量子力学与统计物理

Quantum mechanics and statistical physics

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第三章：量子力学中的力学量

第四、五讲：对易关系
不确定性原理

引入：

$$\hat{F}\hat{G}=\hat{G}\hat{F} \qquad ?$$

问题：1. 哪些算符之间对易，哪些不是？

问题：2. 对易的物理含义是什么？

不对易的物理含义又是什么？

1. 对易关系与对易子

设 $\hat{F}$ 和 $\hat{G}$ 为两个算符

若 $\hat{F}\hat{G}=\hat{G}\hat{F}$， 则称 $\hat{F}$ 与 $\hat{G}$ 对易

若 $\hat{F}\hat{G}\neq\hat{G}\hat{F}$， 则称 $\hat{F}$ 与 $\hat{G}$ 不对易

引入对易子： $\boxed{[\hat{F},\hat{G}]=\hat{F}\hat{G}-\hat{G}\hat{F}}$

若 $[\hat{F},\hat{G}]=0$， 则 $\hat{F}$ 与 $\hat{G}$ 对易

若 $[\hat{F},\hat{G}]\neq 0$， 则 $\hat{F}$ 与 $\hat{G}$ 不对易

2． 对易子的运算法则（重要，要求活学活用）

$\langle 1\rangle [\hat{A},\hat{B}] = -[\hat{B},\hat{A}]$；

$\langle 2\rangle [\hat{A},\hat{A}] = 0$；

$\langle 3\rangle [\hat{A},c] = 0$ （c 为复常数）；

$\langle 4\rangle [\hat{A},\hat{B}+\hat{C}] = [\hat{A},\hat{B}]+[\hat{A},\hat{C}]$；

$\langle 5\rangle [\hat{A},\hat{B}\hat{C}] = \hat{B}[\hat{A},\hat{C}]+[\hat{A},\hat{B}]\hat{C}$；

$\langle 6\rangle [\hat{A}\hat{B},\hat{C}] = \hat{A}[\hat{B},\hat{C}]+[\hat{A},\hat{C}]\hat{B}$。

证明⟨5⟩：等式右边$=\hat{B}\hat{A}\hat{C}-\hat{B}\hat{C}\hat{A}+\hat{A}\hat{B}\hat{C}-\hat{B}\hat{A}\hat{C}=\hat{A}\hat{B}\hat{C}-\hat{B}\hat{C}\hat{A}$

等式左边$=\hat{A}\hat{B}\hat{C}-\hat{B}\hat{C}\hat{A}$，等式成立。

3. 坐标与动量对易关系——基本对易关系

求算符$\hat{x}=x$与$\hat{p}_x=-\mathrm{i}\hbar\dfrac{\partial}{\partial x}$之间的对易关系

解：(1) $x\hat{p}_x\psi=x(-\mathrm{i}\hbar\frac{\partial}{\partial x})\psi=-\mathrm{i}\hbar x\frac{\partial}{\partial x}\psi$

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

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

$\because$ ψ是任意波函数

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

即 $[x,\hat{p}_x]=\mathrm{i}\hbar$

同理可证：$y\hat{p}_y - \hat{p}_y y = \mathrm{i}\hbar,\ z\hat{p}_z - \hat{p}_z z = \mathrm{i}\hbar$

结论：

（1）坐标算符与其共轭动量算符不对易（同一个空间分量）

现证明：

（2）坐标算符与非共轭动量算符对易

$$\begin{cases} x\hat{p}_y - \hat{p}_y x = 0 \\ x\hat{p}_z - \hat{p}_z x = 0 \end{cases},\quad \begin{cases} y\hat{p}_x - \hat{p}_x y = 0 \\ y\hat{p}_z - \hat{p}_z y = 0 \end{cases},\quad \begin{cases} z\hat{p}_x - \hat{p}_x z = 0 \\ z\hat{p}_y - \hat{p}_y z = 0 \end{cases}$$

$$\Leftrightarrow x_i \hat{p}_j - \hat{p}_j x_i = 0,\ i \neq j, x_1 = x, x_2 = y, x_3 = z$$

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

$$\hat{p}_x y\psi = (-\mathrm{i}\hbar\frac{\partial}{\partial x})y\psi = -\mathrm{i}\hbar y\frac{\partial}{\partial x}\psi \qquad \Rightarrow y\hat{p}_x - \hat{p}_x y = 0$$

