# 第4章 力学量用算符表达

2017年4月9日 15:03

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

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

$\psi$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）

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

- [ ] $[\hat{A},\hat{B}] = -[\hat{B},\hat{A}]$
- [ ] $[\hat{A},\hat{A}] = 0$
- [ ] $[\hat{A},c] = 0$
- [ ] $[\hat{A},\hat{B}+\hat{C}] = [\hat{A},\hat{B}] + [\hat{A},\hat{C}]$
- [ ] $[\hat{A},\hat{B}\hat{C}] = [\hat{A},\hat{B}]\hat{C} + \hat{B}[\hat{A},\hat{C}]$
- [ ] $[\hat{A}\hat{B},\hat{C}] = [\hat{A},\hat{C}]\hat{B} + \hat{A}[\hat{B},\hat{C}]$
- [ ] $[\hat{A},[\hat{B},\hat{C}]] = [\hat{B},[\hat{C},\hat{A}]] + [\hat{C},[\hat{A},\hat{B}]]$ (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：$u^2 + v^2 = (iu + v)(-iu + v)$

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

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

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

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

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

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

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

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

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

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 $\psi$ 满足定态 Schrödinger 方程

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

则对于 $\hat{a}_+\psi$ 有

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

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

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

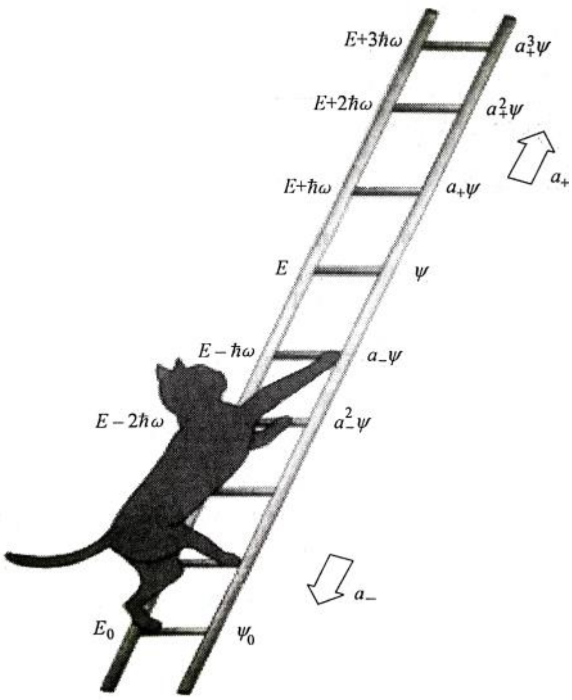
$= \hat{a}_+\hbar\omega\left(\hat{a}_-\hat{a}_+\psi + \frac{1}{2}\psi\right)$

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

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

也就是说如果 $\psi$ 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

$\psi \to E$

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

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

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

$$\hat{H}\hat{a}_+^n\psi_0 = \hbar\omega(n + \frac{1}{2})\hat{a}_+^n\psi_0$$

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

## ★ 常用对易关系

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

## ★ 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

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

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

## 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，$F(x)=e^{ax}$，$\hat{A}=\dfrac{d}{dx}$，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)

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

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

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

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

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

算符的复共轭 $\hat{O}^*$ （算符里的所有量取复共轭）

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

- 算符的转置
- $(\psi, \tilde{\hat{O}}\varphi) = (\varphi^*, \hat{O}\psi^*)$
- $\int d\tau \psi^* \tilde{\hat{O}} \varphi = \int d\tau \varphi \hat{O} \psi^*$
- $\frac{\tilde{\partial}}{\partial x} = -\frac{\partial}{\partial x}$
- $(\widetilde{\hat{A}\hat{B}}) = \tilde{\hat{B}}\tilde{\hat{A}}$
- 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

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

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

! 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