

第四章 态和力学量表象

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§ 4.1 态的表象

量子力学中态和力学量的具体表示方式称为表象，以前所采用的表象是坐标表象，本章将讨论其他的表象。

(1) 动量表象

动量本征函数

$$\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$$

组成完全系，任意态 Ψ
可以由它展开

$$\Psi(x, t) = \int C(p, t) \psi_p(x) dp$$

$$C(p, t) = \int \psi_p^*(x) \Psi(x, t) dx$$

证明

如果 $\Psi(\mathbf{x}, t)$ 已经归一化，则 $C(\mathbf{p}, t)$ 也已经归一化。

$$\begin{aligned} 1 &= \int \Psi^*(x, t) \Psi(x, t) dx \\ &= \int \left[\int C(p', t) \psi_{p'}(x) dp' \right]^* \left[\int C(p, t) \psi_p(x) dp \right] dx \\ &= \iint C(p', t)^* C(p, t) \left[\int \psi_{p'}^*(x) \psi_p(x) dx \right] dp' dp \\ &= \int \int C(p', t)^* C(p, t) \delta(p' - p) dp' dp \\ &= \int C(p, t)^* C(p, t) dp \end{aligned}$$

$\Psi(\mathbf{r}, t)$ 是波函数的坐标表象。 $C(\mathbf{p}, t)$ 是波函数的动量表象。它们为可逆的傅里叶变换。它们是同一个量子态的两种描述。坐标表象描述的是体系处于该态时，测量粒子位置所得结果在 $\mathbf{x} \rightarrow \mathbf{x} + d\mathbf{x}$ 范围内的概率，动量表象描述的是体系处于该态时，测量粒子动量所得结果在 $\mathbf{p} \rightarrow \mathbf{p} + d\mathbf{p}$ 范围内的概率。前者描述坐标与概率关系，后者描述动量与概率关系。但二者描写的是同一状态。

具有确定动量 \mathbf{p}' 的自由粒子的状态用波函数 $\Psi(\mathbf{x}, t)$ 描写，则该状态的动量表象为

$$\Psi(\mathbf{x}, t) = \psi_{p'}(\mathbf{x}) e^{-iE_{p'}t/\hbar}$$

$$E_{p'} = \frac{p'^2}{2\mu}$$

$$\begin{aligned} C(p, t) &= \int \psi_p^*(\mathbf{x}) \Psi(\mathbf{x}, t) d\mathbf{x} = \int \psi_p^*(\mathbf{x}) \psi_{p'}(\mathbf{x}) e^{-iE_{p'}t/\hbar} d\mathbf{x} \\ &= e^{-iE_{p'}t/\hbar} \int \psi_p^*(\mathbf{x}) \psi_{p'}(\mathbf{x}) d\mathbf{x} = e^{-iE_{p'}t/\hbar} \delta(p - p') \end{aligned}$$

同理

坐标 \mathbf{x} 在自身表象中对应于确定值 \mathbf{x}' 的本征函数是 $\delta(\mathbf{x}' - \mathbf{x})$ ，因为

$$x \delta(x' - x) = x' \delta(x' - x)$$

所以
$$\psi_{x'}(x) = \delta(x' - x)$$

所以，在动量表象中，粒子具有确定动量 \mathbf{p}' 的波函数是以动量 \mathbf{p} 为变量的 δ 函数

(2) 力学量表象

(2.1) 分立谱情形

假定算符 Q 的本征值是 $Q_1, Q_2, \dots, Q_n, \dots$,

相应的本征函数是 $u_1(x), u_2(x), \dots, u_n(x), \dots$.

$\Psi(x, t)$ 由 Q 的
本征函数展开:

$$\Psi(x, t) = \sum_n a_n(t) u_n(x)$$

$$a_n(t) = \int u_n^*(x) \Psi(x, t) dx$$

如果 Ψ, u_n 已经归一化,
则 $a_n(t)$ 也已经归一化

证明:

$$1 = \int \Psi^*(x, t) \Psi(x, t) dx$$

$$= \int \left[\sum_m a_m(t) u_m(x) \right]^* \sum_n a_n(t) u_n(x) dx$$

$$= \sum_m \sum_n a_m^*(t) a_n(t) \int u_m^*(x) u_n(x) dx$$

$$= \sum_m \sum_n a_m^*(t) a_n(t) \delta_{mn}$$

$$= \sum_n a_n^*(t) a_n(t)$$

$|a_n|^2$ 表示在状态 $\Psi(x, t)$ 时,
测量力学量 Q 的结果为 Q_n 的概率

$a_1(t), a_2(t), \dots, a_n(t), \dots$ 是对同样状态
 $\Psi(x, t)$ 的 Q 表象表达

可写为矩阵形式

$$\Psi = \begin{pmatrix} a_1(t) \\ a_2(t) \\ \vdots \\ a_n(t) \\ \vdots \end{pmatrix} \quad \Psi^\dagger = \begin{pmatrix} a_1(t)^* & a_2(t)^* & \cdots & a_n(t)^* & \cdots \end{pmatrix}$$

共轭矩阵

$$\Psi^\dagger \Psi = \begin{pmatrix} a_1(t)^* & a_2(t)^* & \cdots & a_n(t)^* & \cdots \end{pmatrix} \begin{pmatrix} a_1(t) \\ a_2(t) \\ \vdots \\ a_n(t) \\ \vdots \end{pmatrix}$$

$$= \sum_n a_n(t)^* a_n(t) = 1$$

(2.2) 连续谱情形

假定算符 Q 的本征值和本征函数是

$$Q_1, Q_2, \dots, Q_n, \dots, \mathbf{q}$$

$$u_1(x), u_2(x), \dots, u_n(x), \dots, \mathbf{u}_q(x)$$

氢原子的能量就是这样一个力学量，既有分立本征值，还有连续本征值

$$\Psi(x, t) = \sum_n a_n(t) u_n(x) + \int a_q(t) u_q(x) dq$$

$$\sum_n a_n^*(t) a_n(t) + \int a_q^*(t) a_q(t) dq = 1$$

$$\begin{cases} a_n(t) = \int u_n^*(x) \Psi(x, t) dx \\ a_q(t) = \int u_q^*(x) \Psi(x, t) dx \end{cases}$$

$$|a_n(t)|^2 \longrightarrow Q_n \longrightarrow Q \longrightarrow \Psi(x, t)$$

$$|a_q(t)|^2 dq \longrightarrow q \rightarrow q + dq \longrightarrow Q \longrightarrow \Psi(x, t)$$