课堂作业！

（3）各动量算符之间相互对易

$$\hat{p}_x\hat{p}_y-\hat{p}_y\hat{p}_x=0,\ \hat{p}_y\hat{p}_z-\hat{p}_z\hat{p}_y=0,\ \hat{p}_z\hat{p}_x-\hat{p}_x\hat{p}_z=0$$

（4）各坐标算符相互对易

$$xy-yx=0,\ xz-zx=0,\ yz-zy=0$$

坐标、动量对易关系小结：

$$\left.\begin{aligned}[\hat{x},\hat{y}]&=0\\ [\hat{y},\hat{z}]&=0\\ [\hat{z},\hat{x}]&=0\end{aligned}\right\} \Rightarrow \quad [x_\alpha,\ x_\beta]=0,\ \ \alpha,\beta=1,2,3 \quad (x_1=x,\ x_2=y,\ x_3=z)$$

$$\left.\begin{aligned}[\hat{p}_x,\hat{p}_y]&=0\\ [\hat{p}_y,\hat{p}_z]&=0\\ [\hat{p}_z,\hat{p}_x]&=0\end{aligned}\right\} \Rightarrow \quad [\hat{p}_\alpha,\hat{p}_\beta]=0,\ \ \alpha,\beta=1,2,3 \quad (\hat{p}_1=\hat{p}_x,\ \hat{p}_2=\hat{p}_y,\ \hat{p}_3=\hat{p}_z)$$

$$\begin{aligned}&[x,\hat{p}_x]=\mathrm{i}\hbar \quad [x,\hat{p}_y]=[x,\hat{p}_z]=0\\ &[y,\hat{p}_y]=\mathrm{i}\hbar,\ [y,\hat{p}_x]=[y,\hat{p}_z]=0\\ &[z,\hat{p}_z]=\mathrm{i}\hbar \quad [z,\hat{p}_x]=[z,\hat{p}_y]=0\end{aligned} \Rightarrow \quad [x_\alpha,\hat{p}_\beta]=\mathrm{i}\hbar\delta_{\alpha\beta}=\begin{cases}\mathrm{i}\hbar, & \alpha=\beta\\ 0, & \alpha\neq\beta\end{cases}$$

$$(\alpha,\beta=1,2,3)$$

基本对易关系通式：

$$\delta_{\alpha\beta}=\begin{cases}1, & \alpha=\beta \\ 0, & \alpha\neq\beta\end{cases},\quad \alpha,\beta=1,2,3$$

$$[x_\alpha, x_\beta]=x_\alpha x_\beta-x_\beta x_\alpha=0$$

$$[\hat{p}_\alpha, \hat{p}_\beta]=\hat{p}_\alpha\hat{p}_\beta-\hat{p}_\beta\hat{p}_\alpha=0$$

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

量子力学基本对易关系

由于力学量一般都是坐标和动量的函数，知道以上基本对易关系，再结合对易子运算法则，可求出其他力学量之间的对易关系。

4. 其他对易关系的推导

坐标与角动量对易关系

例：证明 $[\hat{L}_x, y] = \mathrm{i}\hbar z$

$$[y\hat{p}_z - z\hat{p}_y, y] = -[y, y\hat{p}_z - z\hat{p}_y]$$

$$= -[y, y\hat{p}_z] + [y, z\hat{p}_y]$$

$$= -y[y, \hat{p}_z] - [y, y]\hat{p}_z + z[y, \hat{p}_y] + [y, z]\hat{p}_y$$

$$= -0 - 0 + z(\mathrm{i}\hbar) + 0$$

$$= \mathrm{i}\hbar z$$

坐标与角动量对易关系

$$[\hat{L}_x, y] = i\hbar z \quad [\hat{L}_x, x] = 0 \quad [\hat{L}_x, z] = -i\hbar y$$

$$[\hat{L}_y, z] = i\hbar x \quad [\hat{L}_y, y] = 0 \quad [\hat{L}_y, x] = -i\hbar z$$

$$[\hat{L}_z, z] = 0 \quad [\hat{L}_z, y] = -i\hbar x \quad [\hat{L}_z, x] = i\hbar y$$

$$[\hat{L}_\alpha, x_\beta] = i\hbar \varepsilon_{\alpha\beta\gamma} x_\gamma \equiv \sum_{\gamma=1}^{3} i\hbar \varepsilon_{\alpha\beta\gamma} x_\gamma$$

$$(\alpha, \beta, \gamma = 1, 2, 3)$$

(1) $\varepsilon_{123} = 1$

(2) $\varepsilon_{\alpha\alpha\beta} = \varepsilon_{\alpha\beta\alpha} = \ldots = 0$

