态的表象：

笛卡尔坐标 ⟶ 极坐标

坐标表象 ⟶ 动量表象

$\hat{p}\psi_p = \lambda_p \psi_p$

- 例2：坐标表象的波函数$\Psi(x,t)$→动量表象的函数$c(p,t)$
  - 利用坐标表象下的动量的本征函数 $\phi_p(x)=(2\pi\hbar)^{-1/2}e^{ipx/\hbar}$

$$\Psi(x,t)=\int c(p,t)\phi_p(x)\mathrm{d}p,\quad c(p,t)=\int \phi_p^*(x)\Psi(x,t)\mathrm{d}x$$

  - 利用Ψ的归一化条件

$$1=\int|\Psi(x,t)|^2\,\mathrm{d}x=\int|c(p,t)|^2\,\mathrm{d}p$$

  - $|\Psi(x,t)|^2\mathrm{d}x$：测量粒子的位置，在$x\to x+\mathrm{d}x$范围的概率
    $|c(p,t)|^2\mathrm{d}p$：测量粒子的动量，在$p\to p+\mathrm{d}p$范围的概率
  - 动量表象的具体表示方式指自变量p和基函数ϕ_p，实质上就是动量算符的本征值和本征函数

- 力学量Q的表象：只有分立本征值Q_n，本征函数是$u_n(x)$
  - 利用u_n展开(任意的)波函数Ψ

$$\Psi(x,t)=\sum_n a_n(t)u_n(x),\quad a_n(t)=\int u_n^*(x)\Psi(x,t)\mathrm{d}x$$

  - 利用Ψ的归一化条件

$$1=\int|\Psi(x,t)|^2\,\mathrm{d}x=\sum_n|a_n(t)|^2$$

  - $|a_n(t)|^2$：在$\Psi(x,t)$描写的态中测量力学量Q，结果为Q_n的概率
  - $\{a_1(t),a_2(t),\ldots,a_n(t),\ldots\}$：$\Psi(x,t)$所描写的态在$Q$表象中的表示
  - $\Psi(x,t)$及其共轭在Q表象中的表示写为矩阵形式

$$\Psi=\begin{bmatrix}a_1(t)\\a_2(t)\\\vdots\\a_n(t)\\\vdots\end{bmatrix},\quad \Psi^+=\begin{bmatrix}a_1^*(t) & a_2^*(t) & \cdots & a_n^*(t) & \cdots\end{bmatrix}\Rightarrow \Psi^+\Psi=1$$

- 力学量Q的表象：有分立本征值$Q_n(u_n)$，又有连续本征值$q(u_q)$
  - 利用u_n和u_q展开(任意的)波函数Ψ

$$\Psi(x,t)=\sum_n a_n(t)u_n(x)+\int a_q(t)u_q(x)\mathrm{d}q$$

$$a_n(t)=\int u_n^*(x)\Psi(x,t)\mathrm{d}x,\qquad a_q(t)=\int u_q^*(x)\Psi(x,t)\mathrm{d}x$$

  - 利用Ψ的归一化条件

$$1=\int|\Psi(x,t)|^2\,\mathrm{d}x=\sum_n|a_n(t)|^2+\int|a_q(t)|^2\,\mathrm{d}q$$

  - $|a_n(t)|^2$ ：在$\Psi(x,t)$的态中测量力学量Q，结果为Q_n的概率
  - $|a_n(t)|^2\mathrm{d}q$：结果为$q\to q+\mathrm{d}q$的概率
  - $\Psi(x,t)$及其共轭在Q表象中的表示写为矩阵形式

$$\Psi=\begin{bmatrix}a_1(t)\\a_2(t)\\\vdots\\a_n(t)\\\vdots\\a_q(t)\end{bmatrix},\quad \Psi^+=\begin{bmatrix}a_1^*(t) & a_2^*(t) & \cdots & a_n^*(t) & \cdots & a_q^*(t)\end{bmatrix}\Rightarrow \Psi^+\Psi=1$$

- 基矢
  - 对于展开式$\Psi(x,t)=\sum a_n(t)u_n(x)$和$\Phi(x,t)=\sum b_n(t)u_n(x)$，$u_n(x)$类似于直角坐标系中，$x,y,z$三个方向上的基本单位矢量 $\vec{e}_x,\vec{e}_y,\vec{e}_z$。称力学量$Q$的本征函数$u_n(x)$为基矢
  - 例：动量表象的基矢是动量的本征函数 $\phi_p(x)=(2\pi\hbar)^{-1/2}e^{ipx/\hbar}$
- 态矢量
  - 选定特定的Q表象，相当于选取一组特定的基矢。$\Psi(x,t)$在各个基矢上有各自的分量，类似于直角坐标系的矢量。称态Ψ为态矢量
  - 例：动量表象中，Ψ在各基矢上分量是 $c(p,t)=\int\phi_p^*(x)\Psi(x,t)dx$
- 希耳伯特空间
  - 类似基本单位矢量 $\vec{e}_x,\vec{e}_y,\vec{e}_z$形成三维空间。$Q$表象下的一组基矢(一般是无限个)形成无限维空间，称为希耳伯特空间
  - 例：在动量表象中，动量的本征函数所张开的动量空间