$$\Psi = \begin{pmatrix} a_1(t) \\ a_2(t) \\ \vdots \\ a_n(t) \\ \vdots \\ a_q(t) \end{pmatrix}$$

$$\Psi^+ = (a_1(t)^* \quad a_2(t)^* \quad \dots \quad a_n(t)^* \quad \dots \quad a_q(t)^*)$$

$$\Psi^+ \Psi = 1$$

(3) 讨论

	坐标表象	动量表象
动量本征函数	$\Psi_{p'}(x,t)=[1/(2\pi\hbar)]^{1/2}\exp[i(p'x-E't)/\hbar]$	$C(p,t)=\delta(p'-p)\exp[-iE't/\hbar]$
不含时间的动量 本征函数	$\psi_{p'}(x)=[1/(2\pi\hbar)]^{1/2}\exp[ip'x/\hbar]$	$C(p)=\delta(p'-p)$
本征方程	$p \psi_{p'}(x)=p' \psi_{p'}(x)$	$p \delta(p'-p)=p' \delta(p'-p)$

量子力学中的表象	→	坐标体系
波函数的不同表象		不同坐标体系的一组坐标分量
$u_1(x), u_2(x), \dots, u_n(x), \dots$ 基矢		$i, j, k,$
$a_1(t), a_2(t), \dots, a_n(t), \dots$ 量子态 $\Psi(x,t)$ 希尔伯特 (Hilbert) 空间的 态矢量		A_x, A_y, A_z 矢量 Λ

Q 表象中的基矢量

希尔伯特空间

$$\mathbf{u}_1(\mathbf{x}), \mathbf{u}_2(\mathbf{x}), \dots, \mathbf{u}_n(\mathbf{x}), \dots$$

$$\Psi = \begin{pmatrix} a_1(t) \\ a_2(t) \\ \vdots \\ a_n(t) \\ \vdots \end{pmatrix}$$

§ 4.2 算符的矩阵表示

(1) 力学量的矩阵表示

(2) 算符 F 在表象 Q 中的性质

(3) 力学量 Q 具有连续本征值的情形

(1) 力学量的矩阵表示

坐标 **X** 表象

Q表象

分立本征值,

Ψ 用 $\{u_n(x)\}$ 展开

$$\begin{aligned}\Phi(x,t) &= \hat{F}(x, \hat{p}) \Psi(x,t) \\ &= \hat{F}(x, -i\hbar \frac{\partial}{\partial x}) \Psi(x,t)\end{aligned}$$



$$\begin{cases} \Psi(x,t) = \sum_m a_m(t) u_m(x) \\ \Phi(x,t) = \sum_m b_m(t) u_m(x) \end{cases}$$

$$\sum_m b_m(t) u_m(x) = \hat{F}(x, -i\hbar \frac{\partial}{\partial x}) \sum_m a_m(t) u_m(x)$$

$u_n^*(x) \times$
并 $\int dx$

$$\sum_m b_m(t) \int u_n^* u_m(x) dx = \sum_m [\int u_n^* \hat{F}(x, -i\hbar \frac{\partial}{\partial x}) u_m(x) dx] a_m(t)$$

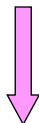
$$\sum_m b_m(t) \delta_{nm} = \sum_m F_{nm} a_m(t) \quad \longrightarrow \quad b_n(t) = \sum_m F_{nm} a_m(t)$$

Q 表象

$$F_{nm} \equiv \int u_n^*(x) \hat{F}(x, -i\hbar \frac{\partial}{\partial x}) u_m(x) dx$$

Q	\longrightarrow	X
$\{A_m(t)\}$		$\Psi(x,t)$
$\{B_n(t)\}$		$\Phi(x,t)$
$H_{nm} \quad F_{nm}$		$\hat{H} \quad F$

$$b_n(t) = \sum_m F_{nm} a_m(t) \quad n = 1, 2, \dots$$



$$\begin{pmatrix} b_1(t) \\ b_2(t) \\ \vdots \\ b_n(t) \\ \vdots \end{pmatrix} = \begin{pmatrix} F_{11} & F_{12} & \dots & F_{1m} & \dots \\ F_{21} & F_{22} & \dots & F_{2m} & \dots \\ \dots & \dots & \dots & \dots & \dots \\ F_{n1} & F_{n2} & \dots & F_{nm} & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix} \begin{pmatrix} a_1(t) \\ a_2(t) \\ \vdots \\ a_m(t) \\ \vdots \end{pmatrix} \quad \Longrightarrow \quad \Phi = F\Psi$$

(2) 算符F在表象Q中的性质

1) 厄米算符F的厄米矩阵

$$\begin{aligned} F_{nm} &= \int u_n^*(x) \hat{F} u_m(x) dx \\ &= [\int u_n(x) (\hat{F} u_m(x))^* dx]^* \\ &= [\int u_m^*(x) \hat{F} u_n(x) dx]^* \\ &= F_{mn}^* = (\tilde{F})_{nm}^* = (F^+)_{nm} \end{aligned}$$

表明：厄米算符对应的矩阵是厄米矩阵

2) 算符在自身表象Q中的形式

$$\begin{aligned} \hat{Q} u_n(x) &= Q_n u_n(x) \\ Q_{nm} &= \int u_n^*(x) \hat{Q} u_m(x) dx \\ &= Q_m \int u_n^*(x) u_m(x) dx = Q_m \delta_{nm} \end{aligned}$$
$$Q = \begin{pmatrix} Q_1 & 0 & \dots & \dots & \dots & \dots \\ 0 & Q_2 & 0 & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \dots & \dots & Q_n \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$

力学量Q的矩阵在自身表象中是对角阵，对角元素是其本征值

(3) 力学量Q具有连续本征值的情形

分立谱

连续谱

$$u_n^*(x), u_m(x) \longrightarrow u_q^*(x), u_q(x)$$

$$a_n(t), b_m(t) \longrightarrow a_q(t), b_q(t)$$

$$\sum_n \longrightarrow \int dq$$

F在 **Q**表象中的矩阵元

$$F_{qq'} = \int u_q^*(x) \hat{F}(x, -i\hbar \frac{\partial}{\partial x}) u_{q'}(x) dx$$

连续矩阵

例题: 在坐标X表象中找到F的矩阵元

$$F_{xx'} = \int \delta(x-x'') \hat{F}(x'', -i\hbar \frac{\partial}{\partial x'}) \delta(x'-x'') dx'' = \hat{F}(x, -i\hbar \frac{\partial}{\partial x}) \delta(x'-x)$$

