第4章 力学量用算符表达

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- ☐ 算符运算规则
- ☐ 谐振子代数解法
- ☐ Hermite 算符，Observable
- ☐ 不确定度关系
- ☐ 共同本征函数，角动量算符
- ☐ 力学量完全集
- ☐ 连续谱本征函数“归一化”

He lies somewhere here

——海森堡 (W. Heisenberg)

坐标空间中的Operator

- ☐ 动量算符 $\hat{p} = -i\hbar\boldsymbol{\nabla}$
- ☐ 动能算符 $\hat{T} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2$
- ☐ 角动量算符 $\hat{l} = r \times \hat{p}$
- ☐ Hamilton量 $\hat{H} = \hat{T} + V(\boldsymbol{r}) = -\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})$

! 在量子力学中，力学量用算符表示。即在某一表象中，所有力学量表示为这一表象中的某种操作。

算符的运算规则

? 态叠加原理中的算符，算符作用在叠加态 $\psi = C_1\psi_1 + C_2\psi_2$ 上会怎样

- ☐ 线性算符：满足 $\hat{O}(C_1\psi_1 + C_2\psi_2) = C_1\hat{O}\psi_1 + C_2\hat{O}\psi_2$ 的算符。线性操作对应的都是线性算符，比如求导。非线性操作，比如开方，平方，取复共轭等不是线性算符。

最简单的算符 → 单位算符：$\hat{I}\psi = \psi$

算符的运算

- ☐ 算符相等：$\hat{A}\psi = \hat{B}\psi \xrightarrow{\psi\text{任意}} \hat{A} = \hat{B}$
- ☐ 算符求和：$(\hat{A} + \hat{B})\psi = \hat{A}\psi + \hat{B}\psi$
- ☐ 算符乘积：$(\hat{A}\hat{B})\psi = \hat{A}(\hat{B}\psi)$

? 乘法交换律 $\hat{A}\hat{B} = \hat{B}\hat{A}$?

两个操作不一定能交换顺序： $\hat{A}\hat{B} \neq \hat{B}\hat{A}$

例：$x\hat{p} - \hat{p}x$

考虑到

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

但

$$\hat{p}_x x\psi = -i\hbar\frac{\partial}{\partial x}(x\psi) = -i\hbar\psi - i\hbar x\frac{\partial}{\partial x}\psi$$

所以

$$(x\hat{p}_x - \hat{p}_x x)\psi = i\hbar\psi$$

ψ是任意的波函数，所以

$$x\hat{p}_x - \hat{p}_x x = i\hbar$$

类似还可以证明

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

但

$$x\hat{p}_y - \hat{p}_y x = 0, \qquad x\hat{p}_z - \hat{p}_z x = 0, \cdots$$

概括起来，就是

$$x_\alpha\hat{p}_\beta - \hat{p}_\beta x_\alpha = i\hbar\delta_{\alpha\beta}$$

对易式（commutator, 对易关系）

$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$

- [ ] $[\hat{A},\hat{B}] = -[\hat{B},\hat{A}]$
- [ ] $[\hat{A},\hat{A}] = 0$
- [ ] $[\hat{A},c] = 0$
- [ ] $[\hat{A},\hat{B}+\hat{C}] = [\hat{A},\hat{B}] + [\hat{A},\hat{C}]$
- [ ] $[\hat{A},\hat{B}\hat{C}] = [\hat{A},\hat{B}]\hat{C} + \hat{B}[\hat{A},\hat{C}]$
- [ ] $[\hat{A}\hat{B},\hat{C}] = [\hat{A},\hat{C}]\hat{B} + \hat{A}[\hat{B},\hat{C}]$
- [ ] $[\hat{A},[\hat{B},\hat{C}]] + [\hat{B},[\hat{C},\hat{A}]] + [\hat{C},[\hat{A},\hat{B}]] = 0$ (Jacobi恒等式)

按照定义，于是有 $[x,\hat{p}] = i\hbar$

? 为什么要讨论对易关系，再论一维谐振子

一维谐振子的代数解法

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

因式分解：$u^2 + v^2 = (iu + v)(-iu + v)$

? $\hat{H} \overset{?}{\to} \frac{1}{2m}(-i\hat{p} + m\omega x)(i\hat{p} + m\omega x)$

$$\frac{1}{2m}(-i\hat{p} + m\omega x)(i\hat{p} + m\omega x)$$
$$= \frac{1}{2m}[\hat{p}^2 + m^2\omega^2x^2 + im\omega(x\hat{p} - \hat{p}x)]$$
$$= \hat{H} + \frac{i\omega}{2}[x,\hat{p}]$$