任意两个下标相同，则为零

(3) $\varepsilon_{\alpha\beta\gamma} = -\varepsilon_{\beta\alpha\gamma} = -\varepsilon_{\alpha\gamma\beta}$

任意两个相邻下标的对换，改变正负符号

$$\left.\begin{aligned} \hat{L}_x &= y\hat{p}_z - z\hat{p}_y \\ \hat{L}_y &= z\hat{p}_x - x\hat{p}_z \\ \hat{L}_z &= x\hat{p}_y - y\hat{p}_x \end{aligned}\right\} \Rightarrow$$

$$\hat{L}_\alpha = \varepsilon_{\alpha\beta\gamma} x_\beta \hat{p}_\gamma \equiv \sum_{\beta,\gamma} \varepsilon_{\alpha\beta\gamma} x_\beta \hat{p}_\gamma$$

$$\begin{cases} x_1 = x,\ x_2 = y,\ x_3 = z \\ \alpha, \beta, \gamma = 1, 2, 3 \end{cases}$$

角动量与动量对易关系

证：$[\hat{L}_x, \hat{p}_y] = \mathrm{i}\hbar\hat{p}_z$, $(\hat{L}_x = y\hat{p}_z - z\hat{p}_y,\ \hat{p}_y = -\mathrm{i}\hbar\frac{\partial}{\partial y})$

$$[\hat{L}_x, \hat{p}_y] = \hat{L}_x\hat{p}_y - \hat{p}_y\hat{L}_x = (y\hat{p}_z - z\hat{p}_y)\hat{p}_y - \hat{p}_y(y\hat{p}_z - z\hat{p}_y)$$

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

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

$$= y\hat{p}_y\hat{p}_z - \hat{p}_y y\hat{p}_z,$$

$$y\hat{p}_y - \hat{p}_y y = \mathrm{i}\hbar \Rightarrow \hat{p}_y y = y\hat{p}_y - \mathrm{i}\hbar,$$

$$[\hat{L}_x, \hat{p}_y] = y\hat{p}_y\hat{p}_z - y\hat{p}_y\hat{p}_z + \mathrm{i}\hbar\hat{p}_z = \mathrm{i}\hbar\hat{p}_z$$

$$[\hat{L}_\alpha, \hat{p}_\beta] = \mathrm{i}\hbar\varepsilon_{\alpha\beta\gamma}\hat{p}_\gamma \equiv \mathrm{i}\hbar\sum_{\gamma=1}^{3}\varepsilon_{\alpha\beta\gamma}\hat{p}_\gamma$$

角动量之间的对易关系

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

矢量形式：

$$\hat{\boldsymbol{L}} \times \hat{\boldsymbol{L}} = \mathrm{i}\hbar\hat{\boldsymbol{L}}$$

证：

$$[\hat{L}_x, \hat{L}_y] = [y\hat{p}_z - z\hat{p}_y, z\hat{p}_x - x\hat{p}_z]$$
$$= [y\hat{p}_z, z\hat{p}_x - x\hat{p}_z] - [z\hat{p}_y, z\hat{p}_x - x\hat{p}_z]$$
$$= [y\hat{p}_z, z\hat{p}_x] - [y\hat{p}_z, x\hat{p}_z] - [z\hat{p}_y, z\hat{p}_x] + [z\hat{p}_y, x\hat{p}_z]$$
$$= [y\hat{p}_z, z\hat{p}_x] + [z\hat{p}_y, x\hat{p}_z]$$
$$= y[\hat{p}_z, z\hat{p}_x] + [y, z\hat{p}_x]\hat{p}_z + z[\hat{p}_y, x\hat{p}_z] + [z, x\hat{p}_z]\hat{p}_y$$
$$= y[\hat{p}_z, z\hat{p}_x] + [z, x\hat{p}_z]\hat{p}_y$$
$$= yz[\hat{p}_z, \hat{p}_x] + y[\hat{p}_z, z]\hat{p}_x + x[z, \hat{p}_z]\hat{p}_y + [z, x]\hat{p}_z\hat{p}_y$$
$$= y[\hat{p}_z, z]\hat{p}_x + x[z, \hat{p}_z]\hat{p}_y$$
$$= -\mathrm{i}\hbar y\hat{p}_x + \mathrm{i}\hbar x\hat{p}_y$$
$$= \mathrm{i}\hbar(x\hat{p}_y - y\hat{p}_x) = \mathrm{i}\hbar\hat{L}_z$$

$$[y\hat{p}_z, x\hat{p}_z] = y\hat{p}_z x\hat{p}_z - x\hat{p}_z y\hat{p}_z$$
$$= (yx - xy)\hat{p}_z\hat{p}_z = 0$$

$$[y, z\hat{p}_x]\hat{p}_z = z[y, \hat{p}_x]\hat{p}_z + [y, z]\hat{p}_z\hat{p}_x$$

$$z[\hat{p}_y, x\hat{p}_z] = zx[\hat{p}_y, \hat{p}_z] + z[\hat{p}_y, x]\hat{p}_z$$