例题: 在动量p表象中找到F的矩阵元

$$F_{pp'} = \int \psi_p^*(x) \hat{F}(x, -i\hbar \frac{\partial}{\partial x}) \psi_{p'}(x) dx$$

$$1) \quad \hat{F} = \hat{p}$$

$$\begin{aligned} p_{pp'} &= \int \psi_p^*(x) \hat{p} \psi_{p'}(x) dx \\ &= p' \int \psi_p^*(x) \psi_{p'}(x) dx \\ &= p' \delta(p - p') \end{aligned}$$

$$2) \quad \hat{F} = x$$

$$\begin{aligned} x_{pp'} &= \int \psi_p^*(x) x \psi_{p'}(x) dx \\ &= \frac{1}{\sqrt{2\pi\hbar}} \int [e^{-ipx/\hbar} x] \psi_{p'}(x) dx \\ &= \frac{1}{\sqrt{2\pi\hbar}} \int (i\hbar \frac{\partial}{\partial p}) e^{-ipx/\hbar} \psi_{p'}(x) dx \\ &= (i\hbar \frac{\partial}{\partial p}) \int \psi_p^*(x) \psi_{p'}(x) dx \\ &= (i\hbar \frac{\partial}{\partial p}) \delta(p - p') \end{aligned}$$

§4.3 量子力学公式的矩阵表达

(1) 平均值公式

(2) 本征函数

(3) 薛定谔方程的矩阵形式

(1) 平均值公式

坐标X表象

力学量Q表象

$$\bar{F} = \int \Psi^*(x, t) \hat{F} \Psi(x, t) dx$$



$$\begin{cases} \Psi(x, t) = \sum_n a_n(t) u_n(x) \\ \Psi^*(x, t) = \sum_n a_n^*(t) u_n^*(x) \end{cases}$$

$$\begin{aligned} \bar{F} &= \int \sum_m a_m^*(t) u_m^*(x) \hat{F} \sum_n a_n(t) u_n(x) dx \\ &= \sum_m \sum_n a_m^*(t) \left[\int u_m^*(x) \hat{F} u_n(x) dx \right] a_n(t) \\ &= \sum_m \sum_n a_m^*(t) F_{mn} a_n(t) \end{aligned}$$

$$\bar{F} = (a_1^*(t), a_2^*(t), \dots, a_m^*(t) \dots)$$

$$\bar{F} = \Psi^+ F \Psi$$

$$\begin{pmatrix} F_{11} & F_{12} & \dots & F_{1n} & \dots \\ F_{21} & F_{22} & \dots & F_{2n} & \dots \\ \dots & \dots & \dots & \dots & \dots \\ F_{m1} & F_{m2} & \dots & F_{mn} & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix} \begin{pmatrix} a_1(t) \\ a_2(t) \\ \vdots \\ a_n(t) \\ \vdots \end{pmatrix}$$

(2) 本征函数

$$\hat{F}\psi(x) = \lambda\psi(x) \quad F\psi = \lambda\psi$$

$$\begin{pmatrix} F_{11} & F_{12} & \cdots & F_{1n} & \cdots \\ F_{21} & F_{22} & \cdots & F_{2n} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ F_{n1} & F_{n2} & \cdots & F_{nn} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \\ \vdots \end{pmatrix} = \lambda \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \\ \vdots \end{pmatrix} \quad \begin{pmatrix} F_{11} - \lambda & F_{12} & \cdots & F_{1n} & \cdots \\ F_{21} & F_{22} - \lambda & \cdots & F_{2n} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ F_{n1} & F_{n2} & \cdots & F_{nn} - \lambda & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \\ \vdots \end{pmatrix} = 0$$

线性齐次代数方程组 $\sum_n (F_{nn} - \lambda \delta_{nn}) a_n = 0$

$m=1, 2, \dots$

方程解 $\lambda_1, \lambda_2, \dots, \lambda_i, \dots, \lambda_n, \dots$ 是 F 的本征值, 对于 λ_i 有函数

$$\psi_i = \begin{pmatrix} a_{1i} \\ a_{2i} \\ \vdots \\ a_{ni} \\ \vdots \end{pmatrix}, i = 1, 2, \dots, n \dots$$

$$\begin{vmatrix} F_{11} - \lambda & F_{12} & \cdots & F_{1n} & \cdots \\ F_{21} & F_{22} - \lambda & \cdots & F_{2n} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ F_{n1} & F_{n2} & \cdots & F_{nn} - \lambda & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{vmatrix} = 0$$

久期方程

(3) 薛定谔方程的矩阵形式

$$i\hbar \frac{\partial}{\partial t} \Psi(x,t) = \hat{H} \Psi(x,t) \quad \Psi(x,t) = \sum_n a_n(t) u_n(x) \quad \mathbf{Q} \text{ 表象}$$

$$i\hbar \frac{\partial}{\partial t} \sum_n a_n(t) u_n(x) = \hat{H} \sum_n a_n(t) u_n(x) \quad \mathbf{u}_m^*(\mathbf{r}) \times \text{且} \int d\mathbf{x}$$

$$i\hbar \frac{\partial}{\partial t} \sum_n a_n(t) \int u_m^*(x) u_n(x) dx = \sum_n a_n(t) \int u_m^*(x) \hat{H} u_n(x) dx$$

$$i\hbar \frac{\partial}{\partial t} \sum_n a_n(t) \delta_{mn} = \sum_n a_n(t) H_{mn} \quad H_{mn} = \int u_m^*(x) \hat{H} u_n(x) dx$$

$$i\hbar \frac{\partial}{\partial t} a_m(t) = \sum_n H_{mn} a_n(t) \quad \begin{matrix} m, n = 1, 2, \dots \end{matrix} \quad i\hbar \frac{\partial}{\partial t} \begin{pmatrix} a_1(t) \\ a_2(t) \\ \vdots \\ a_n(t) \\ \vdots \end{pmatrix} = \begin{pmatrix} H_{11} & H_{12} & \cdots & H_{1n} & \cdots \\ H_{21} & H_{22} & \cdots & H_{2n} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ H_{m1} & H_{m2} & \cdots & H_{mn} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix} \begin{pmatrix} a_1(t) \\ a_2(t) \\ \vdots \\ a_n(t) \\ \vdots \end{pmatrix}$$

