

量子力学题解二百例

(下 册)

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一九八一年八月

§ 4 表象理论

107. (1) 矩阵形式

根据 $F_{\lambda\lambda'} = \int u_{\lambda'}^*(x) \hat{F}(x, \frac{\hbar}{i} \frac{\partial}{\partial x}) u_{\lambda}(x) dx$

有

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

(2) 微分算符形式:

根据 $b(p') = \int F_{pp'} a(p) dp$

有

$$\begin{aligned} b(p') &= \int x_{p'p} a(p) dp \\ &= -i\hbar \int \left[\frac{\partial}{\partial p} \delta(p-p') \right] a(p) dp \\ &= -i\hbar \left[\delta(p-p') a(p) \right]_{-\infty}^{\infty} \\ &\quad - (-i\hbar) \int \delta(p-p') \frac{\partial}{\partial p} a(p) dp \\ &= i\hbar \frac{\partial}{\partial p'} a(p') \end{aligned}$$

故 $\hat{x}$ 在 "p" 表象中的微分算符形式为

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

另法

$$\begin{aligned} \varphi(\vec{r}) &= \int c(\vec{p}) \varphi_{\vec{p}}(\vec{r}) d^3p \\ &= \frac{1}{(2\pi\hbar)^{3/2}} \int c(\vec{p}) e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} d^3p \end{aligned} \quad (1)$$

$$\begin{aligned}
 c(\vec{p}) &= \int \psi(\vec{r}) \psi_p^*(\vec{r}) dV \\
 &= \frac{1}{(2\pi\hbar)^{3/2}} \int \psi(\vec{r}) e^{-\frac{i}{\hbar} \vec{p} \cdot \vec{r}} dV,
 \end{aligned} \quad (2)$$

$c(\vec{p})$ 可看作是“动量表象”中的波函数。在动量表象中，粒子坐标算符 $\hat{\vec{r}}$ 由下式定义：

$$\vec{r} = \int c^*(\vec{p}) \hat{\vec{r}} c(\vec{p}) d^3p \quad (3)$$

另一方面，在“坐标表象”中：

$$\vec{r} = \int \psi^*(\vec{r}) \vec{r} \psi(\vec{r}) dV \quad (4)$$

将 (1) 式代入 (4) 式，得

$$\vec{r} = \frac{1}{(2\pi\hbar)^3} \iiint c^*(\vec{p}') e^{-\frac{i}{\hbar} \vec{p}' \cdot \vec{r}} \vec{r} c(\vec{p}) e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} d^3p' d^3p dV \quad (5)$$

上式中

$$\begin{aligned}
 \int \vec{r} c(\vec{p}) e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} d^3p &= \int \frac{\hbar}{i} c(\vec{p}) \frac{\partial}{\partial \vec{p}} e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} d^3p \\
 &= \frac{\hbar}{i} c(\vec{p}) e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} \Big|_{-\infty}^{\infty} - \frac{\hbar}{i} \int e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} \frac{\partial c(\vec{p})}{\partial \vec{p}} d^3p \\
 &= i\hbar \int e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} \frac{\partial c(\vec{p})}{\partial \vec{p}} d^3p,
 \end{aligned}$$

代入 (5) 式得

$$\begin{aligned}
 \vec{r} &= \frac{1}{(2\pi\hbar)^3} \iiint c^*(\vec{p}') e^{-\frac{i}{\hbar} \vec{p}' \cdot \vec{r}} e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} i\hbar \frac{\partial}{\partial \vec{p}} c(\vec{p}) d^3p' d^3p dV \\
 &= \iiint c^*(\vec{p}') \left[\frac{1}{(2\pi\hbar)^3} \int e^{\frac{i}{\hbar} (\vec{p} - \vec{p}') \cdot \vec{r}} dV \right] i\hbar \frac{\partial}{\partial \vec{p}} c(\vec{p}) d^3p' d^3p \\
 &= \iiint c^*(\vec{p}') \delta(\vec{p} - \vec{p}') i\hbar \frac{\partial}{\partial \vec{p}} c(\vec{p}) d^3p' d^3p \\
 &= \int c^*(\vec{p}) i\hbar \frac{\partial}{\partial \vec{p}} c(\vec{p}) d^3p.
 \end{aligned} \quad (6)$$

将 (3) 式与 (6) 式比较可得

$$\hat{\vec{r}} = i\hbar \frac{\partial}{\partial \vec{p}},$$

这就是动量表象中，粒子坐标算符的微分形式。

108. 算符 $\hat{F}$ 在 Q 表象中的矩阵元是

$$F_{mn} = \int u_m^*(x) \hat{F} u_n(x) dx,$$

其中 $u_n(x)$ 是 $\hat{Q}$ 的本征函数.