$$= \hat{H} - \frac{1}{2}\hbar\omega$$

$$\frac{1}{2m}(i\hat{p} + m\omega x)(-i\hat{p} + m\omega x)$$

$$= \frac{1}{2m}[\hat{p}^2 + m^2\omega^2x^2 - im\omega(x\hat{p} - \hat{p}x)]$$

$$= \hat{H} - \frac{i\omega}{2}[x, \hat{p}]$$

$$= \hat{H} + \frac{1}{2}\hbar\omega$$

定义 $\hat{a}_\pm = \frac{1}{\sqrt{2\hbar m\omega}}(\mp i\hat{p} + m\omega x)$，则有

$$\hat{H} = \hbar\omega\left[(\hat{a}_+\hat{a}_-) + \frac{1}{2}\right] = \hbar\omega\left[(\hat{a}_-\hat{a}_+) - \frac{1}{2}\right]$$

如果波函数 ψ 满足定态 Schrödinger 方程

$$\hat{H}\psi = E\psi$$

则对于 $\hat{a}_+\psi$ 有

$$\hat{H}(\hat{a}_+\psi)$$

$$= \hbar\omega\left[(\hat{a}_+\hat{a}_-) + \frac{1}{2}\right](\hat{a}_+\psi)$$

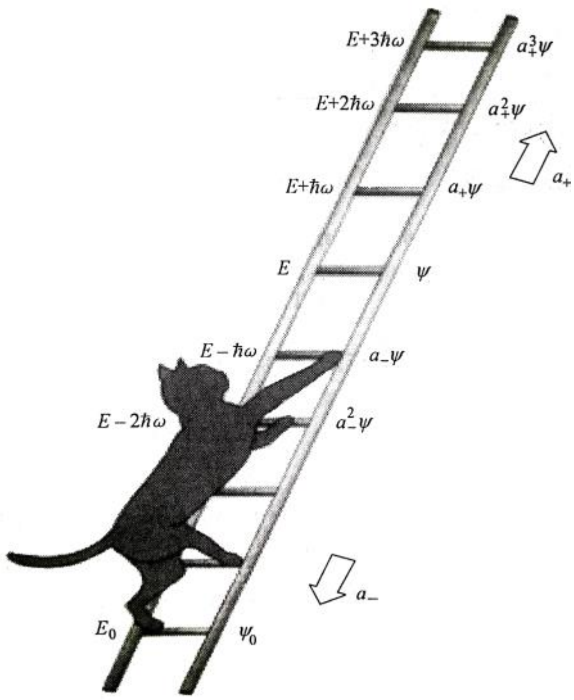
$$= \hbar\omega\left(\hat{a}_+\hat{a}_-a_+\psi + \frac{1}{2}\hat{a}_+\psi\right)$$

$$= \hat{a}_+\hbar\omega\left(\hat{a}_-\hat{a}_+\psi + \frac{1}{2}\psi\right)$$

$$= \hat{a}_+\left(\hat{H} + \frac{1}{2}\hbar\omega\right)\psi$$

$$= \left(E + \frac{1}{2}\hbar\omega\right)\hat{a}_+\psi$$

也就是说如果 ψ 是对应于能量本征值 E 的能量本征态，那么 $\hat{a}_+\psi$ 则是对应于能量本征值 $E + \frac{1}{2}\hbar\omega$ 的能量本征态。



同理有 $\hat{H}(\hat{a}_-\psi) = \left(E - \frac{1}{2}\hbar\omega\right)\hat{a}_-\psi$

于是有

$\psi \rightarrow E$

$\hat{a}_+\psi \rightarrow E + \frac{1}{2}\hbar\omega$

$\hat{a}_-\psi \rightarrow E - \frac{1}{2}\hbar\omega$

所以，这是一种生成新解的极好方法，如果我们得到了一个解，通过升降能量就可以得到其他的解。

升降算符 $\hat{a}_\pm$: 升算符$\hat{a}_+$，降算符 $\hat{a}_-$

如果我们反复应用降算符,能量逐渐下降。然而对于谐振子来说，能量不会小于0，于是必然存在一个本征态（基态）有

$$\hat{a}_-\psi_0 = 0$$

即

$$\frac{1}{\sqrt{2\hbar m\omega}}(i\hat{p} + m\omega x)\psi_0 = 0$$

$$\Rightarrow \left(\frac{\hbar d}{dx}+m\omega x\right)\psi_0 = 0$$
$$\Rightarrow \frac{\hbar d\psi_0}{dx} = -m\omega x\psi_0$$
$$\Rightarrow \frac{d\psi_0}{\psi_0} = -\frac{m\omega}{\hbar}xdx$$
$$\Rightarrow \ln\psi_0 = -\frac{m\omega}{2\hbar}x^2 + C$$
$$\Rightarrow \psi_0 = Ae^{-\frac{\alpha^2}{2}x^2} \quad \left(\alpha = \frac{m\omega}{\hbar}\right)$$