$$i\hbar \frac{\partial}{\partial t} \Psi = H \Psi$$

作业

4.1

4.3

4.4

§ 4.4 么正变换

- (1) 不同表象之间的变换和么正变换矩阵
- (2) 波函数和算符的变换关系
- (3) 么正变换的性质

(1) 不同表象之间的变换和么正变换矩阵

(i) 么正变换矩阵

$$\hat{A}\psi_n(x) = A_n\psi_n(x) \quad n=1,2,\dots$$

$$\hat{B}\varphi_\beta(x) = B_\beta\varphi_\beta(x) \quad \beta=1,2,\dots$$

算符A和B的本征方程
和正交归一的本征函数系

$$F_{nm} = \int \psi_m^*(x) \hat{F} \psi_n(x) dx, \quad m, n = 1, 2, \dots$$

$$F'_{\alpha\beta} = \int \varphi_\alpha^*(x) \hat{F} \varphi_\beta(x) dx, \quad \alpha, \beta = 1, 2, \dots$$

$$\varphi_\beta(x) = \sum_n S_{n\beta} \psi_n(x)$$

将B的基矢按A的完全系展开

$$\varphi_\alpha^*(x) = \sum_m \psi_m^*(x) S_{m\alpha}^*$$

$$S_{n\beta} = \int \psi_n^*(x) \varphi_\beta(x) dx$$

$$S_{m\alpha}^* = \int \psi_m^*(x) \varphi_\alpha^*(x) dx$$

矩阵形式

$$\begin{pmatrix} \varphi_1(x) \\ \varphi_2(x) \\ \vdots \\ \varphi_\beta(x) \\ \vdots \end{pmatrix} = \begin{pmatrix} S_{11} & S_{21} & \cdots & S_{n1} & \cdots \\ S_{12} & S_{22} & \cdots & S_{n2} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ S_{1\beta} & S_{2\beta} & \cdots & S_{n\beta} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix} \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \\ \vdots \\ \psi_n(x) \\ \vdots \end{pmatrix} \Rightarrow \begin{aligned} \Phi &= \tilde{S}\Psi \\ \Phi^+ &= \tilde{\Phi}^* = \Psi^+ S^* \end{aligned}$$

(ii) S矩阵的么正性质

a) $S^+ S = I$

$$\begin{aligned} \delta_{\alpha\beta} &= \int \varphi_\alpha^*(x) \varphi_\beta(x) dx = \sum_{nm} \int \psi_m^*(x) S_{m\alpha}^* S_{n\beta} \psi_n(x) dx = \sum_{nm} S_{m\alpha}^* S_{n\beta} \int \psi_m^*(x) \psi_n(x) dx \\ &= \sum_{nm} S_{m\alpha}^* S_{n\beta} \delta_{mn} = \sum_m S_{m\alpha}^* S_{m\beta} = \sum_m (S^+)_{\alpha m} S_{m\beta} = (S^+ S)_{\alpha\beta} \end{aligned}$$

b) $S S^+ = I$

$$\begin{aligned} (S S^+)_{jk} &= \sum_\alpha S_{j\alpha} (S^+)_{\alpha k} = \sum_\alpha S_{j\alpha} (\tilde{S}^*)_{\alpha k} = \sum_\alpha S_{j\alpha} S_{k\alpha}^* \\ &= \sum_\alpha \int \psi_j^*(x) \varphi_\alpha(x) dx \left[\int \psi_k^*(x') \varphi_\alpha(x') dx' \right]^* = \sum_\alpha \int \psi_j^*(x) \varphi_\alpha(x) dx \int \varphi_\alpha^*(x') \psi_k(x') dx' \\ &= \sum_\alpha \int \psi_j^*(x) \varphi_\alpha(x) dx \bullet c_\alpha = \int \psi_j^*(x) \bullet \left[\sum_\alpha c_\alpha \varphi_\alpha(x) \right] dx = \int \psi_j^*(x) \psi_k(x) dx = \delta_{jk} \end{aligned}$$

综上

$$S^+ S = S S^+ = I \rightarrow S^+ = S^{-1} \rightarrow S \text{ 为么正矩阵}$$

(iii) 么正矩阵的计算方法

方法一：计算所有的矩阵元

$$S_{k\beta} = \int \psi_k^*(x) \varphi_\beta(x) dx$$

方法二：计算基矢的变换系数

$$\varphi_\beta = \sum_k S_{k\beta} \psi_k \quad \varphi_\beta = \begin{pmatrix} S_{1\beta} \\ S_{2\beta} \\ \vdots \\ S_{k\beta} \\ \vdots \end{pmatrix} \quad \mathbf{A} \text{ 表象}$$

假定 \mathbf{A} 和 \mathbf{B} 本征矢的数目是3，即 ψ_1, ψ_2, ψ_3 和 $\varphi_1, \varphi_2, \varphi_3$ 。

若在 \mathbf{A} 表象中已知 $\varphi_\beta, (\beta = 1, 2, 3)$

$$\varphi_1 = S_{11}\psi_1 + S_{21}\psi_2 + S_{31}\psi_3$$

$$\varphi_2 = S_{12}\psi_1 + S_{22}\psi_2 + S_{32}\psi_3$$

$$\varphi_3 = S_{13}\psi_1 + S_{23}\psi_2 + S_{33}\psi_3$$

则在A表象中B的本征矢是

$$\phi_1 = \begin{pmatrix} S_{11} \\ S_{21} \\ S_{31} \end{pmatrix} \quad \phi_2 = \begin{pmatrix} S_{12} \\ S_{22} \\ S_{32} \end{pmatrix} \quad \phi_3 = \begin{pmatrix} S_{13} \\ S_{23} \\ S_{33} \end{pmatrix}$$

$$S = \begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{21} & S_{22} & S_{23} \\ S_{31} & S_{32} & S_{33} \end{pmatrix}$$

A  **B** 的么正变换矩阵

$$\Phi = \tilde{S}\Psi$$

(2) 波函数和算符的变换关系

(a) 波函数(态矢量)的变换关系

对任意态 \mathbf{u}
$$\mathbf{u} = \sum_k a_k \psi_k = \sum_k b_k \phi_k$$

在A表象中 \mathbf{u} 可
写为

$$\mathbf{u} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_k \\ \vdots \end{pmatrix} \equiv \mathbf{a}$$