若 $\hat{Q}$ 的本征值组成连续谱, 则为

$$F_{\lambda\lambda'} = \int u_{\lambda'}^*(x) \hat{F} u_{\lambda}(x) dx. \quad (2)$$

现在要求 $\hat{L}_x$ 在动量表象中的矩阵元, 可设

$$\hat{F} = \hat{L}_x, \quad \hat{Q} = \vec{p}.$$

因为动量算符 $\vec{p}$ 的本征值组成连续谱, 故采用 (2) 式, 且 $u_{\lambda}(x)$ 就是平面波

$$\psi_{\vec{p}} = \frac{1}{(2\pi\hbar)^{3/2}} e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} \quad (3)$$

利用 (2) 式 我们有

$$(L_x)_{\vec{p}\vec{p}'} = \int \psi_{\vec{p}'}^* \hat{L}_x \psi_{\vec{p}} d\tau. \quad (4)$$

将 (3) 式及

$$\hat{L}_x = y\hat{p}_z - z\hat{p}_y$$

代入 (4) 式得

$$(L_x)_{\vec{p}\vec{p}'} = \frac{1}{(2\pi\hbar)^3} \int e^{-\frac{i}{\hbar} \vec{p}' \cdot \vec{r}} (y\hat{p}_z - z\hat{p}_y) e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} d\tau \quad \dots\dots\dots (5)$$

注意到

$$\hat{p}_z = \frac{\hbar}{i} \frac{\partial}{\partial z}, \quad \hat{p}_y = \frac{\hbar}{i} \frac{\partial}{\partial y}$$

及

$$\hat{p}_z e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} = \frac{\hbar}{i} \frac{\partial}{\partial z} e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} = \frac{\hbar}{i} \cdot \frac{z}{\hbar} p_z e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} = p_z e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}}$$

$$\hat{p}_y e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} = p_y e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}}$$

则 (5) 式变成

$$(L_x)_{\vec{p}\vec{p}'} = \frac{1}{(2\pi\hbar)^3} \int e^{-\frac{i}{\hbar} \vec{p}' \cdot \vec{r}} (y p_z - z p_y) e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} d\tau$$

但 $y e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} = \frac{\hbar}{i} \frac{\partial}{\partial p_y} e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}}$

$z e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} = \frac{\hbar}{i} \frac{\partial}{\partial p_z} e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}}$

$$\begin{aligned} \therefore (L_x)_{p'p} &= \frac{p_z}{(2\pi\hbar)^3} \int e^{-\frac{i}{\hbar} \vec{p}' \cdot \vec{r}} \frac{\hbar}{i} \frac{\partial}{\partial p_y} e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} d\tau \\ &\quad - \frac{p_y}{(2\pi\hbar)^3} \int e^{-\frac{i}{\hbar} \vec{p}' \cdot \vec{r}} \frac{\hbar}{i} \frac{\partial}{\partial p_z} e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} d\tau \\ &= \frac{\hbar}{i} (p_z \frac{\partial}{\partial p_y} - p_y \frac{\partial}{\partial p_z}) \cdot \frac{1}{(2\pi\hbar)^3} \int e^{\frac{i}{\hbar} (\vec{p} - \vec{p}') \cdot \vec{r}} d\tau \\ &= \frac{\hbar}{i} (p_z \frac{\partial}{\partial p_y} - p_y \frac{\partial}{\partial p_z}) \delta(\vec{p} - \vec{p}') \\ &= \frac{\hbar}{i} (p_z \frac{\partial}{\partial p_y} - p_y \frac{\partial}{\partial p_z}) \delta(\vec{p}' - \vec{p}) \end{aligned}$$

下面求 $\hat{L}_x^2$ 的矩阵元：

$$\begin{aligned} \text{因 } \hat{L}_x^2 &= \hat{L}_x \hat{L}_x = (\hat{y} \hat{p}_z - \hat{z} \hat{p}_y)(\hat{y} \hat{p}_z - \hat{z} \hat{p}_y) \\ &= \hat{y}^2 \hat{p}_z^2 + \hat{z}^2 \hat{p}_y^2 - \hat{z} \hat{p}_y \hat{y} \hat{p}_z - \hat{y} \hat{p}_z \hat{z} \hat{p}_y \end{aligned}$$

利用对易关系：

$$\hat{y} \hat{p}_y - \hat{p}_y \hat{y} = i\hbar, \quad \hat{z} \hat{p}_z - \hat{p}_z \hat{z} = i\hbar,$$

得

$$\begin{aligned} \hat{L}_x^2 &= \hat{y}^2 \hat{p}_z^2 + \hat{z}^2 \hat{p}_y^2 + i\hbar \hat{z} \hat{p}_z - \hat{z} \hat{y} \hat{p}_y \hat{p}_z \\ &\quad + i\hbar \hat{y} \hat{p}_y - \hat{y} \hat{z} \hat{p}_z \hat{p}_y \\ &= \hat{y}^2 \hat{p}_z^2 + \hat{z}^2 \hat{p}_y^2 + i\hbar \hat{z} \hat{p}_z + i\hbar \hat{y} \hat{p}_y - 2\hat{y} \hat{z} \hat{p}_z \hat{p}_y \end{aligned}$$