- 基态能量本征方程

$$\hat{H}\psi_0 = \hbar\omega\left[(\hat{a}_+\hat{a}_-)+\frac{1}{2}\right]\psi_0 = E_0\psi_0 = \frac{1}{2}\hbar\omega$$

- 激发态能量本征方程

$$\hat{H}\hat{a}_+^n\psi_0 = \hbar\omega(n+\frac{1}{2})\hat{a}_+^n\psi_0$$
$$\begin{cases} \psi_n = \hat{a}_+^n\psi_0 = A\left(-\hbar\frac{d}{dx}+m\omega x\right)^n e^{-\frac{\alpha^2}{2}x^2} \\ E_n = \left(n+\frac{1}{2}\right)\hbar\omega \end{cases}$$

★ 常用对易关系

- $[x,\hat{p}] = i\hbar$
- $[x_\alpha,\hat{p}_\beta] = i\hbar\delta_{\alpha\beta}$
- $[\hat{p},f(x)] = -i\hbar\frac{\partial f}{\partial x}$
- $[\hat{l}_\alpha,x_\beta] = \varepsilon_{\alpha\beta\gamma}i\hbar x_\gamma$ $\left(\text{Levi} - \text{Civita 符号 } \varepsilon_{\alpha\beta\gamma}: \begin{cases} \varepsilon_{123} = \varepsilon_{231} = \varepsilon_{312} = 1 \text{ 正序} \\ \varepsilon_{132} = \varepsilon_{321} = \varepsilon_{213} = -1 \text{ 逆序} \\ \text{other cases} = 0 \end{cases}\right)$
- $[\hat{l}_\alpha,\hat{p}_\beta] = \varepsilon_{\alpha\beta\gamma}i\hbar\hat{p}_\gamma$
- $[\hat{l}_\alpha,\hat{l}_\beta] = \varepsilon_{\alpha\beta\gamma}i\hbar\hat{l}_\gamma$
- $\hat{\boldsymbol{l}}\times\hat{\boldsymbol{l}} = i\hbar\hat{\boldsymbol{l}}$

★ 算符自己叉乘自己可以不为0，原因是分量之间可能不对易

- $[\hat{l}_+,\hat{l}_-] = 2\hbar\hat{l}_z \quad (\hat{l}_\pm = \hat{l}_x \pm i\hat{l}_y)$
- $[\hat{l}_z,\hat{l}_\pm] = \pm\hbar\hat{l}_\pm$
- $[\hat{\boldsymbol{l}},V(\boldsymbol{r})] = 0$

★ 角动量算符

$$\hat{\boldsymbol{l}} = \boldsymbol{r}\times\hat{\boldsymbol{p}}$$

$$\begin{cases} \hat{l}_x = y\hat{p}_z - z\hat{p}_y = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \\ \hat{l}_y = z\hat{p}_x - x\hat{p}_z = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \\ \hat{l}_z = x\hat{p}_y - y\hat{p}_x = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \end{cases}$$

球坐标

$$\begin{cases} x = r\sin\theta\cos\varphi \\ y = r\sin\theta\sin\varphi \\ z = r\cos\theta \end{cases} \qquad \begin{cases} r = \sqrt{x^2+y^2+z^2} \\ \theta = \arctan\left(\dfrac{\sqrt{x^2+y^2}}{z}\right) \\ \varphi = \arctan\left(\dfrac{y}{x}\right) \end{cases}$$

$$\begin{cases} \hat{l}_x = i\hbar\left(\sin\varphi\dfrac{\partial}{\partial\theta} + \cot\theta\cos\varphi\dfrac{\partial}{\partial\varphi}\right) \\ \hat{l}_y = i\hbar\left(-\cos\varphi\dfrac{\partial}{\partial\theta} + \cot\theta\sin\varphi\dfrac{\partial}{\partial\varphi}\right) \\ \hat{l}_z = -i\hbar\dfrac{\partial}{\partial\varphi} \end{cases}$$

$$\hat{l}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]$$

$$\hat{T} = -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{\hat{l}^2}{2mr^2} = \frac{\hat{p}_r^2}{2m} + \frac{\hat{l}^2}{2mr^2}$$

$$\hat{p}_r = -i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)$$

- 逆算符 $\hat{A}^{-1}$

$\hat{A}^{-1}\hat{A} = \hat{A}\hat{A}^{-1} = I \Longrightarrow [\hat{A}, \hat{A}^{-1}] = 0$