动量表象

薛定谔：$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2}+U(x)\right]\psi(x)=E\psi(x)$ // 一维定态

$$\psi(x)=\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}\varphi(p')\underbrace{e^{ip'x/\hbar}}_{\phi_{p'}(x)}dp'$$

代入

$$0=\iint\phi_p^*\varphi\frac{p'^2}{2\mu}\phi_{p'}\mathrm{d}p'\mathrm{d}x+\iint\phi_p^*\varphi U\phi_{p'}\mathrm{d}p'\mathrm{d}x-\iint\phi_p^*\varphi E\phi_{p'}\mathrm{d}p'\mathrm{d}x$$

$$=\int\frac{p'^2}{2\mu}\varphi\int\phi_p^*\phi_{p'}\mathrm{d}x\mathrm{d}p'+\int\varphi\int\phi_p^*U\phi_{p'}\mathrm{d}x\mathrm{d}p'-\int E\varphi\int\phi_p^*\phi_{p'}\mathrm{d}x\mathrm{d}p'$$

$$=\int\frac{p'^2}{2\mu}\varphi\delta(p'-p)\mathrm{d}p'+\int\varphi U_{pp'}\mathrm{d}p'-\int E\varphi\delta(p'-p)\mathrm{d}p' \quad , U_{pp'}=\int\phi_p^*U\phi_p\,dx$$

$$=\frac{p^2}{2\mu}\varphi+\int U_{pp'}\varphi\,\mathrm{d}p'-E\varphi\Rightarrow\frac{p^2}{2\mu}\varphi(p)+\int U_{pp'}\varphi(p')\mathrm{d}p'=E\varphi(p)$$

若 $U(x)$ 展开级数

$$\Rightarrow U_{pp'}=\sum_{n=0}^{\infty}c_n\left(i\hbar\frac{\partial}{\partial p}\right)^n\delta(p-p')$$

$$=U(\hat{x})\delta(p-p'),\quad \hat{x}=i\hbar\frac{\partial}{\partial p}$$ // 动量表象坐标算符

$$\Rightarrow\left[\frac{p^2}{2\mu}+U(\hat{x})\right]\varphi(p)=E\varphi(p)$$

- **例：谐振子势**

$$\left(-\frac{\partial^2}{\partial p^2}+\frac{p^2}{\mu^2\omega^2\hbar^2}\right)\varphi(p)=\frac{2E}{\mu\omega^2\hbar^2}\varphi(p)$$

二阶微分方程，求解过程类似于在坐标表象中，不能简化

- **例：线性势**

$$\left(\frac{\partial}{\partial p}+\frac{p^2}{\mathrm{i}2\hbar F\mu}\right)\varphi(p)=\frac{E}{\mathrm{i}F\hbar}\varphi(p)$$

  - **一阶微分方程，能简化求解过程**

$$\varphi(p)\propto e^{\frac{\mathrm{i}}{F\hbar}\left(\frac{p^3}{6\mu}-Ep\right)},\quad \psi(x)\propto\mathrm{Ai}\left[\left(x-\frac{E}{F}\right)\left(\frac{2\mu F}{\hbar^2}\right)^{1/3}\right]$$

- **例：δ势阱**

$$E\varphi(p)=\frac{p^2}{2\mu}\varphi(p)-\frac{\gamma C}{2\pi\hbar},\quad C=\int\varphi(p')\mathrm{d}p'$$

  - **普通的线性方程**

$$\varphi(p)\propto\frac{\mu\gamma}{\pi\hbar}\frac{1}{p^2-2\mu E},\quad E=-\frac{\mu\gamma^2}{2\hbar^2}$$

- **最适当的表象依赖于具体的问题**

算符矩阵表示：

若 $\Phi=\hat{F}\psi$

$\psi=\sum_m a_m(t)u_m(x)$ 本征函数

$\Phi=\sum_m b_m(t)u_m(x)$

$\Rightarrow\sum_m b_m u_m=\hat{F}\sum_m a_m u_m=\sum_m a_m\hat{F}u_m$

左乘 u_n^* 积分

$b_n=\sum_m b_m\delta_{mn}=\sum_m b_m\int u_n^*u_m dx=\sum_m a_m\int u_n^*\hat{F}u_m dx=\sum_m a_m F_{mn}$

// $F_{mn}=\int u_n^*\hat{F}u_m dx$

$\Rightarrow b_n=\sum_m a_m F_{mn}$

m(无限)

$$
\begin{bmatrix} b_1(t) \\ \cdots \\ b_n(t) \\ \cdots \end{bmatrix} \underbrace{=}_{n\text{（无限）}} \begin{bmatrix} F_{11} & \cdots & F_{1m} & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ F_{n1} & \cdots & F_{nm} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix} \begin{bmatrix} a_1(t) \\ \cdots \\ a_m(t) \\ \cdots \end{bmatrix} \Rightarrow \Phi = F\Psi
$$