于是

$$\begin{aligned} (L_x^2)_{p'p} &= \int \psi_{\vec{p}'}^* \hat{L}_x^2 \psi_{\vec{p}} d\tau \\ &= \frac{1}{(2\pi\hbar)^3} \int e^{-\frac{i}{\hbar} \vec{p}' \cdot \vec{r}} \hat{L}_x^2 e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} d\tau \end{aligned}$$

$$= \frac{1}{(2\pi\hbar)^3} \int e^{-\frac{i}{\hbar} \vec{p} \cdot \vec{r}} (y^2 \hat{p}_y^2 + z^2 \hat{p}_z^2 + i\hbar y \hat{p}_z - i\hbar z \hat{p}_y - 2yz \hat{p}_z \hat{p}_y) e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} d\tau \quad (6)$$

与上面类似, 有

$$\left\{ \begin{aligned} \hat{p}_z^2 e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} &= p_z^2 e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} \\ \hat{p}_y^2 e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} &= p_y^2 e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} \\ \hat{p}_z e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} &= p_z e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} \\ \hat{p}_y e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} &= p_y e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} \\ \hat{p}_z \hat{p}_y e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} &= p_z p_y e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} \end{aligned} \right.$$

及

$$\left\{ \begin{aligned} z e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} &= \frac{\hbar}{i} \frac{\partial}{\partial z} e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} \\ y e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} &= \frac{\hbar}{i} \frac{\partial}{\partial y} e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} \\ y^2 e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} &= -\hbar^2 \frac{\partial^2}{\partial p_y^2} e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} \\ z^2 e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} &= -\hbar^2 \frac{\partial^2}{\partial p_z^2} e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} \\ yz e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} &= -\hbar^2 \frac{\partial^2}{\partial p_y \partial p_z} e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} \end{aligned} \right.$$

又注意到

$$\begin{aligned} \frac{1}{(2\pi\hbar)^3} \int e^{\frac{i}{\hbar} (\vec{p} - \vec{p}') \cdot \vec{r}} d\tau &= \delta(\vec{p} - \vec{p}') \\ &= \delta(\vec{p}' - \vec{p}) \end{aligned}$$

将以上诸式代入(6)式, 最后得到

$$(L_x^2)_{P'P} = \left\{ -\hbar^2 \left(p_z^2 \frac{\partial^2}{\partial p_y^2} + p_y^2 \frac{\partial^2}{\partial p_z^2} \right) \right.$$

$$+ \hbar^2 (p_\delta \frac{\partial}{\partial p_\delta} + p_y \frac{\partial}{\partial p_y}) \\ + 2\hbar^2 p_\delta p_y \frac{\partial^2}{\partial p_y \partial p_\delta} \} \delta(\vec{p}' - \vec{p}).$$

109. 在坐标表象中, 线性 谐振子哈密顿量是

$$\hat{H} = \frac{1}{2\mu} \hat{p}^2 + \frac{1}{2} \mu \omega^2 x^2$$

动量算符的本征函数是

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

在动量表象中哈密顿量的矩阵元是

$$H_{p'p} = \int_{-\infty}^{\infty} \psi_p^* \hat{H} \psi_p dx \\ = \int_{-\infty}^{\infty} \psi_p^* \frac{1}{2\mu} \hat{p}^2 \psi_p dx + \int_{-\infty}^{\infty} \psi_p^* \frac{1}{2} \mu \omega^2 x^2 \psi_p dx$$

注意到

$$\hat{p}^2 \psi_p = \hat{p}^2 \frac{1}{(2\pi\hbar)^{1/2}} e^{\frac{i}{\hbar} p x} = p^2 \frac{1}{(2\pi\hbar)^{1/2}} e^{\frac{i}{\hbar} p x} = p^2 \psi_p$$

$$x^2 \psi_p = x^2 \frac{1}{(2\pi\hbar)^{1/2}} e^{\frac{i}{\hbar} p x} = -\hbar^2 \frac{\partial^2}{\partial p^2} \frac{1}{(2\pi\hbar)^{1/2}} e^{\frac{i}{\hbar} p x} \\ = -\hbar^2 \frac{\partial^2}{\partial p^2} \psi_p$$

$$H_{p'p} = \frac{p^2}{2\mu} \int_{-\infty}^{\infty} \psi_p^* \psi_p dx - \frac{1}{2} \mu \omega^2 \hbar^2 \frac{\partial^2}{\partial p^2} \int_{-\infty}^{\infty} \psi_p^* \psi_p dx \\ = \frac{p^2}{2\mu} \delta(p' - p) - \frac{1}{2} \mu \omega^2 \hbar^2 \frac{\partial^2}{\partial p^2} \delta(p' - p).$$

x

x

x

讨论

上面求出了动量表象中线性谐振子的哈密顿量的矩阵元，利用它可以写出动量表象中振子满足的薛定格方程，设波函数为 $C(p, t)$ 。

在分立谱情况下，薛定格方程在 Q 表象中的形式为

$$i\hbar \frac{\partial a_m(t)}{\partial t} = \sum_n H_{mn} a_n(t), \quad (m = 1, 2, \dots)$$

