2020-2021 第二学期量子力学作业参考答案

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0.1　第一次作业: 2021. 03.25

1. 如图 1 示, 两个质量为 m 的质点由弹簧耦合在一起, 弹簧的劲度系数均为 k. x_1 和 x_2 分别为质点偏离平衡位置的位移. 首先写出其 Lagrangian, 然后求其 E-L 方程.

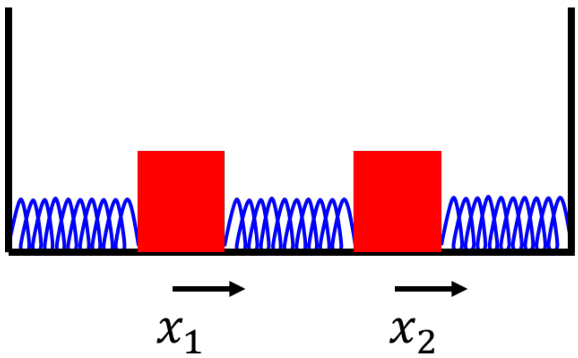

Figure 1: 图 1

解 这个体系的 Lagrangian 可以表示为

$$
\begin{aligned}
L =& T - V \qquad (1)\\
=& \frac{1}{2}m\left(\dot{x}_1^2+\dot{x}_2^2\right)-\frac{1}{2}k\left(x_1^2+x_2^2+\left(x_1-x_2\right)^2\right) \qquad (2)
\end{aligned}
$$

由于 $L = L\left(x_1, x_2, \dot{x}_1, \dot{x}_2\right)$, 故其 E-L 方程为:

$$\frac{\partial L}{\partial x_1}-\frac{d}{dt}\frac{\partial L}{\partial \dot{x}_1}=-k\left(x_1+x_1-x_2\right)-\frac{d}{dt}\left(m\dot{x}_1\right)=0 \qquad (3)$$

$$\frac{\partial L}{\partial x_2}-\frac{d}{dt}\frac{\partial L}{\partial \dot{x}_2}=-k\left(x_2+x_2-x_1\right)-\frac{d}{dt}\left(m\dot{x}_2\right)=0 \qquad (4)$$

即

$$
\begin{aligned}
m\ddot{x}_1 &= -k\left(2x_1-x_2\right) \qquad (5)\\
m\ddot{x}_2 &= -k\left(2x_2-x_1\right) \qquad (6)
\end{aligned}
$$

2. 利用 Hamiltonian 形式, 求解第 1 题的正则方程.

解 利用 Legendre 变换, 1 中问题的 Hamiltonian 可以表示为:

$$H=\sum_{i=1}^{2} p_i \dot{x}_i - L \tag{7}$$

而

$$p_i=\frac{\partial L}{\partial \dot{x}_i}=m\dot{x}_i, \quad i=1,2 \tag{8}$$

于是

$$H=\sum_{i=1}^{n}\frac{p_i^2}{m}-L=\frac{p_1^2}{2m}+\frac{p_2^2}{2m}+\frac{1}{2}k\left(x_1^2+x_2^2+(x_1-x_2)^2\right) \tag{9}$$

其正则方程为

$$\dot{x}_1=\frac{\partial H}{\partial p_1}=\frac{p_1}{m} \tag{10}$$

$$\dot{p}_1=-\frac{\partial H}{\partial x_1}=-kx_1-k\left(x_1-x_2\right)=-2kx_1+kx_2 \tag{11}$$

和

$$\dot{x}_2=\frac{\partial H}{\partial p_2}=\frac{p_2}{m} \tag{12}$$

$$\dot{p}_2=-\frac{\partial H}{\partial x_2}=-kx_2-k\left(x_2-x_1\right)=-2kx_2+kx_1 \tag{13}$$

注意: $H=H\left(x_1,x_2,p_1,p_2\right)$; 不需要把 H 分成两部分; 这两组正则方程分别和题 1 中的 E-L 方程等价.

3. 利用能量守恒, 证明: 在 (x,p) 空间, 简谐振子的轨道为 $\left(\frac{x}{a}\right)^2+\left(\frac{p}{b}\right)^2=1$. 这里 $a^2=\frac{2E}{k}$, $b^2=2mE$.

解 在 (x,p) 空间, 简谐振子的 Hamiltonian 为

$$H=\frac{p^2}{2m}+\frac{1}{2}kx^2 \tag{14}$$

由于能量守恒, 可令

$$\frac{p^2}{2m}+\frac{1}{2}kx^2=E \tag{15}$$

能量 E 是常量, 于是

$$\frac{p^2}{2mE}+\frac{x^2}{\frac{2E}{k}}=1 \tag{16}$$

令 $a^2=\frac{2E}{k}$, $b^2=2mE$, 可得

$$\left(\frac{x}{a}\right)^2+\left(\frac{p}{b}\right)^2=1 \tag{17}$$

注意: E 是常量, a, b 也是.

4. 证明: 普朗克黑体辐射公式在高频和低频极限下分别给出维恩公式和瑞利 -金斯公式.

证: Planck 黑体辐射公式为:

$$u_\nu(T) = \frac{8\pi\nu^2}{c^3}\frac{h\nu}{\exp\left(\frac{h\nu}{k_BT}\right)-1} \tag{18}$$

在高频极限下, $\frac{h\nu}{k_BT} \gg 1$, 即 $\exp\left(\frac{h\nu}{k_BT}\right) \gg 1$, 所以

$$u_\nu(T) \approx \frac{8\pi h\nu^3}{c^3}\exp\left(-\frac{h\nu}{k_BT}\right) \tag{19}$$

即 Wien 公式;

在低频极限下, $\frac{h\nu}{k_BT} \ll 1$, 则 $\exp\left(\frac{h\nu}{k_BT}\right) \approx 1 + \frac{h\nu}{k_BT}$, 所以

$$u_\nu(T) \approx \frac{8\pi\nu^2}{c^3}\frac{h\nu}{1+\frac{h\nu}{k_BT}-1} = \frac{8\pi\nu^2}{c^3}k_BT \tag{20}$$

0.2 第二次作业: 2021.03.30

1. 教材第 8 页练习 1

解: 由 $\int|\psi(x)|^2dx = 1$ 得:

$$\begin{aligned}
\int_{-\infty}^{\infty}|\psi(x)|^2dx =& A^2\int_{-\infty}^{\infty}e^{-\alpha^2x^2}dx && (21)\\
=& A^2\sqrt{\int_{-\infty}^{\infty}e^{-\alpha^2x^2}dx\int_{-\infty}^{\infty}e^{-\alpha^2y^2}dy} && (22)\\
=& A^2\sqrt{\int_0^{\infty}rdr\int_0^{2\pi}d\theta e^{-\alpha^2r^2}} && (23)\\
=& A^2\sqrt{2\pi\int_0^{\infty}rdre^{-\alpha^2r^2}} && (24)\\
=& A^2\sqrt{2\pi\left.\frac{e^{-\alpha^2r^2}}{-2\alpha^2}\right|_0^{\infty}} && (25)\\
=& A^2\sqrt{\frac{\pi}{\alpha^2}} = 1 && (26)
\end{aligned}$$

所以, $A = (\frac{\alpha^2}{\pi})^{\frac{1}{4}}$.

2. 教材第 8 页练习 5

解

(1) 在球壳 $(r, r+dr)$ 中被观测到的概率, 对角度无限制, 所以它可表示为 $r^2dr\int_0^{\pi}\sin\theta d\theta\int_0^{2\pi}d\varphi\,|\psi(r,\theta,\varphi)|^2$.

(2) 在 (θ,φ) 方向立体角元中找到粒子的概率为 $d\Omega\int_0^{\infty}r^2dr\,|\psi(r,\theta,\varphi)|^2$.

3. 考虑波函数

$$\Psi(x,t) = Ae^{-2\lambda|x|}e^{-i\omega t} \tag{27}$$

这里, A, λ, ω 均为实的. 求归一化常数 A.

解 由 $\int dx|\psi(x,t)|^2=1$ 得,

$$\int dx|\psi(x,t)|^2 = A^2\int_{-\infty}^{\infty} dx e^{-4\lambda|x|} = A^2\left(\int_{-\infty}^{0} dx e^{4\lambda x} + \int_{0}^{\infty} dx e^{-4\lambda x}\right) \tag{28}$$

$$= A^2\left(\left.\frac{e^{4\lambda x}}{4\lambda}\right|_{-\infty}^{0} + \left.\frac{e^{-4\lambda x}}{-4\lambda}\right|_{0}^{\infty}\right) \tag{29}$$

$$= \frac{A^2}{2\lambda} = 1 \tag{30}$$

所以 $A=\sqrt{2\lambda}$.

4. 25 页 1.4(a)

解: (a) 容易验证，$\psi(x,0)$ 已经归一化,

$$\bar{x} = \int_{-\infty}^{\infty} dx\psi^*(x,0)\,x\psi(x,0) \tag{31}$$

$$= \int_{-\infty}^{\infty} dx x\frac{1}{(\pi\alpha^2)^{1/2}}e^{-\frac{x^2}{\alpha^2}} \tag{32}$$

由于被积函数是 x 的奇函数，所以 $\bar{x}=0$.

$$\bar{p} = \int_{-\infty}^{\infty} dx\psi^*(x,0)\,\hat{p}\psi(x,0) \tag{33}$$

$$= \int_{-\infty}^{\infty} dx\psi^*(x,0)\,\frac{\hbar}{i}\frac{d}{dx}\psi(x,0) \tag{34}$$

$$= \int_{-\infty}^{\infty} dx\psi^*(x,0)\left(p_0-\frac{\hbar x}{i\alpha^2}\right)\psi(x,0) \tag{35}$$

$$= \int_{-\infty}^{\infty} dx\left(p_0-\frac{\hbar x}{i\alpha^2}\right)\frac{1}{(\pi\alpha^2)^{1/2}}e^{-\frac{x^2}{\alpha^2}} \tag{36}$$

$$= p_0\int_{-\infty}^{\infty} dx\frac{1}{(\pi\alpha^2)^{1/2}}e^{-\frac{x^2}{\alpha^2}} - \int_{-\infty}^{\infty} dx\frac{\hbar x}{i\alpha^2}\frac{1}{(\pi\alpha^2)^{1/2}}e^{-\frac{x^2}{\alpha^2}} \tag{37}$$

上式中第二项是 x 的奇函数，所以 $\bar{p}=p_0$.

$$\overline{x^2} = \int_{-\infty}^{\infty} dx\psi^*(x,0)\,x^2\psi(x,0) \tag{38}$$

$$= \frac{1}{(\pi\alpha^2)^{1/2}}\int_{-\infty}^{\infty} dx x^2 e^{-\frac{x^2}{\alpha^2}} \tag{39}$$

$$= \frac{1}{(\pi\alpha^2)^{1/2}}\int_{-\infty}^{\infty} dx\left(-\frac{d}{du}\right)e^{-ux^2} \tag{40}$$

$$= -\frac{1}{(\pi\alpha^2)^{1/2}}\frac{d}{du}\int_{-\infty}^{\infty} dx e^{-ux^2} \tag{41}$$

这里令 $u=\frac{1}{\alpha^2}$, $\overline{x^2}=-\frac{1}{(\pi\alpha^2)^{1/2}}\frac{d}{du}\sqrt{\frac{\pi}{u}}=\frac{\alpha^2}{2}$.

$$\overline{p^2} = \int_{-\infty}^{\infty} dx\psi^*(x,0)\,\hat{p}^2\psi(x,0) \tag{42}$$

$$= \int_{-\infty}^{\infty} dx\psi^*(x,0)\left(-\hbar^2\frac{d^2}{dx^2}\right)\psi(x,0) \tag{43}$$

$$\frac{\hbar}{i}\frac{d}{dx}\psi\left(x,0\right)=\left(p_0-\frac{\hbar x}{i\alpha^2}\right)\psi\left(x,0\right) \tag{44}$$

$$\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2\psi\left(x,0\right)=\frac{\hbar^2}{\alpha^2}\psi\left(x,0\right)+\left(p_0-\frac{\hbar x}{i\alpha^2}\right)^2\psi\left(x,0\right) \tag{45}$$

$$=\left(\frac{\hbar^2}{\alpha^2}+p_0^2-\frac{2p_0\hbar x}{i\alpha^2}-\frac{\hbar^2x^2}{\alpha^4}\right)\psi\left(x,0\right) \tag{46}$$

所以

$$\overline{p^2}=\frac{1}{\left(\pi\alpha^2\right)^{1/2}}\int_{-\infty}^{\infty}dx\left(\frac{\hbar^2}{\alpha^2}+p_0^2-\frac{2p_0\hbar x}{i\alpha^2}-\frac{\hbar^2x^2}{\alpha^4}\right)e^{-\frac{x^2}{\alpha^2}} \tag{47}$$

$$=\frac{\hbar^2}{\alpha^2}+p_0^2-\frac{\hbar^2}{\alpha^4}\frac{\alpha^2}{2}=p_0^2+\frac{\hbar^2}{2\alpha^2} \tag{48}$$

我们最终得到

$$\overline{\left(x-\bar{x}\right)^2}=\overline{x^2}-\left(\bar{x}\right)^2=\frac{\alpha^2}{2} \tag{49}$$

$$\overline{\left(\hat{p}-\bar{p}\right)^2}=\overline{p^2}-\left(\bar{p}\right)^2=\frac{\hbar^2}{2\alpha^2} \tag{50}$$

即 $\Delta x=\frac{\alpha}{\sqrt{2}}$，$\Delta p=\frac{\hbar}{\sqrt{2}\alpha}$，$\Delta x\Delta p=\frac{\hbar}{2}$.

讨论： 对任意算符 $\hat{A}$

$$\overline{\left(\hat{A}-\bar{\hat{A}}\right)^2}=\int dx\psi^*\left(x\right)\left(\hat{A}-\bar{\hat{A}}\right)^2\psi\left(x\right) \tag{51}$$

$$=\int dx\psi^*\left(x\right)\left(\hat{A}^2-\bar{\hat{A}}\hat{A}-\hat{A}\bar{\hat{A}}+\overline{\hat{A}}^2\right)\psi\left(x\right) \tag{52}$$

$$=\int dx\psi^*\left(x\right)\left(\hat{A}^2-2\bar{\hat{A}}\hat{A}+\overline{\hat{A}}^2\right)\psi\left(x\right) \tag{53}$$

$$=\int dx\psi^*\left(x\right)\hat{A}^2\psi\left(x\right)-2\bar{\hat{A}}\int dx\psi^*\left(x\right)\hat{A}\psi\left(x\right)+\overline{\hat{A}}^2\int dx\psi^*\left(x\right)\psi\left(x\right) \tag{54}$$

$$=\overline{\hat{A}^2}-2\overline{\hat{A}}^2+\overline{\hat{A}}^2 \tag{55}$$

$$=\overline{\hat{A}^2}-\overline{\hat{A}}^2 \tag{56}$$

0.3 第三次作业: 2021.04.06

1 已知 $t=0$ 时, 一维粒子的波函数为

$$\Psi\left(x,0\right)=\begin{cases}A\left(a^2-x^2\right), & -a\le x\le a\\ 0, & \text{其它}\end{cases} \tag{57}$$

(1) 确定归一化常数 A;

(2) 计算 $\langle\hat{x}\rangle$ 和 $\langle\hat{x}-\langle\hat{x}\rangle\rangle^2$;

(3) 计算 $\langle\hat{p}\rangle$ 和 $\langle\hat{p}-\langle\hat{p}\rangle\rangle^2$.

提示: 对任意算符 $\hat{A}$, $\left\langle \hat{A}-\left\langle \hat{A}\right\rangle \right\rangle^2=\left\langle \hat{A}^2\right\rangle -\left\langle \hat{A}\right\rangle^2$.

解

(1)

$$\int_{-\infty}^{\infty}\left|\Psi\left(x,0\right)\right|^2dx=\int_{-a}^{a}\left|A\right|^2\left(a^2-x^2\right)^2dx \tag{58}$$

令 $x=a\sin\theta$, ($-\frac{\pi}{2}\leq\theta\leq\frac{\pi}{2}$) , 于是,

$$\begin{aligned}
\int_{-\infty}^{\infty}\left|\Psi\left(x,0\right)\right|^2dx=&\left|A\right|^2\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}a^4\cos^4\theta d\left(a\sin\theta\right) &(59)\\
=&\left|A\right|^2a^5\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\cos^5\theta d\theta &(60)\\
=&\left|A\right|^2a^5\left(\cos^4\theta\sin\theta\Big|_{-\frac{\pi}{2}}^{\frac{\pi}{2}}+4\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\cos^3\theta\sin^2\theta d\theta\right) &(61)\\
=&\left|A\right|^2a^5\left(4\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\cos^2\theta\sin^2\theta d\left(\sin\theta\right)\right) &(62)\\
=&\left|A\right|^2a^5\left(4\int_{-1}^{1}\left(1-x^2\right)x^2dx\right) &(63)\\
=&4\left|A\right|^2a^5\left(\frac{x^3}{3}-\frac{x^5}{5}\right)\Big|_{-1}^{1} &(64)\\
=&\frac{16a^5}{15}\left|A\right|^2 &(65)
\end{aligned}$$

所以可取 $A=\frac{1}{4a^2}\sqrt{\frac{15}{a}}$.

(2)

$$\begin{aligned}
\left\langle x\right\rangle =&\int_{-\infty}^{\infty}\Psi^*\left(x,0\right)x\Psi\left(x,0\right)dx &(66)\\
=&\int_{-a}^{a}\left|A\right|^2x\left(a^2-x^2\right)^2dx &(67)
\end{aligned}$$

被积函数在积分区间上是奇函数, 所以 $\langle x\rangle = 0$.

$$\begin{aligned}
\left\langle x^2\right\rangle =&\int_{-\infty}^{\infty}\Psi^*\left(x,0\right)x^2\Psi\left(x,0\right)dx && (68)\\
=&\int_{-a}^{a}\left|A\right|^2x^2\left(a^2-x^2\right)^2dx && (69)\\
=&\left|A\right|^2a^7\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\sin^2\theta\cos^5\theta d\theta && (70)\\
=&\left|A\right|^2a^7\left(\left.\frac{\sin^3\theta\cos^4\theta}{3}\right|_{-\frac{\pi}{2}}^{\frac{\pi}{2}}+\frac{4}{3}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\sin^4\theta\cos^3\theta d\theta\right) && (71)\\
=&\left|A\right|^2a^7\left(\frac{4}{3}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\sin^4\theta\cos^2\theta d\left(\sin\theta\right)\right) && (72)\\
=&\left|A\right|^2a^7\left(\frac{4}{3}\int_{-1}^{1}x^4\left(1-x^2\right)dx\right) && (73)\\
=&\frac{4}{3}\left|A\right|^2a^7\left.\left(\frac{x^5}{5}-\frac{x^7}{7}\right)\right|_{-1}^{1} && (74)\\
=&\frac{a^2}{7} && (75)
\end{aligned}$$

所以

$$\left\langle\hat{x}-\left\langle\hat{x}\right\rangle\right\rangle^2=\left\langle\hat{x}^2\right\rangle-\left\langle\hat{x}\right\rangle^2=\frac{a^2}{7} \tag{76}$$

(3)

$$\begin{aligned}
\left\langle\hat{p}\right\rangle =&\int_{-\infty}^{\infty}\Psi^*\left(x,0\right)\hat{p}\Psi\left(x,0\right)dx && (77)\\
=&\int_{-a}^{a}\left|A\right|^2\left(a^2-x^2\right)\frac{\hbar}{i}\frac{d}{dx}\left(a^2-x^2\right)dx && (78)\\
=&-2\left|A\right|^2\frac{\hbar}{i}\int_{-a}^{a}\left(a^2-x^2\right)xdx && (79)
\end{aligned}$$

被积函数在积分区间上是奇函数, 所以 $\langle\hat{p}\rangle = 0$.

$$\begin{aligned}
\left\langle\hat{p}^2\right\rangle =&\int_{-\infty}^{\infty}\Psi^*\left(x,0\right)\hat{p}^2\Psi\left(x,0\right)dx && (80)\\
=&\int_{-a}^{a}\left|A\right|^2\left(a^2-x^2\right)\left(-\hbar^2\right)\frac{d^2}{dx^2}\left(a^2-x^2\right)dx && (81)\\
=&2\hbar^2\left|A\right|^2\int_{-a}^{a}\left(a^2-x^2\right)dx && (82)\\
=&\frac{5\hbar^2}{2a^2} && (83)
\end{aligned}$$

所以

$$\left\langle\hat{p}-\left\langle\hat{p}\right\rangle\right\rangle^2=\left\langle\hat{p}^2\right\rangle-\left\langle\hat{p}\right\rangle^2=\frac{5\hbar^2}{2a^2} \tag{84}$$

注意: 不能省略关键计算步骤; 运用量纲判断计算结果是否正确.

2. 一维量子体系满足 Schrödinger 方程 $i\hbar\frac{\partial}{\partial t}\psi(x,t)=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x,t)\right)\psi(x,t)$, 这里 $V(x,t)$ 是实的. 证明

$$\frac{d}{dt}\langle\hat{p}\rangle=-\left\langle\frac{\partial V}{\partial x}\right\rangle \tag{85}$$

这里 $\langle\hat{p}\rangle=\int_{-\infty}^{\infty}\psi^*(x,t)\frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x,t)\,dx$ 和 $\left\langle\frac{\partial V}{\partial x}\right\rangle=\int_{-\infty}^{\infty}\psi^*(x,t)\frac{\partial V}{\partial x}\psi(x,t)\,dx$.

解 利用 Schrödinger 方程,

$$\begin{aligned}\frac{d}{dt}\langle\hat{p}\rangle=&\frac{d}{dt}\int_{-\infty}^{\infty}\psi^*(x,t)\frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x,t)\,dx &(86)\\=&\int_{-\infty}^{\infty}(-i\hbar)\frac{\partial\psi^*(x,t)}{\partial t}\frac{d}{dx}\psi(x,t)\,dx+\int_{-\infty}^{\infty}\psi^*(x,t)\frac{\partial}{\partial x}(-i\hbar)\frac{\partial\psi(x,t)}{\partial t}dx &(87)\end{aligned}$$

对 Schrödinger 方程取复共轭得:

$$-i\hbar\frac{\partial}{\partial t}\psi^*(x,t)=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x,t)\right)\psi^*(x,t) \tag{88}$$

于是

$$\begin{aligned}\frac{d}{dt}\langle\hat{p}\rangle=&\int_{-\infty}^{\infty}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x,t)\right)\psi^*(x,t)\frac{\partial}{\partial x}\psi(x,t)\,dx &(89)\\&-\int_{-\infty}^{\infty}\psi^*(x,t)\frac{\partial}{\partial x}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x,t)\right)\psi(x,t)\,dx &(90)\end{aligned}$$

在方程 (89) 中,

$$\begin{aligned}&\int_{-\infty}^{\infty}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\psi^*(x,t)\frac{\partial}{\partial x}\psi(x,t)\,dx &(91)\\=&\left(-\frac{\hbar^2}{2m}\frac{\partial\psi^*(x,t)}{\partial x}\right)\frac{\partial\psi(x,t)}{\partial x}\bigg|_{-\infty}^{\infty}+\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\frac{\partial\psi^*(x,t)}{\partial x}\frac{\partial^2}{\partial x^2}\psi(x,t)\,dx &(92)\\=&\frac{\hbar^2}{2m}\psi^*(x,t)\frac{\partial^2}{\partial x^2}\psi(x,t)\bigg|_{-\infty}^{\infty}-\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\psi^*(x,t)\frac{\partial^3}{\partial x^3}\psi(x,t)\,dx &(93)\\=&-\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\psi^*(x,t)\frac{\partial^3}{\partial x^3}\psi(x,t)\,dx &(94)\end{aligned}$$

这里利用了 $\psi(x,t)$ 在无穷远处的渐近行为, 对于满足平方可积条件的波函数, $\psi(x,t)$ 和 $\frac{\partial\psi(x,t)}{\partial x}$ (及其复共轭) 在无穷远处趋于零. 并且 $-\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\psi^*(x,t)\frac{\partial^3}{\partial x^3}\psi(x,t)\,dx$ 与方程 (90) 中的第一项相抵消. 下面考察方程 (89) 和 (90) 中和势能有关的项,

$$\begin{aligned}\frac{d}{dt}\langle\hat{p}\rangle=&\int_{-\infty}^{\infty}V(x,t)\psi^*(x,t)\frac{\partial}{\partial x}\psi(x,t)\,dx-\int_{-\infty}^{\infty}\psi^*(x,t)\frac{\partial}{\partial x}(V(x,t)\psi(x,t))\,dx &(95)\\=&\int_{-\infty}^{\infty}V(x,t)\psi^*(x,t)\frac{\partial}{\partial x}\psi(x,t)\,dx-\int_{-\infty}^{\infty}\psi^*(x,t)\frac{\partial V(x,t)}{\partial x}\psi(x,t)\,dx &(96)\\&-\int_{-\infty}^{\infty}\psi^*(x,t)V(x,t)\frac{\partial}{\partial x}\psi(x,t)\,dx &(97)\\=&\int_{-\infty}^{\infty}\psi^*(x,t)\left(-\frac{\partial V(x,t)}{\partial x}\right)\psi(x,t)\,dx &(98)\end{aligned}$$

即

$$\frac{d}{dt}\langle\hat{p}\rangle=-\left\langle\frac{\partial V}{\partial x}\right\rangle \tag{99}$$

3. 25 页 1.1

解

(a) 由题意能量算符可以写为 $\hat{H}=-\frac{\hbar^2}{2m}\nabla^2+V(\boldsymbol{r})$:

$$E=\int d^3r\psi^*(\boldsymbol{r},t)\hat{H}\psi(\boldsymbol{r},t) \tag{100}$$

$$=\int d^3r\psi^*(\boldsymbol{r},t)\left(-\frac{\hbar^2}{2m}\nabla^2+V(\boldsymbol{r})\right)\psi(\boldsymbol{r},t) \tag{101}$$

$$=-\frac{\hbar^2}{2m}\int d^3r\psi^*(\boldsymbol{r},t)\nabla\cdot\nabla\psi(\boldsymbol{r},t)+\int d^3r\psi^*(\boldsymbol{r},t)V(\boldsymbol{r})\psi(\boldsymbol{r},t) \tag{102}$$

$$=-\frac{\hbar^2}{2m}\left(\int d^3r\nabla\cdot(\psi^*(\boldsymbol{r},t)\nabla\psi(\boldsymbol{r},t))-\int d^3r\nabla\psi^*(\boldsymbol{r},t)\cdot\nabla\psi(\boldsymbol{r},t)\right)+\int d^3r\psi^*(\boldsymbol{r},t)V(\boldsymbol{r})\psi(\boldsymbol{r},t) \tag{103}$$

$$=-\frac{\hbar^2}{2m}\int d^3r\nabla\cdot(\psi^*(\boldsymbol{r},t)\nabla\psi(\boldsymbol{r},t))+\int d^3r\left(\frac{\hbar^2}{2m}\nabla\psi^*(\boldsymbol{r},t)\cdot\nabla\psi(\boldsymbol{r},t)+\psi^*(\boldsymbol{r},t)V(\boldsymbol{r})\psi(\boldsymbol{r},t)\right) \tag{104}$$

