{\partial y}$$

$$\hat{p}_z = \frac{\hbar}{i}\frac{\partial}{\partial z}$$

$$\left(\hat{\vec{p}} = \frac{\hbar}{i}\vec{\nabla}\right)$$

$$\hat{\vec{p}}\, u_{\vec{p}} = \vec{p}\, u_{\vec{p}}$$

$$\frac{\hbar}{i}\frac{\partial}{\partial x} u_{\vec{p}}(x, y, z)$$

$$= p_x\, u_{\vec{p}}(x, y, z)$$

$$(x, y, z) = \vec{r}$$

$$\frac{\hbar}{i}\frac{\partial}{\partial y}u_{\vec{p}}(\vec{r}) = p_y u_{\vec{p}}(\vec{r})$$

$$\frac{\hbar}{i}\frac{\partial}{\partial z}u_{\vec{p}}(\vec{r}) = p_z u_{\vec{p}}(\vec{r})$$

$$u_{\vec{p}}(\vec{r}) = Ce^{i(\vec{p}\cdot\vec{r})/\hbar}$$

$$= Ce^{i(p_x x + p_y y + p_z z)/\hbar}$$

$$\frac{\vec{p}}{\hbar} = \vec{k} \quad \checkmark$$

$$u_{\vec{p}}(\vec{r}) = Ce^{i\vec{k}\cdot\vec{r}}$$

$$= Ce^{i(k_x x + k_y y + k_z z)}$$

(in 1D, $\hat{p}_x u_p(x) = p_x u_p(x)$)

$$u_{\vec{k}}(\vec{r}) = C e^{i\vec{k}\cdot\vec{r}}$$

$$\hat{\vec{p}}\, u_{\vec{k}}(\vec{r}) = (\hbar \vec{k})\, u_{\vec{k}}(\vec{r})$$

$$\langle f_\mu | f_\nu \rangle = \delta(\mu - \nu)$$

$$\langle u_{\vec{\ell}} | u_{\vec{k}} \rangle = \int_{\mathbb{R}^3} u_{\vec{\ell}}(\vec{r})^* u_{\vec{k}}(\vec{r})\, dx\, dy\, dz$$

$$= |C|^2 \int_{-\infty}^{\infty} e^{i(k_x - \ell_x)x}\, dx$$

$2\pi\delta(k_x - \ell_x)$

$$\times \int_{-\infty}^{\infty} e^{i(k_y - \ell_y)y}\, dy$$

$2\pi\delta(k_y - \ell_y)$

$$\times \int_{-\infty}^{\infty} e^{i(k_z - l_z)z}\, dz$$

$$2\pi\,\delta(k_z - l_z)$$

$$u_{\vec{k}}(\vec{r}) = C e^{ik_x x} e^{ik_y y} \times e^{ik_z z}$$

$$\int_{-\infty}^{\infty} e^{iax}\, dx = 2\pi\,\delta(a)$$

$$\langle u_{\vec{l}} | u_{\vec{k}} \rangle = (2\pi)^3 |C|^2 \times \delta(k_x - l_x)\,\delta(k_y - l_y) \times \delta(k_z - l_z)$$

$$= \delta(\vec{k} - \vec{l})$$

$$\langle u_{\vec{l}} | u_{\vec{k}} \rangle = (2\pi)^3 |C|^2$$

$$\times \delta(\vec{k} - \vec{l})$$

$$= \delta(\vec{k} - \vec{l})$$

$$(2\pi)^3 |C|^2 = 1$$

$$C = \frac{1}{(2\pi)^{3/2}}$$

$$u_{\vec{k}}(\vec{r}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{r}} \leftarrow$$

$$\langle u_{\vec{l}} | u_{\vec{k}} \rangle = \delta(\vec{k} - \vec{l})$$

$\checkmark$

In 1D,

$$\hat{p}_x u_k(x) = \hbar k\, u_k(x)$$

$$u_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

$$\langle u_\ell | u_k \rangle = \delta(k-\ell)$$

Closure:

$$\int f_\mu^*(q') f_\mu(q)\, d\mu$$
$$= \delta(q'-q)$$

$$\int u_{\vec{k}}^*(\vec{r}\,')\, u_{\vec{k}}(\vec{r})\, dk_x dk_y dk_z$$

$$= \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} e^{ik_x(x-x')} dk_x$$

$$\times \int_{-\infty}^{\infty} e^{ik_y(y-y')} dk_y$$

$$\times \int_{-\infty}^{\infty} e^{ik_z(z-z')} dk_z$$

$$\int_{-\infty}^{\infty} e^{iax} dx = 2\pi\,\delta(a)$$

$$= \frac{1}{\cancel{(2\pi)^3}} \cancel{2\pi}\,\delta(x-x')$$

$$\times \cancel{2\pi}\,\delta(y-y')$$

$$\times \cancel{2\pi}\, \delta(z-z')$$

$$= \delta(x-x')\,\delta(y-y')\,\times\,\delta(z-z')$$

$$= \delta(\vec{r}-\vec{r}\,')$$

$$\int u_{\vec{k}}(\vec{r}\,')^{*}\, u_{\vec{k}}(\vec{r})\, dk_x\, dk_y\, dk_z = \delta(\vec{r}-\vec{r}\,')$$

In 1D,

$$\int_{-\infty}^{\infty} u_k(x')^{*}\, u_k(x)\, dk = \delta(x'-x)$$