对连续谱，总和应被积分代替，对动量表象，应为

$$i\hbar \frac{\partial C(p, t)}{\partial t} = \int H_{p'p} C(p', t) dp'$$

将已求得的 $H_{p'p}$ 代入上式得

$$\begin{aligned} i\hbar \frac{\partial C(p, t)}{\partial t} &= \int \left[\frac{p'^2}{2\mu} \delta(p' - p) - \frac{1}{2} \mu \omega^2 \hbar^2 \frac{\partial^2}{\partial p'^2} \delta(p' - p) \right] \times \\ &\quad \times C(p', t) dp' \\ &= \frac{p^2}{2\mu} C(p, t) - \frac{1}{2} \mu \omega^2 \hbar^2 \frac{\partial^2}{\partial p^2} C(p, t) \end{aligned}$$

$$\text{即 } i\hbar \frac{\partial C(p, t)}{\partial t} = \left(\frac{p^2}{2\mu} - \frac{1}{2} \mu \omega^2 \hbar^2 \frac{\partial^2}{\partial p^2} \right) C(p, t)$$

$$\text{令 } \frac{1}{\mu} = \mu' \omega'^2, \quad \mu \omega^2 = \frac{1}{\mu'}$$

$$\text{则 } i\hbar \frac{\partial C(p, t)}{\partial t} = \left(-\frac{\hbar^2}{2\mu'} \frac{\partial^2}{\partial p^2} + \frac{1}{2} \mu' \omega'^2 p^2 \right) C(p, t).$$

此方程与坐标表象中振子的薛定格方程形式完全相同，只须作如下代换：

$$C(p, t) \rightarrow \Psi(x, t) \quad \mu' \rightarrow \mu$$

$$\frac{\partial^2}{\partial p^2} \rightarrow \frac{\partial^2}{\partial x^2}$$

$$p^2 \rightarrow x^2$$

因此，坐标表象中振子薛定格方程的解

$$H_n\left(\frac{x}{\beta}\right) = \sqrt{\frac{\alpha}{n! \pi^{1/2} n! 2^n}} e^{-\frac{x^2}{2}} H_n\left(\frac{x}{\beta}\right)$$

依上述代换便是动量表象中振子薛定谔方程的解。

注意: $\alpha \rightarrow \alpha'$

因 $\alpha = \sqrt{\frac{\mu\omega}{\hbar}}$

故 $\alpha' = \sqrt{\frac{\mu'\omega}{\hbar}} = \sqrt{\frac{1}{\mu\omega^2} \cdot \frac{\omega}{\hbar}} \quad (\mu' = \frac{1}{\mu\omega^2})$

$$= \sqrt{\frac{1}{\mu\omega} \cdot \frac{1}{\hbar}} = \sqrt{\frac{\hbar}{\mu\omega} \cdot \frac{1}{\hbar^2}} = \frac{1}{\alpha\hbar} \equiv \beta$$

又 $\xi \rightarrow \xi'$

因 $\xi = \alpha x$

故 $\xi' = \alpha' p = \frac{p}{\alpha\hbar} \equiv \eta$

这样便可得

$$C(\eta) = \sqrt{\frac{\beta}{\pi^{1/2} n! 2^n}} e^{-\frac{\eta^2}{2}} H_n(\eta)$$

与上题结果差一常数因子 $(-i)^n$, 但两者表示同一状态

110 在坐标表象中谐振子的能量本征函数为

$$\psi_n = \sqrt{\frac{\alpha}{\pi^{1/2} n! 2^n}} e^{-\frac{\xi^2}{2}} H_n(\xi) = N_n e^{-\frac{\xi^2}{2}} H_n(\xi)$$

其中 $\alpha = \sqrt{\frac{\mu\omega}{\hbar}} \quad \xi = \alpha x$

在坐标表象中, 动量算符的本征函数是

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

设

$$\psi_n = \int C(p) \psi_p(x) dp$$

其中

$$C(p) = \int \psi_n \psi_p^* dx$$

就是动量表象中谐振子能量的本征函数

$$C(p) = \int_{-\infty}^{\infty} \psi_n(x) \psi_p^*(x) dx$$

$$= \frac{N_n}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{\infty} e^{-\frac{x^2}{2}} H_n\left(\frac{x}{\alpha}\right) e^{-\frac{i}{\hbar} p x} dx$$