上式中第一项 $-\frac{\hbar^2}{2m}\int d^3r\nabla\cdot(\psi^*(\boldsymbol{r},t)\nabla\psi(\boldsymbol{r},t))=-\frac{\hbar^2}{2m}\int(\psi^*(\boldsymbol{r},t)\nabla\psi(\boldsymbol{r},t))\cdot d\boldsymbol{S}$。由于当 $r\to\infty$ 时，平方可积函数的渐近行为 $\psi\sim r^{-\left(\frac{3}{2}+s\right)}$, $s>0$，

$$\int(\psi^*(\boldsymbol{r},t)\nabla\psi(\boldsymbol{r},t))\cdot d\boldsymbol{S}\sim\left(-\frac{3}{2}-s\right)r^{-4-2s}\left(4\pi r^2\right)\xrightarrow{r\to\infty}0 \tag{105}$$

因此，

$$E=\int d^3r\left(\frac{\hbar^2}{2m}\nabla\psi^*(\boldsymbol{r},t)\cdot\nabla\psi(\boldsymbol{r},t)+\psi^*(\boldsymbol{r},t)V(\boldsymbol{r})\psi(\boldsymbol{r},t)\right)\equiv\int d^3rw \tag{106}$$

(b) 根据 w 的定义，

$$i\hbar\frac{\partial w}{\partial t}=\frac{\hbar^2}{2m}\nabla\frac{i\hbar\partial\psi^*(\boldsymbol{r},t)}{\partial t}\cdot\nabla\psi(\boldsymbol{r},t)+\frac{\hbar^2}{2m}\nabla\psi^*(\boldsymbol{r},t)\cdot\nabla\frac{i\hbar\partial\psi(\boldsymbol{r},t)}{\partial t} \tag{107}$$

$$+\frac{i\hbar\partial\psi^*(\boldsymbol{r},t)}{\partial t}V(\boldsymbol{r})\psi(\boldsymbol{r},t)+\psi^*(\boldsymbol{r},t)V(\boldsymbol{r})\frac{i\hbar\partial\psi(\boldsymbol{r},t)}{\partial t} \tag{108}$$

由于

$$\nabla\frac{i\hbar\partial\psi^*(\boldsymbol{r},t)}{\partial t}\cdot\nabla\psi(\boldsymbol{r},t)=\nabla\cdot\left(\frac{i\hbar\partial\psi^*(\boldsymbol{r},t)}{\partial t}\nabla\psi(\boldsymbol{r},t)\right)-\frac{i\hbar\partial\psi^*(\boldsymbol{r},t)}{\partial t}\nabla^2\psi(\boldsymbol{r},t)$$

$$\nabla\psi^*(\boldsymbol{r},t)\cdot\nabla\frac{i\hbar\partial\psi(\boldsymbol{r},t)}{\partial t}=\nabla\cdot\left(\nabla\psi^*(\boldsymbol{r},t)\frac{i\hbar\partial\psi(\boldsymbol{r},t)}{\partial t}\right)-\left(\nabla^2\psi^*(\boldsymbol{r},t)\right)\frac{i\hbar\partial\psi(\boldsymbol{r},t)}{\partial t}$$

可得到：

$$i\hbar\frac{\partial w}{\partial t}=\frac{\hbar^2}{2m}\nabla\cdot\left(\frac{i\hbar\partial\psi^*(\boldsymbol{r},t)}{\partial t}\nabla\psi(\boldsymbol{r},t)\right)+\frac{\hbar^2}{2m}\nabla\cdot\left(\nabla\psi^*(\boldsymbol{r},t)\frac{i\hbar\partial\psi(\boldsymbol{r},t)}{\partial t}\right) \tag{109}$$

$$-\left(\frac{i\hbar\partial\psi^*(\boldsymbol{r},t)}{\partial t}\frac{\hbar^2}{2m}\nabla^2\psi(\boldsymbol{r},t)+\left(\frac{\hbar^2}{2m}\nabla^2\psi^*(\boldsymbol{r},t)\right)\frac{i\hbar\partial\psi(\boldsymbol{r},t)}{\partial t}\right) \tag{110}$$

$$+\frac{i\hbar\partial\psi^*(\boldsymbol{r},t)}{\partial t}V(\boldsymbol{r})\psi(\boldsymbol{r},t)+\psi^*(\boldsymbol{r},t)V(\boldsymbol{r})\frac{i\hbar\partial\psi(\boldsymbol{r},t)}{\partial t} \tag{111}$$

利用 Schrödinger 方程 $i\hbar\frac{\partial\psi}{\partial t}=\left(-\frac{\hbar^2}{2m}\nabla^2+V(\boldsymbol{r})\right)\psi$ 及其复共轭合并最后四项，可得：

$$
\begin{aligned}
i\hbar\frac{\partial w}{\partial t}=&\frac{\hbar^2}{2m}\nabla\cdot\left(\frac{i\hbar\partial\psi^*(\boldsymbol{r},t)}{\partial t}\cdot\nabla\psi(\boldsymbol{r},t)+\nabla\psi^*(\boldsymbol{r},t)\frac{i\hbar\partial\psi(\boldsymbol{r},t)}{\partial t}\right) &(112)\\
&+\left(\frac{i\hbar\partial\psi^*(\boldsymbol{r},t)}{\partial t}\left(-\frac{\hbar^2}{2m}\nabla^2+V(\boldsymbol{r})\right)\psi(\boldsymbol{r},t)+\left(\left(-\frac{\hbar^2}{2m}\nabla^2+V(\boldsymbol{r})\right)\psi^*(\boldsymbol{r},t)\right)\frac{i\hbar\partial\psi(\boldsymbol{r},t)}{\partial t}\right) &(113)\\
=&\frac{\hbar^2}{2m}\nabla\cdot\left(\frac{i\hbar\partial\psi^*(\boldsymbol{r},t)}{\partial t}\cdot\nabla\psi(\boldsymbol{r},t)+\nabla\psi^*(\boldsymbol{r},t)\frac{i\hbar\partial\psi(\boldsymbol{r},t)}{\partial t}\right) &(114)\\
&+\frac{i\partial\psi^*(\boldsymbol{r},t)}{\partial t}\frac{i\hbar\partial\psi(\boldsymbol{r},t)}{\partial t}+\left(-i\frac{\partial\psi^*(\boldsymbol{r},t)}{\partial t}\right)\frac{i\hbar\partial\psi(\boldsymbol{r},t)}{\partial t} &(115)\\
=&\frac{\hbar^2}{2m}\nabla\cdot\left(\frac{i\hbar\partial\psi^*(\boldsymbol{r},t)}{\partial t}\cdot\nabla\psi(\boldsymbol{r},t)+\nabla\psi^*(\boldsymbol{r},t)\frac{i\hbar\partial\psi(\boldsymbol{r},t)}{\partial t}\right) &(116)\\
\equiv&-i\hbar\nabla\cdot\boldsymbol{s} &(117)
\end{aligned}
$$

所以

$$\frac{\partial w}{\partial t}+\nabla\cdot\boldsymbol{s}=0 \tag{118}$$

注意：

1. 方程113中，$\left(-\frac{\hbar^2}{2m}\nabla^2+V(\boldsymbol{r})\right)\psi(\boldsymbol{r},t)\neq E\psi(\boldsymbol{r},t)$。$\psi(\boldsymbol{r},t)$ 是含时 Schrödinger 方程 $i\hbar\frac{\partial\psi(\boldsymbol{r},t)}{\partial t}=\hat{H}\psi(\boldsymbol{r},t)$ 的一般解。分离变量后，$\psi_E(\boldsymbol{r})e^{-iEt/\hbar}$ 称为本征解，需要把特解叠加在一起才能得到含时 Schrödinger 方程 $i\hbar\frac{\partial\psi(\boldsymbol{r},t)}{\partial t}=\hat{H}\psi(\boldsymbol{r},t)$ 的一般解; 利用初始条件确定叠加系数.
2. 只有对于定态 $\psi(\boldsymbol{r},t)=\psi_E(\boldsymbol{r})e^{-iEt/\hbar}$ 才有 $\left(-\frac{\hbar^2}{2m}\nabla^2+V(\boldsymbol{r})\right)\psi(\boldsymbol{r},t)=i\hbar\frac{\partial\psi(\boldsymbol{r},t)}{\partial t}=E\psi(\boldsymbol{r},t)$。但是，一般的，对于非定态 $\psi(\boldsymbol{r},t)=\sum_E c_E\psi_E e^{-iEt/\hbar}$，满足 $i\hbar\frac{\partial\psi(\boldsymbol{r},t)}{\partial t}=\hat{H}\psi(\boldsymbol{r},t)$，它不满足 $i\hbar\frac{\partial\psi(\boldsymbol{r},t)}{\partial t}=E\psi(\boldsymbol{r},t)$。
3. 粒子的初态 $\psi(\boldsymbol{r},0)$ 可以不满足定态 Schrödinger 方程，即 $\psi(\boldsymbol{r},0)$ 不是能量本征态。
4. 不含时的 Schrödinger 方程确定的能量本征态是一个完备函数族。任意时刻的粒子的量子态都可以用它来展开。

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证： 首先

$$\nabla\times\left(\frac{1}{\psi}\nabla\psi\right)=\epsilon_{ijk}\nabla_i\left(\frac{1}{\psi}\nabla\psi\right)_j\boldsymbol{e}_k \tag{119}$$

$$=\epsilon_{ijk}\nabla_i\left(\frac{1}{\psi}\nabla_j\psi\right)\boldsymbol{e}_k \tag{120}$$

$$=\epsilon_{ijk}\left(\nabla_i\left(\frac{1}{\psi}\right)\nabla_j\psi+\frac{1}{\psi}\nabla_i\nabla_j\psi\right)\boldsymbol{e}_k \tag{121}$$

$$=\epsilon_{ijk}\left(-\frac{1}{\psi^2}\nabla_i\psi\nabla_j\psi+\frac{1}{\psi}\nabla_i\nabla_j\psi\right)\boldsymbol{e}_k \tag{122}$$

$$=-\frac{1}{\psi^2}\nabla\psi\times\nabla\psi+\frac{1}{\psi}\nabla\times(\nabla\psi) \tag{123}$$

$$=0 \tag{124}$$

对于同一个矢量，$\nabla\psi\times\nabla\psi=0$，梯度的旋度为零，所以 $\nabla\times(\nabla\psi)=0$。类似的，$\nabla\times\left(\frac{1}{\psi^*}\nabla\psi^*\right)=0$，所以 $\nabla\times\boldsymbol{v}=0$。

另外一种方法是 $\boldsymbol{v}=-\frac{i\hbar}{2m}(\nabla\ln\psi-\nabla\ln\psi^*)=-\frac{i\hbar}{2m}\nabla\ln\frac{\psi}{\psi^*}$。利用的梯度的旋度为零，所以 $\nabla\times\boldsymbol{v}=-\frac{i\hbar}{2m}\nabla\times\left(\nabla\ln\frac{\psi}{\psi^*}\right)=0$。

第三种方法是计算任一分量，比如计算 x 分量，$\nabla\times\left(\frac{1}{\psi}\nabla\psi\right)$ 的 x 分量为：$\frac{\partial}{\partial y}\left(\frac{1}{\psi}\frac{\partial\psi}{\partial z}\right)-\frac{\partial}{\partial z}\left(\frac{1}{\psi}\frac{\partial\psi}{\partial y}\right)=\frac{\partial}{\partial y}\left(\frac{\partial\ln\psi}{\partial z}\right)-\frac{\partial}{\partial z}\left(\frac{\partial\ln\psi}{\partial y}\right)=0$，同理可证 $\nabla\times\left(\frac{1}{\psi}\nabla\psi\right)$ 的其它分量为 0。类似的，$\nabla\times\left(\frac{1}{\psi^*}\nabla\psi^*\right)=0$。

5. 考虑一维情形, 粒子状态由波函数 $\psi(x,t)$ 描述, 设 P_{ab} 是在 t 时刻发现粒子处于区间 ($a<x<b$) 内的概率.

(1) 证明 $\frac{dP_{ab}}{dt}=J(a,t)-J(b,t)$. 这里概率流密度 $J(x,t)=\frac{i\hbar}{2m}(\psi(x,t)\frac{\partial\psi^*(x,t)}{\partial x}-\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x})$.

(2) 利用归一化条件确定 $\psi(x,t)$ 的单位, 并进而确定 $J(x,t)$ 的单位.

(3) 若 $\psi(x,t)=Ae^{-\lambda(x-a)^2-i\omega t}$, 这里 A, λ, a, ω 均为实数. 利用 $J(x,t)$ 的公式确定其概率流密度.

解

(1) 对处于状态 $\psi(x,t)$ 的波函数, 它处于区间 ($a<x<b$) 的概率为

$$P_{ab}=\int_a^b\psi^*(x,t)\psi(x,t)dx \tag{125}$$

则

$$i\hbar\frac{dP_{ab}}{dt}=\int_a^b i\hbar\frac{\partial\psi^*(x,t)}{\partial t}\psi(x,t)dx+\int_a^b\psi^*(x,t)i\hbar\frac{\partial\psi(x,t)}{\partial t}dx \tag{126}$$

粒子的状态满足 Schrödinger 方程

$$i\hbar\frac{\partial\psi(x,t)}{\partial t}=\hat{H}\psi(x,t)=(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x))\psi(x,t) \tag{127}$$

它的复共轭为,

$$-i\hbar\frac{\partial\psi^*(x,t)}{\partial t}=(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x))\psi^*(x,t) \tag{128}$$

所以

$$\begin{aligned}
i\hbar\frac{dP_{ab}}{dt}&=\int_a^b\left[-\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right)\psi^*(x,t)\right]\psi(x,t)dx \qquad (129)\\
&+\int_a^b\psi^*(x,t)\left[\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right)\psi(x,t)\right]dx \qquad (130)\\
&=\int_a^b\frac{\hbar^2}{2m}\frac{\partial^2\psi^*(x,t)}{\partial x^2}\psi(x,t)dx-\int_a^b\psi^*(x,t)\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}dx \qquad (131)\\
&=\frac{\hbar^2}{2m}\frac{\partial\psi^*(x,t)}{\partial x}\psi(x,t)\bigg|_a^b-\frac{\hbar^2}{2m}\int_a^b\frac{\partial\psi^*(x,t)}{\partial x}\frac{\partial\psi(x,t)}{\partial x}dx \qquad (132)\\
&-\frac{\hbar^2}{2m}\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x}\bigg|_a^b+\frac{\hbar^2}{2m}\int_a^b\frac{\partial\psi^*(x,t)}{\partial x}\frac{\partial\psi(x,t)}{\partial x}dx \qquad (133)\\
&=\frac{\hbar^2}{2m}\left[\frac{\partial\psi^*(x,t)}{\partial x}\psi(x,t)-\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x}\right]\bigg|_a^b \qquad (134)\\
&=i\hbar\,\frac{-i\hbar}{2m}\left[\frac{\partial\psi^*(x,t)}{\partial x}\psi(x,t)-\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x}\right]\bigg|_a^b \qquad (135)\\
&=i\hbar\,(-J(x,t))|_a^b \qquad (136)\\
&=i\hbar\,(J(a,t)-J(b,t)) \qquad (137)
\end{aligned}$$

(2) 由归一化条件得 $\int dx\,|\psi(x,t)|^2=1$: 从量纲的角度看, $L\,[\psi]^2=1$, 那么 $[\psi]=L^{-1/2}$. 由概率流密度 $J(x,t)=\frac{i\hbar}{2m}(\psi(x,t)\frac{\partial\psi^*(x,t)}{\partial x}-\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x})$ 的公式得: $[J]=\frac{[\hbar]}{[m]}\,[\psi]\,[\frac{\partial\psi^*}{\partial x}]=\frac{L^2MT^{-2}T}{M}L^{-1/2}\frac{L^{-1/2}}{L}=T^{-1}$.

(3) 对于 $\psi(x,t)=Ae^{-\lambda(x-a)^2-i\omega t}$, 可得

$$\frac{\partial\psi^*(x,t)}{\partial x}=\frac{\partial}{\partial x}\left(Ae^{-\lambda(x-a)^2+i\omega t}\right)=-2A\lambda\,(x-a)\,e^{-\lambda(x-a)^2+i\omega t} \tag{138}$$

$$\frac{\partial\psi(x,t)}{\partial x}=\frac{\partial}{\partial x}\left(Ae^{-\lambda(x-a)^2-i\omega t}\right)=-2A\lambda\,(x-a)\,e^{-\lambda(x-a)^2-i\omega t} \tag{139}$$

所以概率流密度 $\frac{i\hbar}{2m}(\psi(x,t)\frac{\partial\psi^*(x,t)}{\partial x}-\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x})=0$.

讨论:

(1) 这是一个一维问题, 需要使用一维的微商符号 $\frac{\partial}{\partial x}$;

(2) 波函数的量纲和空间的维度有关: n 维空间 $[\psi]=L^{-n/2}$;

(3) 利用 $\frac{dP_{ab}}{dt}$ 判断 J 的量纲也是一个好办法.

0.4 第四次作业 2021.04.13

1. 第 25 页 1.3

解：

(a) 该一维自由粒子的波函数为 $\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$，则

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_p(x) = -\frac{\hbar^2}{2m}\frac{d}{dx}\frac{d}{dx}\frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar} \tag{140}$$

$$= -\frac{\hbar^2}{2m}\frac{1}{\sqrt{2\pi\hbar}}\frac{ip}{\hbar}\frac{d}{dx}e^{ipx/\hbar} \tag{141}$$

$$= -\frac{\hbar^2}{2m}\frac{1}{\sqrt{2\pi\hbar}}\left(\frac{ip}{\hbar}\right)^2 e^{ipx/\hbar} \tag{142}$$

$$= \frac{p^2}{2m}\psi_p(x) \tag{143}$$

(b) 由于初态是本征能量为 $\frac{p^2}{2m}$ 的本征态，所以 t 时刻粒子处于定态

$$\psi(x,t) = \psi_p(x)\, e^{-i\frac{p^2}{2m}\frac{t}{\hbar}} \tag{144}$$

(c) 粒子的初态为 $\psi(x) = \delta(x)$，则

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\delta(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\frac{1}{2\pi\hbar}\int e^{ipx/\hbar}dp \tag{145}$$

$$= -\frac{\hbar^2}{2m}\frac{1}{2\pi\hbar}\int \frac{d}{dx}\frac{d}{dx}e^{ipx/\hbar}dp \tag{146}$$

$$= -\frac{\hbar^2}{2m}\frac{1}{2\pi\hbar}\int \left(\frac{ip}{\hbar}\right)^2 e^{ipx/\hbar}dp \tag{147}$$

$$= \frac{1}{2\pi\hbar}\int \frac{p^2}{2m}e^{ipx/\hbar}dp \tag{148}$$

$$\neq E\delta(x) \tag{149}$$

所以 $\psi(x) = \delta(x)$ 不是能量本征态.

(d) 由 (a, c) 可知 $\delta(x)$ 是能量本征态的叠加，所以在时刻 t，粒子处于非定态，

$$\psi(x,t) = \frac{1}{2\pi\hbar}\int e^{ipx/\hbar}e^{-i\frac{p^2}{2m}\frac{t}{\hbar}}dp \tag{150}$$

$$= \frac{1}{2\pi\hbar}\int dp\, \mathrm{exp}\left[-\frac{it}{2m\hbar}\left(p - \frac{mx}{t}\right)^2 + \frac{imx^2}{2\hbar t}\right] \tag{151}$$

$$= \frac{1}{2\pi\hbar}\sqrt{\frac{2m\pi\hbar}{it}}\,\mathrm{exp}\left(\frac{imx^2}{2\hbar t}\right) \tag{152}$$

这里利用了积分公式 $\int_{-\infty}^{\infty} dx e^{i\alpha x^2} = \sqrt{\frac{i\pi}{\alpha}}$ ($\mathrm{Im}\alpha \geq 0$).

讨论： 当 $t \to 0$ 时，利用公式 $\lim_{\alpha\to\infty}(1 \mp i)\sqrt{\frac{\alpha}{2\pi}}e^{\pm i\alpha x^2} = \delta(x)$，可回到初态.

2. 假设 $t=0$ 时刻, 一个粒子的初始状态是能量本征态 $\psi_1(x)$, $\psi_2(x)$,$\cdots$, $\psi_n(x)$ 的线性叠加: $\psi(x,0)=\sum_{i=1}^n c_i\psi_i(x)$ (已归一化). c_i 是复常数. $\psi_i(x)$ 对应的本征能量为 E_i, 满足 $E_i\neq E_j$, 并且 $(\psi_i,\psi_j)=0$.

(1) 已知粒子 Hamiltonian 算符为 $\hat{H}$, 计算它在 $\psi(x,0)$ 上的能量平均值;

(2) 写出 $t>0$ 时刻粒子的波函数 $\psi(x,t)$, 验证它满足 Schrödinger 方程, 并计算能量的平均值;

(3) 若在 $t=0$ 时刻测量粒子的能量, 测量值为 E_1, 写出粒子在 $t>0$ 时刻的波函数, 并解释原因.

解:

(1) Hamiltonian 算符 $\hat{H}$ 在 $\psi(x,0)$ 上的能量平均值为

$$\begin{aligned}\left(\psi,\hat{H}\psi\right)&=\left(\psi,\hat{H}\sum_{i=1}^n c_i\psi_i(x)\right) &(153)\\ &=\left(\psi,\sum_{i=1}^n c_iE_i\psi_i(x)\right) &(154)\\ &=\left(\sum_{j=1}^n c_j\psi_j(x),\sum_{i=1}^n c_iE_i\psi_i(x)\right) &(155)\\ &=\sum_{j=1}^n\sum_{i=1}^n c_j^*c_iE_i\left(\psi_j,\psi_i\right) &(156)\\ &=\sum_{j=1}^n\sum_{i=1}^n c_j^*c_iE_i\delta_{ij} &(157)\\ &=\sum_{i=1}^n\left|c_i\right|^2E_i &(158)\end{aligned}$$

(2) $t>0$ 时刻粒子的波函数 $\psi(x,t)$ 为:

$$\psi\left(x,t\right)=\sum_{i=1}^n c_i\psi_ie^{-iE_it/\hbar} \tag{159}$$

这里 $c_i=\left(\psi_i,\psi\left(x,0\right)\right)$. 验证它满足 Schrödinger 方程:

$$i\hbar\frac{\partial\psi\left(x,t\right)}{\partial t}=\sum_{i=1}^n c_i\psi_iE_ie^{-iE_it/\hbar} \tag{160}$$

$$\begin{aligned}\hat{H}\psi\left(x,t\right)&=\sum_{i=1}^n c_i\hat{H}\psi_ie^{-iE_it/\hbar} &(161)\\ &=\sum_{i=1}^n c_iE_i\psi_ie^{-iE_it/\hbar} &(162)\end{aligned}$$

即

$$i\hbar\frac{\partial\psi\left(x,t\right)}{\partial t}=\hat{H}\psi\left(x,t\right) \tag{163}$$

(3) 在 $t>0$ 时刻的波函数为:

$$\psi\left(x,t\right)=\psi_1\left(x\right)e^{-iE_1t/\hbar} \tag{164}$$

$t=0$ 时刻的能量测量使粒子坍缩到能量为 E_1 的能量本征态上. 下面的演化以 $\psi_1\left(x\right)$ 为初态.

3. 在一维问题中, 考虑一个质量为 m 的粒子, 它的波函数在 t 时刻为 $\psi\left(x,t\right)$:

(1) 设想在时刻 t 测量粒子到原点 O 的距离 d. 试求测得的结果大于给定长度 d_0 的概率 $P\left(d_0\right)$ (用 $\psi\left(x,t\right)$ 表示). 并求 $P\left(d_0\right)$ 在 $d_0\to 0$ 及 $d_0\to\infty$ 时的极限.

(2) 不做 (1) 中的测量, 而测量粒子在时刻 t 的速度 v. 试求测得的结果大于给定速度值 v_0 的概率 (用 $\psi\left(x,t\right)$ 表示).

解

(1) 在 x 处测量到粒子的概率密度为 $\left|\psi\left(x,t\right)\right|^2$. 测得的结果大于给定长度 d_0 的概率即 $x>d_0$ 或 $x<-d_0$ 的概率:

$$\int_{d_0}^{\infty}dx\left|\psi\left(x,t\right)\right|^2+\int_{-\infty}^{-d_0}dx\left|\psi\left(x,t\right)\right|^2=1-\int_{-d_0}^{d_0}dx\left|\psi\left(x,t\right)\right|^2 \tag{165}$$

当 $d_0\to 0$ 时,

$$P\left(d_0\to 0\right)=\lim_{d_0\to 0}\left(\int_{d_0}^{\infty}dx+\int_{-\infty}^{-d_0}dx\right)\left|\psi\left(x,t\right)\right|^2=\int_{-\infty}^{\infty}dx\left|\psi\left(x,t\right)\right|^2=1 \tag{166}$$

当 $d_0\to\infty$ 时,

$$P\left(d_0\to\infty\right)=1-\lim_{d_0\to\infty}\int_{-d_0}^{d_0}dx\left|\psi\left(x,t\right)\right|^2=0 \tag{167}$$

(2) 粒子的速度为 v_0 时, 动量为 $p_0=mv_0$. 粒子的动量为 p_0 的概率密度为

$$\left|\varphi\left(p_0,t\right)\right|^2 \tag{168}$$

粒子的动量大于 p_0 的概率密度为

$$\left(\int_{p_0}^{\infty}dp+\int_{-\infty}^{p_0}dp\right)\left|\varphi\left(p,t\right)\right|^2=1-\int_{-p_0}^{p_0}dp\left|\varphi\left(p,t\right)\right|^2 \tag{169}$$

而

$$\begin{aligned}\int_{-p_0}^{p_0}dp\left|\varphi\left(p,t\right)\right|^2&=\int_{-p_0}^{p_0}dp\varphi^*\left(p,t\right)\varphi\left(p,t\right) &(170)\\&=\int_{-p_0}^{p_0}dp\int_{-\infty}^{\infty}dx'\psi^*\left(x',t\right)e^{ipx'/\hbar}\int_{-\infty}^{\infty}dx\psi\left(x,t\right)e^{-ipx/\hbar} &(171)\\&=\int_{-p_0}^{p_0}dp\int_{-\infty}^{\infty}dx'\int_{-\infty}^{\infty}dx\psi^*\left(x',t\right)\psi\left(x,t\right)e^{ip\left(x'-x\right)/\hbar} &(172)\end{aligned}$$

4. 已知质量为 m 的微观粒子处于状态 $\psi\left(\boldsymbol{r}\right)$, 其概率密度为 $\rho\left(\boldsymbol{r}\right)$ 和概率流密度为 $\boldsymbol{J}\left(\boldsymbol{r}\right)$. 设 $\xi\left(\boldsymbol{r}\right)$ 为 $\psi\left(\boldsymbol{r}\right)$ 的辐角, 则

$$\psi\left(\boldsymbol{r}\right)=\sqrt{\rho\left(\boldsymbol{r}\right)}e^{i\xi\left(\boldsymbol{r}\right)}$$

(1) 求证 $\boldsymbol{J}(\boldsymbol{r})=\frac{\hbar}{m}\rho(\boldsymbol{r})\nabla\xi(\boldsymbol{r})$.