在B表象中 \mathbf{u} 可
写为

$$\mathbf{u} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_\alpha \\ \vdots \end{pmatrix} \equiv \mathbf{b}$$

$$\begin{aligned} b_\alpha(t) &= \int \phi_\alpha^*(x) u(x, t) dx = \int \left[\sum_m \psi_m^*(x) S_{m\alpha}^* \right] u(x, t) dx \\ &= S_{m\alpha}^* \sum_m \int \psi_m^*(x) u(x, t) dx = S_{m\alpha}^* \sum_m a_m(t) = \sum_m S_{m\alpha}^* a_m(t) \\ &= \sum_m S_{\alpha m}^+ a_m(t) = (S^+ \mathbf{a})_\alpha \end{aligned}$$



$$\mathbf{b} = \mathbf{S}^+ \mathbf{a} = \mathbf{S}^{-1} \mathbf{a}$$

(b) 算符F的变换关系

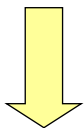
A: $F_{jk} = \int \psi_j^*(x) \hat{F} \psi_k(x) dx$

$$\varphi_\beta(x) = \sum_n S_{n\beta} \psi_n(x)$$

$$\varphi_\alpha^*(x) = \sum_m \psi_m^*(x) S_{m\alpha}^*$$

B:

$$\begin{aligned} F'_{\alpha\beta} &= \int \varphi_\alpha^*(x) \hat{F} \varphi_\beta(x) dx = \int \left[\sum_m \psi_m^*(x) S_{m\alpha}^* \right] \hat{F} \left[\sum_n S_{n\beta} \psi_n(x) \right] dx \\ &= \sum_{mn} \int \psi_m^*(x) S_{m\alpha}^* \hat{F} S_{n\beta} \psi_n(x) dx = \sum_{mn} S_{m\alpha}^* \int \psi_m^*(x) \hat{F} \psi_n(x) dx S_{n\beta} \\ &= \sum_{mn} S_{m\alpha}^* F_{mn} S_{n\beta} = \sum_{mn} S_{\alpha m}^+ F_{mn} S_{n\beta} = (S^+ F S)_{\alpha\beta} \end{aligned}$$



$$\mathbf{F}' = \mathbf{S}^+ \mathbf{F} \mathbf{S} = \mathbf{S}^{-1} \mathbf{F} \mathbf{S}$$

(3) 么正变换的性质

(a) 本征值不变

F 在 **A** 表象中: $\mathbf{F} \mathbf{a} = \lambda \mathbf{a}$

在 **B** 表象 $\mathbf{F}' \mathbf{b} = \mathbf{S}^{-1} \mathbf{F} \mathbf{S} \mathbf{S}^{-1} \mathbf{a} = \mathbf{S}^{-1} \mathbf{F} \mathbf{a} = \mathbf{S}^{-1} \lambda \mathbf{a}$
中:
 $\quad \quad \quad = \lambda \mathbf{S}^{-1} \mathbf{a} = \lambda \mathbf{b}$

(b) 矩阵的迹不变

矩阵的迹 $Sp F = \sum_k F_{kk}$

$$\begin{aligned} Sp(F') &= Sp(S^{-1}FS) \\ &= Sp(SS^{-1}F) \\ &= Sp(F) \end{aligned}$$

作业

4.5

§ 4.5 狄拉克符号

- (1) 引论
- (2) 态矢量
- (3) 算符
- (4) 小结

(1) 引论

- 表象：坐标 X , 力学量 Q
- 状态矢量 A 不涉及具体表象(A_x, A_y, A_z)
- 量子力学中描写态和力学量可以不用具体表象，这种描写的方式是狄拉克最先引用的，这样的一套符号就称为狄拉克符号。

(2) 态矢量

(a) 右矢 $|>$

线性谐振子状态 $\psi_n(\mathbf{x})$ 的量子数 n ;氢原子状态 $\psi_{nlm}(\mathbf{r}, \theta, \varphi)$ 的量子数 n, l, m 可用于标记体系状态, 如下所示

$$\psi_n(\mathbf{x}) \rightarrow |\psi_n\rangle \rightarrow |n\rangle; \quad \psi_{nlm} \rightarrow |\psi_{nlm}\rangle \rightarrow |n, l, m\rangle$$

本征态 $|x\rangle, |p\rangle, |Q_n\rangle \dots$

完全右矢集合(或基组), 基矢

如

$$|\psi\rangle = \sum_n a_n |n\rangle$$

(b) 左矢 $\langle |$

狄拉克符号

左矢	右矢
$\langle n $	$ n \rangle$
$\langle n, l, m $	$ n, l, m \rangle$
$\langle x' $	$ x' \rangle$
$\langle A $	$ A \rangle$
$\langle l, m $	$ l, m \rangle$
$\langle p' $	$ p' \rangle$
$\langle Qn $	$ Qn \rangle$
bra	ket

$\langle | = (| \rangle)^+$ 共轭矢量

$\langle \psi |$ 和 $|\psi \rangle$ 共轭矢量, $\langle p' |, \langle x' |, \langle Qn |$ 组成左矢完全系 (基组)

$$\langle \psi | \phi \rangle \equiv (\psi, \phi) = \int \psi^*(x) \phi(x) dx = (\langle \psi |) \bullet (| \phi \rangle)$$

$$\langle \psi | \phi \rangle^* \equiv (\psi, \phi)^* = (\phi, \psi) = \langle \phi | \psi \rangle^+$$

$\langle \psi | \phi \rangle = 0$, 正交; $\langle \psi | \psi \rangle = 1$, 归一

本征方程 $\hat{F}|n\rangle = f_n|n\rangle$, $\langle n|n'\rangle = \delta_{nn'}$ 正交归一 $\{|n\rangle\}$ 构成 F 表象希尔伯特空间基矢, 则

任意态矢在 F 表象展开 (完全性)

$$|\psi \rangle = \sum_n a_n |n \rangle$$

F表
象

$$|1\rangle = \begin{pmatrix} a_1=1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad |2\rangle = \begin{pmatrix} 0 \\ a_2=1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad \dots \quad |n\rangle = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ a_n=1 \\ 0 \end{pmatrix} \quad \dots$$

$$\langle n' | \psi \rangle = \sum_n a_n \langle n' | n \rangle = \sum_n a_n \delta_{n'n} = a_{n'}$$

$$a_n = \langle n | \psi \rangle$$

$$\{a_n\} = \{\langle n | \psi \rangle\}$$



$$|\psi\rangle = \begin{pmatrix} \langle 1 | \psi \rangle \\ \langle 2 | \psi \rangle \\ \vdots \\ \langle n | \psi \rangle \\ \vdots \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \\ \vdots \end{pmatrix} = a_1 \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + a_2 \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \dots + a_n \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} + \dots$$

$$= \sum_n a_n |n\rangle$$

$$= \sum_n (\langle n | \psi \rangle) \cdot |n\rangle = \sum_n |n\rangle (\langle n | \psi \rangle) = \sum_n |n\rangle \langle n | \psi \rangle$$