令 $\eta = \frac{p}{\alpha\hbar}$

则 $\frac{p}{\hbar} x = \frac{p}{\hbar} \cdot \frac{x}{\alpha} = \eta \xi$

$$d\xi = d(\alpha x) = \alpha dx$$

于是 $C(\eta) = \frac{N_n}{\alpha \sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{\xi^2}{2}} H_n\left(\frac{\xi}{\alpha}\right) e^{-i\eta\xi} d\xi$

上式的积分计算如下：

利用厄米多项式的母函数

$$e^{-t^2+2t\xi} = \sum_{\ell} \frac{H_{\ell}(\xi)}{\ell!} t^{\ell}$$

两边乘以 $e^{-\frac{\xi^2}{2}} e^{-i\eta\xi}$ 并对 ξ 积分得

$$\begin{aligned} \sum_{\ell} \int_{-\infty}^{\infty} e^{-\frac{\xi^2}{2}} H_{\ell}(\xi) \frac{t^{\ell}}{\ell!} e^{-i\eta\xi} d\xi \\ &= \int_{-\infty}^{\infty} e^{-\frac{\xi^2}{2}} e^{-t^2+2t\xi} e^{-i\eta\xi} d\xi \\ &= e^{-t^2} \int_{-\infty}^{\infty} e^{-\frac{1}{2}[\xi - (2t - i\eta)]^2} d\xi \cdot e^{\frac{1}{2}(2t - i\eta)^2} \\ &= e^{-t^2 + \frac{1}{2}(2t - i\eta)^2} \sqrt{\frac{\pi}{\frac{1}{2}}} \\ &= \sqrt{2\pi} e^{t^2 - 2it\eta - \frac{\eta^2}{2}} \\ &= \sqrt{2\pi} e^{-\frac{\eta^2}{2}} e^{-(it)^2 + 2(it)(-\eta)} \\ &= \sqrt{2\pi} e^{-\frac{\eta^2}{2}} \sum_{\ell} \frac{H_{\ell}(-\eta)}{\ell!} (it)^{\ell} \end{aligned}$$

比较两边 t^{ℓ} 项的系数得

$$\int_{-\infty}^{\infty} e^{-\frac{\xi^2}{2}} H_n(\xi) e^{-i\eta\xi} d\xi = \sqrt{2\pi} e^{-\frac{\eta^2}{2}} H_n(-\eta) i^n$$

$$\therefore C(\eta) = \frac{1/\sqrt{2}}{\sqrt{\pi}^{1/2} n! 2^n} e^{-\frac{\eta^2}{2}} H_n(-\eta) i^n$$

式中

$$\beta = \frac{1}{2\pi}$$

但

$$H_n(\xi) = (-1)^n H_n(-\xi)$$

$$\begin{aligned} \therefore C(\eta) &= \frac{\sqrt{\beta}}{\sqrt{\pi^{1/2} n! 2^n}} (-1)^n i^n e^{-\frac{\eta^2}{2}} H_n(\eta) \\ &= \frac{\sqrt{\beta}}{\sqrt{\pi^{1/2} n! 2^n}} (-i)^n e^{-\frac{\eta^2}{2}} H_n(\eta) \end{aligned}$$

111. 在 E 表象中, 算符 $\hat{L}$ 可表示为一矩阵, 矩阵元为

$$L_{mn} = \int \psi_m^* \hat{L} \psi_n dx$$

其中

$$\psi_n = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

(1) 坐标的矩阵元:

$$\text{令 } \hat{L} = \hat{x} = x$$

则当 $m \neq n$ 时,

$$\begin{aligned} x_{mn} &= \frac{2}{a} \int_0^a x \sin \frac{m\pi x}{a} \sin \frac{n\pi x}{a} dx \\ &= \frac{2}{a} \int_0^a \frac{x}{2} \cos \left[\frac{(m-n)\pi x}{a} \right] dx \\ &\quad - \frac{2}{a} \int_0^a \frac{x}{2} \cos \left[\frac{(m+n)\pi x}{a} \right] dx \\ &= \frac{1}{a} \cdot \frac{a}{(m-n)\pi} \int_0^a x d \sin \frac{(m-n)\pi}{a} x \\ &\quad - \frac{1}{a} \cdot \frac{a}{(m+n)\pi} \int_0^a x d \sin \frac{(m+n)\pi}{a} x \\ &= \frac{1}{(m-n)\pi} \left[x \sin \frac{(m-n)\pi}{a} x \right]_0^a \\ &\quad - \frac{1}{(m-n)\pi} \int_0^a \sin \frac{(m-n)\pi}{a} x dx \\ &\quad - \frac{1}{(m+n)\pi} \left[x \sin \frac{(m+n)\pi}{a} x \right]_0^a \end{aligned}$$