(2) 如果两个波函数给出同一个概率密度为 $\rho(\boldsymbol{r})$ 和同一个概率流密度为 $\boldsymbol{J}(\boldsymbol{r})$, 则这两个波函数只相差一个总的相位因子.

解

(1) 证：已知概率流密度为

$$\begin{aligned}\boldsymbol{J}=&\frac{1}{2m}\left(\psi^*(\boldsymbol{r},t)\hat{\boldsymbol{p}}\psi(\boldsymbol{r},t)-\psi(\boldsymbol{r},t)\hat{\boldsymbol{p}}\psi^*(\boldsymbol{r},t)\right) &(173)\\ =&\frac{1}{m}\text{Re}\left(\psi^*(\boldsymbol{r},t)\hat{\boldsymbol{p}}\psi(\boldsymbol{r},t)\right) &(174)\\ =&\frac{1}{m}\text{Re}\left(\psi^*(\boldsymbol{r},t)\hat{\boldsymbol{p}}\left(\sqrt{\rho(\boldsymbol{r})}e^{i\xi(\boldsymbol{r})}\right)\right) &(175)\end{aligned}$$

这里

$$\begin{aligned}\hat{\boldsymbol{p}}\left(\sqrt{\rho(\boldsymbol{r})}e^{i\xi(\boldsymbol{r})}\right)=&\frac{\hbar}{i}\nabla\left(\sqrt{\rho(\boldsymbol{r})}e^{i\xi(\boldsymbol{r})}\right) &(176)\\ =&\frac{\hbar}{i}\left(\frac{1}{2}\frac{\nabla\rho}{\sqrt{\rho}}+i\sqrt{\rho}\nabla\xi\right)e^{i\xi} &(177)\end{aligned}$$

所以

$$\begin{aligned}\boldsymbol{J}=&\frac{1}{m}\text{Re}\left(\sqrt{\rho}e^{-i\xi}\frac{\hbar}{i}\left(\frac{1}{2}\frac{\nabla\rho}{\sqrt{\rho}}+i\sqrt{\rho}\nabla\xi\right)e^{i\xi}\right) &(178)\\ =&\frac{1}{m}\text{Re}\left(\frac{\hbar}{i}\frac{1}{2}\nabla\rho+\hbar\rho\nabla\xi\right) &(179)\\ =&\frac{\hbar}{m}\rho\nabla\xi &(180)\end{aligned}$$

(2) 两个波函数的概率密度相同, 则可令 $\psi_1(\boldsymbol{r})=\sqrt{\rho}e^{i\xi_1}$, $\psi_2(\boldsymbol{r})=\sqrt{\rho}e^{i\xi_2}$. 如果两者的概率密度相同, 则

$$\frac{\hbar}{m}\rho\nabla\xi_1=\frac{\hbar}{m}\rho\nabla\xi_2 \tag{181}$$

即

$$\nabla(\xi_1-\xi_2)=0 \tag{182}$$

所以 $\xi_1-\xi_2=C$. C 为常数, 即 $\psi_1(\boldsymbol{r})$ 和 $\psi_1(\boldsymbol{r})$ 只差一个相位因子.

0.5 第五次作业 2021.04.20

1. 设 $\psi_1(x)$ 和 $\psi_2(x)$ 是两个函数, 定义它们的朗斯基行列式为 $W(\psi_1,\psi_2)=\begin{vmatrix}\psi_1 & \psi_2\\ \psi_1' & \psi_2'\end{vmatrix}$, 证明它有下列性质:

(1) 反称性: $W(\psi_1,\psi_2)=-W(\psi_2,\psi_1)$

(2) 线性: $W(\psi_1,C_2\psi_2+C_3\psi_3)=C_2W(\psi_1,\psi_2)+C_3W(\psi_1,\psi_3)$, C_2, C_3 为常数;

(3) 雅可比恒等式 $W(\psi_1,W(\psi_2,\psi_3))+W(\psi_2,W(\psi_3,\psi_1))+W(\psi_3,W(\psi_1,\psi_2))=0$;

(4) 若 $W(\psi_1,\psi_2)=0$, 则 ψ_1,ψ_2 线性相关.

证

(1) 由于 $W(\psi_1,\psi_2) = \begin{vmatrix} \psi_1 & \psi_2 \\ \psi_1' & \psi_2' \end{vmatrix} = \psi_1\psi_2' - \psi_2\psi_1'$, $W(\psi_2,\psi_1) = \begin{vmatrix} \psi_2 & \psi_1 \\ \psi_2' & \psi_1' \end{vmatrix} = \psi_2\psi_1' - \psi_1\psi_2'$. 所以 $W(\psi_1,\psi_2) = -W(\psi_2,\psi_1)$.

(2) $W(\psi_1, C_2\psi_2 + C_3\psi_3) = \begin{vmatrix} \psi_1 & C_2\psi_2 + C_3\psi_3 \\ \psi_1' & C_2\psi_2' + C_3\psi_3' \end{vmatrix}$. 由行列式的性质 (拆分定理) 可得:

$$(\psi_1, C_2\psi_2 + C_3\psi_3) = \begin{vmatrix} \psi_1 & C_2\psi_2 + C_3\psi_3 \\ \psi_1' & C_2\psi_2' + C_3\psi_3' \end{vmatrix} = \begin{vmatrix} \psi_1 & C_2\psi_2 \\ \psi_1' & C_2\psi_2' \end{vmatrix} + \begin{vmatrix} \psi_1 & C_3\psi_3 \\ \psi_1' & C_3\psi_3' \end{vmatrix} \tag{183}$$

$$= C_2\begin{vmatrix} \psi_1 & \psi_2 \\ \psi_1' & \psi_2' \end{vmatrix} + C_3\begin{vmatrix} \psi_1 & \psi_3 \\ \psi_1' & \psi_3' \end{vmatrix} \tag{184}$$

$$= C_2W(\psi_1,\psi_2) + C_3W(\psi_1,\psi_3) \tag{185}$$

(3) 首先注意到

$$W(\psi_1, W(\psi_2,\psi_3)) = W(\psi_1, \psi_2\psi_3' - \psi_3\psi_2') \tag{186}$$

$$= W(\psi_1, \psi_2\psi_3') - W(\psi_1, \psi_3\psi_2') \tag{187}$$

$$= \psi_1(\psi_2'\psi_3' + \psi_2\psi_3'') - \psi_2\psi_3'\psi_1' - \psi_1(\psi_3'\psi_2' + \psi_3\psi_2'') + \psi_3\psi_2'\psi_1' \tag{188}$$

$$= \psi_1\psi_2\psi_3'' - \psi_2\psi_3'\psi_1' - \psi_1\psi_3\psi_2'' + \psi_3\psi_2'\psi_1' \tag{189}$$

$$= \psi_2W(\psi_1,\psi_3') - \psi_3W(\psi_1,\psi_2') \tag{190}$$

所以

$$W(\psi_1, W(\psi_2,\psi_3)) + W(\psi_2, W(\psi_3,\psi_1)) + W(\psi_3, W(\psi_1,\psi_2)) \tag{191}$$

$$=\psi_2W(\psi_1,\psi_3') - \psi_3W(\psi_1,\psi_2') + \psi_3W(\psi_2,\psi_1') - \psi_1W(\psi_2,\psi_3') + \psi_1W(\psi_3,\psi_2') - \psi_2W(\psi_3,\psi_1') \tag{192}$$

$$=\psi_2\left(W(\psi_1,\psi_3') - W(\psi_3,\psi_1')\right) - \psi_3\left(W(\psi_1,\psi_2') - W(\psi_2,\psi_1')\right) - \psi_1\left(W(\psi_2,\psi_3') - W(\psi_3,\psi_2')\right) \tag{193}$$

$$=\psi_2\left(\psi_1\psi_3'' - \psi_3\psi_1''\right) - \psi_3\left(\psi_1\psi_2'' - \psi_2\psi_1''\right) - \psi_1\left(\psi_2\psi_3'' - \psi_3\psi_2''\right) \tag{194}$$

$$=0 \tag{195}$$

(4) 由 $W(\psi_1,\psi_2) = 0$ 得:

$$W(\psi_1,\psi_2) = \psi_1\psi_2' - \psi_2\psi_1' = 0 \tag{196}$$

两边同除以 $\psi_1\psi_2$ 得到 (当然需要 $\psi_1\psi_2 \neq 0$):

$$\frac{\psi_2'}{\psi_2} = \frac{\psi_1'}{\psi_1} \tag{197}$$

$$\frac{d\ln\psi_2}{dx} = \frac{d\ln\psi_1}{dx} \tag{198}$$

$$\frac{d\left(\ln\psi_2 - \ln\psi_1\right)}{dx} = 0 \tag{199}$$

于是 $\ln\psi_2 - \ln\psi_1 = C$, ($C$ 为任意常数) 即 $\psi_2 = e^C\psi_1$, 所以两者线性相关.

讨论:

(i) (1) 和 (2) 的证明也可以用行列式的性质.

(ii) (4) 的证明也可以利用 $\frac{\psi_1\psi_2'-\psi_2\psi_1'}{\psi_1^2}=\left(\frac{\psi_1}{\psi_2}\right)'=0$.

2 设有一维势 $V(x)$, 满足 $V(\pm\infty)\to+\infty$, 考虑定态 Schrödinger 方程的两个实的归一化解: $\psi_n(x)$ 和 $\psi_m(x)$, 相应的本征能量 $E_n>E_m$.

(1) 证明:

$$\frac{d}{dx}\left(\frac{d\psi_m}{dx}\psi_n-\psi_m\frac{d\psi_n}{dx}\right)=\frac{2m}{\hbar^2}(E_n-E_m)\psi_m\psi_n$$

(2) 设 x_1 和 x_2 是 $\psi_m(x)$ 的两个相邻的节点 ($x_1<x_2$), 证明

$$\psi_m'(x_2)\psi_n(x_2)-\psi_m'(x_1)\psi_n(x_1)=\frac{2m}{\hbar^2}(E_n-E_m)\int_{x_1}^{x_2}\psi_m\psi_n dx \tag{200}$$

(3) 证明: 在 $\psi_m(x)$ 的任两个相邻节点 x_1 和 x_2 之间, $\psi_n(x)$ 至少有一个节点. (提示: 如果 $\psi_n(x)$ 在 x_1 和 x_2 之间无节点, 则它在这个区间上不变号, 结合 (2) 的结论利用反证法.)

证

(1) 定态 Schrödinger 方程为 $\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right)\psi(x)=E\psi(x)$, 即

$$\psi''(x)=\frac{2m(V-E)}{\hbar^2}\psi(x) \tag{201}$$

已知 $\psi_n(x)$ 和 $\psi_m(x)$ 满足上述方程, 于是:

$$\begin{aligned}\frac{d}{dx}\left(\frac{d\psi_m}{dx}\psi_n-\psi_m\frac{d\psi_n}{dx}\right)=&\psi_m''\psi_n+\psi_m'\psi_n'-\psi_m'\psi_n'-\psi_m\psi_n'' &(202)\\ =&\psi_m''\psi_n-\psi_m\psi_n'' &(203)\\ =&\frac{2m(V-E_m)}{\hbar^2}\psi_m(x)\psi_n(x)-\psi_m(x)\frac{2m(V-E_n)}{\hbar^2}\psi_n(x) &(204)\\ =&0 &(205)\end{aligned}$$

于是原命题得证.

(2) 对 (1) 中结论两端在区间 $[x_1,x_2]$ 上进行积分,

$$\int_{x_1}^{x_2}dx\frac{d}{dx}\left(\frac{d\psi_m}{dx}\psi_n-\psi_m\frac{d\psi_n}{dx}\right)=\frac{2m}{\hbar^2}(E_n-E_m)\int_{x_1}^{x_2}\psi_m\psi_n dx \tag{206}$$

左端可化为

$$\left.\frac{d\psi_m}{dx}\psi_n-\psi_m\frac{d\psi_n}{dx}\right|_{x_1}^{x_2} \tag{207}$$

由于 x_1 和 x_2 是 $\psi_m(x)$ 的节点, $\psi_m(x_1)=\psi_m(x_2)=0$,

$$\left.\frac{d\psi_m}{dx}\psi_n-\psi_m\frac{d\psi_n}{dx}\right|_{x_1}^{x_2}=\psi_m'(x_2)\psi_n(x_2)-\psi_m'(x_1)\psi_n(x_1) \tag{208}$$

于是

$$\psi_m'(x_2)\psi_n(x_2)-\psi_m'(x_1)\psi_n(x_1)=\frac{2m}{\hbar^2}(E_n-E_m)\int_{x_1}^{x_2}\psi_m\psi_n dx \tag{209}$$

(3) 假设 $\psi_n(x)$ 在区间 (x_1, x_2) 上无节点, 则 $\psi_n(x)$ ($x_1 < x < x_2$) 与 $\psi_n(x_1)$, $\psi_n(x_2)$ 符号相同, 又由于 $E_n > E_m$, 所以, 对于 (2) 中等式 (209), 两端符号是否相同取决于 $\psi_m(x)$. 如图示, , 可知, 在区间

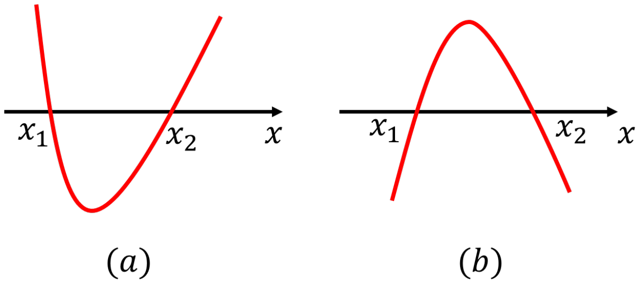

Figure 2: $\psi_m(x)$ 的节点

(x_1, x_2) 上,

- 如果 $\psi_m(x) < 0$, 那么 $\psi_m'(x_2)$, $-\psi_m'(x_1)$ 与 $\psi_m(x)$ 符号相反;
- 如果 $\psi_m(x) > 0$, 那么 $\psi_m'(x_2)$, $-\psi_m'(x_1)$ 与 $\psi_m(x)$ 符号也相反.

即对于 (2) 中等式两边的符号相反, 即不可能相等. 于是, 假设不成立, 所以在 $\psi_m(x)$ 的任两个相邻节点 x_1 和 x_2 之间, $\psi_n(x)$ 至少有一个节点.

3 证明定理 8.

证: 设束缚态波函数 $\psi(x)$ 已经归一化，则

$$E = \int dx\psi^* \hat{H}\psi = \int dx\psi^* \left(-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi\right) \tag{210}$$

$$= -\frac{\hbar^2}{2m}\psi^*\frac{d\psi}{dx}\bigg|_{-\infty}^{\infty} + \frac{\hbar^2}{2m}\int dx\psi^{*\prime}\psi' + \int dxV|\psi|^2 \tag{211}$$

$$\geq \int dxV_{\text{min}}|\psi|^2 \tag{212}$$

这里方程 (211) 中 $-\frac{\hbar^2}{2m}\psi^*\frac{d\psi}{dx}\Big|_{-\infty}^{\infty} = 0$ 是由于束缚态的性质, 而 $\frac{\hbar^2}{2m}\int dx\psi^{*\prime}\psi' = \frac{\hbar^2}{2m}\int dx|\psi'|^2 \geq 0$.

0.6 第六次作业 2021.04.27

1. 质量为 m 的粒子在宽为 a 的一维无限深势阱中, 设粒子处于能量本征态 $\psi_n(x)$, 计算其坐标的平均值 $\langle\hat{x}\rangle$ 和动量平均值 $\langle\hat{p}\rangle$.

解 设一维无限深势阱分布在区间 $[0,a]$, 已知其能量本征态 $\psi_n(x)=\begin{cases}0, & x<0,x>a\\ \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}, & 0<x<a\end{cases}$. 处于能量本征态 $\psi_n(x)$ 的粒子, 坐标的平均值为

$$\langle x\rangle=\int_{-\infty}^{\infty}\psi_n^*(x)\,x\psi_n(x)\,dx \tag{213}$$

$$=\frac{2}{a}\int_0^a x\sin^2\frac{n\pi x}{a}dx \tag{214}$$

$$=\frac{2}{a}\int_0^a x\frac{1-\cos\frac{2n\pi x}{a}}{2}dx \tag{215}$$

$$=\frac{1}{a}\frac{a^2}{2}-\frac{1}{a}\int_0^a x\cos\frac{2n\pi x}{a}dx \tag{216}$$

$$=\frac{a}{2}-\frac{1}{a}\left(x\frac{\sin\frac{2n\pi x}{a}}{\frac{2n\pi}{a}}\bigg|_0^a-\int_0^a\frac{\sin\frac{2n\pi x}{a}}{\frac{2n\pi}{a}}dx\right) \tag{217}$$

$$=\frac{a}{2}+\frac{1}{2n\pi}\frac{-\cos\frac{2n\pi x}{a}}{\frac{2n\pi}{a}}\bigg|_0^a \tag{218}$$

$$=\frac{a}{2} \tag{219}$$

动量平均值:

$$\langle\hat{p}\rangle=\int_{-\infty}^{\infty}\psi_n^*(x)\frac{\hbar}{i}\frac{d}{dx}\psi_n(x)\,dx \tag{220}$$

$$=\frac{2}{a}\frac{n\pi}{a}\int_0^a\sin\frac{n\pi x}{a}\cos\frac{n\pi x}{a}dx \tag{221}$$

$$=\frac{n\pi}{a^2}\int_0^a\sin\frac{2n\pi x}{a}dx \tag{222}$$

$$=\frac{n\pi}{a^2}\frac{-\cos\frac{2n\pi x}{a}}{\frac{2n\pi}{a}}\bigg|_0^a \tag{223}$$

$$=0 \tag{224}$$

注意: 正确使用符号: 对于一维情形, $\hat{p}=\frac{\hbar}{i}\frac{d}{dx}$.

2. (49 页) 2.3

解 由于 $V(x)=V(-x)$, 所以能量本征函数有确定的宇称. 根据 $V(x)$, 可以分为三个区域: I: $x<-\frac{a}{2}$, II: $|x|<\frac{a}{2}$, 和 III: $x>\frac{a}{2}$. 显然在区域 I 和 III, 概率幅为 0. 在区域 II, 定态 Schrödinger 方程可以写为:

$$\psi''+k^2\psi=0 \tag{225}$$

这里 $k=\sqrt{\frac{2mE}{\hbar^2}}$. 先考虑偶宇称的解,

$$\psi_n=A\cos kx \tag{226}$$

和 $x=-\frac{a}{2}$ 处的衔接条件:

$$\psi_n\left(-\frac{a}{2}\right)=0 \tag{227}$$

即

$$A\cos\frac{ka}{2}=0 \tag{228}$$

$$\frac{ka}{2}=\left(n+\frac{1}{2}\right)\pi,\quad n=0,1,2,\cdots$$

于是

$$E_n=\frac{(2n+1)^2\pi^2\hbar^2}{2ma^2} \tag{229}$$

然后考虑奇宇称的解

$$\psi_n=A\sin kx \tag{230}$$

和 $x=-\frac{a}{2}$ 处的衔接条件:

$$\psi_n\left(-\frac{a}{2}\right)=0 \tag{231}$$

即

$$A\sin\frac{ka}{2}=0 \tag{232}$$

$$\frac{ka}{2}=n\pi,\quad n=1,2,\cdots$$

于是

$$E_n=\frac{(2n)^2\pi^2\hbar^2}{2ma^2} \tag{233}$$

能量本征态可以一般的表示为 $\psi_n(x)=\begin{cases}0, & |x|>\frac{a}{2}\\ \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{2}-\frac{n\pi}{a}x\right), & |x|<\frac{a}{2}\end{cases}$, 可见基态波函数为:

$$\psi_1=A\cos\frac{\pi x}{a},\quad |x|<\frac{a}{2} \tag{234}$$

由归一化可以确定 $A=\sqrt{\frac{2}{a}}$, 所以 $\psi_1(x)=\sqrt{\frac{2}{a}}\cos\frac{\pi x}{a}$ ($|x|<\frac{a}{2}$). 于是动量空间波函数可以表示

为:

$$
\begin{aligned}
\varphi_1(p) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi_1(x)\,e^{-i\frac{p}{\hbar}x}dx && (235)\\
&= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\frac{a}{2}}^{\frac{a}{2}}\sqrt{\frac{2}{a}}\cos\frac{\pi x}{a}e^{-i\frac{p}{\hbar}x}dx && (236)\\
&= \frac{1}{\sqrt{2\pi\hbar}}\sqrt{\frac{1}{2a}}\int_{-\frac{a}{2}}^{\frac{a}{2}}\left(e^{\frac{i\pi x}{a}}+e^{-\frac{i\pi x}{a}}\right)e^{-i\frac{p}{\hbar}x}dx && (237)\\
&= \frac{1}{2\sqrt{\pi\hbar a}}\left(\left.\frac{e^{i\left(\frac{\pi}{a}-\frac{p}{\hbar}\right)x}}{i\left(\frac{\pi}{a}-\frac{p}{\hbar}\right)}\right|_{-\frac{a}{2}}^{\frac{a}{2}}+\left.\frac{e^{-i\left(\frac{\pi}{a}+\frac{p}{\hbar}\right)x}}{-i\left(\frac{\pi}{a}+\frac{p}{\hbar}\right)}\right|_{-\frac{a}{2}}^{\frac{a}{2}}\right) && (238)\\
&= \frac{1}{2\sqrt{\pi\hbar a}}\left(\frac{e^{-i\frac{pa}{2\hbar}}+e^{i\frac{pa}{2\hbar}}}{\frac{\pi}{a}-\frac{p}{\hbar}}+\frac{e^{-i\frac{pa}{2\hbar}}+e^{i\frac{pa}{2\hbar}}}{\frac{\pi}{a}+\frac{p}{\hbar}}\right) && (239)\\
&= \frac{1}{\sqrt{\pi\hbar a}}\cos\frac{pa}{2\hbar}\left(\frac{1}{\frac{\pi}{a}-\frac{p}{\hbar}}+\frac{1}{\frac{\pi}{a}+\frac{p}{\hbar}}\right) && (240)\\
&= 2\sqrt{\frac{\pi}{a^3\hbar}}\cos\frac{pa}{2\hbar}\frac{1}{\left(\frac{\pi}{a}\right)^2-\left(\frac{p}{\hbar}\right)^2} && (241)
\end{aligned}
$$

基态的动量密度为 $|\varphi_1(p)|^2 = \frac{4\pi}{a^3\hbar}\cos^2\frac{pa}{2\hbar}\frac{1}{\left(\left(\frac{\pi}{a}\right)^2-\left(\frac{p}{\hbar}\right)^2\right)^2}$.

讨论:

- 这个题目表明
$$\psi_1(x) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\varphi_1(p)\,e^{ipx/\hbar}dp \tag{242}$$
基态是很多个平面波的叠加. 尽管我们说 $\psi_1(x)$ 是驻波. 但它并不是严格意义上的驻波. 严格意义上的驻波是无穷长的波列, 而无限深势阱中只有半个波长. 当 n 越来越大, $\psi_n(x)$ 对应的驻波波数越来越大, 也就越来越接近严格的驻波, 从而在动量空间的分布越来越接近两个 δ 函数.

- 具体推导和计算如下: 对于能量本征态 $\psi_n(x)$,

$$\varphi_n(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi_n(x) e^{-i\frac{p}{\hbar}x} dx \tag{243}$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\frac{a}{2}}^{\frac{a}{2}} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{2} - \frac{n\pi}{a}x\right) e^{-i\frac{p}{\hbar}x} dx \tag{244}$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \sqrt{\frac{2}{a}} \int_{-\frac{a}{2}}^{\frac{a}{2}} \frac{e^{i\left(\frac{n\pi}{2} - \frac{n\pi}{a}x\right)} - e^{-i\left(\frac{n\pi}{2} - \frac{n\pi}{a}x\right)}}{2i} e^{-i\frac{p}{\hbar}x} dx \tag{245}$$

$$= \frac{1}{2i\sqrt{\pi\hbar a}} \left(e^{i\frac{n\pi}{2}} \left. \frac{e^{-i\left(\frac{n\pi}{a}+\frac{p}{\hbar}\right)x}}{-i\left(\frac{n\pi}{a}+\frac{p}{\hbar}\right)} \right|_{-\frac{a}{2}}^{\frac{a}{2}} - e^{-i\frac{n\pi}{2}} \left. \frac{e^{i\left(\frac{n\pi}{a}-\frac{p}{\hbar}\right)x}}{i\left(\frac{n\pi}{a}-\frac{p}{\hbar}\right)} \right|_{-\frac{a}{2}}^{\frac{a}{2}} \right) \tag{246}$$

$$= \frac{1}{2\sqrt{\pi\hbar a}} \left(e^{i\frac{n\pi}{2}} \frac{e^{-i\left(\frac{n\pi}{a}+\frac{p}{\hbar}\right)\frac{a}{2}} - e^{i\left(\frac{n\pi}{a}+\frac{p}{\hbar}\right)\frac{a}{2}}}{\frac{n\pi}{a}+\frac{p}{\hbar}} + e^{-i\frac{n\pi}{2}} \frac{e^{i\left(\frac{n\pi}{a}-\frac{p}{\hbar}\right)\frac{a}{2}} - e^{-i\left(\frac{n\pi}{a}-\frac{p}{\hbar}\right)\frac{a}{2}}}{\frac{n\pi}{a}-\frac{p}{\hbar}} \right) \tag{247}$$

$$= \frac{1}{2\sqrt{\pi\hbar a}} \left(\frac{e^{-i\frac{pa}{2\hbar}} - e^{in\pi + i\frac{pa}{2\hbar}}}{\frac{n\pi}{a}+\frac{p}{\hbar}} + \frac{e^{-i\frac{pa}{2\hbar}} - e^{-in\pi + i\frac{pa}{2\hbar}}}{\frac{n\pi}{a}-\frac{p}{\hbar}} \right) \tag{248}$$

$$= \frac{e^{-i\frac{pa}{2\hbar}} - (-1)^n e^{i\frac{pa}{2\hbar}}}{2\sqrt{\pi\hbar a}} \left(\frac{1}{\frac{n\pi}{a}+\frac{p}{\hbar}} + \frac{1}{\frac{n\pi}{a}-\frac{p}{\hbar}} \right) \tag{249}$$

如图3示, 可以看到对于高激发态, 其动量分布 $|\varphi_n(p)|^2$ 接近两个 δ 函数.