★ $(\hat{A}\hat{B})^{-1} = \hat{B}^{-1}\hat{A}^{-1}$

- 算符的函数

$$F(\hat{A}) = \sum_{n=0}^{\infty}\frac{F^{(n)}(0)}{n!}\hat{A}^n$$

例如，$F(x)=e^{ax}$，$\hat{A}=\dfrac{\mathrm{d}}{\mathrm{d}x}$，则可定义

$$F(\hat{A}) = \exp\left(a\frac{\mathrm{d}}{\mathrm{d}x}\right) = \sum_{n=0}^{\infty}\frac{a^n}{n!}\frac{\mathrm{d}^n}{\mathrm{d}x^n}$$

波函数的标积 (scalar product)

$$(\psi, \varphi) \equiv \int \mathrm{d}\tau\,\psi^*\varphi$$

$(\psi,\psi) \geqslant 0$

$(\psi,\varphi)^* = (\varphi,\psi)$

$(\psi, c_1\varphi_1 + c_2\varphi_2) = c_1(\psi,\varphi_1) + c_2(\psi,\varphi_2)$

$(c_1\psi_1 + c_2\psi_2, \varphi) = c_1^*(\psi_1,\varphi) + c_2^*(\psi_2,\varphi)$

算符的复共轭 $\hat{O}^*$ （算符里的所有量取复共轭）

$\hat{\boldsymbol{p}}^* = -\hat{\boldsymbol{p}}$

- 算符的转置
- $(\psi, \tilde{\hat{O}}\varphi) = (\varphi^*, \hat{O}\psi^*)$
- $\int d\tau \psi^* \tilde{\hat{O}} \varphi = \int d\tau \varphi \hat{O} \psi^*$
- $\dfrac{\tilde{\partial}}{\partial x} = -\dfrac{\partial}{\partial x}$
- $(\widetilde{\hat{A}\hat{B}}) = \tilde{\hat{B}}\tilde{\hat{A}}$
- 算符的厄米 (Hermite) 共轭: 转置复共轭
- $(\psi, \hat{O}^+\varphi) = (\hat{O}\psi, \varphi)$
- $\hat{O}^+ = \tilde{\hat{O}}^*$
- $(\hat{A}\hat{B}\hat{C}\cdots)^* = \hat{A}^*\hat{B}^*\hat{C}^*\cdots$

  $(\hat{A}\hat{B}\hat{C}\cdots)^+ = \cdots\hat{C}^+\hat{B}^+\hat{A}^+$
- 厄米算符
- $\hat{O}^\dagger = \hat{O}$ or $(\psi, \hat{O}\psi) = (\hat{O}\psi, \psi)$ †: dagger
- ? 若 Â, B̂ 都是厄米算符,那么乘积 ÂB̂ 是否是厄米算符?

  $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger = \hat{B}\hat{A}$,

  所以需要 $[\hat{A},\hat{B}] = 0$, 才有 $(\hat{A}\hat{B})^\dagger = \hat{A}\hat{B}$
- 在任何量子态下，厄米算符的平均值必为实数。
- 在体系的任何量子态下平均值均为实数的算符， 必为厄米算符。
- 实验上可以观测的力学量：可观测量（Observable）要求平均值为实数。

  可观测量的算符必然为厄米算符
- 对于厄米算符有

  $\overline{\hat{O}^2} = (\psi, \hat{O}^2\psi) \geqslant 0$

- 幺正算符 (Unitary operator)

$\hat{A}^{-1} = \hat{A}^{\dagger} \Longrightarrow \hat{A}\hat{A}^{\dagger} = \hat{A}^{\dagger}\hat{A} = 1$

- 幺正算符乘积还是幺正算符

$\hat{A}\hat{B}(\hat{A}\hat{B})^{\dagger} = \hat{A}\hat{B}\hat{B}^{\dagger}\hat{A}^{\dagger} = \hat{A}\hat{A}^{\dagger} = 1$

! 若$\hat{O}$为厄米算符，则 $\hat{A} = e^{i\hat{O}}$ 为幺正算符

$\left(e^{i\hat{O}}\right)^{\dagger} e^{i\hat{O}} = e^{-i\hat{O}} e^{i\hat{O}} = 1$