$|\psi\rangle$ 为任意态矢，求和与之 无关，可得

$\sum_n |n\rangle \langle n| = 1 \Rightarrow$ 本征矢的封闭性，使表 象变换大为简化

$|n\rangle\langle n|$ 和 $|q\rangle\langle q|$ 可定义为投影算符

$$|n\rangle\langle n|\psi\rangle = |\psi\rangle \rightarrow |n\rangle\langle n|\psi\rangle$$

$$|q\rangle\langle q|\psi\rangle = |\psi\rangle \rightarrow |q\rangle\langle q|\psi\rangle$$

$\psi(x, t)$ 表示坐标 X 表象中的状态 $|\psi\rangle$, 则

$$\begin{cases} \langle x|\psi\rangle = \psi(x, t) \\ \langle\psi|x\rangle = \langle x|\psi\rangle^* = \psi^*(x, t) \end{cases}$$

$\langle x|x\rangle = 1$
 $\langle x|x'\rangle = 0$

$$\sum_n |n\rangle\langle n| = 1$$

坐标表象中的封闭性

$$\sum_n \langle x|n\rangle\langle n|x'\rangle = \langle x|x'\rangle \longrightarrow \sum_n u_n^*(x')u_n(x) = \delta(x-x')$$

$$\int |q\rangle dq \langle q| = 1 \longrightarrow \int \langle x|q\rangle dq \langle q|x'\rangle = \langle x|x'\rangle \longrightarrow \int u_q^*(x')u_q(x) dq = \delta(x-x')$$

正交归一性

(本征值不同)

$$\int u_n^*(x)u_m(x)dx = \delta_{nm}$$

$$\int u_{q'}^*(x)u_q(x)dx = \delta(q-q')$$

dx

$$\sum_n u_n^*(x')u_n(x) = \delta(x-x')$$

$$\int u_q^*(x')u_q(x) dq = \delta(x-x')$$

n 或 dq

本征值既有分立

又有联系谱的封闭性表示

$$\sum_n |n\rangle\langle n| + \int |q\rangle dq \langle q| = 1$$

(3) 算符

(a) 右矢

$$\psi(x,t) = \hat{F}(x, \hat{p})\phi(x,t)$$

坐标X表象

$$|\psi\rangle = \hat{F}|\phi\rangle$$

F_{mn} —
F在Q表象的矩阵元

$$\langle m|\psi\rangle = \langle m|\hat{F}|\phi\rangle = \sum_n \langle m|\hat{F}|n\rangle \langle n|\phi\rangle$$

$$\sum_n |n\rangle \langle n| = 1$$



矩阵

$$\begin{pmatrix} \langle 1|\psi\rangle \\ \langle 2|\psi\rangle \\ \vdots \\ \langle n|\psi\rangle \\ \vdots \end{pmatrix} = \begin{pmatrix} \langle 1|\hat{F}|1\rangle, \langle 1|\hat{F}|2\rangle, \dots \\ \langle 2|\hat{F}|1\rangle, \langle 2|\hat{F}|2\rangle, \dots \\ \vdots \\ \langle n|\hat{F}|1\rangle, \dots \\ \vdots \end{pmatrix} \begin{pmatrix} \langle 1|\phi\rangle \\ \langle 2|\phi\rangle \\ \vdots \\ \langle n|\phi\rangle \\ \vdots \end{pmatrix}$$

Q表象



$$\psi = F \phi$$

$$\begin{aligned} \bar{F} = \langle \psi | \hat{F} | \psi \rangle &\longrightarrow \bar{F} = \sum_{mn} \langle \psi | m \rangle \langle m | \hat{F} | n \rangle \langle n | \psi \rangle \\ &= \sum_{mn} a_m^* F_{mn} a_n \end{aligned}$$

(b) 左矢

$$\begin{aligned} \langle \psi | m \rangle &= \langle m | \psi \rangle^* = \left(\sum_n \langle m | \hat{F} | n \rangle \langle n | \phi \rangle \right)^* = \left(\sum_n F_{mn} \langle n | \phi \rangle \right)^* \\ &= \sum_n F_{mn}^* \langle n | \phi \rangle^* = \sum_n \tilde{F}_{nm}^* \langle \phi | n \rangle = \sum_n (F^+)_{nm} \langle \phi | n \rangle \\ &= \sum_n \langle \phi | n \rangle \langle n | \hat{F}^+ | m \rangle = \langle \phi | \hat{F}^+ | m \rangle \end{aligned}$$

$$\longrightarrow \langle \psi | = \langle \phi | \hat{F}^+$$

若 \mathbf{F} 是厄米算符

$$\langle \psi | = \langle \phi | \hat{F}$$

$$\langle \psi | = \langle \phi | \hat{F} \qquad \hat{F} | \phi \rangle = | \psi \rangle$$

$$|\psi\rangle = \hat{x} |\phi\rangle \quad \langle p|\psi\rangle = \langle p|\hat{x}|\phi\rangle = \int \langle p|\hat{x}|p'\rangle dp' \langle p'|\phi\rangle$$

$$\begin{aligned} \langle p|\hat{x}|p'\rangle &= \iint \langle p|x\rangle dx \langle x|\hat{x}|x'\rangle dx' \langle x'|p'\rangle \\ &= \iint \langle p|x\rangle dx x' \langle x|x'\rangle dx' \langle x'|p'\rangle \\ &= \iint \langle p|x\rangle dx x' \delta(x-x') dx' \langle x'|p'\rangle \\ &= \iint \langle p|x\rangle x dx \langle x|p'\rangle = \frac{1}{2\pi\hbar} \iint e^{-\frac{i}{\hbar}px} x e^{\frac{i}{\hbar}p'x} dx \\ &= \frac{1}{2\pi\hbar} \iint i\hbar \frac{\partial}{\partial p} e^{-\frac{i}{\hbar}px} e^{\frac{i}{\hbar}p'x} dx = \frac{1}{2\pi\hbar} i\hbar \frac{\partial}{\partial p} \iint e^{-\frac{i}{\hbar}px} e^{\frac{i}{\hbar}p'x} dx \\ &= i\hbar \frac{\partial}{\partial p} \delta(p-p') \end{aligned}$$

$$\begin{aligned} \langle p|\psi\rangle &= \langle p|\hat{x}|\phi\rangle = \int \langle p|\hat{x}|p'\rangle dp' \langle p'|\phi\rangle \\ &= \int i\hbar \frac{\partial}{\partial p} \delta(p-p') dp' \langle p'|\phi\rangle = i\hbar \frac{\partial}{\partial p} \langle p|\phi\rangle \end{aligned} \quad \hat{x} = i\hbar \frac{\partial}{\partial p}$$