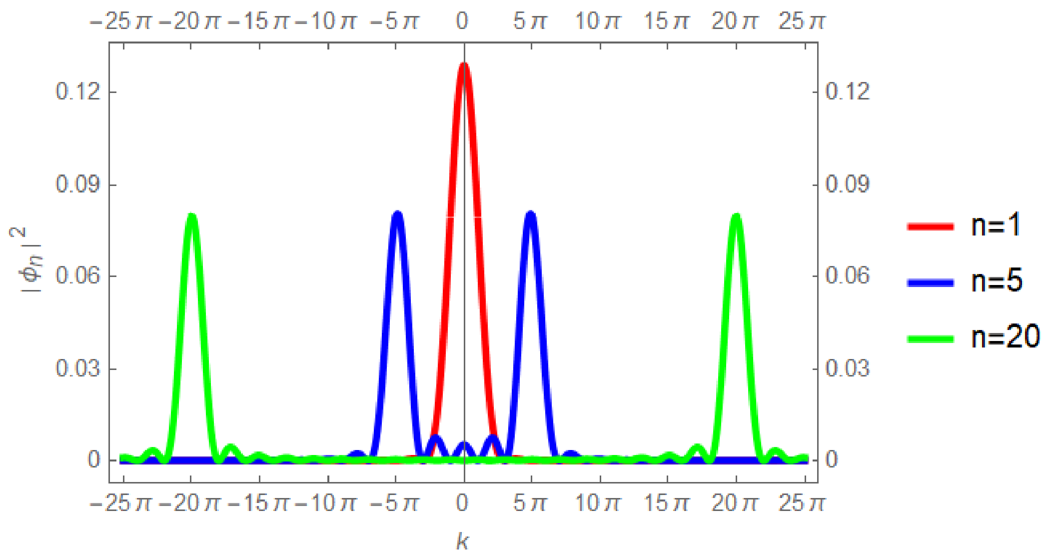

Figure 3: 一维无限深方势阱中的动量分布

3. (50 页) 2.4

解 (a) 归一化要求

$$\int_0^a |\psi(x)|^2 dx = 1 \tag{250}$$

$$|A|^2 \int_0^a |x(x-a)|^2 dx = |A|^2 \int_0^a |x(x-a)|^2 dx = |A|^2 \int_0^a dx \left(x^4 - 2ax^3 + a^2x^2\right) \tag{251}$$

$$= |A|^2 \left(\frac{x^5}{5} - 2a\frac{x^4}{4} + a^2\frac{x^3}{3} \right) \Big|_0^a = |A|^2 \frac{a^5}{30} \tag{252}$$

所以 A 可取为 $\sqrt{\frac{30}{a^5}}$.

(b) 粒子在势阱中的能量本征态是正交完备的, 所以 $\psi(x)$ 可以用 $\psi_n(x)$ 展开:

$$\psi(x)=\sum_{n=1}^{\infty}c_n\psi_n(x) \tag{253}$$

$$\begin{aligned}
c_n&=\int_{-\infty}^{\infty}dx\psi_n^*(x)\psi(x)=\int_0^a dx\sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}Ax(x-a) &(254)\\
&=A\sqrt{\frac{2}{a}}\int_0^a dx\sin\frac{n\pi x}{a}x(x-a) &(255)\\
&=A\sqrt{\frac{2}{a}}\left(-\frac{1}{\frac{n\pi}{a}}\cos\frac{n\pi x}{a}x(x-a)\bigg|_0^a+\int_0^a dx\frac{1}{\frac{n\pi}{a}}\cos\frac{n\pi x}{a}(2x-a)\right) &(256)\\
&=A\sqrt{\frac{2}{a}}\int_0^a dx\frac{1}{\frac{n\pi}{a}}\cos\frac{n\pi x}{a}(2x-a) &(257)\\
&=A\sqrt{\frac{2}{a}}\left(\frac{\sin\frac{n\pi x}{a}}{\left(\frac{n\pi}{a}\right)^2}(2x-a)\bigg|_0^a-2\int_0^a dx\frac{\sin\frac{n\pi x}{a}}{\left(\frac{n\pi}{a}\right)^2}\right) &(258)\\
&=A\sqrt{\frac{2}{a}}(-2)\frac{\cos\frac{n\pi x}{a}}{\left(\frac{n\pi}{a}\right)^3}\bigg|_0^a=A\sqrt{\frac{2}{a}}2\frac{(-1)^n-1}{\left(\frac{n\pi}{a}\right)^3} &(259)
\end{aligned}$$

所以, 粒子处于 ψ_n 的概率 $P_n=|c_n|^2=\frac{240((-1)^n-1)^2}{n^6\pi^6}$. 其中 $P_1=\frac{960}{\pi^6}\approx 0.9986$.

(c) 如图4示, 可看出 $\psi(x)$ 与 $\psi_1(x)$ 非常接近. 为了进行比较, 由于波函数有一个相位的自由度, $\psi(x)$

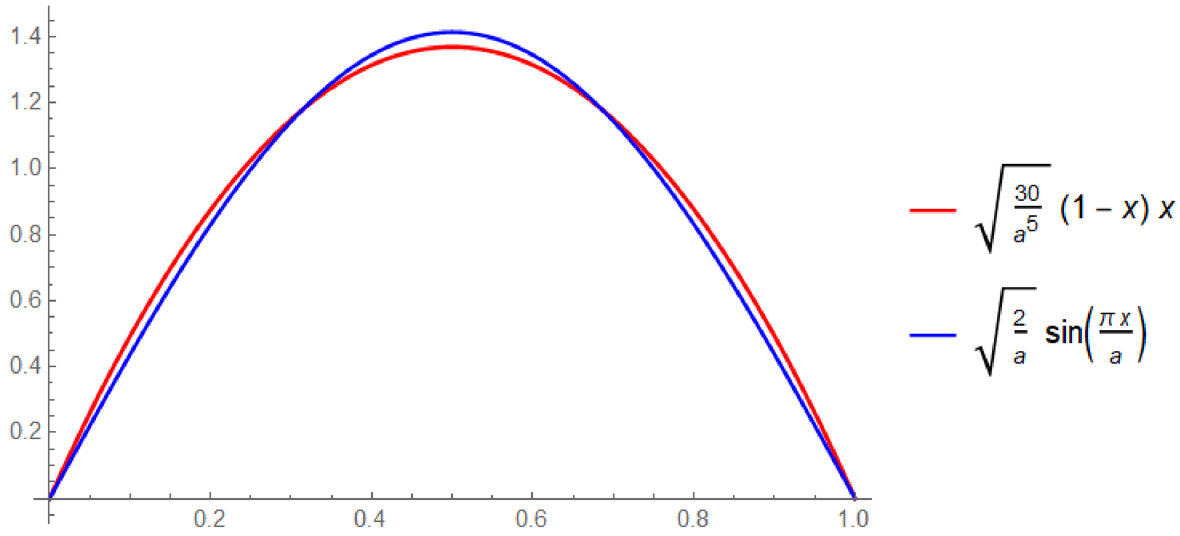

Figure 4: $\psi(x)$ 与 $\psi_1(x)$

前加了一个负号.

4. (50 页) 2.5

解: 对于加宽的势阱, 粒子的能量本征态为

$$\psi_{n,2a}(x) = \begin{cases} \sqrt{\frac{2}{2a}}\sin\left(\frac{n\pi x}{2a}\right) = \sqrt{\frac{1}{a}}\sin\left(\frac{n\pi x}{2a}\right), & 0 < x < 2a \\ 0, & x < 0, x > 2a \end{cases} \tag{260}$$

$$E_{n,2a} = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}, \quad n = 1, 2, 3 \tag{261}$$

粒子处于原来势阱的基态

$$\psi_1(x) = \begin{cases} \sqrt{\frac{2}{a}}\sin\frac{\pi x}{a}, & 0 < x < a \\ 0, & x < 0, x > a \end{cases} \tag{262}$$

本征能量 $E_1 = \frac{\pi^2\hbar^2}{2ma^2}$. 此时的 $\psi_1(x)$ 在 $0 < x < 2a$ 区域, 不再满足能量本征方程, 因此不再是本征态.

势阱突然变宽时, 粒子仍处于 ψ_1, 若测得其能量为 E_1, 对应的本征态为 $\psi_{2,2a}$. 在 $0 < x < a$ 区域

$$\psi_1 = \sum_{n=1}^{\infty} c_n\psi_{n,2a}(x) \tag{263}$$

$$c_2 = \int_{-\infty}^{\infty} dx\psi_{2,2a}^*(x)\psi_1(x) \tag{264}$$

$$= \int_0^a dx\sqrt{\frac{1}{a}}\sin\left(\frac{\pi x}{a}\right)\sqrt{\frac{2}{a}}\sin\frac{\pi x}{a} \tag{265}$$

$$= \frac{\sqrt{2}}{a}\int_0^a dx\frac{1-\cos\frac{2\pi x}{a}}{2} \tag{266}$$

$$= \frac{\sqrt{2}}{2} \tag{267}$$

所以测得粒子能量为 E_1 的概率为 $|c_2|^2 = \frac{1}{2}$.

5. 质量为 m 的粒子在下列势阱中运动:

$$V(x) = \begin{cases} 0, & x < 0 \\ -\frac{40\hbar^2}{ma^2}, & 0 \le x \le a \\ \infty, & x > a \end{cases}$$

求势阱中有多少个束缚态? 写出推理过程.

解: 势阱可以分为三个区域

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_{\text{I}} = E\psi_{\text{I}}, x < 0 \tag{268}$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_{\text{II}} - V_0\psi_{\text{II}} = E\psi_{\text{II}}, 0 \le x \le a \tag{269}$$

$$\psi_{\text{III}}(x) = 0, x > a \tag{270}$$

这里 $V_0=\frac{40\hbar^2}{ma^2}$. 束缚态能量 $E<0$. 首先在第 III 区, 由于势能无限大, 唯一有意义的解是 $\psi_{\text{III}}(x)=0$. 下面考察第 I 区和第 II 区,

$$\psi_{\text{I}}''-\frac{2m(-E)}{\hbar^2}\psi_{\text{I}}=0 \tag{271}$$

$$\psi_{\text{II}}''+\frac{2m(V_0+E)}{\hbar^2}\psi_{\text{II}}=0 \tag{272}$$

由于束缚态能量 $-V_0<E<0$, 所以

$$\psi_{\text{I}}=Ce^{-\kappa x}+De^{\kappa x},\kappa=\sqrt{\frac{2m(-E)}{\hbar^2}} \tag{273}$$

$$\psi_{\text{II}}=A\sin(kx+\delta),k=\sqrt{\frac{2m(V_0+E)}{\hbar^2}} \tag{274}$$

对于束缚态, ψ_{I} 中的 $Ce^{-\kappa x}$ 应舍去:

$$\psi_{\text{I}}=De^{\kappa x} \tag{275}$$

考虑 $x=0$ 和 $x=a$ 处边界条件

$$\psi_{\text{I}}(0)=\psi_{\text{II}}(0) \tag{276}$$

$$\psi_{\text{I}}'(0)=\psi_{\text{II}}'(0) \tag{277}$$

$$\psi_{\text{II}}(a)=0 \tag{278}$$

即

$$D=A\sin\delta \tag{279}$$

$$D\kappa=Ak\cos\delta \tag{280}$$

$$A\sin(ka+\delta)=0 \tag{281}$$

于是,

$$\tan\delta=\frac{k}{\kappa} \tag{282}$$

显然, $A\neq 0$. 于是, $ka+\delta=n\pi$ ($n=0,1,2,\cdots$). 所以

$$\tan\delta=\tan(n\pi-ka)=-\tan ka=\frac{k}{\kappa}=\frac{ka}{\kappa a} \tag{283}$$

令 $\xi=ka$, $\eta=\kappa a$, 则 $\tan\xi=-\frac{\xi}{\eta}$, 并且 $\xi^2+\eta^2=\frac{2mV_0a^2}{\hbar^2}$. 利用图解法 (图5), 可得到原方程有 3 个根.

讨论: 由于 $V(x)\neq V(-x)$, 不能分奇和偶宇称讨论.

6. 如图6示, 质量为 m 的粒子流从右边入射, 碰到如图所示的阶梯势, 粒子能量 $E>V_0$, 求反射系数和透射系数.

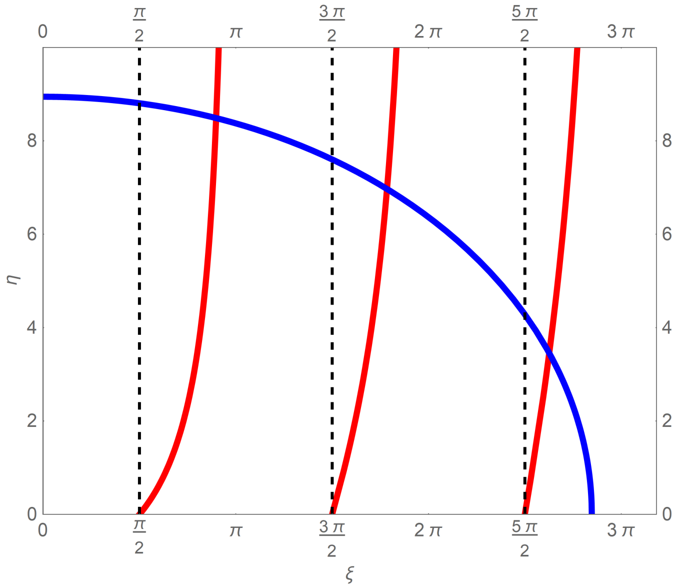

Figure 5: 3 个束缚态解

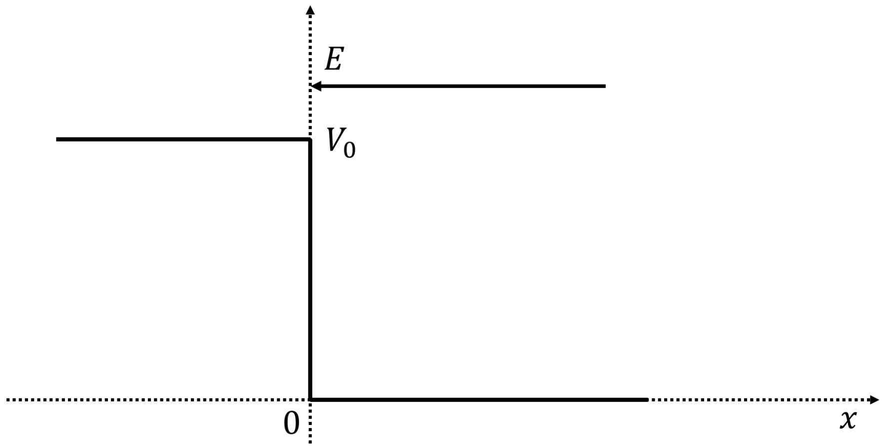

Figure 6: 第 6 题图

解: 粒子从右边入射. 势阱可以分为 $x<0$ 和 $x>0$ 两个区域:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V_0\right)\psi_{\text{I}}(x)=E\psi_{\text{I}}(x) \tag{284}$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_{\text{II}}(x)=E\psi_{\text{II}}(x) \tag{285}$$

化简得到

$$\frac{d^2}{dx^2}\psi_{\text{I}}(x)+k_1^2\psi_{\text{I}}(x)=0,\qquad k_1=\sqrt{\frac{2m(E-V_0)}{\hbar^2}} \tag{286}$$

$$\frac{d^2}{dx^2}\psi_{\text{II}}(x)+k_2^2\psi_{\text{II}}(x)=0,\qquad k_2=\sqrt{\frac{2mE}{\hbar^2}} \tag{287}$$

所以

$$\psi_{\text{I}}(x)=Fe^{-ik_1x} \tag{288}$$

$$\psi_{\text{II}}(x)=Ae^{ik_2x}+Be^{-ik_2x} \tag{289}$$

在 $x=0$ 处，由波函数和波函数一阶导数的连续性得

$$F = A + B \tag{290}$$

$$-ik_1F = Aik_2 - Bik_2 \tag{291}$$

所以

$$A = \frac{1}{2}F\left(1 - \frac{k_1}{k_2}\right) \tag{292}$$

$$B = \frac{1}{2}F\left(1 + \frac{k_1}{k_2}\right) \tag{293}$$

入射粒子 $\psi_i = Be^{-ik_2x}$, 流密度:

$$j_i = \frac{1}{2m}\left(\psi_i^* \frac{\hbar}{i}\frac{d}{dx}\psi_i + \psi_i \frac{\hbar}{i}\frac{d}{dx}\psi_i^*\right) = -\frac{1}{m}\hbar k_2 \left|B\right|^2 \tag{294}$$

反射粒子 $\psi_r = Ae^{ik_2x}$, 流密度:

$$j_r = \frac{1}{2m}\left(\psi_r^* \frac{\hbar}{i}\frac{d}{dx}\psi_r + \psi_r \frac{\hbar}{i}\frac{d}{dx}\psi_r^*\right) = \frac{1}{m}\hbar k_2 \left|A\right|^2 \tag{295}$$

透射粒子 $\psi_t = Fe^{-ik_1x}$, 流密度:

$$j_t = \frac{1}{2m}\left(\psi_t^* \frac{\hbar}{i}\frac{d}{dx}\psi_t + \psi_t \frac{\hbar}{i}\frac{d}{dx}\psi_t^*\right) = -\frac{1}{m}\hbar k_1 \left|F\right|^2 \tag{296}$$

反射系数

$$R = \frac{|j_r|}{|j_i|} = \frac{|A|^2}{|B|^2} = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 \tag{297}$$

透射系数

$$T = \frac{|j_t|}{|j_i|} = \frac{k_1}{k_2}\left(\frac{2k_2}{k_1 + k_2}\right)^2 \tag{298}$$

讨论: 粒子是从右边入射的. 波 $e^{i(kx-\omega t)}$, 令 $kx - \omega t = \phi_0$, 则 $x = \frac{\omega t + \phi_0}{k}$, 所以它是右行波, 类似的, $e^{-i(kx+\omega t)}$ 是左行波. 与行波法中的结论一致: $f_1(x - vt)$ 是右行波, $f_2(x + vt)$ 是左行波.

0.7 第七次作业 2021.05.06

1. 如图7示的势 $V(x)$, 只分布在区域 II, 在区域 I 和 III 为 0. 各个区域的波函数如图所示. 在区域 II 中, 由于没有给定 $V(x)$ 的具体形式, 其波函数表示为 $\psi_{II}(x) = Cf(x) + Dg(x)$. $\psi_I(x)$ 和 $\psi_{II}(x)$ 的形式使得我们既能处理粒子从左边入射的情形, 也能处理粒子从右边入射的情形. 利用连续性条件, 可以得到:

$$\begin{pmatrix} F \\ G \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix}$$

这里 $M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}$ 称为转移矩阵 (transfer matrix).

(1) 利用 I 区和 III 区的概率流守恒, 证明: $|A|^2 - |B|^2 = |F|^2 - |G|^2$;

(2) 根据本章第一节定理 1, $\psi_I^*(x) = A^* e^{-ikx} + B^* e^{ikx}$ 也是定态 Schrödinger 方程的散射解, 相应的 $\psi_{III}^*(x) = F^* e^{-ikx} + G^* e^{ikx}$, 于是 $\begin{pmatrix} G^* \\ F^* \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} B^* \\ A^* \end{pmatrix}$, 证明: $M_{11} = M_{22}^*$, $M_{12} = M_{21}^*$.

(3) 结合步骤 (1) 和 (2) 的结论证明: $|M| = 1$.

(4) 考虑能量为 E 的粒子流, $E > 0$, 对于势垒 $V(x) = \begin{cases} V_0, & 0 \le x \le a \\ 0, & x > a, \text{或} x < 0 \end{cases}$, $E > V_0 > 0$, 构造相应的转移矩阵 M. 写出推理过程. 令 $G = 0$, 求从左边入射粒子流的反射系数和透射系数.

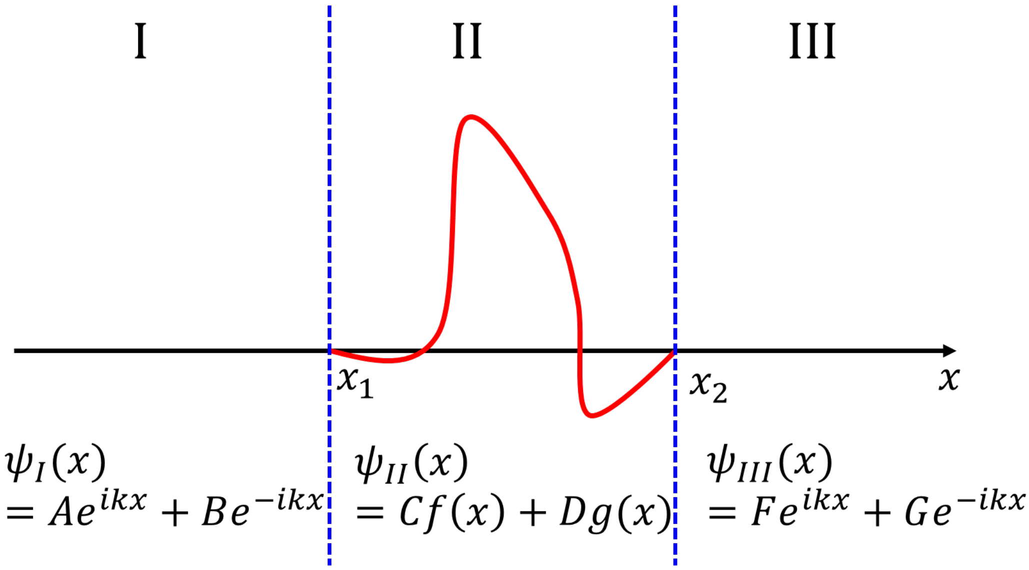

Figure 7: 转移矩阵

解:

(1) I 区的概率流密度为:

$$\begin{aligned}
J_I =& \frac{1}{m}\text{Re}\left(\psi_I^*\hat{p}\psi_I\right) && (299)\\
=& \frac{1}{m}\text{Re}\left(\left(A^*e^{-ikx}+B^*e^{ikx}\right)\hbar k\left(Ae^{ikx}-Be^{-ikx}\right)\right) && (300)\\
=& \frac{\hbar k}{m}\text{Re}\left(|A|^2-|B|^2-A^*Be^{-2ikx}+B^*Ae^{2ikx}\right) && (301)\\
=& \frac{\hbar k}{m}\left(|A|^2-|B|^2\right) && (302)
\end{aligned}$$

$$\begin{aligned}
J_{III} =& \frac{1}{m}\text{Re}\left(\psi_{III}^*\hat{p}\psi_{III}\right) && (303)\\
=& \frac{1}{m}\text{Re}\left(\left(C^*e^{-ikx}+D^*e^{ikx}\right)\hbar k\left(Ce^{ikx}-De^{-ikx}\right)\right) && (304)\\
=& \frac{\hbar k}{m}\text{Re}\left(|C|^2-|D|^2-C^*De^{-2ikx}+D^*Ce^{2ikx}\right) && (305)\\
=& \frac{\hbar k}{m}\left(|C|^2-|D|^2\right) && (306)
\end{aligned}$$

由概率流守恒可得:

$$J_I = J_{III} \tag{307}$$

所以

$$|A|^2-|B|^2=|C|^2-|D|^2 \tag{308}$$

(2) 由于

$$\begin{pmatrix} G^* \\ F^* \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}\begin{pmatrix} B^* \\ A^* \end{pmatrix} \tag{309}$$

$$\begin{aligned}
\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} G^* \\ F^* \end{pmatrix} &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} B^* \\ A^* \end{pmatrix} && (310)\\
\begin{pmatrix} F^* \\ G^* \end{pmatrix} &= \begin{pmatrix} M_{22} & M_{21} \\ M_{12} & M_{11} \end{pmatrix}\begin{pmatrix} A^* \\ B^* \end{pmatrix} && (311)
\end{aligned}$$

两边取复共轭得到:

$$\begin{pmatrix} F \\ G \end{pmatrix} = \begin{pmatrix} M_{22}^* & M_{21}^* \\ M_{12}^* & M_{11}^* \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} \tag{312}$$

与 $\begin{pmatrix} F \\ G \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix}$ 比较得到:

$$M_{11}=M_{22}^*, M_{12}=M_{21}^* \tag{313}$$

(3) 由于 $\begin{pmatrix} F \\ G \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix}$, 于是

$$\begin{aligned}
|F|^2-|G|^2 &= |M_{11}A+M_{12}B|^2-|M_{21}A+M_{22}B|^2 && (314)\\
&= \left(M_{11}^*A^*+M_{12}^*B^*\right)\left(M_{11}A+M_{12}B\right)-\left(M_{21}^*A^*+M_{22}^*B^*\right)\left(M_{21}A+M_{22}B\right) && (315)
\end{aligned}$$

利用 (2) 的结论,

$$
\begin{aligned}
|F|^2-|G|^2 &= \left(M_{22}A^*+M_{21}B^*\right)\left(M_{11}A+M_{12}B\right)-\left(M_{12}A^*+M_{11}B^*\right)\left(M_{21}A+M_{22}B\right) && (316)\\
&= M_{11}M_{22}|A|^2+M_{21}M_{12}|B|^2+M_{21}M_{11}B^*A+M_{22}M_{12}A^*B-M_{12}M_{21}|A|^2 && (317)\\
&-M_{11}M_{22}|B|^2-M_{12}M_{22}A^*B-M_{11}M_{21}B^*A && (318)\\
&= \left(M_{11}M_{22}-M_{12}M_{21}\right)\left(|A|^2-|B|^2\right) && (319)
\end{aligned}
$$

由 (1) 的结论, 可得

$$
M_{11}M_{22}-M_{12}M_{21}=1 \tag{320}
$$

即 $|M|=1$.