$$\begin{aligned}
& + \frac{1}{(m+n)\pi} \int_0^a \sin \frac{(m+n)\pi}{a} x dx \\
& = \frac{a}{(m-n)^2 \pi^2} \cos \frac{(m-n)\pi}{a} x \Big|_0^a \\
& \quad - \frac{a}{(m+n)^2 \pi^2} \cos \frac{(m+n)\pi}{a} x \Big|_0^a \\
& = (-1)^{m-n} \frac{a}{(m-n)^2 \pi^2} - \frac{a}{(m-n)^2 \pi^2} \\
& \quad - (-1)^{m+n} \frac{a}{(m+n)^2 \pi^2} + \frac{a}{(m+n)^2 \pi^2} \\
& = \frac{a}{\pi^2} \left\{ (-1)^{m+n} \frac{1}{(m-n)^2} - \frac{1}{(m-n)^2} \right. \\
& \quad \left. - (-1)^{m+n} \frac{1}{(m+n)^2} + \frac{1}{(m+n)^2} \right\}, \quad (-1)^{m+n} = (-1)^m \\
& = \frac{a}{\pi^2} \{ (-1)^{m+n} - 1 \} \left\{ \frac{1}{(m-n)^2} - \frac{1}{(m+n)^2} \right\} \\
& = \frac{a}{\pi^2} \cdot \frac{4mn}{(m^2 - n^2)^2} [(-1)^{m+n} - 1] \\
& = \begin{cases} 0, & \text{当 } m+n \text{ 为偶数时} \\ -\frac{a}{\pi^2} \cdot \frac{8mn}{(m^2 - n^2)^2}, & \text{当 } m+n \text{ 为奇数时} \end{cases}
\end{aligned}$$

$$\begin{aligned}
\text{当 } m=n \text{ 时 } \chi_{nn} &= \frac{2}{a} \int_0^a x \sin^2 \frac{n\pi}{a} x dx = \frac{1}{a} \int_0^a x dx - \frac{1}{a} \int_0^a x \cos \frac{2n\pi}{a} x dx \\
&= \frac{1}{a} \int_0^a x dx - \frac{1}{a} \int_0^a x \cos \frac{2n\pi}{a} x dx = \frac{a}{2} - 0 = \frac{a}{2}
\end{aligned}$$

$$\text{例如 } \chi_{11} = \chi_{22} = \cdots = \chi_{nn} = \cdots = \frac{a}{2}$$

$$\chi_{12} = \chi_{21} = -\frac{16}{9\pi^2} a$$

$$\chi_{13} = \chi_{31} = 0, \cdots$$

$$\chi_{14} = \chi_{41} = -\frac{32}{(15\pi)^2} a \cdots$$

可见所求矩阵为对称矩阵，又因矩阵元为实数，故又是厄米矩阵，矩阵形式为

$$\begin{pmatrix}
 \frac{a}{2} & -\frac{16}{9\pi^2}a & 0 & -\frac{32}{(15\pi)^2}a & \cdots \\
 -\frac{16}{9\pi^2}a & \frac{a}{2} & & & \\
 0 & & \frac{a}{2} & & \\
 -\frac{32}{(15\pi)^2}a & & & \frac{a}{2} & \\
 & & & & \frac{a}{2}
 \end{pmatrix}$$

(2) 动量的矩阵元:

$$\text{今 } \hat{L} = \hat{p}_x = -i\hbar \frac{\partial}{\partial x}$$

则当 $m \neq n$ 时

$$\begin{aligned}
 (p_x)_{mn} &= \frac{2}{a} \int_0^a \sin \frac{m\pi x}{a} (-i\hbar \frac{\partial}{\partial x}) \sin \frac{n\pi x}{a} dx \\
 &= -\frac{2i\hbar}{a} \cdot \frac{n\pi}{a} \int_0^a \sin \frac{m\pi x}{a} \cos \frac{n\pi x}{a} dx \\
 &= -\frac{2i\hbar n\pi}{a^2} \int_0^a \frac{1}{2} \left[\sin \frac{(m+n)\pi}{a} x + \sin \frac{(m-n)\pi}{a} x \right] dx \\
 &= -\frac{i\hbar n\pi}{a^2} \cdot \frac{a}{(m+n)\pi} \int_0^a \sin \frac{(m+n)\pi}{a} x d\frac{(m+n)\pi}{a} x \\
 &\quad - \frac{i\hbar n\pi}{a^2} \cdot \frac{a}{(m-n)\pi} \int_0^a \sin \frac{(m-n)\pi}{a} x d\frac{(m-n)\pi}{a} x \\
 &= -\frac{i\hbar n}{a(m+n)} \left[-\cos \frac{m+n}{a} \pi x \right]_0^a - \frac{i\hbar n}{a(m-n)} \left[-\cos \frac{m-n}{a} \pi x \right]_0^a \\
 &= -\frac{i\hbar n}{a(m+n)} [1 - \cos(m+n)\pi] - \frac{i\hbar n}{a(m-n)} [1 - \cos(m-n)\pi] \\
 &= -\frac{i\hbar n}{a(m+n)} [1 - (-1)^{m+n}] - \frac{i\hbar n}{a(m-n)} [1 - (-1)^{m-n}] \\
 &= -\frac{i\hbar n}{a} [1 - (-1)^{m+n}] \times \left[\frac{1}{n+n} + \frac{1}{m-n} \right] \\
 &= \frac{2mn i\hbar}{a(m^2 - n^2)} [(-1)^{m+n} - 1]
 \end{aligned}$$