角动量与角动量平方的对易关系

$$\left.\begin{aligned}[\hat{L}_x,\hat{L}^2]=0\\ [\hat{L}_y,\hat{L}^2]=0\\ [\hat{L}_z,\hat{L}^2]=0\end{aligned}\right\}$$

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

【证明】

$$[\hat{L}^2,\hat{L}_x]=[\hat{L}_x{}^2,\hat{L}_x]+[\hat{L}_y{}^2,\hat{L}_x]+[\hat{L}_z{}^2,\hat{L}_x]$$

$$=\hat{L}_y[\hat{L}_y,\hat{L}_x]+[\hat{L}_y,\hat{L}_x]\hat{L}_y+\hat{L}_z[\hat{L}_z,\hat{L}_x]+[\hat{L}_z,\hat{L}_x]\hat{L}_z$$

$$=-\mathrm{i}\hbar\hat{L}_y\hat{L}_z-\mathrm{i}\hbar\hat{L}_z\hat{L}_y+\mathrm{i}\hbar\hat{L}_z\hat{L}_y+\mathrm{i}\hbar\hat{L}_y\hat{L}_z$$

$$=0$$

小结：

$\langle 1\rangle [\hat{A},\hat{B}]=-[\hat{B},\hat{A}]$；

$\langle 2\rangle [\hat{A},\hat{A}]=0$；

$\langle 3\rangle [\hat{A},c]=0$ （c 为复常数）；

$\langle 4\rangle [\hat{A},\hat{B}+\hat{C}]=[\hat{A},\hat{B}]+[\hat{A},\hat{C}]$；

$\langle 5\rangle [\hat{A},\hat{B}\hat{C}]=\hat{B}[\hat{A},\hat{C}]+[\hat{A},\hat{B}]\hat{C}$；

$\langle 6\rangle [\hat{A}\hat{B},\hat{C}]=\hat{A}[\hat{B},\hat{C}]+[\hat{A},\hat{C}]\hat{B}$。

$$[x_\alpha, x_\beta]=0$$

$$[\hat{p}_\alpha, \hat{p}_\beta]=0$$

$$[\hat{L}_i, \hat{L}^2]=0$$

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

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

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

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

例：试证明　(1) $[\hat{L}_z, \hat{L}_\pm] = \pm\hbar\hat{L}_\pm$

(2) $[\hat{L}^2, \hat{L}_\pm] = 0$, 式中 $\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$

证：

$$(1)\ [\hat{L}_z, \hat{L}_\pm] = [\hat{L}_z, \hat{L}_x \pm i\hat{L}_y]$$

$$= [\hat{L}_z, \hat{L}_x] \pm [\hat{L}_z, i\hat{L}_y]$$

$$= [\hat{L}_z, \hat{L}_x] \pm i[\hat{L}_z, \hat{L}_y]$$

$$= i\hbar\hat{L}_y \pm i(-i\hbar\hat{L}_x) = \pm\hbar\hat{L}_\pm$$

$$(2)\ [\hat{L}^2, \hat{L}_\pm] = [\hat{L}^2, \hat{L}_x \pm i\hat{L}_y] = [\hat{L}^2, \hat{L}_x] \pm i[\hat{L}^2, \hat{L}_y]$$

$$= 0 \pm i0 = 0$$

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

练习：令 $\hat{l}_\pm = \hat{l}_x \pm \mathrm{i}\hat{l}_y$ （升、降算符）

证明 $[\hat{l}_+, \hat{l}_-] = 2\hbar\hat{l}_z$

$$\hat{l}_\pm \hat{l}_\mp = \hat{l}^2 - \hat{l}_z^2 \pm \hbar\hat{l}_z$$

作业

1． 试证明：

$$[\hat{L}_z, \hat{L}^2] = 0$$

2． 求 $\hat{L}_x$ 与 $\hat{p}_z$ 的对易子