(4) 我们首先写出三个区域的 Schrödinger 方程:

$$
\begin{cases}
\mathrm{I}: & -\frac{\hbar^2}{2m}\frac{d^2\psi_{\mathrm{I}}}{dx^2}=E\psi_{\mathrm{I}},\ (x\le 0)\\
\mathrm{II}: & -\frac{\hbar^2}{2m}\frac{d^2\psi_{\mathrm{II}}}{dx^2}+V_0\psi_{\mathrm{II}}=E\psi_{\mathrm{II}},\ (0<x<a)\\
\mathrm{III}: & -\frac{\hbar^2}{2m}\frac{d^2\psi_{\mathrm{III}}}{dx^2}=E\psi_{\mathrm{III}},\ (x\ge a)
\end{cases} \tag{321}
$$

和方程的解:

$$
\begin{cases}
\psi_{\mathrm{I}}(x)= & Ae^{ik_1x}+Be^{-ik_1x}, & k_1=\sqrt{\frac{2mE}{\hbar^2}}\\
\psi_{\mathrm{II}}(x)= & Ce^{ik_2x}+De^{-ik_2x}, & k_2=\sqrt{\frac{2m(E-V_0)}{\hbar^2}}\\
\psi_{\mathrm{III}}(x)= & Fe^{ik_1x}+Ge^{-ik_1x}
\end{cases} \tag{322}
$$

由 $x=0,a$ 处波函数及其一阶导数的连续性条件可得:

$$
A+B=C+D \tag{323}
$$

$$
ik_1(A-B)=ik_2(C-D) \tag{324}
$$

$$
Ce^{ik_2a}+De^{-ik_2a}=Fe^{ik_1a}+Ge^{-ik_1a} \tag{325}
$$

$$
ik_2\left(Ce^{k_2a}-De^{-k_2a}\right)=ik_1Fe^{ik_1a}-ik_1Ge^{-ik_1a} \tag{326}
$$

写成矩阵的形式:

$$
\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}A\\ B\end{pmatrix}=\begin{pmatrix}1 & 1\\ \frac{k_2}{k_1} & -\frac{k_2}{k_1}\end{pmatrix}\begin{pmatrix}C\\ D\end{pmatrix} \tag{327}
$$

$$
\begin{pmatrix}e^{ik_2a} & e^{-ik_2a}\\ e^{ik_2a} & -e^{-ik_2a}\end{pmatrix}\begin{pmatrix}C\\ D\end{pmatrix}=\begin{pmatrix}e^{ik_1a} & e^{-ik_1a}\\ \frac{k_1}{k_2}e^{ik_1a} & -\frac{k_1}{k_2}e^{-ik_1a}\end{pmatrix}\begin{pmatrix}F\\ G\end{pmatrix} \tag{328}
$$

所以

$$
\begin{pmatrix}A\\ B\end{pmatrix}=\frac{1}{2}\begin{pmatrix}1+\frac{k_2}{k_1} & 1-\frac{k_2}{k_1}\\ 1-\frac{k_2}{k_1} & 1+\frac{k_2}{k_1}\end{pmatrix}\begin{pmatrix}C\\ D\end{pmatrix} \tag{329}
$$

$$
\begin{pmatrix}C\\ D\end{pmatrix}=\frac{1}{2}\begin{pmatrix}\left(1+\frac{k_1}{k_2}\right)e^{i(k_1-k_2)a} & \left(1-\frac{k_1}{k_2}\right)e^{-i(k_1+k_2)a}\\ \left(1-\frac{k_1}{k_2}\right)e^{i(k_1+k_2)a} & \left(1+\frac{k_1}{k_2}\right)e^{-i(k_1-k_2)a}\end{pmatrix}\begin{pmatrix}F\\ G\end{pmatrix} \tag{330}
$$

最终得到:

$$M_{11}=\frac{1}{4}\left(\left(1+\frac{k_2}{k_1}\right)\left(1+\frac{k_1}{k_2}\right)e^{i(k_1-k_2)a}+\left(1-\frac{k_2}{k_1}\right)\left(1-\frac{k_1}{k_2}\right)e^{i(k_1+k_2)a}\right) \tag{331}$$

$$=\frac{e^{ik_1a}}{4}\left(\left(1+\frac{k_2}{k_1}\right)\left(1+\frac{k_1}{k_2}\right)e^{-ik_2a}+\left(1-\frac{k_2}{k_1}\right)\left(1-\frac{k_1}{k_2}\right)e^{ik_2a}\right) \tag{332}$$

$$=\frac{e^{ik_1a}}{4}\left(4\cos\left(k_2a\right)-2i\left(\frac{k_2}{k_1}+\frac{k_1}{k_2}\right)\sin\left(k_2a\right)\right) \tag{333}$$

$$M_{12}=\frac{1}{4}\left(\left(1+\frac{k_2}{k_1}\right)\left(1-\frac{k_1}{k_2}\right)e^{-i(k_1+k_2)a}+\left(1-\frac{k_2}{k_1}\right)\left(1+\frac{k_1}{k_2}\right)e^{-i(k_1-k_2)a}\right) \tag{334}$$

$$=\frac{e^{-ik_1a}}{4}\left(\left(1+\frac{k_2}{k_1}\right)\left(1-\frac{k_1}{k_2}\right)e^{-ik_2a}+\left(1-\frac{k_2}{k_1}\right)\left(1+\frac{k_1}{k_2}\right)e^{ik_2a}\right) \tag{335}$$

$$=\frac{e^{-ik_1a}}{4}\left(-2i\left(\frac{k_1}{k_2}-\frac{k_2}{k_1}\right)\sin\left(k_2a\right)\right) \tag{336}$$

而 $M_{21}=M_{12}^*$, $M_{22}=M_{11}^*$.

下面计算透射系数和反射系数. 令 $G=0$, 则

$$F=M_{11}A+M_{12}B \tag{337}$$

$$0=M_{21}A+M_{22}B \tag{338}$$

于是,

$$B=-\frac{M_{21}A}{M_{22}} \tag{339}$$

$$F=M_{11}A-M_{12}\frac{M_{21}A}{M_{22}} \tag{340}$$

$$=\frac{1}{M_{22}}A \tag{341}$$

则反射系数

$$R=\frac{|B|^2}{|A|^2}=\left|\frac{M_{21}}{M_{22}}\right|^2 \tag{342}$$

$$=\frac{\frac{1}{4}\left(\frac{k_2}{k_1}-\frac{k_1}{k_2}\right)^2\sin^2\left(k_2a\right)}{\cos^2\left(k_2a\right)+\frac{1}{4}\left(\frac{k_2}{k_1}+\frac{k_1}{k_2}\right)^2\sin^2\left(k_2a\right)} \tag{343}$$

$$=\frac{\frac{1}{4}\left(\frac{k_2}{k_1}-\frac{k_1}{k_2}\right)^2\sin^2\left(k_2a\right)}{1+\frac{1}{4}\left(\frac{k_2}{k_1}-\frac{k_1}{k_2}\right)^2\sin^2\left(k_2a\right)} \tag{344}$$

透射系数

$$T=\frac{|F|^2}{|A|^2}=\frac{1}{|M_{22}|^2} \tag{345}$$

$$=\frac{1}{\cos^2\left(k_2a\right)+\frac{1}{4}\left(\frac{k_2}{k_1}+\frac{k_1}{k_2}\right)^2\sin^2\left(k_2a\right)} \tag{346}$$

$$=\frac{1}{1+\frac{1}{4}\left(\frac{k_2}{k_1}-\frac{k_1}{k_2}\right)^2\sin^2\left(k_2a\right)} \tag{347}$$

0.8 第八次作业 2021.05.11

1. 一个质量为 m 的粒子在一维 δ 函数势场 $V(x) = -A[\delta(x-a)+\delta(x+a)]$ 中运动, 常数 $a>0$, $A>0$. 考察其束缚态, 求基态波函数, 并导出联系 A 和能量本征值 E 的方程.

解 由于 $V(x)=V(-x)$, 束缚态解具有确定的宇称, 分偶宇称和奇宇称讨论. 且束缚态能量满足 $E<0$.

首先分区域写出定态 Schrödinger 方程:

$$-\frac{\hbar^2}{2m}\psi_I''(x) = E\psi_I(x), \quad x<-a \tag{348}$$

$$-\frac{\hbar^2}{2m}\psi_{II}''(x) = E\psi_{II}(x), \quad -a<x<a \tag{349}$$

$$-\frac{\hbar^2}{2m}\psi_{III}''(x) = E\psi_{III}(x), \quad x>a \tag{350}$$

进一步化简为:

$$\psi_I''+\kappa^2\psi_I=0, \quad x<-a, \tag{351}$$

$$\psi_{II}''+\kappa^2\psi_{II}=0, \quad -a<x<a \tag{352}$$

$$\psi_{III}''+\kappa^2\psi_{III}=0, \quad x>a \tag{353}$$

这里 $\kappa=\sqrt{\frac{-2mE}{\hbar^2}}$.

(1) 偶宇称: 第 I 区

$$\psi_I(x)=Be^{\kappa x}, \quad x<-a \tag{354}$$

这里舍去了不满足束缚态要求的解 $e^{-\kappa x}$. 第 II 区的解满足 $\psi_{II}(x)=\psi_{II}(-x)$:

$$\psi_{II}(x)=C\left(e^{\kappa x}+e^{-\kappa x}\right), \quad -a<x<a \tag{355}$$

第 III 区:

$$\psi_{III}(x)=\psi_I(-x)=Be^{-\kappa x}, \quad x>a \tag{356}$$

考虑 $x=-a$ 处的波函数连续条件和一阶导数不连续条件:

$$Be^{-\kappa a} = C\left(e^{-\kappa a}+e^{\kappa a}\right) \tag{357}$$

$$C\kappa\left(e^{-\kappa a}-e^{\kappa a}\right)-\kappa Be^{-\kappa a} = -\frac{2mA}{\hbar^2}Be^{-\kappa a} \tag{358}$$

化简得:

$$e^{-2\kappa a}=\frac{\hbar^2\kappa}{mA}-1 \tag{359}$$

上式左右两端是关于 κ 的函数, 两者在第一象限总是有一个交点, 对应着一个束缚态的解. 归一化:

$$\int_{-\infty}^{\infty}dx\,|\psi(x)|^2 = 2|B|^2\left.\frac{e^{2\kappa x}}{2\kappa}\right|_{-\infty}^{-a}+4|C|^2\left(a+\left.\frac{\sinh 2\kappa x}{4\kappa}\right|_{-a}^{a}\right)=1 \tag{360}$$

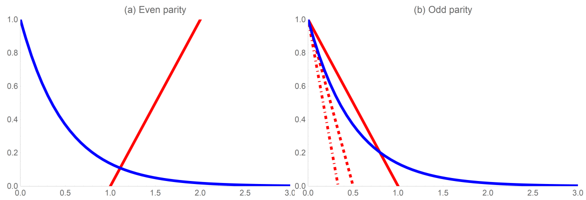

Figure 8: 双 δ 势阱的偶宇称和奇宇称解

而 $|B|^2 = e^{2\kappa a}4|C|^2\cosh^2\kappa a$,

$$4|C|^2\left(\frac{\cosh^2\kappa a}{\kappa}+a+\frac{\sinh 2\kappa a}{2\kappa}\right)=1 \tag{361}$$

即

$$\frac{4|C|^2}{2\kappa}\left(e^{2\kappa a}+1+2\kappa a\right)=1 \tag{362}$$

取

$$2C=\left(\frac{2\kappa}{e^{2\kappa a}+1+2\kappa a}\right)^{-\frac{1}{2}} \tag{363}$$

所以

$$\psi(x)=\begin{cases}2C\sinh\kappa a e^{\kappa(a+|x|)}, & |x|>a\\ 2C\cosh\kappa a, & |x|<a\end{cases} \tag{364}$$

(2) 类似的, 奇宇称的解在各个分区可写为:

$$\begin{cases}\psi_I(x)=De^{\kappa x}, & x<-a\\ \psi_{II}(x)=F\left(e^{\kappa x}-e^{-\kappa x}\right), & -a<x<a\\ \psi_{III}(x)=-De^{-\kappa x}, & x>a\end{cases} \tag{365}$$

考虑 $x=-a$ 处的波函数连续条件和一阶导数不连续条件:

$$De^{-\kappa a}=F\left(e^{-\kappa a}-e^{\kappa a}\right) \tag{366}$$

$$F\kappa\left(e^{-\kappa a}+e^{\kappa a}\right)-\kappa De^{-\kappa a}=-\frac{2mA}{\hbar^2}De^{-\kappa a} \tag{367}$$

化简得:

$$e^{-2\kappa a}=-\frac{\hbar^2\kappa}{mA}+1 \tag{368}$$

上式左右两端是关于 κ 的函数. 由于 $(e^{-2\kappa a})'=-2ae^{-2\kappa a}$, $(e^{-2\kappa a})''=4a^2e^{-2\kappa a}>0$, 可见其斜率逐渐变大, 即由 $\kappa=0$ 处的 $-2a$ 逐渐增加. 于是, 当 $\frac{\hbar^2\kappa}{mA}=2a$ 时, 只有一个平庸解; 当 $\frac{\hbar^2\kappa}{mA}<2a$ 时, 有一个非平庸解. 可以看出: 束缚态能量为 $E=-\frac{\hbar^2\kappa^2}{2m}$. 因此, κ 越大, 基态能量越低, 偶宇称的 κ 不受限制, 可以任意大, 而奇宇称的有上限. 所以偶宇称的能量更低.

2. 51 页 2.12.

解

(a) $\psi(x,0)$ 已经归一化. 对于一维无限深势阱中的粒子, 设势阱宽度为 a, 处于区间 $[0,a]$. 粒子本征能量为 $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$, 能量本征态 $\psi_n(x) = \begin{cases} 0 & x<0, x>a \\ \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}, & 0<x<a \end{cases}$, $(n=0,1,2,\cdots)$, 且 $(\psi_n,\psi_m)=\delta_{mn}$. 于是

$$\psi(x,t) = \frac{1}{\sqrt{2}}\left(\psi_1(x)e^{-\frac{iE_1 t}{\hbar}} + \psi_2(x)e^{-\frac{iE_2 t}{\hbar}}\right) \tag{369}$$

$$\begin{aligned}
\rho(x,t) =& \psi^*(x,t)\psi(x,t) && (370)\\
=& \frac{1}{\sqrt{2}}\left(\psi_1^*(x)e^{\frac{iE_1 t}{\hbar}} + \psi_2^*(x)e^{\frac{iE_2 t}{\hbar}}\right)\frac{1}{\sqrt{2}}\left(\psi_1(x)e^{-\frac{iE_1 t}{\hbar}} + \psi_2(x)e^{-\frac{iE_2 t}{\hbar}}\right) && (371)\\
=& \frac{1}{2}\left(\psi_1^*(x)\psi_1(x) + \psi_2^*(x)\psi_2(x) + \psi_1^*(x)\psi_2(x)e^{-i\frac{E_2-E_1}{\hbar}t} + \psi_1(x)\psi_2^*(x)e^{i\frac{E_2-E_1}{\hbar}t}\right) && (372)\\
=& \frac{1}{2}\left(\psi_1^2(x) + \psi_2^2(x) + 2\psi_1(x)\psi_2(x)\cos\left(\frac{E_2-E_1}{\hbar}t\right)\right) && (373)
\end{aligned}$$

(b) 能量平均值

$$\begin{aligned}
\left\langle \hat{H}\right\rangle =& \left(\psi(x,t), \hat{H}\psi(x,t)\right) && (374)\\
=& \left(\psi(x,t), \hat{H}\frac{1}{\sqrt{2}}\left(\psi_1(x)e^{-\frac{iE_1 t}{\hbar}} + \psi_2(x)e^{-\frac{iE_2 t}{\hbar}}\right)\right) && (375)\\
=& \left(\psi(x,t), \frac{1}{\sqrt{2}}\left(E_1\psi_1(x)e^{-\frac{iE_1 t}{\hbar}} + E_2\psi_2(x)e^{-\frac{iE_2 t}{\hbar}}\right)\right) && (376)\\
=& \left(\frac{1}{\sqrt{2}}\psi_1(x)e^{-\frac{iE_1 t}{\hbar}}, \frac{1}{\sqrt{2}}E_1\psi_1(x)e^{-\frac{iE_1 t}{\hbar}}\right) + \left(\frac{1}{\sqrt{2}}\psi_2(x)e^{-\frac{iE_2 t}{\hbar}}, \frac{1}{\sqrt{2}}E_2\psi_2(x)e^{-\frac{iE_2 t}{\hbar}}\right) && (377)\\
=& \frac{E_1}{2} + \frac{E_2}{2} && (378)
\end{aligned}$$

这里利用了 $(\psi_n,\psi_m)=\delta_{mn}$.

(c) 能量平方平均值

$$\begin{aligned}
\left\langle \hat{H}^2\right\rangle =& \left(\psi(x,t), \hat{H}^2\psi(x,t)\right) && (379)\\
=& \left(\psi(x,t), \hat{H}^2\frac{1}{\sqrt{2}}\left(\psi_1(x)e^{-\frac{iE_1 t}{\hbar}} + \psi_2(x)e^{-\frac{iE_2 t}{\hbar}}\right)\right) && (380)\\
=& \left(\psi(x,t), \frac{1}{\sqrt{2}}\left(E_1^2\psi_1(x)e^{-\frac{iE_1 t}{\hbar}} + E_2^2\psi_2(x)e^{-\frac{iE_2 t}{\hbar}}\right)\right) && (381)\\
=& \frac{E_1^2}{2} + \frac{E_2^2}{2} && (382)
\end{aligned}$$

这里的计算过程和 (b) 中类似.

(d) 于是能量的涨落:

$$\Delta E = \left[\overline{\left(\hat{H} - \bar{H}\right)^2}\right]^{\frac{1}{2}} \tag{383}$$

$$= \left[\bar{\hat{H}^2} - \bar{H}^2\right]^{\frac{1}{2}} \tag{384}$$

$$= \left[\frac{E_1^2}{2} + \frac{E_2^2}{2} - \left(\frac{E_1}{2} + \frac{E_2}{2}\right)^2\right]^{\frac{1}{2}} \tag{385}$$

$$= \frac{E_2 - E_1}{2} \tag{386}$$

(e) 体系的特征时间可以用概率密度的变化周期来表示

$$T = \frac{2\pi}{\frac{E_2 - E_1}{\hbar}} \tag{387}$$

于是

$$\Delta E \cdot T = \pi\hbar \tag{388}$$

讨论: 粒子的概率密度以 T 为周期在两个极值 (对应 cos $\left(\frac{E_2-E_1}{\hbar}t\right) = \pm 1$) 之间振荡.

3. 50 页 2.9

解 对于一维谐振子, 其能量本征态 $\psi_n(x)$ 满足

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} \mathsf{H}_n(\xi)\, e^{-\xi^2/2} \tag{389}$$

这里 $\xi = \sqrt{\frac{m\omega}{\hbar}}x$, $\mathsf{H}_n(\xi)$ 满足

$$\frac{d\mathsf{H}_n(\xi)}{d\xi} = 2n\mathsf{H}_{n-1}(\xi) \tag{390}$$

$$\mathsf{H}_{n+1}(\xi) + 2n\mathsf{H}_{n-1}(\xi) = 2\xi\mathsf{H}_n(\xi) \tag{391}$$

于是

$$x\psi_n(x) = \sqrt{\frac{\hbar}{m\omega}}\xi\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} \mathsf{H}_n(\xi)\, e^{-\xi^2/2} \tag{392}$$

$$= \sqrt{\frac{\hbar}{m\omega}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} \frac{1}{2}\left(\mathsf{H}_{n+1}(\xi) + 2n\mathsf{H}_{n-1}(\xi)\right) e^{-\xi^2/2} \tag{393}$$

$$= \frac{1}{2}\sqrt{\frac{\hbar}{m\omega}}\left(\sqrt{2(n+1)}\psi_{n+1} + \frac{2n}{\sqrt{2n}}\psi_{n-1}\right) \tag{394}$$

$$= \sqrt{\frac{\hbar}{m\omega}}\left(\sqrt{\frac{n+1}{2}}\psi_{n+1} + \sqrt{\frac{n}{2}}\psi_{n-1}\right) \tag{395}$$

$$x^2\psi_n(x) = x\sqrt{\frac{\hbar}{m\omega}}\left(\sqrt{\frac{n+1}{2}}\psi_{n+1}+\sqrt{\frac{n}{2}}\psi_{n-1}\right) \tag{396}$$

$$= \sqrt{\frac{\hbar}{m\omega}}\left(\sqrt{\frac{n+1}{2}}x\psi_{n+1}+\sqrt{\frac{n}{2}}x\psi_{n-1}\right) \tag{397}$$

$$= \sqrt{\frac{\hbar}{m\omega}}\left(\sqrt{\frac{n+1}{2}}\sqrt{\frac{\hbar}{m\omega}}\left(\sqrt{\frac{n+2}{2}}\psi_{n+2}+\sqrt{\frac{n+1}{2}}\psi_n\right)\right. \tag{398}$$

$$\left.+\sqrt{\frac{n}{2}}x\sqrt{\frac{\hbar}{m\omega}}\left(\sqrt{\frac{n}{2}}\psi_n+\sqrt{\frac{n-1}{2}}\psi_{n-2}\right)\right) \tag{399}$$

$$= \frac{\hbar}{2m\omega}\left(\sqrt{(n+1)(n+2)}\psi_{n+2}+(2n+1)\psi_n+\sqrt{n(n-1)}\psi_{n-2}\right) \tag{400}$$

所以

$$\langle x\rangle = (\psi_n, \hat{x}\psi_n) \tag{401}$$

$$= \left(\psi_n, \sqrt{\frac{\hbar}{m\omega}}\left(\sqrt{\frac{n+1}{2}}\psi_{n+1}+\sqrt{\frac{n}{2}}\psi_{n-1}\right)\right) \tag{402}$$

$$= \sqrt{\frac{\hbar}{m\omega}}\sqrt{\frac{n+1}{2}}(\psi_n,\psi_{n+1})+\sqrt{\frac{\hbar}{m\omega}}\sqrt{\frac{n}{2}}(\psi_n,\psi_{n-1}) \tag{403}$$

$$= 0 \tag{404}$$

这里利用了 $(\psi_n, \psi_m) = \delta_{mn}$.

$$\langle x^2\rangle = \left(\psi_n, x^2\psi_n(x)\right) \tag{405}$$

$$= \left(\psi_n, \frac{\hbar}{2m\omega}\left(\sqrt{(n+1)(n+2)}\psi_{n+2}+(2n+1)\psi_n+\sqrt{n(n-1)}\psi_{n-2}\right)\right) \tag{406}$$

$$= \frac{\hbar}{2m\omega}\sqrt{(n+1)(n+2)}(\psi_n,\psi_{n+2})+\frac{\hbar}{2m\omega}(2n+1)(\psi_n,\psi_n)+\frac{\hbar}{2m\omega}\sqrt{n(n-1)}(\psi_n,\psi_{n-2}) \tag{407}$$

$$= \frac{\hbar}{2m\omega}(2n+1) \tag{408}$$

这里利用了 $(\psi_n, \psi_m) = \delta_{mn}$. 所以

$$\Delta x = \left[\left\langle x^2\right\rangle - \langle x\rangle^2\right]^{\frac{1}{2}} \tag{409}$$

$$= \sqrt{\frac{\hbar}{2m\omega}(2n+1)} \tag{410}$$

另一方面，

$$\frac{d}{dx}\psi_n(x)=\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}\sqrt{\frac{m\omega}{\hbar}}\frac{d\mathsf{H}_n(\xi)}{d\xi}e^{-\xi^2/2}+\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}\mathsf{H}_n(\xi)\left(-\frac{m\omega}{\hbar}x\right)e^{-\xi^2/2} \tag{411}$$

$$=\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}\sqrt{\frac{m\omega}{\hbar}}2n\mathsf{H}_{n-1}(\xi)e^{-\xi^2/2}-\frac{m\omega}{\hbar}x\psi_n \tag{412}$$

$$=\sqrt{\frac{m\omega}{\hbar}}\sqrt{2n}\psi_{n-1}-\frac{m\omega}{\hbar}\sqrt{\frac{\hbar}{m\omega}}\left(\sqrt{\frac{n+1}{2}}\psi_{n+1}+\sqrt{\frac{n}{2}}\psi_{n-1}\right) \tag{413}$$

$$=\sqrt{\frac{m\omega}{\hbar}}\left(\sqrt{\frac{n}{2}}\psi_{n-1}-\sqrt{\frac{n+1}{2}}\psi_{n+1}\right) \tag{414}$$

$$\frac{d^2}{dx^2}\psi_n(x)=\sqrt{\frac{m\omega}{\hbar}}\frac{d}{dx}\left(\sqrt{\frac{n}{2}}\psi_{n-1}-\sqrt{\frac{n+1}{2}}\psi_{n+1}\right) \tag{415}$$

$$=\sqrt{\frac{m\omega}{\hbar}}\left(\left(\sqrt{\frac{n}{2}}\sqrt{\frac{m\omega}{\hbar}}\left(\sqrt{\frac{n-1}{2}}\psi_{n-2}-\sqrt{\frac{n}{2}}\psi_n\right)\right)\right) \tag{416}$$

$$-\sqrt{\frac{n+1}{2}}\sqrt{\frac{m\omega}{\hbar}}\left(\sqrt{\frac{n+1}{2}}\psi_n-\sqrt{\frac{n+2}{2}}\psi_{n+2}\right)\Bigg)\Bigg) \tag{417}$$

$$=\frac{m\omega}{2\hbar}\left(\sqrt{n(n-1)}\psi_{n-2}-(2n+1)\psi_n+\sqrt{(n+1)(n+2)}\psi_{n+2}\right) \tag{418}$$

所以

$$(\psi_n,\hat{p}\psi_n)=\left(\psi_n,\frac{\hbar}{i}\sqrt{\frac{m\omega}{\hbar}}\left(\sqrt{\frac{n}{2}}\psi_{n-1}-\sqrt{\frac{n+1}{2}}\psi_{n+1}\right)\right) \tag{419}$$

$$=0 \tag{420}$$

$$\left(\psi_n,\hat{p}^2\psi_n\right)=\left(\psi_n,-\hbar^2\frac{m\omega}{2\hbar}\left(\sqrt{n(n-1)}\psi_{n-2}-(2n+1)\psi_n+\sqrt{(n+1)(n+2)}\psi_{n+2}\right)\right) \tag{421}$$

$$=\left(\psi_n,\hbar^2\frac{m\omega}{2\hbar}(2n+1)\psi_n\right) \tag{422}$$

$$=\hbar^2\frac{m\omega}{2\hbar}(2n+1) \tag{423}$$

于是

$$\Delta p=\left[\left\langle p^2\right\rangle-\langle p\rangle^2\right]^{\frac{1}{2}} \tag{424}$$

$$=\hbar\sqrt{\frac{m\omega}{2\hbar}(2n+1)} \tag{425}$$

$$\Delta x\Delta p=\sqrt{\frac{\hbar}{2m\omega}(2n+1)}\hbar\sqrt{\frac{m\omega}{2\hbar}(2n+1)} \tag{426}$$

$$=(2n+1)\frac{\hbar}{2} \tag{427}$$

4. 51 页 2.10

解 带电谐振子的 Hamiltonian 为

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 - q\mathscr{E}\hat{x} \tag{428}$$

$$= \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\left(\hat{x}^2 - \frac{2q\mathscr{E}}{m\omega^2}\hat{x}\right) \tag{429}$$

$$= \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\left(\hat{x} - \frac{q\mathscr{E}}{m\omega^2}\right)^2 - \frac{q^2\mathscr{E}^2}{2m\omega^2} \tag{430}$$

由于 $x_0 = \frac{q\mathscr{E}}{m\omega^2}$ 为常量, 可以定义 $\tilde{x} = x - x_0$, 并且动量算符 $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x} = \frac{\hbar}{i}\frac{\partial}{\partial \tilde{x}}$. 于是

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\tilde{x}^2 - \frac{q^2\mathscr{E}^2}{2m\omega^2} \tag{431}$$

已经解得 $\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\tilde{x}^2$ 的本征态和能量本征值分别为 $\psi_n(x)$, $E_n = \left(n+\frac{1}{2}\right)\hbar\omega$, $n = 0, 1, 2, \cdots$. 于是

$$\hat{H}\psi_n(x) = \left(\hat{H}_0 - \frac{q^2\mathscr{E}^2}{2m\omega^2}\right)\psi_n(x) \tag{432}$$

$$= \left(\left(n+\frac{1}{2}\right)\hbar\omega - \frac{q^2\mathscr{E}^2}{2m\omega^2}\right)\psi_n(x) \tag{433}$$

即带电谐振子的本征态和能量本征值分别为 $\psi_n(x)$, $E_n = \left(n+\frac{1}{2}\right)\hbar\omega - \frac{q^2\mathscr{E}^2}{2m\omega^2}$, $n = 0, 1, 2, \cdots$.