厄米算符对应厄米共厄矩阵（$F_{mn}^* = F_{mn}$，$\hat{F}^* = \hat{F}$）

$$F_{mn}^* = \int u_n [\hat{F} u_m]^* dx$$
$$= \int u_m^* \hat{F} u_n \, dx = F_{mn}$$

$$F_{mn} = F_{mn}^\dagger \quad \text{or} \quad F = F^\dagger$$

- **算符Q在自身的表象中是对角矩阵——求解薛定谔方程**

$$\hat{H}\psi = E\psi$$
$$(H - EI)\psi = 0$$
$$\begin{cases} ① \ \psi = 0, \ \text{平凡} \\ ② \ |H - EI| = 0 \quad \text{久期方程} \end{cases}$$

// 求解特征值

$$Q_{mn} = \int u_n^* \hat{Q} u_m \, dx$$

↓自身算符

$$= \int u_n^* Q_m u_m \, dx = Q_m \delta_{mn}$$

  - **Q的表象(只有连续本征值q，本征函数是$u_q(x)$)下的算符**

$$n \to q, \quad m \to q', \quad \sum(\cdots) \to \int(\cdots)\mathrm{d}q'$$
$$\Phi(x,t) = \int b_{q'}(t) u_{q'}(x) \mathrm{d}q', \quad \Psi(x,t) = \int a_{q'}(t) u_{q'}(x) \mathrm{d}q'$$
$$\int b_{q'} u_{q'} \mathrm{d}q' = \Phi(x,t) = \hat{F}(x,\hat{p})\Psi(x,t) = \hat{F}\int a_{q'} u_{q'} \mathrm{d}q' = \int a_{q'} \hat{F} u_{q'} \mathrm{d}q'$$
$$\int u_q^* \int b_{q'} u_{q'} \mathrm{d}q' \mathrm{d}x = \int u_q^* \int a_{q'} \hat{F} u_{q'} \mathrm{d}q' \mathrm{d}x$$

$\bullet$ Left $= \int b_{q'} \int u_q^* u_{q'} \mathrm{d}x \, \mathrm{d}q' = \int b_{q'} \delta(q - q') \mathrm{d}q' = b_q$

$\bullet$ Right $= \int a_{q'} \int u_q^* \hat{F} u_{q'} \mathrm{d}x \, \mathrm{d}q' = \int F_{qq'} a_{q'} \mathrm{d}q', \quad F_{qq'} = \int u_q^* \hat{F} u_{q'} \mathrm{d}x$

$$b_q(t) = \int F_{qq'} a_{q'}(t) \mathrm{d}q'$$

$$
\begin{bmatrix} b_q(t) \\ \cdots \\ \cdots \end{bmatrix} = \begin{bmatrix} F_{qq'} & \cdots & \cdots \\ \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots \end{bmatrix} \begin{bmatrix} a_{q'}(t) \\ \cdots \\ \cdots \end{bmatrix} \mathrm{d}q' \Rightarrow \Phi = F\Psi
$$

$$\Phi(x,t) = \int b_{q'}(t) u_{q'}(x) \mathrm{d}q', \quad \Psi(x,t) = \int a_{q'}(t) u_{q'}(x) \mathrm{d}q'$$
$$b_q = \int F_{qq'} a_{q'} \mathrm{d}q', \quad F_{qq'} = \int u_q^* \hat{F} u_{q'} \mathrm{d}x, \quad \Phi = F\Psi$$

  - **例：$\hat{F}$在坐标表象和动量表象中的矩阵元**
    - **坐标表象**

$$F_{xx'} = \int u_x^* \hat{F}(\hat{x},\hat{p}) u_{x'} \mathrm{d}x'', \quad u_{x'}(x'') = \delta(x'' - x')$$
$$= \int \delta(x'' - x)[\hat{F}(x'', -\mathrm{i}\hbar\frac{\partial}{\partial x''})\delta(x'' - x')]\mathrm{d}x''$$
$$= \hat{F}(x, -\mathrm{i}\hbar\frac{\partial}{\partial x})\delta(x - x')$$

    - **动量表象**

$$F_{pp'} = \int u_p^* \hat{F}(\hat{x},\hat{p}) u_{p'} \mathrm{d}x = \int \phi_p^* \hat{F}(x, -\mathrm{i}\hbar\frac{\partial}{\partial x})\phi_{p'} \mathrm{d}x \qquad \phi_{p'} = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$$

$$F_{pp'} = \int u_p^* \hat{F}\left(i\hbar\frac{\partial}{\partial p}, \hat{p}\right) u_{p'}\, dp \qquad u_{p'} = \delta(p - p')$$

$$= \hat{F}\left(i\hbar\frac{\partial}{\partial p}, \hat{p}\right) \delta(p - p')$$