★ 算符的指数乘积不等于算符乘积的指数，除非二者对易

★ Schrödinger方程的形式解，时间演化算符

$$i\hbar \frac{\partial \psi(t)}{\partial t} = \hat{H}\psi(t)$$

假设有时间演化算符 $\hat{U}(t)$, 使得 $\psi(t) = \hat{U}(t)\psi(0)$, 则有

$$i\hbar \frac{\partial \hat{U}(t)}{\partial t}\psi(0) = \hat{H}\hat{U}(t)\psi(0)$$

$$\Longrightarrow i\hbar \frac{\partial \hat{U}(t)}{\partial t} = \hat{H}\hat{U}(t)$$

$$\Longrightarrow \frac{1}{\hat{U}(t)} \frac{\partial \hat{U}(t)}{\partial t} = -\frac{i\hat{H}}{\hbar}$$

$$\Longrightarrow \hat{U}(t) = e^{-\frac{iHt}{\hbar}}$$

由于 $\hat{H} = \hat{H}^{\dagger}$, 所以$\hat{U}\hat{U}^{\dagger} = 1$

★ 时间演化算符 $\hat{U}(t) = e^{-iHt/\hbar}$ 是幺正算符

★ 厄米算符的本征问题

■ 平均值与涨落 (fluctuation)

力学量的平均值是由多次测量得到的结果，趋于一个确定值。然而每次测量结果围绕平均值有一个涨落.其定义为（均方差，标准差）

$$\overline{\Delta O^2} = \overline{(\hat{O} - \bar{O})^2} = \int \psi^*(\hat{O} - \bar{O})^2 \psi d\tau = \int \left|(\hat{O} - \bar{O})\psi\right|^2 d\tau \geq 0$$

与能量对应类似，总可以找到特殊的态，使得 $\overline{\Delta O^2} = 0$。即 $(\hat{O} - \bar{O})\psi = 0$

于是有

★ $\hat{O}\psi_n = O_n\psi_n$

★ 此即厄米算符的本征方程

- 厄米算符的本征值必为实数
- 厄米算符对应于不同本征值的本征函数，彼此正交

上面两个性质证明见课本136页。137-139页4个例子页需要掌握。

■ 力学量的本征问题与简并

如果算符 $\hat{O}$ 的第 n 个本征态有 f_n 重简并，则有

$\hat{O}\psi_{n\alpha} = O_n\psi_{n\alpha} \quad (\alpha = 1,2,\dots,f_n)$

此时这 f_n 个本征态不一定正交，但总可以通过线性叠加

$\phi_{n\beta} = \sum_{\alpha=1}^{f_n} a_{\beta\alpha}\psi_{n\alpha}$，

使得彼此正交

$(\phi_{n\beta}, \phi_{n\gamma}) = \delta_{\beta\gamma}$

在处理实际问题 时，如出现简并 时，为了要把 $\hat{O}$ 的本征态确定下来，往往是用 $\hat{O}$ 以外的其他某力学量的本征值来区分这些简并态．此时，正交性问题可自动 得到解决．这 就涉及两个（或多个）力学 量的共同本征态,也涉及不同 的 力学量的不确定度的关系．

不确定度关系的严格证明

回想一下谐振子的代数解法，假设有两个厄米算符组成的算符 $\hat{A}+i\gamma\hat{B}$ 作用在量子态 $\varphi=(\hat{A}+i\gamma\hat{B})\psi$上

则其模必为正，即

$(\varphi,\varphi)=\left((\hat{A}+i\gamma\hat{B})\psi,(\hat{A}+i\gamma\hat{B})\psi\right)$

$=\left(\psi,\hat{A}^2\psi\right)+\left(\psi,i\gamma[\hat{A},\hat{B}]\psi\right)+\left(\psi,\gamma^2\hat{B}^2\psi\right)$

$=\overline{\hat{A}^2}+i\gamma\overline{[\hat{A},\hat{B}]}+\gamma^2\overline{\hat{B}^2}\geq 0$

于是有

$\bar{\hat{C}}^2-4\overline{\hat{A}^2}\,\overline{\hat{B}^2}\leq 0\quad \hat{C}=i\left[\hat{A},\hat{B}\right]$ 为厄米算符

即 $\sqrt{\overline{\hat{A}^2}\,\overline{\hat{B}^2}}\geq\frac{1}{2}\left|\bar{\hat{C}}\right|$

定义新厄米算符

$\hat{A}‘=\hat{A}-\bar{\hat{A}}$

$\hat{B}‘=\hat{B}-\bar{\hat{B}}$

同样满足 $\hat{C}=i\left[\hat{A}‘,\hat{B}’\right]$

于是有

$\Delta A\cdot\Delta B\geq\frac{1}{2}\left|\overline{[\hat{A},\hat{B}]}\right|$

此即推广的 Heisenberg 不确定度关系