5. 一维谐振子在 $t = 0$ 时刻处于归一化波函数:

$$\psi(x, 0) = \sqrt{\frac{1}{2}}\psi_0(x) + \sqrt{\frac{1}{3}}\psi_1(x) + c\psi_4(x)$$

式中 $\psi_n(x)$ ($n = 0, 1, 4$) 均为一维谐振子的定态波函数, 求:

(1) 待定系数 c ;

(2) $t = 0$ 时能量, 和宇称的可能取值和相应的概率;

(3) $t > 0$ 时, 体系的状态波函数 $\psi(x, t) =$? 写出推理过程.

解:

(1) 由归一化要求和 $(\psi_n, \psi_m) = \delta_{mn}$ 得

$$1 = (\psi(x,0), \psi(x,0)) \tag{434}$$

$$= \left(\sqrt{\frac{1}{2}}\psi_0(x) + \sqrt{\frac{1}{3}}\psi_1(x) + c\psi_4(x), \sqrt{\frac{1}{2}}\psi_0(x) + \sqrt{\frac{1}{3}}\psi_1(x) + c\psi_4(x)\right) \tag{435}$$

$$= \left(\sqrt{\frac{1}{2}}\psi_0(x), \sqrt{\frac{1}{2}}\psi_0(x)\right) + \left(\sqrt{\frac{1}{3}}\psi_1(x), \sqrt{\frac{1}{3}}\psi_1(x)\right) + (c\psi_4(x), c\psi_4(x)) \tag{436}$$

$$= \frac{1}{2} + \frac{1}{3} + |c|^2 \tag{437}$$

所以 $|c|^2 = \frac{1}{6}$, 可以取 $|c| = \sqrt{\frac{1}{6}}$.

(2) 由于

$$\psi\left(x,0\right)=\sqrt{\frac{1}{2}}\psi_0\left(x\right)+\sqrt{\frac{1}{3}}\psi_1\left(x\right)+\sqrt{\frac{1}{6}}\psi_4\left(x\right) \tag{438}$$

于是

$$\left(\psi_0,\psi\left(x,0\right)\right)=\sqrt{\frac{1}{2}} \tag{439}$$

$$\left(\psi_1,\psi\left(x,0\right)\right)=\sqrt{\frac{1}{3}} \tag{440}$$

$$\left(\psi_4,\psi\left(x,0\right)\right)=\sqrt{\frac{1}{6}} \tag{441}$$

所以粒子处于能量本征态 ψ_0, ψ_1 和 ψ_4 的概率分别为 $\frac{1}{2}$, $\frac{1}{3}$ 和 $\frac{1}{6}$, 相应的能量测量值为 E_0, E_1 和 E_4. 对于宇称相应的测量值分别为 1, -1, 1, 所以宇称测量值为 1 的概率为 $\frac{1}{2}+\frac{1}{6}=\frac{2}{3}$, 测量值为 -1 的概率为 $\frac{1}{3}$.

(3) $t>0$ 时, 粒子所处状态为本征解的线性叠加

$$\psi\left(x,t\right)=\sum_{n=0}^{\infty}a_n\psi_n e^{-iE_nt/\hbar} \tag{442}$$

而

$$\psi\left(x,0\right)=\sum_{n=0}^{\infty}a_n\psi_n \tag{443}$$

$$a_n=\left(\psi_n,\psi\left(x,0\right)\right) \tag{444}$$

可见 $a_0=\sqrt{\frac{1}{2}}$, $a_1=\sqrt{\frac{1}{3}}$, $a_4=\sqrt{\frac{1}{6}}$, 其余系数为 0. 于是

$$\psi\left(x,0\right)=\sqrt{\frac{1}{2}}\psi_0\left(x\right)e^{-iE_0t/\hbar}+\sqrt{\frac{1}{3}}\psi_1\left(x\right)e^{-iE_1t/\hbar}+\sqrt{\frac{1}{6}}\psi_4\left(x\right)e^{-iE_4t/\hbar} \tag{445}$$

0.9 第九次作业 2021.05.18

1. 证明算符 $\hat{A}$, $\hat{B}$, $\hat{C}$ 对易关系的 Jacobi 恒等式.

证:

$$\left[\hat{A},\left[\hat{B},\hat{C}\right]\right]=\left[\hat{A},\hat{B}\hat{C}-\hat{C}\hat{B}\right]=\hat{A}\left(\hat{B}\hat{C}-\hat{C}\hat{B}\right)-\left(\hat{B}\hat{C}-\hat{C}\hat{B}\right)\hat{A} \tag{446}$$

$$=\hat{A}\hat{B}\hat{C}-\hat{A}\hat{C}\hat{B}-\hat{B}\hat{C}\hat{A}+\hat{C}\hat{B}\hat{A} \tag{447}$$

类似的,

$$\left[\hat{B},\left[\hat{C},\hat{A}\right]\right]=\hat{B}\hat{C}\hat{A}-\hat{B}\hat{A}\hat{C}-\hat{C}\hat{A}\hat{B}+\hat{A}\hat{C}\hat{B} \tag{448}$$

$$\left[\hat{C},\left[\hat{A},\hat{B}\right]\right]=\hat{C}\hat{A}\hat{B}-\hat{C}\hat{B}\hat{A}-\hat{A}\hat{B}\hat{C}+\hat{B}\hat{A}\hat{C} \tag{449}$$

所以 $\left[\hat{A},\left[\hat{B},\hat{C}\right]\right]+\left[\hat{B},\left[\hat{C},\hat{A}\right]\right]+\left[\hat{C},\left[\hat{A},\hat{B}\right]\right]=0$.

2. 利用基本对易关系 $[\hat{x},\hat{p}]=i\hbar$,

(1) 证明 $[\hat{x},\hat{p}^2]=2i\hbar\hat{p}$;

(2) 证明 $[\hat{x},\hat{p}^n]=ni\hbar\hat{p}^{n-1}$ ($n\in\mathbb{Z}$, $n\geq 1$);

(3) 已知连续可微函数 $f(x)=\sum_{n=0}^{\infty}\frac{f^{(n)}(0)}{n!}x^n$, 证明对于动量算符 $\hat{p}$ 的函数 $f(\hat{p})$: $[\hat{x},f(\hat{p})]=i\hbar\frac{\partial f}{\partial\hat{p}}$.

证:

(1) $[\hat{x},\hat{p}^2]=[\hat{x},\hat{p}]\,\hat{p}+\hat{p}\,[\hat{x},\hat{p}]=2i\hbar\hat{p}$.

(2)

$$\begin{aligned}
[\hat{x},\hat{p}^n]=&\hat{p}\left[\hat{x},\hat{p}^{n-1}\right]+[\hat{x},\hat{p}]\,\hat{p}^{n-1} && (450)\\
=&\hat{p}\left(\hat{p}\left[\hat{x},\hat{p}^{n-2}\right]+[\hat{x},\hat{p}]\,\hat{p}^{n-2}\right)+i\hbar\hat{p}^{n-1} && (451)\\
=&\hat{p}^2\left[\hat{x},\hat{p}^{n-2}\right]+2i\hbar\hat{p}^{n-1} && (452)\\
=&\hat{p}^2\left(\hat{p}\left[\hat{x},\hat{p}^{n-3}\right]+[\hat{x},\hat{p}]\,\hat{p}^{n-3}\right)+2i\hbar\hat{p}^{n-1} && (453)\\
=&\hat{p}^3\left[\hat{x},\hat{p}^{n-3}\right]+3i\hbar\hat{p}^{n-1} && (454)\\
&\cdots && (455)\\
=&ni\hbar\hat{p}^{n-1} && (456)
\end{aligned}$$

(3)

$$\begin{aligned}
[\hat{x},f(\hat{p})]=&\left[\hat{x},\sum_{n=0}^{\infty}\frac{f^{(n)}(0)}{n!}\hat{p}^n\right] && (457)\\
=&\sum_{n=0}^{\infty}\frac{f^{(n)}(0)}{n!}[\hat{x},\hat{p}^n] && (458)\\
=&\sum_{n=0}^{\infty}\frac{f^{(n)}(0)}{n!}ni\hbar\hat{p}^{n-1} && (459)\\
=&i\hbar\frac{\partial}{\partial\hat{p}}\sum_{n=0}^{\infty}\frac{f^{(n)}(0)}{n!}\hat{p}^n && (460)\\
==&i\hbar\frac{\partial f(\hat{p})}{\partial\hat{p}} && (461)
\end{aligned}$$

3. 教材 56 页练习 3

证:

$$\left[\hat{\boldsymbol{l}},r^2\right]=\left[\hat{l}_\alpha\hat{\boldsymbol{e}}_\alpha,\hat{r}_\beta^2\right] \tag{462}$$
$$=\left[\hat{l}_\alpha,\hat{r}_\beta^2\right]\hat{\boldsymbol{e}}_\alpha \tag{463}$$
$$=\left(\hat{r}_\beta\left[\hat{l}_\alpha,\hat{r}_\beta\right]+\left[\hat{l}_\alpha,\hat{r}_\beta\right]\hat{r}_\beta\right)\hat{\boldsymbol{e}}_\alpha \tag{464}$$
$$=\left(\hat{r}_\beta i\hbar\epsilon_{\alpha\beta\gamma}\hat{r}_\gamma+i\hbar\epsilon_{\alpha\beta\gamma}\hat{r}_\gamma\hat{r}_\beta\right)\hat{\boldsymbol{e}}_\alpha \tag{465}$$
$$=2i\hbar\epsilon_{\alpha\beta\gamma}\hat{r}_\beta\hat{r}_\gamma\hat{\boldsymbol{e}}_\alpha \tag{466}$$
$$=2i\hbar\epsilon_{\alpha\gamma\beta}\hat{r}_\gamma\hat{r}_\beta\hat{\boldsymbol{e}}_\alpha \tag{467}$$
$$=-2i\hbar\epsilon_{\alpha\beta\gamma}\hat{r}_\beta\hat{r}_\gamma\hat{\boldsymbol{e}}_\alpha \tag{468}$$
$$=0 \tag{469}$$

方程466里, $\epsilon_{\alpha\beta\gamma}$ 关于 β, γ 反对称, 而 $\hat{r}_\beta\hat{r}_\gamma$ 关于 β, γ 对称. 由方程466和468得原式为零. 下面的几个对易式都利用了这一性质.

$$\left[\hat{\boldsymbol{l}},p^2\right]=\left[\hat{l}_\alpha\hat{\boldsymbol{e}}_\alpha,\hat{p}_\beta^2\right] \tag{470}$$
$$=\left(\hat{p}_\beta\left[\hat{l}_\alpha,\hat{p}_\beta\right]+\left[\hat{l}_\alpha,\hat{p}_\beta\right]\hat{p}_\beta\right)\hat{\boldsymbol{e}}_\alpha \tag{471}$$
$$=\left(\hat{p}_\beta i\hbar\epsilon_{\alpha\beta\gamma}\hat{p}_\gamma+i\hbar\epsilon_{\alpha\beta\gamma}\hat{p}_\gamma\hat{p}_\beta\right)\hat{\boldsymbol{e}}_\alpha \tag{472}$$
$$=2i\hbar\epsilon_{\alpha\beta\gamma}\hat{p}_\beta\hat{p}_\gamma\hat{\boldsymbol{e}}_\alpha \tag{473}$$
$$=0 \tag{474}$$

$$\left[\hat{\boldsymbol{l}},\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}}\right]=\left[\hat{l}_\alpha\hat{\boldsymbol{e}}_\alpha,\hat{r}_\beta\hat{p}_\beta\right] \tag{475}$$
$$=\left(\hat{r}_\beta\left[\hat{l}_\alpha,\hat{p}_\beta\right]+\left[\hat{l}_\alpha,\hat{r}_\beta\right]\hat{p}_\beta\right)\hat{\boldsymbol{e}}_\alpha \tag{476}$$
$$=\left(\hat{r}_\beta i\hbar\epsilon_{\alpha\beta\gamma}\hat{p}_\gamma+i\hbar\epsilon_{\alpha\beta\gamma}\hat{r}_\gamma\hat{p}_\beta\right)\hat{\boldsymbol{e}}_\alpha \tag{477}$$
$$=i\hbar\epsilon_{\alpha\beta\gamma}\left(\hat{r}_\beta\hat{p}_\gamma+\hat{r}_\gamma\hat{p}_\beta\right)\hat{\boldsymbol{e}}_\alpha \tag{478}$$
$$=0 \tag{479}$$

$$\left[\hat{\boldsymbol{l}},V\left(r\right)\right]=\left[\hat{l}_\alpha\hat{\boldsymbol{e}}_\alpha,V\left(r\right)\right] \tag{480}$$
$$=\left[\epsilon_{\alpha\beta\gamma}\hat{r}_\beta\hat{p}_\gamma,V\left(r\right)\right]\hat{\boldsymbol{e}}_\alpha \tag{481}$$
$$=\epsilon_{\alpha\beta\gamma}\hat{r}_\beta\left[\hat{p}_\gamma,V\left(r\right)\right]\hat{\boldsymbol{e}}_\alpha \tag{482}$$
$$=\epsilon_{\alpha\beta\gamma}\hat{r}_\beta\left(-i\hbar\right)\frac{dV}{dr}\frac{r_\gamma}{r}\hat{\boldsymbol{e}}_\alpha \tag{483}$$
$$=-i\hbar\frac{1}{r}\frac{dV}{dr}\epsilon_{\alpha\beta\gamma}\hat{r}_\beta r_\gamma\hat{\boldsymbol{e}}_\alpha \tag{484}$$
$$=0 \tag{485}$$

4. 令 $\hat{D}=\frac{d}{dx}$, 计算 (1) $\cos\left(\hat{D}\right)x^4$; (2) $\left(\frac{1}{1-\lambda\hat{D}}\right)\sin\left(x\right)$, 这里非零实常数 λ 满足 $|\lambda|<1$.

解:

(1) 由于 $\cos x = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} x^{2n}$, 于是 $\cos\left(\hat{D}\right) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} \hat{D}^{2n} = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} \frac{d^{2n}}{dx^{2n}} = \hat{I} - \frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{4!}\frac{d^4}{dx^4} + \cdots$, 并且

$$\frac{d^2}{dx^2} x^4 = 12x^2, \qquad \frac{d^4}{dx^4} x^4 = 24, \qquad \frac{d^{2n}}{dx^{2n}} x^4 = 0, n > 2 \tag{486}$$

所以

$$\cos\left(\hat{D}\right) x^4 = \hat{x}^4 - 6x^2 + 1 \tag{487}$$

(2) 由于 $\frac{1}{1-x} = \sum_{n=0}^{\infty} x^n$, 于是 $\frac{1}{1-\lambda\hat{D}} = \sum_{n=0}^{\infty} \lambda^n \hat{D}^n = \sum_{n=0}^{\infty} \lambda^n \frac{d^n}{dx^n}$, 并且

$$\frac{d}{dx}\sin x = \cos x, \qquad \frac{d^2}{dx^2}\sin x = -\sin x, \qquad \frac{d^3}{dx^3}\sin x = -\cos x, \qquad \frac{d^4}{dx^4}\sin x = \sin x, \cdots \tag{488}$$

并且

$$\frac{d^{2n+1}}{dx^{2n+1}} \sin x = (-1)^n \cos x, n = 0, 1, \cdots \tag{489}$$

$$\frac{d^{2n}}{dx^{2n}} \sin x = (-1)^n \sin x, n = 0, 1, \cdots \tag{490}$$

所以

$$\begin{aligned} \frac{1}{1-\lambda\hat{D}} \sin x &= \left(\sum_{n=0}^{\infty} \lambda^{2n} \frac{d^{2n}}{dx^{2n}} + \sum_{n=0}^{\infty} \lambda^{2n+1} \frac{d^{2n+1}}{dx^{2n+1}}\right) \sin x & (491) \\ &= \sum_{n=0}^{\infty} \lambda^{2n} (-1)^n \sin x + \sum_{n=0}^{\infty} \lambda^{2n+1} (-1)^n \cos x & (492) \\ &= \sum_{n=0}^{\infty} \left(-\lambda^2\right)^n \sin x + \lambda \sum_{n=0}^{\infty} \left(-\lambda^2\right)^n \cos x & (493) \\ &= \frac{\sin x}{1+\lambda^2} + \frac{\lambda \cos x}{1+\lambda^2} & (494) \end{aligned}$$

5. 教材 75-76 页 3.2, 3.6, 3.8

3.2 解: $\hat{l}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y$, 由于坐标算符和动量算符为 Hermite 算符, 且 $[\hat{y}, \hat{p}_z] = [\hat{z}, \hat{p}_y] = 0$, 所以 $\hat{l}_x$ 是 Hermite 算符, 同理可判断 $\hat{l}_y$ 和 $\hat{l}_z$ 也是 Hermite 算符. 所以 $\hat{\boldsymbol{l}}$ 是 Hermite 算符.

$$\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{p}} = \hat{x}\hat{p}_x + \hat{y}\hat{p}_y + \hat{z}\hat{p}_z \tag{495}$$

而

$$(\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{p}})^\dagger = \hat{p}_x\hat{x} + \hat{p}_y\hat{y} + \hat{p}_z\hat{z} \tag{496}$$

且 $\hat{p}_\alpha$ 与 $\hat{r}_\alpha$ 不对易, 所以 $(\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{p}})^\dagger \neq \hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{p}}$, $\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{p}}$ 不是 Hermite 算符.

$$\left(\hat{\boldsymbol{p}} \times \hat{\boldsymbol{l}}\right)_x = \hat{p}_y\hat{l}_z - \hat{p}_z\hat{l}_y \tag{497}$$

$$\left(\hat{\boldsymbol{p}} \times \hat{\boldsymbol{l}}\right)_x^\dagger = \hat{l}_z\hat{p}_y - \hat{l}_y\hat{p}_z = \hat{p}_y\hat{l}_z - i\hbar\hat{p}_x - \left(\hat{p}_z\hat{l}_y + i\hbar\hat{p}_x\right) = \left(\hat{\boldsymbol{p}} \times \hat{\boldsymbol{l}}\right)_x - 2i\hbar\hat{p}_x \tag{498}$$

可以看出 $\left(\hat{\boldsymbol{p}}\times\hat{\boldsymbol{l}}\right)_x$ 不是 Hermite 算符. 同理, 可判断其它分量也不是 Hermite 算符. 所以 $\hat{\boldsymbol{p}}\times\hat{\boldsymbol{l}}$ 不是 Hermite 算符.

$$\left(\hat{\boldsymbol{r}}\times\hat{\boldsymbol{l}}\right)_x=\hat{y}\hat{l}_z-\hat{z}\hat{l}_y \tag{499}$$

$$\left(\hat{\boldsymbol{r}}\times\hat{\boldsymbol{l}}\right)_x^\dagger=\hat{l}_z\hat{y}-\hat{l}_y\hat{z}=\hat{y}\hat{l}_z-i\hbar\hat{x}-\left(\hat{z}\hat{l}_y+i\hbar\hat{x}\right)=\left(\hat{\boldsymbol{r}}\times\hat{\boldsymbol{l}}\right)_x-2i\hbar\hat{x} \tag{500}$$

可以看出 $\left(\hat{\boldsymbol{r}}\times\hat{\boldsymbol{l}}\right)_x$ 不是 Hermite 算符. 同理, 可判断其它分量也不是 Hermite 算符. 所以 $\hat{\boldsymbol{r}}\times\hat{\boldsymbol{l}}$ 不是 Hermite 算符.

对于非厄米算符, 可以利用对称化的方法构造厄米算符, $\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}}\to\frac{\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}}+\hat{\boldsymbol{p}}\cdot\hat{\boldsymbol{r}}}{2}$, $\hat{\boldsymbol{p}}\times\hat{\boldsymbol{l}}\to\frac{\hat{\boldsymbol{p}}\times\hat{\boldsymbol{l}}+\hat{\boldsymbol{l}}\times\hat{\boldsymbol{p}}}{2}$, $\hat{\boldsymbol{r}}\times\hat{\boldsymbol{l}}\to\frac{\hat{\boldsymbol{r}}\times\hat{\boldsymbol{l}}+\hat{\boldsymbol{l}}\times\hat{\boldsymbol{r}}}{2}$.

3.6 解:

$$\begin{aligned}\left[\hat{F},\hat{\boldsymbol{A}}\cdot\hat{\boldsymbol{B}}\right]&=\left[\hat{F},\sum_{\alpha=x,y,z}\hat{A}_\alpha\hat{B}_\alpha\right] &(501)\\ &=\sum_\alpha\left[\hat{F},\hat{A}_\alpha\hat{B}_\alpha\right] &(502)\\ &=\sum_\alpha\hat{A}_\alpha\left[\hat{F},\hat{B}_\alpha\right]+\left[\hat{F},\hat{A}_\alpha\right]\hat{B}_\alpha &(503)\\ &=\hat{\boldsymbol{A}}\cdot\left[\hat{F},\hat{\boldsymbol{B}}\right]+\left[\hat{F},\hat{\boldsymbol{A}}\right]\cdot\hat{\boldsymbol{B}} &(504)\end{aligned}$$

$$\begin{aligned}\left[\hat{F},\hat{\boldsymbol{A}}\times\hat{\boldsymbol{B}}\right]&=\left[\hat{F},\sum_{\alpha,\beta,\gamma}\epsilon_{\alpha\beta\gamma}\hat{A}_\alpha\hat{B}_\beta\hat{\boldsymbol{e}}_\gamma\right] &(505)\\ &=\sum_{\alpha,\beta,\gamma}\epsilon_{\alpha\beta\gamma}\left[\hat{F},\hat{A}_\alpha\hat{B}_\beta\right]\hat{\boldsymbol{e}}_\gamma &(506)\\ &=\sum_{\alpha,\beta,\gamma}\epsilon_{\alpha\beta\gamma}\hat{A}_\alpha\left[\hat{F},\hat{B}_\beta\right]\hat{\boldsymbol{e}}_\gamma+\epsilon_{\alpha\beta\gamma}\left[\hat{F},\hat{A}_\alpha\right]\hat{B}_\beta\hat{\boldsymbol{e}}_\gamma &(507)\\ &=\hat{\boldsymbol{A}}\times\left[\hat{F},\hat{\boldsymbol{B}}\right]+\left[\hat{F},\hat{\boldsymbol{A}}\right]\times\hat{\boldsymbol{B}} &(508)\end{aligned}$$

3.8 证

$$\hat{\boldsymbol{p}}\times\hat{\boldsymbol{l}}+\hat{\boldsymbol{l}}\times\hat{\boldsymbol{p}}=\epsilon_{\alpha\beta\gamma}\left(\hat{p}_\alpha\hat{l}_\beta+\hat{l}_\alpha\hat{p}_\beta\right)\boldsymbol{e}_\gamma \tag{509}$$

$$=\left(\epsilon_{\alpha\beta\gamma}\hat{p}_\alpha\hat{l}_\beta+\epsilon_{\alpha\beta\gamma}\hat{l}_\alpha\hat{p}_\beta\right)\boldsymbol{e}_\gamma \tag{510}$$

$$=\left(\epsilon_{\beta\alpha\gamma}\hat{p}_\beta\hat{l}_\alpha+\epsilon_{\alpha\beta\gamma}\hat{l}_\alpha\hat{p}_\beta\right)\boldsymbol{e}_\gamma \tag{511}$$

$$=\left(-\epsilon_{\alpha\beta\gamma}\hat{p}_\beta\hat{l}_\alpha+\epsilon_{\alpha\beta\gamma}\hat{l}_\alpha\hat{p}_\beta\right)\boldsymbol{e}_\gamma \tag{512}$$

$$=\epsilon_{\alpha\beta\gamma}\left[\hat{l}_\alpha,\hat{p}_\beta\right]\boldsymbol{e}_\gamma \tag{513}$$

$$=\epsilon_{\alpha\beta\gamma}\epsilon_{\alpha\beta\gamma'}i\hbar\hat{p}_{\gamma'}\boldsymbol{e}_\gamma \tag{514}$$

$$=2\delta_{\gamma\gamma'}i\hbar\hat{p}_{\gamma'}\boldsymbol{e}_\gamma \tag{515}$$

$$=2i\hbar\hat{\boldsymbol{p}} \tag{516}$$

$$i\hbar\left(\boldsymbol{p}\times\boldsymbol{l}-\boldsymbol{l}\times\boldsymbol{p}\right)=\left(i\hbar\epsilon_{\alpha\beta\gamma}\hat{p}_\alpha\hat{l}_\beta-i\hbar\epsilon_{\alpha\beta\gamma}\hat{l}_\alpha\hat{p}_\beta\right)\boldsymbol{e}_\gamma \tag{517}$$

$$=\left(\left[\hat{l}_\beta,\hat{p}_\gamma\right]\hat{l}_\beta+i\hbar\epsilon_{\beta\alpha\gamma}\hat{l}_\alpha\hat{p}_\beta\right)\boldsymbol{e}_\gamma \tag{518}$$

$$=\left(\left[\hat{l}_\beta,\hat{p}_\gamma\right]\hat{l}_\beta+\hat{l}_\alpha\left[\hat{l}_\alpha,\hat{p}_\gamma\right]\right)\boldsymbol{e}_\gamma \tag{519}$$

$$=\left(\left[\hat{l}_\alpha,\hat{p}_\gamma\right]\hat{l}_\alpha+\hat{l}_\alpha\left[\hat{l}_\alpha,\hat{p}_\gamma\right]\right)\boldsymbol{e}_\gamma \tag{520}$$

$$=\left[\hat{l}_\alpha\hat{l}_\alpha,\hat{p}_\gamma\boldsymbol{e}_\gamma\right] \tag{521}$$

$$=\left[\hat{\boldsymbol{l}}^2,\hat{\boldsymbol{p}}\right] \tag{522}$$

0.10 第十次作业 2021.05.25

1. 3.9

解

$$\left[\left[\nabla^2,x^ly^mz^n\right],r^2\right]=-\left[\left[x^ly^mz^n,r^2\right],\nabla^2\right]-\left[\left[r^2,\nabla^2\right],x^ly^mz^n\right] \tag{523}$$

$$=-\left[\left[r^2,\nabla^2\right],x^ly^mz^n\right] \tag{524}$$

$$\left[r^2,\nabla^2\right]=-\left[\nabla^2,r^2\right] \tag{525}$$

$$=-\left[\nabla_\alpha,r^2\right]\nabla_\alpha-\nabla_\alpha\left[\nabla_\alpha,r^2\right] \tag{526}$$

$$=-2r_\alpha\nabla_\alpha-\nabla_\alpha 2r_\alpha \tag{527}$$

$$=-4r_\alpha\nabla_\alpha-6 \tag{528}$$

$$\left[\left[r^2,\nabla^2\right],x^ly^mz^n\right]=\left[-4r_\alpha\nabla_\alpha-6,x^ly^mz^n\right] \tag{529}$$

$$=-4r_\alpha\nabla_\alpha x^ly^mz^n \tag{530}$$

$$=-4\left(l+m+n\right)x^ly^mz^n \tag{531}$$

所以

$$\left[\left[\nabla^2,x^ly^mz^n\right],r^2\right]=4\left(l+m+n\right)x^ly^mz^n \tag{532}$$

