

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

! 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

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

但

$$x\hat{p}_y - \hat{p}_y x = 0, \quad x\hat{p}_z - \hat{p}_z x = 0, \dots$$

概括起来, 就是

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

对易 (commutator, 对易关系)

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

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

$$\square [\hat{A}, \hat{A}] = 0$$

$$\square [\hat{A}, c] = 0$$

$$\square [\hat{A}, \hat{B} + \hat{C}] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}]$$

$$\square [\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$$

$$\square [\hat{A}\hat{B}, \hat{C}] = [\hat{A}, \hat{C}]\hat{B} + \hat{A}[\hat{B}, \hat{C}]$$

$$\square [\hat{A}, [\hat{B}, \hat{C}]] + [\hat{B}, [\hat{C}, \hat{A}]] + [\hat{C}, [\hat{A}, \hat{B}]] = 0 \quad (\text{Jacobi 恒等式})$$

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

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

因式分解: $u^2 + v^2 = (iu + v)(-iu + v)$

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

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

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

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

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

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

$$\begin{aligned}
&\hat{H}(\hat{a}_+\psi) \\
&= \hbar\omega \left[(\hat{a}_+ \hat{a}_-) + \frac{1}{2} \right] (\hat{a}_+\psi) \\
&= \hbar\omega \left(\hat{a}_+ \hat{a}_- \hat{a}_+\psi + \frac{1}{2} \hat{a}_+\psi \right) \\
&= \hat{a}_+ \hbar\omega \left(\hat{a}_- \hat{a}_+\psi + \frac{1}{2} \psi \right) \\
&= \hat{a}_+ \left(\hat{H} + \frac{1}{2}\hbar\omega \right) \psi \\
&= \left(E + \frac{1}{2}\hbar\omega \right) \hat{a}_+\psi
\end{aligned}$$

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。

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

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。

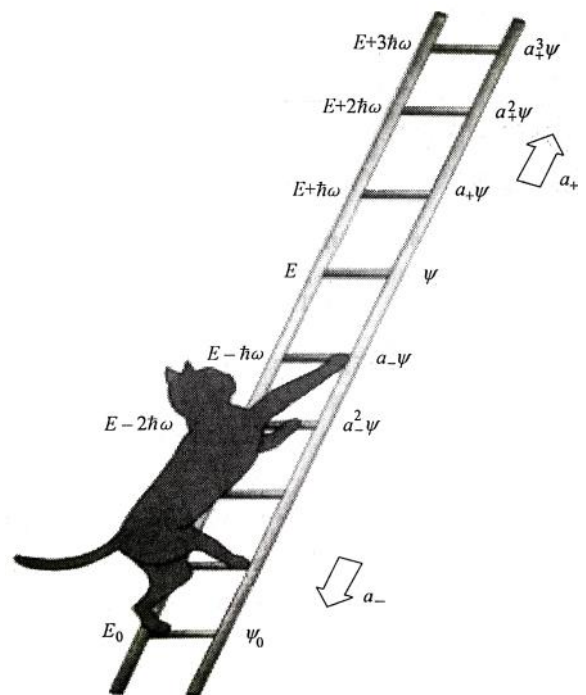
! 升降算符 \hat{a}_{\pm} : 升算符 \hat{a}_+ , 降算符 \hat{a}_-

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

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



$$\begin{aligned} \Rightarrow \left(\frac{\hbar d}{dx} + m\omega x \right) \psi_0 &= 0 \\ \Rightarrow \frac{\hbar d\psi_0}{dx} &= -m\omega x \psi_0 \\ \Rightarrow \frac{d\psi_0}{\psi_0} &= -\frac{m\omega}{\hbar} x dx \\ \Rightarrow \ln \psi_0 &= -\frac{m\omega}{2\hbar} x^2 + C \\ \Rightarrow \psi_0 &= A e^{-\frac{\alpha^2}{2} x^2} \quad \left(\alpha = \frac{m\omega}{\hbar} \right) \end{aligned}$$

■ 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

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

★ 常用对易关系

$$\square [x, \hat{p}] = i\hbar$$

$$\square [x_\alpha, \hat{p}_\beta] = i\hbar \delta_{\alpha\beta}$$

$$\square [\hat{p}, f(x)] = -i\hbar \frac{\partial f}{\partial x}$$

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

$$\square [\hat{l}_\alpha, \hat{p}_\beta] = \varepsilon_{\alpha\beta\gamma} i\hbar \hat{p}_\gamma$$

$$\square [\hat{l}_\alpha, \hat{l}_\beta] = \varepsilon_{\alpha\beta\gamma} i\hbar \hat{l}_\gamma$$

$$\square \hat{\mathbf{l}} \times \hat{\mathbf{l}} = i\hbar \hat{\mathbf{l}}$$

★ 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

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

$$\square [\hat{l}_z, \hat{l}_\pm] = \pm \hbar \hat{l}_\pm$$

$$\square [\hat{\mathbf{l}}, V(\mathbf{r})] = 0$$

★ 角动量算符

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

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

球坐标

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

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

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

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

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

□ 逆算符 \hat{A}^{-1}

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

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

□ 算符的函数

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

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

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

波函数的标积 (scalar product)

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

$$(\psi, \psi) \geq 0$$

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

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

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

算符的复共轭 \hat{O}^* (算符里的所有量取复共轭)

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

★ 算符的转置

$$\square (\psi, \tilde{\hat{O}} \varphi) = (\varphi^*, \hat{O} \psi^*)$$

$$\square \int d\tau \psi^* \tilde{\hat{O}} \varphi = \int d\tau \varphi \hat{O} \psi^*$$

$$\square \frac{\tilde{\partial}}{\partial x} = -\frac{\partial}{\partial x}$$

$$\square \widetilde{(\hat{A} \hat{B})} = \tilde{\hat{B}} \tilde{\hat{A}}$$

★ 算符的厄米 (Hermite) 共轭: 转置复共轭

$$\square (\psi, \hat{O}^+ \varphi) = (\hat{O} \psi, \varphi)$$

$$\square \hat{O}^- = \tilde{\hat{O}}^*$$

$$\square (\hat{A} \hat{B} \hat{C} \dots)^* = \hat{A}^* \hat{B}^* \hat{C}^* \dots$$

$$\square (\hat{A} \hat{B} \hat{C} \dots)^+ = \dots \hat{C}^+ \hat{B}^+ \hat{A}^+$$

💡 厄米算符

$$\star \hat{O}^\dagger = \hat{O} \text{ or } (\psi, \hat{O} \psi) = (\hat{O} \psi, \psi) \quad \dagger: \text{dagger}$$

? 若 \hat{A}, \hat{B} 都是厄米算符, 那么乘积 $\hat{A}\hat{B}$ 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 $(\hat{A}\hat{B})^\dagger = \hat{A}\hat{B}$

\square 在任何量子态下, 厄米算符的平均值必为实数。

\square 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

\square 对于厄米算符有

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

💡 么正算符 (Unitary operator)

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

□ 么正算符乘积还是么正算符

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

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

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

★ 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

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

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

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

$$\Rightarrow \hat{U}(t) = e^{-\frac{i\hat{H}t}{\hbar}}$$

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

★ 时间演化算符 $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$ 是么正算符