$$= \begin{cases} 0, & \text{当 } m+n \text{ 为偶数时} \\ -\frac{4mn i \hbar}{a(m^2-n^2)}, & \text{当 } m+n \text{ 为奇数时} \end{cases}$$

$$\begin{aligned} \text{当 } m=n \text{ 时 } (P_x)_{nn} &= \frac{2}{a} \int_0^a \sin \frac{n\pi x}{a} (-i\hbar \frac{\partial}{\partial x}) \sin \frac{n\pi x}{a} dx \\ &= -\frac{2i\hbar}{a} \int_0^a \sin \frac{n\pi x}{a} x \sin \frac{n\pi x}{a} dx \\ &= -\frac{i\hbar}{a} \sin^2 \frac{n\pi x}{a} \Big|_0^a = 0. \end{aligned}$$

$$\text{例如 } (P_x)_{11} = 0, \quad (P_x)_{22} = 0, \quad (P_x)_{33} = 0, \dots$$

$$(P_x)_{12} = \frac{8i\hbar}{3a}, \quad (P_x)_{21} = -\frac{8i\hbar}{3a} = (P_x)_{12}^*$$

$$(P_x)_{13} = (P_x)_{31} = 0, \dots$$

$$(P_x)_{14} = \frac{16i\hbar}{15a}, \quad (P_x)_{41} = -\frac{16i\hbar}{15a} = (P_x)_{14}^*$$

可见所求矩阵为厄米矩阵，矩阵形式为

$$P_x = \begin{pmatrix} 0 & \frac{8i\hbar}{3a} & 0 & \frac{16i\hbar}{15a} & \dots \\ -\frac{8i\hbar}{3a} & 0 & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & \dots \\ -\frac{16i\hbar}{15a} & \dots & \dots & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$

$$112 \quad \dot{x} = \frac{1}{i\hbar} (x\hat{H} - \hat{H}x)$$

$$\begin{aligned} \therefore (\dot{x})_{nm} &= \frac{1}{i\hbar} (x\hat{H} - \hat{H}x)_{nm} \\ &= \frac{1}{i\hbar} \sum_k (x_{nk} H_{km} - H_{nk} x_{km}). \end{aligned}$$

因为哈密顿量在能量表象中是对角矩阵，即

$$H_{km} = E_k \delta_{km}, \quad H_{nk} = E_k \delta_{nk}$$

于是

$$\begin{aligned}
 (\dot{\chi})_{nm} &= \frac{1}{i\hbar} \sum_k (\chi_{nk} E_k \delta_{km} - E_k \delta_{nk} \chi_{km}) \\
 &= \frac{1}{i\hbar} (\chi_{nm} E_m - E_n \chi_{nm}) \\
 &= \frac{1}{i\hbar} (E_m - E_n) \chi_{nm}
 \end{aligned}$$

或

$$\chi_{nm} = \frac{-i\hbar}{E_n - E_m} (\dot{\chi})_{nm} \quad (1)$$

同理

$$(\dot{\chi}^*)_{nm} = \frac{1}{-i\hbar} (E_m - E_n) \chi_{nm}^*$$

或

$$\chi_{nm}^* = \frac{i\hbar}{E_n - E_m} (\dot{\chi}^*)_{nm} \quad (2)$$

现将 $\sum_n (E_n - E_m) |\chi_{nm}|^2$ 写成 I 即

$$\begin{aligned}
 I &= \sum_n (E_n - E_m) |\chi_{nm}|^2 \\
 &= \sum_n (E_n - E_m) \chi_{nm}^* \chi_{nm}
 \end{aligned} \quad (3)$$