2. 3.10

解 (a)

$$\hat{p}_r = \frac{1}{2}\left(\frac{\hat{\boldsymbol{r}}}{r}\cdot\hat{\boldsymbol{p}} + \hat{\boldsymbol{p}}\cdot\frac{\hat{\boldsymbol{r}}}{r}\right) \tag{533}$$

$$(\hat{p}_r)^\dagger = \frac{1}{2}\left(\left(\frac{\hat{\boldsymbol{r}}}{r}\cdot\hat{\boldsymbol{p}}\right)^\dagger + \left(\hat{\boldsymbol{p}}\cdot\frac{\hat{\boldsymbol{r}}}{r}\right)^\dagger\right) = \frac{1}{2}\left(\hat{\boldsymbol{p}}\cdot\frac{\hat{\boldsymbol{r}}}{r} + \frac{\hat{\boldsymbol{r}}}{r}\cdot\hat{\boldsymbol{p}}\right) = \hat{p}_r \tag{534}$$

(b)

$$\hat{\boldsymbol{p}}\cdot\frac{\hat{\boldsymbol{r}}}{r} = \hat{p}_\alpha\frac{\hat{r}_\alpha}{r} = \frac{\hbar}{i}\nabla_\alpha\frac{\hat{r}_\alpha}{r} = \frac{\hbar}{i}\left(\nabla_\alpha\frac{r_\alpha}{r}\right) + \frac{\hbar}{i}\frac{\hat{r}_\alpha}{r}\nabla_\alpha \tag{535}$$

$$= \frac{\hbar}{i}\left(\frac{3}{r} - \frac{1}{2}\frac{r_\alpha}{r^3}2r_\alpha\right) + \frac{\hbar}{i}\frac{\hat{r}_\alpha}{r}\nabla_\alpha = 2\frac{\hbar}{i}\frac{1}{r} + \frac{\hbar}{i}\frac{\hat{r}_\alpha}{r}\nabla_\alpha \tag{536}$$

并且注意到, $\frac{\hat{r}_\alpha}{r} = \frac{\partial\hat{r}_\alpha}{\partial r}$ (利用球坐标的具体形式验证)

$$\frac{\hat{r}_\alpha}{r}\nabla_\alpha = \frac{\partial\hat{r}_\alpha}{\partial r}\frac{\partial}{\partial r_\alpha} = \frac{\partial}{\partial r} \tag{537}$$

$$\hat{p}_r = \frac{\hbar}{i}\frac{1}{r} + \frac{\hbar}{i}\frac{\hat{r}_\alpha}{r}\nabla_\alpha = \frac{\hbar}{i}\frac{1}{r} + \frac{\hbar}{i}\boldsymbol{e}_{\boldsymbol{r}}\cdot\nabla = \frac{\hbar}{i}\frac{1}{r} + \frac{\hbar}{i}\frac{\partial}{\partial r} \tag{538}$$

(c)

$$[\hat{r}, \hat{p}_r] = \left[\hat{r}, \frac{\hbar}{i}\frac{1}{r} + \frac{\hbar}{i}\frac{\partial}{\partial r}\right] = \left[\hat{r}, \frac{\hbar}{i}\frac{\partial}{\partial r}\right] = \hat{r}\frac{\hbar}{i}\frac{\partial}{\partial r} - \frac{\hbar}{i}\frac{\partial}{\partial r}r - \frac{\hbar}{i}\hat{r}\frac{\partial}{\partial r} = i\hbar \tag{539}$$

(d)

$$\hat{p}_r^2 = \left(\frac{\hbar}{i}\frac{1}{r} + \frac{\hbar}{i}\frac{\partial}{\partial r}\right)\left(\frac{\hbar}{i}\frac{1}{r} + \frac{\hbar}{i}\frac{\partial}{\partial r}\right) \tag{540}$$

$$= -\hbar^2\left(\frac{1}{r} + \frac{\partial}{\partial r}\right)\left(\frac{1}{r} + \frac{\partial}{\partial r}\right) \tag{541}$$

$$= -\hbar^2\left(\frac{1}{r^2} + \frac{\partial}{\partial r}\frac{1}{r} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2}\right) \tag{542}$$

$$= -\hbar^2\left(\frac{1}{r^2} - \frac{1}{r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2}\right) \tag{543}$$

$$= -\hbar^2\left(2\frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2}\right) \tag{544}$$

$$= -\hbar^2\frac{1}{r^2}\left(2r\frac{\partial}{\partial r} + \frac{\partial}{\partial r}\right)\frac{\partial}{\partial r} \tag{545}$$

$$= -\hbar^2\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} \tag{546}$$

(e)

$$\hat{\boldsymbol{l}}\cdot\hat{\boldsymbol{l}} = \epsilon_{\alpha\beta\gamma}\hat{r}_\alpha\hat{p}_\beta\epsilon_{\alpha'\beta'\gamma}\hat{r}_{\alpha'}\hat{p}_{\beta'} \tag{547}$$
$$= \left(\delta_{\alpha\alpha'}\delta_{\beta\beta'} - \delta_{\alpha\beta'}\delta_{\beta\alpha'}\right)\hat{r}_\alpha\hat{p}_\beta\hat{r}_{\alpha'}\hat{p}_{\beta'} \tag{548}$$
$$= \hat{r}_\alpha\hat{p}_\beta\hat{r}_\alpha\hat{p}_\beta - \hat{r}_\alpha\hat{p}_\beta\hat{r}_\beta\hat{p}_\alpha \tag{549}$$
$$= \hat{r}_\alpha\left(\hat{r}_\alpha\hat{p}_\beta - i\hbar\delta_{\alpha\beta}\right)\hat{p}_\beta - \hat{r}_\alpha\hat{p}_\beta\left(i\hbar\delta_{\alpha\beta} + \hat{p}_\alpha\hat{r}_\beta\right) \tag{550}$$
$$= \hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{r}}\hat{\boldsymbol{p}}\cdot\hat{\boldsymbol{p}} - i\hbar\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}} - i\hbar\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}} - \hat{r}_\alpha\hat{p}_\beta\hat{p}_\alpha\hat{r}_\beta \tag{551}$$
$$= \hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{r}}\hat{\boldsymbol{p}}\cdot\hat{\boldsymbol{p}} - 2i\hbar\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}} - \hat{r}_\alpha\hat{p}_\alpha\hat{p}_\beta\hat{r}_\beta \tag{552}$$
$$= \hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{r}}\hat{\boldsymbol{p}}\cdot\hat{\boldsymbol{p}} - 2i\hbar\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}} - \hat{r}_\alpha\hat{p}_\alpha\left(\hat{r}_\beta\hat{p}_\beta - 3i\hbar\right) \tag{553}$$
$$= r^2\hat{\boldsymbol{p}}\cdot\hat{\boldsymbol{p}} - \hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}}\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}} + i\hbar\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}} \tag{554}$$

由于 $\hat{p}_\beta\hat{r}_\beta = \sum_{\beta=x,y,z}\hat{p}_\beta\hat{r}_\beta$, 每一个交换时都会贡献 $i\hbar$. 由$\hat{r}_\alpha\nabla_\alpha = r\frac{\partial}{\partial r}$ 得,

$$\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}}\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}} - i\hbar\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}} = r^2\left(-\hbar^2\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r} - \hbar^2\frac{1}{r}\frac{\partial}{\partial r}\right) = r^2\hat{p}_r^2 \tag{555}$$

所以

$$\frac{\hat{\boldsymbol{l}}^2}{r^2} = \hat{\boldsymbol{p}}^2 - \hat{p}_r^2 \tag{556}$$

3. 满足下列关系的算符 $\hat{Q}$ 称为斜厄米算符或反厄米算符:

$$\hat{Q}^\dagger = -\hat{Q} \tag{557}$$

(1) 证明斜厄米算符的平均值为纯虚数;

(2) 证明斜厄米算符的本征值为纯虚数;

(3) 证明对应不同本征值的斜厄米算符的本征向量是正交的;

证:

(1) $\left(\psi,\hat{Q}\psi\right) = \left(\hat{Q}\psi,\psi\right)^* = \left(\psi,\hat{Q}^\dagger\psi\right)^* = -\left(\psi,\hat{Q}\psi\right)^*$, 即其平均值为纯虚数.

(2) 令 $\hat{Q}\psi_1 = \lambda_1\psi_1$, 则 $\left(\psi_1,\hat{Q}^\dagger\psi_1\right) = \left(\hat{Q}\psi_1,\psi_1\right)$, 即 $\left(\psi_1,-\hat{Q}\psi_1\right) = \left(\hat{Q}\psi_1,\psi_1\right)$, 于是 $(\psi_1,-\lambda_1\psi_1) = (\lambda_1\psi_1,\psi_1)$,

$$\left(\lambda_1+\lambda_1^*\right)(\psi_1,\psi_1) = 0 \tag{558}$$

所以 $\lambda_1+\lambda_1^* = 0$, 即其本征值 λ_1 是纯虚的.

(3) 令 $\hat{Q}\psi_1 = \lambda_1\psi_1$, $\hat{Q}\psi_2 = \lambda_2\psi_2$, 则 $\left(\psi_1,\hat{Q}^\dagger\psi_2\right) = \left(\hat{Q}\psi_1,\psi_2\right)$, 即 $\left(\psi_1,-\hat{Q}\psi_2\right) = \left(\hat{Q}\psi_1,\psi_2\right)$, 于是 $(\psi_1,-\lambda_2\psi_2) = (\lambda_1\psi_1,\psi_2)$,

$$\left(\lambda_2+\lambda_1^*\right)(\psi_1,\psi_2) = 0 \tag{559}$$

$$\left(\lambda_2-\lambda_1\right)(\psi_1,\psi_2) = 0 \tag{560}$$

由于 $\lambda_2 \neq \lambda_1$ 所以 $(\psi_1,\psi_2) \neq 0$, 即不同本征值的斜厄米算符的本征向量是正交的.

4. 3.12

证: 设量子体系的 Hamiltonian 为 $\hat{H}=\frac{\hat{p}^2}{2m}+V(x)$, 体系的能量本征态 ψ_n, 满足 $\hat{H}\psi_n=E_n\psi_n$. 则

$$\left[\hat{x},\hat{H}\right]=\left[\hat{x},\frac{\hat{p}^2}{2m}+V(x)\right]=i\hbar\frac{\hat{p}}{m} \tag{561}$$

所以

$$\left(\psi_n,\ \left[\hat{x},\hat{H}\right]\psi_n\right)=\frac{i\hbar}{m}\langle\hat{p}\rangle \tag{562}$$

$$\left(\psi_n,\ \left(\hat{x}\hat{H}-\hat{H}\hat{x}\right)\psi_n\right)=\frac{i\hbar}{m}\langle\hat{p}\rangle \tag{563}$$

$$\left(\psi_n,\ \hat{x}\hat{H}\psi_n\right)-\left(\psi_n,\ \hat{H}\hat{x}\psi_n\right)=\frac{i\hbar}{m}\langle\hat{p}\rangle \tag{564}$$

$$E_n\left(\psi_n,\ \hat{x}\psi_n\right)-\left(\hat{H}\psi_n,\ \hat{x}\psi_n\right)=\frac{i\hbar}{m}\langle\hat{p}\rangle \tag{565}$$

$$E_n\left(\psi_n,\ \hat{x}\psi_n\right)-E_n\left(\psi_n,\ \hat{x}\psi_n\right)=\frac{i\hbar}{m}\langle\hat{p}\rangle \tag{566}$$

$$0=\frac{i\hbar}{m}\langle\hat{p}\rangle \tag{567}$$

讨论:

1. 在分立的能量本征态即束缚态上, $(\psi_n,\ \hat{x}\psi_n)$ 是有意义的.

2. 要学会使用内积的符号, 以后内积的符号又会被全部换成 Dirac 符号.

5. 3.13

证: 由不确定度关系可得

$$\sqrt{\left\langle(\Delta x)^2(\Delta F)^2\right\rangle}\geq\frac{1}{2}\left|\left\langle\left[\hat{x},F(\hat{p})\right]\right\rangle\right| \tag{568}$$

由 $[\hat{x},F(\hat{p})]=i\hbar\frac{\partial F(\hat{p})}{\partial p}$ 得,

$$\sqrt{\left\langle(\Delta x)^2(\Delta F)^2\right\rangle}\geq\frac{\hbar}{2}\left|\left\langle\frac{\partial F(\hat{p})}{\partial p}\right\rangle\right| \tag{569}$$

当 $F(\hat{p})$ 为能量算符 $\hat{H}=\frac{\hat{p}^2}{2m}+V(x)$ 时, $\left\langle\frac{\partial F(\hat{p})}{\partial p}\right\rangle=\frac{1}{m}\langle\hat{p}\rangle=0$. 在 $\hat{H}$ 的离散能量本征态 ψ_m 上, $\left\langle(\Delta H)^2\right\rangle=0$. 此时上式中的等号成立, 即使 $\hat{x}$ 与 $\hat{H}$ 不对易, 但是量子态取为 ψ_m 时, 上式中的等号仍然成立.

6. 证明在 $\hat{l}_z$ 的本征态下, $\bar{l}_x=\bar{l}_y=0$.

证: $\hat{l}_z$ 的本征态 ψ_m, 满足 $\hat{l}_z\psi_m=m\hbar\psi_m$, $m=0,\pm1,\pm2,\cdots$. $\left[\hat{l}_y,\ \hat{l}_z\right]=i\hbar\hat{l}_x$, 则

$$\left(\psi_m,\left[\hat{l}_y,\ \hat{l}_z\right]\psi_m\right)=\left(\psi_m,i\hbar\hat{l}_x\psi_m\right) \tag{570}$$

$$\left(\psi_m,\left(\hat{l}_y\hat{l}_z-\hat{l}_z\hat{l}_y\right)\psi_m\right)=i\hbar\left\langle\hat{l}_x\right\rangle \tag{571}$$

$$\left(\psi_m,\hat{l}_y\hat{l}_z\psi_m\right)-\left(\psi_m,\hat{l}_z\hat{l}_y\psi_m\right)=i\hbar\left\langle\hat{l}_x\right\rangle \tag{572}$$

$$\left(\psi_m,\hat{l}_y\hat{l}_z\psi_m\right)-\left(\hat{l}_z\psi_m,\hat{l}_y\psi_m\right)=i\hbar\left\langle\hat{l}_x\right\rangle \tag{573}$$

$$m\hbar\left(\psi_m,\hat{l}_y\psi_m\right)-m\hbar\left(\psi_m,\hat{l}_y\psi_m\right)=i\hbar\left\langle\hat{l}_x\right\rangle \tag{574}$$

$$0=i\hbar\left\langle\hat{l}_x\right\rangle \tag{575}$$

所以 $\left\langle\hat{l}_x\right\rangle=0$. 同理 $\left\langle\hat{l}_y\right\rangle=0$.

7. 3.16 (a), (b)

解: 由 $\hat{\boldsymbol{l}}^2Y_{lm}=l\left(l+1\right)\hbar^2Y_{lm}$, $\hat{l}_zY_{lm}=m\hbar Y_{lm}$ 得, 在态 $\psi=c_1Y_{11}+c_2Y_{20}$ 下,

(a) 测量 l_z 时, 体系坍缩到 Y_{11} 的概率为 $|c_1|^2$, 测量值为 $\hbar$; 体系坍缩到 Y_{20} 的概率为 $|c_2|^2$, 测量值为 0. 所以平均值为 $|c_1|^2$.

(b) 测量 $\boldsymbol{l}^2$ 时, 体系坍缩到 Y_{11} 的概率为 $|c_1|^2$, 测量值为 $2\hbar^2$; 体系坍缩到 Y_{20} 的概率为 $|c_2|^2$, 测量值为 $6\hbar^2$. 所以平均值为 $2\left|c_1\right|^2\hbar^2+6\left|c_2\right|^2\hbar^2$.

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1. 7.1

解:

(1) $iAB + iBA = [B, C]\,B + B\,[B, C] = [B^2, C]$, 由于 $B^2 = 1$, 所以 $[B^2, C] = 0$, 即 $AB + BA = 0$.

类似的, $iAC + iCA = [B, C]\,C + C\,[B, C] = [B, C^2] = [B, I] = 0$.

(2) A 的本征方程为 $Av = \lambda v$, 由于 $A^2 = i$, $A^2 v = \lambda^2 v = v$, 故 $\lambda = \pm 1$, 本征值不简并, 分别对应着两个本征向量. 故在 A 的表象里, A 为对角矩阵: $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. 设在 A 的表象里, B 和 C 的矩阵表示分别为 $\begin{pmatrix} b_1 & b_2 \\ b_3 & b_4 \end{pmatrix}$ 和 $\begin{pmatrix} c_1 & c_2 \\ c_3 & c_4 \end{pmatrix}$.

由于 $BA + AB = 0$, 即 $\begin{pmatrix} b_1 & b_2 \\ b_3 & b_4 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} b_1 & b_2 \\ b_3 & b_4 \end{pmatrix} = 0$, 得到 $b_1 = b_4 = 0$. 于是 $B = \begin{pmatrix} 0 & b_2 \\ b_3 & 0 \end{pmatrix}$. 由于 $B^2 = 1$, 得到 $b_2 b_3 = 0$. 所以可令 $B = \begin{pmatrix} 0 & b \\ b^{-1} & 0 \end{pmatrix}$. 类似的, 利用 $CA + AC = 0$ 和 $C^2 = 1$, 可以得到 $C = \begin{pmatrix} 0 & c \\ c^{-1} & 0 \end{pmatrix}$.

由于 $BC - CA = iA$, 所以

$$\begin{pmatrix} 0 & b \\ b^{-1} & 0 \end{pmatrix}\begin{pmatrix} 0 & c \\ c^{-1} & 0 \end{pmatrix} - \begin{pmatrix} 0 & c \\ c^{-1} & 0 \end{pmatrix}\begin{pmatrix} 0 & b \\ b^{-1} & 0 \end{pmatrix} = i\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{576}$$

即

$$\begin{pmatrix} bc^{-1} - cb^{-1} & 0 \\ 0 & b^{-1}c - c^{-1}b \end{pmatrix} = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} \tag{577}$$

得: $bc^{-1} - cb^{-1} = i$.

所以, 在 A 的表象里, $B = \begin{pmatrix} 0 & b \\ b^{-1} & 0 \end{pmatrix}$, $C = \begin{pmatrix} 0 & c \\ c^{-1} & 0 \end{pmatrix}$, b, c 满足 $bc^{-1} - cb^{-1} = i$.

讨论:

(1) 在这个问题里, 应该明确说明 A, B, C 都是 Hermitian 算符对应的矩阵. 在这个前提下, 进行下面的讨论.

(2) B 和 C 都是 Hermitian 矩阵, 要求 $B^\dagger = B$, $C^\dagger = C$, 故 $b^* = b^{-1}$, $c^* = c^{-1}$. 即 $|b| = |c| = 1$, 可以令 $b = e^{i\alpha}$, $c = e^{i\beta}$, $\alpha, \beta \in \mathbb{R}$. 代入 $bc^{-1} - cb^{-1} = i$ 得到 $e^{i(\alpha-\beta)} - e^{i(\beta-\alpha)} = i$, 于是 $\sin(\alpha - \beta) = \frac{1}{2}$, 所以 $\alpha = \beta + \frac{\pi}{6}$ 或 $\alpha = \beta + \frac{5\pi}{6}$.

(3) B 的本征值为 $\lambda_{1,2} = \pm 1$, 在 A 的表象里, B 的本征向量为 $v_1 = \frac{1}{\sqrt{2}}\left(e^{i\alpha}, 1\right)^T$, $v_2 = \frac{1}{\sqrt{2}}\left(-e^{i\alpha}, 1\right)^T$.

(4) 于是 $B = \begin{pmatrix} 0 & b \\ b^{-1} & 0 \end{pmatrix} = \begin{pmatrix} v_1 & v_2 \end{pmatrix}\begin{pmatrix} 1 & \\ & -1 \end{pmatrix}\begin{pmatrix} v_1^\dagger \\ v_2^\dagger \end{pmatrix} \equiv U\begin{pmatrix} 1 & \\ & -1 \end{pmatrix}U^\dagger$, 所以 $\begin{pmatrix} 1 & \\ & -1 \end{pmatrix} = U^\dagger\begin{pmatrix} 0 & b \\ b^{-1} & 0 \end{pmatrix}U$, 所以从 A 表象到 B 表象的变换矩阵为 U. 相应的, 矩阵 A 从 A 表象变换到 B 表象为 $\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} = U^\dagger\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}U$.

2. 7.2

解: (a) 由于 $AA^\dagger + A^\dagger A = I$ 和 $A^2 = 0$, 所以

$$B^2 = \left(A^\dagger A\right)^2 = A^\dagger A A^\dagger A = A^\dagger A\left(1 - AA^\dagger\right) = A^\dagger A - A^\dagger A^2 A^\dagger = A^\dagger A = B \tag{578}$$

(b) 在矩阵 B 的本征态张开的表象里, 设 $B\psi = \lambda\psi$, 则

$$B^2\psi = BB\psi = \lambda^2\psi \tag{579}$$

由 $B^2\psi = B\psi$ 得

$$\lambda^2\psi = \lambda\psi \tag{580}$$

所以 $\lambda^2 = \lambda$, $\lambda = 0$ 或 1. 由于 B 的本征态无简并, 所以两个不同的本征值对应着两个本征态, ψ_1 和 ψ_2:

$$B\psi_1 = \psi_1 \tag{581}$$

$$B\psi_2 = 0 \tag{582}$$

在 ψ_1 和 ψ_2 张开的空间内, 可得 B 的矩阵表示为 $B = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$.

设 $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$, 由 $A^\dagger A = B$ 得到

$$A^\dagger A = \begin{pmatrix} a^* & c^* \\ b^* & d^* \end{pmatrix}\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} |a|^2 + |c|^2 & a^*b + c^*d \\ b^*a + d^*c & |b|^2 + |d|^2 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{583}$$

可得

$$|a|^2 + |c|^2 = 0 \tag{584}$$

即 $a = c = 0$. 另外,

$$AA^\dagger = I - A^\dagger A = \begin{pmatrix} 0 & b \\ 0 & d \end{pmatrix}\begin{pmatrix} 0 & 0 \\ b^* & d^* \end{pmatrix} = \begin{pmatrix} |b|^2 & bd^* \\ db^* & |d|^2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{585}$$

所以 $|b|^2 = 1$, $|d|^2 = 0$, 即 $b = e^{i\alpha}$ (α 为实数), $d = 0$. 我们最终得到 $A = \begin{pmatrix} 0 & e^{i\alpha} \\ 0 & 0 \end{pmatrix}$.

3. 考虑一个量子体系, 其正交完备归一的基矢为 $\{u_i(\boldsymbol{r})\}$, $i = 1, 2$. 利用此基矢, 体系 Hamiltonian 的矩阵表示为

$$H = \begin{pmatrix} h & g \\ g & h \end{pmatrix} \tag{586}$$

这里 g, h 为实数.

(1) 求体系 Hamiltonian 的本征值和本征向量;

(2) $t = 0$ 时, 体系处于初态 $u_1(\boldsymbol{r})$, 求 $t > 0$ 时体系的波函数.

解:

(1) 令 $\det(H - \lambda I) = 0$ 得: $(h - \lambda)^2 - g^2 = 0$, 所以本征值 $\lambda = h \pm g$.

当 $\lambda_1 = h + g$ 时,

$$\begin{pmatrix} h-\lambda_1 & g \\ g & h-\lambda_1 \end{pmatrix} \to \begin{pmatrix} -g & g \\ g & -g \end{pmatrix} \to \begin{pmatrix} -g & g \\ 0 & 0 \end{pmatrix} \to \begin{pmatrix} -1 & 1 \\ 0 & 0 \end{pmatrix} \tag{587}$$

所以本征向量可取为 $v_1 = \frac{1}{\sqrt{2}}(1,1)^T$.

当 $\lambda_2 = h - g$ 时,

$$\begin{pmatrix} h-\lambda_2 & g \\ g & h-\lambda_2 \end{pmatrix} \to \begin{pmatrix} g & g \\ g & g \end{pmatrix} \to \begin{pmatrix} g & g \\ 0 & 0 \end{pmatrix} \to \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix} \tag{588}$$

所以本征向量可取为 $v_2 = \frac{1}{\sqrt{2}}(1,-1)^T$.

(2) 在基矢 $\{u_1, u_2\}$ 下, 体系的初态为 $v_0 = (1,0)^T = \frac{1}{\sqrt{2}}v_1 + \frac{1}{\sqrt{2}}v_2$, 为非定态. 在 $t > 0$ 时, 非定态波函数为 $v(t) = \frac{1}{\sqrt{2}}v_1 e^{-i(h+g)t/\hbar} + \frac{1}{\sqrt{2}}v_2 e^{i(h-g)t/\hbar}$.

4. 一个三能级体系的 Hamiltonian 由下列矩阵表示

$$H = \begin{pmatrix} a & 0 & b \\ 0 & a & 0 \\ b & 0 & a \end{pmatrix}$$

这里 a, b 是非零实数, 且 $a \neq b$.

(1) 求该 Hamiltonian 的本征值和本征向量;

(2) 若体系的初态为 $S(0) = (0,1,0)^T$, 求 $t > 0$ 时体系的状态 $S(t)$.

(3) 若体系的初态为 $S(0) = \frac{1}{\sqrt{3}}(1,1,1)^T$, 求 $t > 0$ 时体系的状态 $S(t)$.

解:

(1) 令 $\det(H - \lambda I) = 0$, 得 $(a-\lambda)(a-\lambda-b)(a-\lambda+b) = 0$, 所以 $\lambda_1 = a$, $\lambda_2 = a-b$, $\lambda_3 = a+b$.

当 $\lambda_1 = a$ 时,

$$H - \lambda_1 I = \begin{pmatrix} 0 & 0 & b \\ 0 & 0 & 0 \\ b & 0 & 0 \end{pmatrix} \to \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \tag{589}$$

所以本征向量可取为 $v_1 = (0,1,0)^T$.

当 $\lambda_2 = a - b$ 时,

$$H - \lambda_2 I = \begin{pmatrix} b & 0 & b \\ 0 & b & 0 \\ b & 0 & b \end{pmatrix} \to \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{590}$$

所以本征向量可取为 $v_2 = \frac{1}{\sqrt{2}}(1,0,-1)^T$.

当 $\lambda_3 = a + b$ 时,

$$H - \lambda_3 I = \begin{pmatrix} -b & 0 & b \\ 0 & -b & 0 \\ b & 0 & -b \end{pmatrix} \to \begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{591}$$

所以本征向量可取为 $v_3 = \frac{1}{\sqrt{2}}(1,0,1)^T$.

(2) 由于初态 $S(0)$ 为体系的本征态, 所以 $S(t)$ 为定态 $S(t)=S(0)e^{-iat/\hbar}$.

(3) 由于 $v_1^\dagger S(0)=\frac{1}{\sqrt{3}}$, $v_2^\dagger S(0)=0$, $v_3^\dagger S(0)=\frac{2}{\sqrt{6}}$, 所以 $S(0)=\frac{1}{\sqrt{3}}v_1+\frac{2}{\sqrt{6}}v_3$, 即非定态, 所以 $S(t)=\frac{1}{\sqrt{3}}v_1e^{-iat/\hbar}+\frac{2}{\sqrt{6}}v_3e^{-i(a+b)t/\hbar}$.