(4) 小结

性质	坐标X表象	狄拉克符号
状态波函数	$\Psi(x, t)$	$ \Psi\rangle$
算符	$\hat{F}(\vec{r}, -i\hbar\nabla)$	\hat{F}
归一化	$\int u_m^*(x) u_n(x) dx = \delta_{mn}$	$\langle m n \rangle = \delta_{mn}$
波函数	$\int \Psi^*(x, t) \Psi(x, t) dx = 1$	$\langle \Psi \Psi \rangle = 1$
正交归一性	$\int u_q^*(x) u_{q''}(x) dx = \delta(q' - q'')$	$\langle q' q'' \rangle = \delta(q' - q'')$
本征函数封闭性	$\sum_n u_n(x) u_n^*(x') = \delta(x' - x)$ $\int_n u_q(x) u_q^*(x') dq = \delta(x' - x)$	$\sum_n n\rangle \langle n = 1$ $\int q\rangle \langle q = 1$
公式	$\Psi(x, t) = \hat{F}(x, \hat{p}_x) \Phi(x, t)$	$ \Psi\rangle = \hat{F} \Phi\rangle$
本征函数	$\hat{F}(\vec{r}, \hat{p}) \psi(\vec{r}) = \lambda \psi(\vec{r})$	$\hat{F} \psi\rangle = \lambda \psi\rangle$
平均值	$\bar{F} = \int \psi^* \hat{F} \psi dx$	$\bar{F} = \langle \psi \hat{F} \psi \rangle$
矩阵元	$F_{mn} = \int \psi_m^* \hat{F} \psi_n dx$	$F_{mn} = \langle m \hat{F} n \rangle$
薛定谔方程	$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) = \hat{H}(\vec{r}, -i\hbar\nabla) \Psi(\vec{r}, t)$	$i\hbar \frac{d}{dt} \Psi(t)\rangle = \hat{H} \Psi(t)\rangle$

§ 4.6 线性谐振子和占有数表象

(1) 算符 \mathbf{a} , \mathbf{a}^+ , \mathbf{N}

(2) 占有数表象

(1) 算符 \mathbf{a} , \mathbf{a}^+ , \mathbf{N}

(a) 坐标表象中的线性谐振子

$$\begin{cases} \hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 \\ \psi_n = N_n e^{-\alpha^2 x^2 / 2} H_n(\alpha x) \\ E_n = (n + \frac{1}{2}) \hbar \omega \end{cases} \quad \begin{aligned} \alpha &= \sqrt{\frac{m\omega}{\hbar}} \\ n &= 0, 1, 2, \dots \end{aligned}$$

(b) 算符 \mathbf{a} , \mathbf{a}^+ , \mathbf{N} 的定义

假定

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \left[\hat{x} + \frac{i}{m\omega} \hat{p} \right] = \frac{\alpha}{\sqrt{2}} \left[\hat{x} - \frac{1}{i\hbar\alpha^2} \hat{p} \right]$$

$$\hat{a}^+ = \sqrt{\frac{m\omega}{2\hbar}} \left[\hat{x} - \frac{i}{m\omega} \hat{p} \right] = \frac{\alpha}{\sqrt{2}} \left[\hat{x} + \frac{1}{i\hbar\alpha^2} \hat{p} \right]$$

$$[\hat{a}, \hat{a}^+] = 1$$

证明 $[\hat{a}, \hat{a}^+] = 1$

$$\begin{aligned}
 [\hat{a}, \hat{a}^+] &= \left[\frac{\alpha}{\sqrt{2}} \left(\hat{x} - \frac{1}{i\hbar\alpha^2} \hat{p} \right), \frac{\alpha}{\sqrt{2}} \left(\hat{x} + \frac{1}{i\hbar\alpha^2} \hat{p} \right) \right] \\
 &= \frac{\alpha^2}{2} \left[\hat{x} - \frac{1}{i\hbar\alpha^2} \hat{p}, \hat{x} + \frac{1}{i\hbar\alpha^2} \hat{p} \right] \\
 &= \frac{\alpha^2}{2} \{ [\hat{x}, \hat{x}] + [\hat{x}, \frac{1}{i\hbar\alpha^2} \hat{p}] - [\frac{1}{i\hbar\alpha^2} \hat{p}, \hat{x}] - [\frac{1}{i\hbar\alpha^2} \hat{p}, \frac{1}{i\hbar\alpha^2} \hat{p}] \} \\
 &= \frac{\alpha^2}{2} \frac{1}{i\hbar\alpha^2} \{ [\hat{x}, \hat{p}] - [\hat{p}, \hat{x}] \} \\
 &= \frac{\alpha^2}{2} \frac{1}{i\hbar\alpha^2} \{ 2i\hbar \} \\
 &= 1
 \end{aligned}$$

(c) \hat{a} , \hat{a}^+ 及线性谐振子的哈密顿算符

$$\hat{a} = \frac{\alpha}{\sqrt{2}} \left[\hat{x} - \frac{1}{i\hbar\alpha^2} \hat{p} \right] \quad (1)$$

$$\hat{a}^+ = \frac{\alpha}{\sqrt{2}} \left[\hat{x} + \frac{1}{i\hbar\alpha^2} \hat{p} \right] \quad (2)$$

$$\Rightarrow \begin{cases} x = \frac{1}{\sqrt{2}\alpha} [(2) + (1)] = \frac{1}{\alpha\sqrt{2}} [\hat{a}^+ + \hat{a}] \\ \hat{p} = i\hbar \frac{\alpha}{\sqrt{2}} [(2) - (1)] = i\hbar \frac{\alpha}{\sqrt{2}} [\hat{a}^+ - \hat{a}] \end{cases}$$