将(1)式代入(3)式得

$$\begin{aligned}
 I &= -i\hbar \sum_n \chi_{nm}^* (\dot{\chi})_{nm} \\
 &= -\frac{i\hbar}{\mu} \sum_n \chi_{nm}^* p_{nm} \quad \left(\hat{\chi} = \frac{\hat{p}}{\mu} \right) \\
 &= -\frac{i\hbar}{\mu} \sum_n \chi_{mn} p_{nm}
 \end{aligned} \quad (4)$$

其中利用了 χ 的厄米性质

$$\chi_{nm}^* = \chi_{mn}$$

将(2)式代入(3)式得

$$\begin{aligned}
 I &= i\hbar \sum_n (\dot{\chi}^*)_{nm} \chi_{nm} \\
 &= \frac{i\hbar}{\mu} \sum_n p_{nm}^* \chi_{nm} \\
 &= \frac{i\hbar}{\mu} \sum_n p_{mn} \chi_{nm} \quad (p_{nm}^* = p_{mn})
 \end{aligned} \quad (5)$$

(4) 式与 (5) 式相加, 得

$$\begin{aligned} 2I &= \frac{-i\hbar}{\mu} \sum_n (\chi_{mn} p_{nm} - p_{mn} \chi_{nm}) \\ &= \frac{-i\hbar}{\mu} (\hat{x}\hat{p} - \hat{p}\hat{x})_{mm} = \frac{-i\hbar}{\mu} \cdot i\hbar = \frac{\hbar^2}{\mu} \end{aligned}$$

$$\therefore I = \sum_n (E_n - E_m) |\chi_{nm}|^2 = \frac{\hbar^2}{2\mu}$$

113. (1) 在 A 表象中, 算符 $\hat{A}$ 的矩阵为对角矩阵, 对角元素就是算符的本征值, 现因

$$\hat{A}^2 = 1$$

故 $\hat{A}$ 的本征值为 ± 1 , 因而 $\hat{A}$ 可用二阶矩阵表示,

由此得 $\hat{A}$ 在 A 表象中的矩阵表示为

$$A = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

设 $\hat{B}$ 的矩阵表示为

$$B = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$$

由于 $\hat{A}\hat{B} + \hat{B}\hat{A} = 0$, 故

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} + \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = 0$$

$$\text{即 } \begin{pmatrix} b_{11} & b_{12} \\ -b_{21} & -b_{22} \end{pmatrix} + \begin{pmatrix} b_{11} & -b_{12} \\ b_{21} & -b_{22} \end{pmatrix} = \begin{pmatrix} 2b_{11} & 0 \\ 0 & -2b_{22} \end{pmatrix} = 0$$

$$\therefore b_{11} = b_{22} = 0,$$

于是

$$B = \begin{pmatrix} 0 & b_{12} \\ b_{21} & 0 \end{pmatrix}$$

再利用 $\hat{B}^2 = 1$, 有

$$\begin{pmatrix} 0 & b_{12} \\ b_{21} & 0 \end{pmatrix} \begin{pmatrix} 0 & b_{12} \\ b_{21} & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

即

$$\begin{pmatrix} b_{12} & b_{21} & 0 \\ 0 & b_{21} & b_{12} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$\begin{cases} b_{12} \cdot b_{21} = 1 \\ b_{21} \cdot b_{12} = 1 \end{cases}$$

由此得

$$b_{12} = \frac{1}{b_{21}}$$

于是

$$B = \begin{pmatrix} 0 & b_{12} \\ \frac{1}{b_{12}} & 0 \end{pmatrix}$$

因 B 是厄米矩阵, 即 $B^+ = B$, 故

$$\begin{pmatrix} 0 & \frac{1}{b_{12}^*} \\ b_{12}^* & 0 \end{pmatrix} = \begin{pmatrix} 0 & b_{12} \\ \frac{1}{b_{12}} & 0 \end{pmatrix}$$

由此得

$$b_{12} = \frac{1}{b_{12}^*}$$

一般地选

$$b_{12} = e^{i\theta}$$

于是得算符 $\hat{B}$ 在 A 表象中的矩阵表示为

$$B = \begin{pmatrix} 0 & e^{i\theta} \\ e^{-i\theta} & 0 \end{pmatrix}$$

(2) 同理, 在 B 表象中, $\hat{B}$ 的矩阵表示为

$$B = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$\hat{A}$ 的矩阵表示为

$$A = \begin{pmatrix} 0 & e^{i\theta} \\ e^{-i\theta} & 0 \end{pmatrix}$$

(3) 设 $\hat{B}$ 的本征值为 β , 本征函数为 $\begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix}$

已知在 A 表象中 $\hat{B}$ 的矩阵表示为

$$B = \begin{pmatrix} 0 & e^{i\theta} \\ e^{-i\theta} & 0 \end{pmatrix}$$

故本征方程为

$$\begin{pmatrix} 0 & e^{i\theta} \\ e^{-i\theta} & 0 \end{pmatrix} \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix} = \beta \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix}$$