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 x^2 = \frac{1}{2m} i\hbar \frac{\alpha}{\sqrt{2}} [\hat{a}^+ - \hat{a}] i\hbar \frac{\alpha}{\sqrt{2}} [\hat{a}^+ - \hat{a}] + \frac{1}{2} m \omega^2 \frac{1}{\alpha\sqrt{2}} [\hat{a}^+ + \hat{a}] \frac{1}{\alpha\sqrt{2}} [\hat{a}^+ + \hat{a}]$$

$$\begin{aligned} \boxed{\alpha^2 = m\omega/\hbar} & \Rightarrow -\frac{\alpha^2 \hbar^2}{4m} [\hat{a}^+ \hat{a}^+ + \hat{a} \hat{a} - \hat{a}^+ \hat{a} - \hat{a} \hat{a}^+] + \frac{1}{4\alpha^2} m \omega^2 [\hat{a}^+ \hat{a}^+ + \hat{a} \hat{a} + \hat{a}^+ \hat{a} + \hat{a} \hat{a}^+] \\ &= -\frac{\hbar\omega}{4} [\hat{a}^+ \hat{a}^+ + \hat{a} \hat{a} - \hat{a}^+ \hat{a} - \hat{a} \hat{a}^+] + \frac{1}{4} \hbar\omega [\hat{a}^+ \hat{a}^+ + \hat{a} \hat{a} + \hat{a}^+ \hat{a} + \hat{a} \hat{a}^+] \\ &= \frac{1}{2} \hbar\omega [\hat{a}^+ \hat{a} + \hat{a} \hat{a}^+] \quad \boxed{[\hat{a} \quad \hat{a}^+] = 1} \\ &= \frac{1}{2} \hbar\omega [\hat{a}^+ \hat{a} + \hat{a}^+ \hat{a} + 1] = \hbar\omega [\hat{a}^+ \hat{a} + \frac{1}{2}] = \hbar\omega [\hat{N} + \frac{1}{2}] \end{aligned}$$

$\hat{N} = \hat{a}^+ \hat{a}$ 为粒子数算符

(d) 算符 \hat{a} , \hat{a}^\dagger , \hat{N} 的物理意义

d.I \hat{a} , \hat{a}^\dagger 的物理意义

$$\hat{a} = \frac{\alpha}{\sqrt{2}} \left[\hat{x} - \frac{1}{i\hbar\alpha} \hat{p} \right] = \frac{\alpha}{\sqrt{2}} \left[\hat{x} + \frac{1}{\alpha^2} \frac{\partial}{\partial \alpha} \right] = \frac{\alpha}{\sqrt{2}} \hat{x} + \frac{1}{\alpha\sqrt{2}} \frac{\partial}{\partial \alpha} = \frac{1}{\sqrt{2}} \left(\xi + \frac{\partial}{\partial \xi} \right)$$

$$\hat{a} \psi_n = \frac{1}{\sqrt{2}} \left(\xi + \frac{\partial}{\partial \xi} \right) \psi_n \quad \hat{a}^\dagger = \frac{\alpha}{\sqrt{2}} \left[\hat{x} + \frac{1}{i\hbar\alpha} \hat{p} \right] = \frac{\alpha}{\sqrt{2}} \hat{x} - \frac{1}{\alpha\sqrt{2}} \frac{\partial}{\partial \alpha} = \frac{1}{\sqrt{2}} \left(\xi - \frac{\partial}{\partial \xi} \right), \quad \xi = \alpha x$$
$$= \sqrt{n} \psi_{n-1}$$

同理, $\hat{a}^\dagger \psi_n = \sqrt{n+1} \psi_{n+1}$

$$\xi \psi_n(\xi) = \sqrt{\frac{n}{2}} \psi_{n-1}(\xi) + \sqrt{\frac{n+1}{2}} \psi_{n+1}(\xi)$$

$$\frac{d}{d\xi} \psi_n(\xi) = \sqrt{\frac{n}{2}} \psi_{n-1}(\xi) - \sqrt{\frac{n+1}{2}} \psi_{n+1}(\xi)$$

粒子湮灭

$$\hat{a} |n\rangle = \sqrt{n} |n-1\rangle$$

粒子产生

$$\hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$$

$|n\rangle$, $|n-1\rangle$, $|n+1\rangle$ 是 \hat{H} 的本征基矢, E_n , E_{n-1} , E_{n+1} 是本征值.

振子能量 $\hbar\omega$ --- 声子
状态 $|n\rangle$ --- 第 n 声子态

且 $\hat{a} |0\rangle = 0$

基态

$$\hat{a}^+ |0\rangle = \sqrt{0+1} |0+1\rangle \rightarrow |1\rangle = \frac{1}{\sqrt{1}} \hat{a}^+ |0\rangle$$

$$\hat{a}^+ |1\rangle = \sqrt{1+1} |1+1\rangle \rightarrow |2\rangle = \frac{1}{\sqrt{2}} \hat{a}^+ |1\rangle = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{1}} \hat{a}^+ \hat{a}^+ |0\rangle = \frac{1}{\sqrt{2!}} (\hat{a}^+)^2 |0\rangle$$

$$\dots\dots\dots |n\rangle = \frac{1}{\sqrt{n!}} (\hat{a}^+)^n |0\rangle$$

d.II 算符N的意义

$$\begin{aligned} \hat{N} |n\rangle &= \hat{a}^+ \hat{a} |n\rangle = \hat{a}^+ \sqrt{n} |n-1\rangle \\ &= \sqrt{n} \sqrt{(n-1)+1} |n\rangle \\ &= n |n\rangle \end{aligned}$$

n 是算符**N**的本征值，描述粒子数目，定义为粒子数算符

(2) 占有数表象

基于 $|n\rangle$ 的表象称为占有数表象

算符 a 的矩阵元 $\langle n' | \hat{a} | n \rangle = \sqrt{n} \langle n' | n-1 \rangle = \sqrt{n} \delta_{n'n-1}$

算符 a^+ 的矩阵元 $\langle n' | \hat{a}^+ | n \rangle = \sqrt{n+1} \langle n' | n+1 \rangle = \sqrt{n+1} \delta_{n'n+1}$

$$a = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \cdots & \cdots \\ 0 & 0 & \sqrt{2} & 0 & 0 & \cdots & \cdots \\ 0 & 0 & 0 & \sqrt{3} & 0 & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix} \quad a^+ = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \cdots & \cdots \\ \sqrt{1} & 0 & 0 & 0 & 0 & \cdots & \cdots \\ 0 & \sqrt{2} & 0 & 0 & 0 & \cdots & \cdots \\ 0 & 0 & \sqrt{3} & 0 & 0 & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}$$

$$N = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 2 & 0 & \cdots \\ 0 & 0 & 0 & 3 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}$$