5. 考虑一个由基矢 $|1\rangle$, $|2\rangle$, $|3\rangle$ 张开的向量空间, 这组基矢满足正交归一和完备性关系. 右矢 $|\alpha\rangle$ 与 $|\beta\rangle$ 如下定义

$$|\alpha\rangle=\frac{i}{2}|1\rangle-i|2\rangle+|3\rangle,\qquad|\beta\rangle=2|2\rangle-i|3\rangle$$

(1) 求相应的左矢 $\langle\alpha|$ 和 $\langle\beta|$.

(2) 计算 $\langle\alpha|\beta\rangle$ 和 $\langle\beta|\alpha\rangle$.

(3) 求算符 $|\alpha\rangle\langle\beta|$ 在基矢 $\{|1\rangle,|2\rangle,|3\rangle\}$ 下的矩阵表示.

解:

(1) $\langle\alpha|=(|\alpha\rangle)^\dagger=-\frac{i}{2}\langle1|+i\langle2|+\langle3|$. $\langle\beta|=(|\beta\rangle)^\dagger=2\langle2|+i\langle3|$.

(2) 内积

$$\langle\alpha|\beta\rangle=\left(-\frac{i}{2}\langle1|+i\langle2|+\langle3|\right)(2|2\rangle-i|3\rangle)=2i-i=i \tag{592}$$

$$\langle\beta|\alpha\rangle=(2\langle2|+i\langle3|)\left(\frac{i}{2}|1\rangle-i|2\rangle+|3\rangle\right)=-i \tag{593}$$

(3) 由于 $|\alpha\rangle\langle\beta|1\rangle=0$, 所以 $|\alpha\rangle\langle\beta|$ 矩阵表示的第 1 列为 $(0,0,0)^T$; $|\alpha\rangle\langle\beta|2\rangle=2|\alpha\rangle$, 所以 $|\alpha\rangle\langle\beta|$ 矩阵表示的第 2 列为 $(i,-2i,1)^T$; $|\alpha\rangle\langle\beta|3\rangle=i|\alpha\rangle$, 所以 $|\alpha\rangle\langle\beta|$ 矩阵表示的第 3 列为 $\left(-\frac{1}{2},1,i\right)^T$; 所以 $|\alpha\rangle\langle\beta|$ 在基矢 $\{|1\rangle,|2\rangle,|3\rangle\}$ 下的矩阵表示为 $\begin{pmatrix}0&i&-\frac{1}{2}\\0&-2i&1\\0&2&i\end{pmatrix}$.

6. 某量子体系正交归一完备的基矢为 $\{|e_n\rangle\}$. n 是体系一组 CSCO 的本征值数组集合. 体系的某 Hermitian 算符 $\hat{Q}$ 表示为 $\hat{Q}=\sum_n q_n|e_n\rangle\langle e_n|$. 证明下列问题:

(1) 证明 $\hat{Q}|e_n\rangle=q_n|e_n\rangle$.

(2) 体系的任一向量 $|\psi\rangle=\sum_n c_n|e_n\rangle$, 证明 $\hat{Q}|\psi\rangle=\sum_n c_nq_n|e_n\rangle$.

(3) 证明: $\hat{Q}^m=\sum_n q_n^m|e_n\rangle\langle e_n|$. m 为正整数.

(4) 已知函数 $f(x)$ 为连续可微函数, 证明 $\hat{Q}$ 的函数 $f\left(\hat{Q}\right)$ 可以表示为 $f\left(\hat{Q}\right)=\sum_n f(q_n)|e_n\rangle\langle e_n|$.

解:

(1) $\hat{Q}|e_n\rangle=\sum_{n'}q_{n'}|e_{n'}\rangle\langle e_{n'}|e_n\rangle=\sum_{n'}q_{n'}|e_{n'}\rangle\delta_{nn'}=q_n|e_n\rangle$.

(2) $\hat{Q}|\psi\rangle=\hat{Q}\sum_n c_n|e_n\rangle=\sum_n c_n\hat{Q}|e_n\rangle=\sum_n c_nq_n|e_n\rangle$.

(3) 方法 1: $\hat{Q}^2|e_n\rangle=q_n^2|e_n\rangle$, 一般的 $\hat{Q}^m|e_n\rangle=q_n^m|e_n\rangle$,

$$\hat{Q}^m|\psi\rangle=\hat{Q}^m\sum_n c_n|e_n\rangle=\sum_n c_n\hat{Q}^m|e_n\rangle=\sum_n c_nq_n^m|e_n\rangle \tag{594}$$

$$\sum_n q_n^m|e_n\rangle\langle e_n|\psi\rangle=\sum_n q_n^m|e_n\rangle\langle e_n|\sum_{n'}c_{n'}|e_{n'}\rangle=\sum_n q_n^m|e_n\rangle\sum_{n'}c_{n'}\delta_{nn'}=\sum_n c_nq_n^m|e_n\rangle \tag{595}$$

所以 $\hat{Q}^m|\psi\rangle=\sum_n q_n^m|e_n\rangle\langle e_n|\psi\rangle$, 由于 $|\psi\rangle$ 的任意性, 所以 $\hat{Q}^m=\sum_n q_n^m|e_n\rangle\langle e_n|$.

方法 2:

$$\hat{Q}^2=\sum_n q_n|e_n\rangle\langle e_n|\sum_{n'}q_{n'}|e_{n'}\rangle\langle e_{n'}|=\sum_n q_n|e_n\rangle\sum_{n'}q_{n'}\delta_{nn'}\langle e_{n'}|=\sum_n q_n^2|e_n\rangle\langle e_n| \tag{596}$$

$$\hat{Q}^3 = \sum_n q_n^2 \left|e_n\right\rangle \left\langle e_n\right| \sum_{n'} q_{n'} \left|e_{n'}\right\rangle \left\langle e_{n'}\right| = \sum_n q_n^2 \left|e_n\right\rangle \sum_{n'} q_{n'} \delta_{nn'} \left\langle e_{n'}\right| = \sum_n q_n^3 \left|e_n\right\rangle \left\langle e_n\right| \tag{597}$$

一般的, 可以归纳证明 $\hat{Q}^m = \sum_n q_n^m \left|e_n\right\rangle \left\langle e_n\right|$.

(4) 对于连续可微函数 $f(x)$, $f(x) = \sum_{n'=0}^{\infty} \frac{f^{(n')}(0)}{n'!} x^{n'}$, 则

$$f\left(\hat{Q}\right) = \sum_{n'=0}^{\infty} \frac{f^{(n')}(0)}{n'!} \hat{Q}^{n'} = \sum_{n'=0}^{\infty} \frac{f^{(n')}(0)}{n'!} \sum_n q_n^{n'} \left|e_n\right\rangle \left\langle e_n\right| \tag{598}$$

$$= \sum_n \left(\sum_{n'=0}^{\infty} \frac{f^{(n')}(0)}{n'!} q_n^{n'} \right) \left|e_n\right\rangle \left\langle e_n\right| = \sum_n f(q_n) \left|e_n\right\rangle \left\langle e_n\right| \tag{599}$$

0.12 第十二次作业

1. 考察一个量子系统, 其 Hamiltonian 可写为:

$$\hat{H}=\hat{a}^{\dagger}\hat{a}+\alpha\hat{a}+\beta\hat{a}^{\dagger}$$

其中 α, β 为复常数, 而算符 $\hat{a}$ 及其厄米共轭算符 $\hat{a}^{\dagger}$ 满足对易关系: $\left[\hat{a},\hat{a}^{\dagger}\right]=1$, 求此系统的能量本征值.

提示: 首先根据 Hamiltonian 的厄米性找到 α 与 β 的关系, 然后令 $\hat{\tilde{a}}^{\dagger}=\hat{a}^{\dagger}+\alpha$.

解: 由哈密顿量的厄米性可得 $\beta=\alpha^*$. 令 $\hat{\tilde{a}}^{\dagger}=\hat{a}^{\dagger}+\alpha$, 则

$$\hat{H}=\left(\hat{a}^{\dagger}+\alpha\right)\left(\hat{a}+\alpha^*\right)-\alpha^*\alpha \tag{600}$$

$$=\hat{\tilde{a}}^{\dagger}\hat{\tilde{a}}-\alpha^*\alpha \tag{601}$$

并且

$$\left[\hat{\tilde{a}},\hat{\tilde{a}}^{\dagger}\right]=\left[\hat{a}+\alpha^*,\hat{a}^{\dagger}+\alpha\right]=\left[\hat{a},\hat{a}^{\dagger}\right]=1 \tag{602}$$

且

$$\left[\hat{\tilde{a}},\hat{H}\right]=\hat{\tilde{a}},\qquad\left[\hat{\tilde{a}}^{\dagger},\hat{H}\right]=-\hat{\tilde{a}}^{\dagger} \tag{603}$$

与谐振子哈密顿量中梯算符的对易关系相同, 与之类比, 得此体系的能量本征值为 $E_n=n-\alpha^*\alpha$. $n=0,1,2,\cdots$.

2. 一量子谐振子的本征态记作 $|n\rangle$, $n=0,1,2,\cdots$

(1) 构造一个由 $|0\rangle$ 和 $|1\rangle$ 线性叠加而成的态, 使得坐标算符 $\hat{x}$ 在这个态中的平均值为最大.

(2) 设 $t=0$ 时的量子态为 (1) 中所得结果, 求 $t>0$ 时系统的态是怎样的?

(3) 求 $t>0$ 时, $\hat{x}$ 的平均值.

解:

(1) 令 $|\psi\rangle=\sin\theta e^{i\varphi}|0\rangle+\cos\theta|1\rangle$. $\theta,\varphi\in\mathbb{R}$. 由于 $\hat{x}=\sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}^{\dagger}+\hat{a}\right)$, 则

$$\langle\psi|\hat{x}|\psi\rangle=\sqrt{\frac{\hbar}{2m\omega}}\left(\sin\theta e^{-i\varphi}\langle 0|+\cos\theta\langle 1|\right)\left(\hat{a}^{\dagger}+\hat{a}\right)\left(\sin\theta e^{i\varphi}|0\rangle+\cos\theta|1\rangle\right) \tag{604}$$

$$=\sqrt{\frac{\hbar}{2m\omega}}\left(\sin\theta e^{-i\varphi}\langle 0|+\cos\theta\langle 1|\right)\left(\sin\theta e^{i\varphi}|1\rangle+\cos\theta|0\rangle\right) \tag{605}$$

$$=\sqrt{\frac{\hbar}{2m\omega}}\left(\sin\theta\cos\theta e^{-i\varphi}+\sin\theta\cos\theta e^{i\varphi}\right) \tag{606}$$

$$=\sqrt{\frac{\hbar}{2m\omega}}\sin 2\theta\cos\varphi \tag{607}$$

可见 $\theta=\frac{\pi}{4}$, $\varphi=0$ 时, 坐标算符 $\hat{x}$ 的平均值最大. 此时 $|\psi\rangle=\frac{1}{\sqrt{2}}\left(|0\rangle+|1\rangle\right)$.

(2) $t=0$ 时, $|\psi\rangle=\frac{1}{\sqrt{2}}\left(|0\rangle+|1\rangle\right)$. $t>0$ 时, 根据非定态的一般形式 $|\psi\rangle=\sum_n a_n e^{-iE_nt/\hbar}|n\rangle$, $E_n=\left(n+\frac{1}{2}\right)\hbar\omega$, 于是 $|\psi(t)\rangle=\frac{1}{\sqrt{2}}\left(e^{-iE_0t/\hbar}|0\rangle+e^{-iE_1t/\hbar}|1\rangle\right)$.

(3) $t>0$ 时, $\hat{x}$ 的平均值

$$\begin{aligned}
\langle\psi(t)|\hat{x}|\psi(t)\rangle &= \langle\psi(t)|\sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}^{\dagger}+\hat{a}\right)\frac{1}{\sqrt{2}}\left(e^{-iE_0t/\hbar}|0\rangle+e^{-iE_1t/\hbar}|1\rangle\right) &(608)\\
&= \frac{1}{\sqrt{2}}\left(e^{iE_0t/\hbar}\langle 0|+e^{iE_1t/\hbar}\langle 1|\right)\sqrt{\frac{\hbar}{2m\omega}}\frac{1}{\sqrt{2}}\left(e^{-iE_0t/\hbar}|1\rangle+e^{-iE_1t/\hbar}|0\rangle\right) &(609)\\
&= \sqrt{\frac{\hbar}{2m\omega}}\cos\frac{(E_1-E_0)t}{\hbar} &(610)\\
&= \sqrt{\frac{\hbar}{2m\omega}}\cos(\omega t) &(611)
\end{aligned}$$

3. 一维量子谐振子的相干态 $|\alpha\rangle$ 满足 $\hat{a}|\alpha\rangle=\alpha|\alpha\rangle$. α 为复常数. $|\alpha\rangle$ 可以表示为能量本征态 $|n\rangle$ 的叠加

$$|\alpha\rangle=\sum_{n=0}^{\infty}c_n|n\rangle$$

(1) 证明 $c_n=\frac{\alpha^n}{\sqrt{n!}}c_0$.

(2) 证明 $|\alpha\rangle$ 的归一化因子 c_0 可取为 $\exp\left(-\frac{|\alpha|^2}{2}\right)$.

(3) 设 $t=0$ 时, 体系处于 $|\alpha\rangle$, 求 $t>0$ 时的 $|\alpha(t)\rangle$, 并证明它仍然是 $\hat{a}|\alpha(t)\rangle=\alpha e^{-i\omega t}|\alpha(t)\rangle$.

(4) 基态 $|\alpha\rangle$ 是否相干态? 为什么?

(5) (选做) 证明在相干态上 $\sqrt{\left\langle(\hat{x}-\langle\hat{x}\rangle)^2\right\rangle\left\langle(\hat{p}-\langle\hat{p}\rangle)^2\right\rangle}=\frac{\hbar}{2}$.

解:

(1) 由已知,

$$\begin{aligned}
\hat{a}|\alpha\rangle &= \hat{a}\sum_{n=0}^{\infty}c_n|n\rangle &(612)\\
&= \sum_{n=0}^{\infty}c_n\sqrt{n}|n-1\rangle &(613)
\end{aligned}$$

于是

$$\sum_{n=0}^{\infty}c_n\sqrt{n}|n-1\rangle=\alpha\sum_{n=0}^{\infty}c_n|n\rangle \tag{614}$$

两边与 $|m\rangle$ 做内积得:

$$\sum_{n=0}^{\infty}c_n\sqrt{n}\delta_{m,n-1}=\alpha\sum_{n=0}^{\infty}c_n\delta_{m,n} \tag{615}$$

所以

$$c_{m+1}\sqrt{m+1}=\alpha c_m \tag{616}$$

即

$$c_{m+1}=\frac{\alpha}{\sqrt{m+1}}c_m \tag{617}$$

所以

$$c_m=\frac{\alpha}{\sqrt{m}}c_{m-1}=\frac{\alpha^2}{\sqrt{m(m-1)}}c_{m-2}=\frac{\alpha^3}{\sqrt{m(m-1)(m-2)}}c_{m-3}=\cdots=\frac{\alpha^m}{\sqrt{m!}}c_0 \tag{618}$$

(2) 由于 $|\alpha\rangle=\sum_{n=0}^{\infty}c_n|n\rangle=c_0\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle$, 根据归一化,

$$\langle\alpha|\alpha\rangle=c_0^*\sum_{n'=0}^{\infty}\frac{\alpha^{*n'}}{\sqrt{n'!}}\langle n'|c_0\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle=|c_0|^2\sum_{n'=0}^{\infty}\sum_{n=0}^{\infty}\frac{\alpha^{*n'}}{\sqrt{n'!}}\frac{\alpha^n}{\sqrt{n!}}\delta_{nn'}=|c_0|^2\sum_{n=0}^{\infty}\frac{|\alpha|^{2n}}{n!}=1 \tag{619}$$

即

$$|c_0|^2e^{-|\alpha|^2}=1 \tag{620}$$

所以 c_0 可取为 exp $\left(-\frac{|\alpha|^2}{2}\right)$.

(3) $t=0$ 时, 体系处于 $|\alpha\rangle=c_0\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle$. $t>0$ 时, 根据非定态的一般公式, $|\alpha(t)\rangle=c_0\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}e^{-iE_nt/\hbar}|n\rangle$. 于是,

$$\hat{a}|\alpha(t)\rangle=\hat{a}c_0\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}e^{-iE_nt/\hbar}|n\rangle \tag{621}$$

$$=c_0\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}e^{-iE_nt/\hbar}\sqrt{n}|n-1\rangle \tag{622}$$

$$=c_0\sum_{n=1}^{\infty}\frac{\alpha^n}{\sqrt{(n-1)!}}e^{-iE_nt/\hbar}|n-1\rangle \tag{623}$$

令 $n'=n-1$, 则

$$\hat{a}|\alpha(t)\rangle=c_0\sum_{n'=0}^{\infty}\frac{\alpha^{n'+1}}{\sqrt{n'!}}e^{-iE_{n'+1}t/\hbar}|n'\rangle \tag{624}$$

$$=\alpha e^{-i\omega t}c_0\sum_{n'=0}^{\infty}\frac{\alpha^{n'}}{\sqrt{n'!}}e^{-iE_{n'}t/\hbar}|n'\rangle \tag{625}$$

$$=\alpha e^{-i\omega t}|\alpha(t)\rangle \tag{626}$$

(4) $\hat{a}|0\rangle=0|0\rangle$, 所以 $|0\rangle$ 是相干态, 此时 $\alpha=0$.

(5) 由 $\hat{a}|\alpha\rangle=\alpha|\alpha\rangle$ 得到 $\langle\alpha|\hat{a}^\dagger=\langle\alpha|\alpha^*$. 由于 $\hat{x}=\sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}^\dagger+\hat{a}\right)$, 则

$$\langle\alpha|\hat{x}|\alpha\rangle=\sqrt{\frac{\hbar}{2m\omega}}\langle\alpha|\left(\hat{a}^\dagger+\hat{a}\right)|\alpha\rangle=\sqrt{\frac{\hbar}{2m\omega}}\left(\alpha+\alpha^*\right) \tag{627}$$

$$\langle\alpha|\hat{x}^2|\alpha\rangle=\frac{\hbar}{2m\omega}\langle\alpha|\left(\hat{a}^\dagger+\hat{a}\right)^2|\alpha\rangle \tag{628}$$

$$=\frac{\hbar}{2m\omega}\langle\alpha|\hat{a}^{\dagger2}+\hat{a}^2+\hat{a}^\dagger\hat{a}+\hat{a}\hat{a}^\dagger|\alpha\rangle \tag{629}$$

$$=\frac{\hbar}{2m\omega}\langle\alpha|\hat{a}^{\dagger2}+\hat{a}^2+2\hat{a}^\dagger\hat{a}+1|\alpha\rangle \tag{630}$$

$$=\frac{\hbar}{2m\omega}\left(\alpha^{*2}+\alpha^2+2\alpha^*\alpha+1\right) \tag{631}$$

所以

$$\left\langle(\hat{x}-\langle\hat{x}\rangle)^2\right\rangle=\left\langle\hat{x}^2\right\rangle-\langle\hat{x}\rangle^2=\frac{\hbar}{2m\omega}\left(\alpha^{*2}+\alpha^2+2\alpha^*\alpha+1\right)-\frac{\hbar}{2m\omega}\left(\alpha+\alpha^*\right)^2=\frac{\hbar}{2m\omega} \tag{632}$$

类似的, 对 $\hat{p}=i\sqrt{\frac{\hbar m\omega}{2}}\left(\hat{a}^{\dagger}-\hat{a}\right)$, 有

$$\langle\alpha|\,\hat{p}\,|\alpha\rangle=i\sqrt{\frac{\hbar m\omega}{2}}\,\langle\alpha|\left(\hat{a}^{\dagger}-\hat{a}\right)|\alpha\rangle=i\sqrt{\frac{\hbar m\omega}{2}}\left(\alpha^{*}-\alpha\right)\tag{633}$$

$$\begin{aligned}\langle\alpha|\,\hat{p}^{2}\,|\alpha\rangle&=-\frac{\hbar m\omega}{2}\,\langle\alpha|\left(\hat{a}^{\dagger}-\hat{a}\right)^{2}|\alpha\rangle&(634)\\&=-\frac{\hbar m\omega}{2}\,\langle\alpha|\,\hat{a}^{\dagger 2}+\hat{a}^{2}-\hat{a}^{\dagger}\hat{a}-\hat{a}\hat{a}^{\dagger}\,|\alpha\rangle&(635)\\&=-\frac{\hbar m\omega}{2}\,\langle\alpha|\,\hat{a}^{\dagger 2}+\hat{a}^{2}-2\hat{a}^{\dagger}\hat{a}-1\,|\alpha\rangle&(636)\\&=-\frac{\hbar m\omega}{2}\left(\alpha^{*2}+\alpha^{2}-2\alpha^{*}\alpha-1\right)&(637)\end{aligned}$$

$$\left\langle\left(\hat{p}-\langle\hat{p}\rangle\right)^{2}\right\rangle=-\frac{\hbar m\omega}{2}\left(\alpha^{*2}+\alpha^{2}-2\alpha^{*}\alpha-1\right)+\frac{\hbar m\omega}{2}\left(\alpha^{*}-\alpha\right)^{2}=\frac{\hbar m\omega}{2}\tag{638}$$

所以 $\sqrt{\left\langle\left(\hat{x}-\langle\hat{x}\rangle\right)^{2}\right\rangle\left\langle\left(\hat{p}-\langle\hat{p}\rangle\right)^{2}\right\rangle}=\frac{\hbar}{2}$.

4. 取 $\left(\hat{\boldsymbol{l}}^{2},\hat{l}_{z}\right)$ 的共同本征态作为基矢 $\{|lm\rangle\}$,

(1) 计算 $\hat{l}_{-}$ 的矩阵元 $\langle l'm'|\,\hat{l}_{-}\,|lm\rangle$, 和 $\hat{l}_{x}$ 的矩阵元 $\langle l'm'|\,\hat{l}_{x}\,|lm\rangle$;

(2) 当 $l=1$ 时, 这个子空间的基矢为 $\{|11\rangle,|10\rangle,|1-1\rangle\}$, 写出 $\hat{l}_{-}$ 和 $\hat{l}_{x}$ 在这个子空间中的矩阵表示, 并计算 $\hat{l}_{x}$ 所对应矩阵的本征值和本征向量;

(3) 在 $l=1$ 子空间中, 计算 $\exp\left(-i\beta\hat{l}_{x}/\hbar\right)$ 的矩阵表示 ($\beta\in\mathbb{R}$ 为常数).

解 (1) $\hat{l}_{-}\,|lm\rangle=\hbar\sqrt{l\left(l+1\right)-m\left(m-1\right)}\,|l,m-1\rangle$, 则

$$\begin{aligned}n\,\langle l'm'|\,\hat{l}_{-}\,|lm\rangle&=\langle l'm'|\,\hbar\sqrt{l\left(l+1\right)-m\left(m-1\right)}\,|l,m-1\rangle&(639)\\&=\delta_{l'l}\delta_{m'm-1}\hbar\sqrt{l\left(l+1\right)-m\left(m-1\right)}&(640)\end{aligned}$$

由于 $\hat{l}_{x}=\frac{\hat{l}_{+}+\hat{l}_{-}}{2}$, 则

$$\begin{aligned}\hat{l}_{x}\,|lm\rangle=&\frac{\hat{l}_{+}+\hat{l}_{-}}{2}\,|lm\rangle&(641)\\=&\frac{\hbar}{2}\sqrt{l\left(l+1\right)-m\left(m+1\right)}\,|l,m+1\rangle+\frac{\hbar}{2}\sqrt{l\left(l+1\right)-m\left(m-1\right)}\,|l,m-1\rangle&(642)\end{aligned}$$

于是,

$$\langle l'm'|\,\hat{l}_{x}\,|lm\rangle=\frac{\hbar}{2}\sqrt{l\left(l+1\right)-m\left(m+1\right)}\delta_{ll'}\delta_{m',m+1}+\frac{\hbar}{2}\sqrt{l\left(l+1\right)-m\left(m-1\right)}\delta_{m',m-1}\tag{643}$$

(2) 当 $l=1$ 时,

$$\hat{l}_{x}\,|1m\rangle=\frac{\hbar}{2}\sqrt{2-m\left(m+1\right)}\,|1,m+1\rangle+\frac{\hbar}{2}\sqrt{2-m\left(m-1\right)}\,|1,m-1\rangle\tag{644}$$

于是

$$\begin{aligned}\hat{l}_{x}\,|11\rangle&=\frac{\hbar}{2}\sqrt{2}\,|1,0\rangle&(645)\\\hat{l}_{x}\,|10\rangle&=\frac{\hbar}{2}\sqrt{2}\,|1,1\rangle+\frac{\hbar}{2}\sqrt{2}\,|1,-1\rangle&(646)\\\hat{l}_{x}\,|1-1\rangle&=\frac{\hbar}{2}\sqrt{2}\,|1,0\rangle&(647)\end{aligned}$$

所以

$$\hat{l}_x \to L_x = \frac{\sqrt{2}\hbar}{2}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \tag{648}$$

令 $\det\left(\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} - \lambda I\right) = 0$ 得: $\lambda = \sqrt{2}, 0, -\sqrt{2}$. 于是 L_x 的本征值为 $\hbar, 0, -\hbar$. 当本征值为 $\hbar$ 时,

$$\begin{pmatrix} -\sqrt{2} & 1 & 0 \\ 1 & -\sqrt{2} & 1 \\ 0 & 1 & -\sqrt{2} \end{pmatrix} \to \begin{pmatrix} 1 & -\frac{1}{\sqrt{2}} & 0 \\ 1 & -\sqrt{2} & 1 \\ 0 & 1 & -\sqrt{2} \end{pmatrix} \to \begin{pmatrix} 1 & -\frac{1}{\sqrt{2}} & 0 \\ 0 & -\frac{1}{\sqrt{2}} & 1 \\ 0 & 1 & -\sqrt{2} \end{pmatrix} \to \begin{pmatrix} 1 & -\frac{1}{\sqrt{2}} & 0 \\ 0 & 1 & -\sqrt{2} \\ 0 & 1 & -\sqrt{2} \end{pmatrix} \tag{649}$$

$$\to \begin{pmatrix} 1 & -\frac{1}{\sqrt{2}} & 0 \\ 0 & 1 & -\sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \to \begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & -\sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \tag{650}$$

所以本征向量可以取为 $v_1 = \frac{1}{2}\left(1, \sqrt{2}, 1\right)$. 类似的, 可以确定 $v_2 = \frac{1}{\sqrt{2}}(1, 0, -1)$, $v_3 = \frac{1}{2}\left(1, -\sqrt{2}, 1\right)$.

(3) 在 $l = 1$ 的子空间 v_1 对应的态矢为

$$|\psi_1\rangle = \frac{1}{2}\left(|11\rangle + \sqrt{2}|10\rangle + |1-1\rangle\right) \tag{651}$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}(|11\rangle - |1-1\rangle) \tag{652}$$

$$|\psi_3\rangle = \frac{1}{2}\left(|11\rangle - \sqrt{2}|10\rangle + |1-1\rangle\right) \tag{653}$$

$\hat{l}_x$ 可以表示为 $\hat{l}_x = \hbar|\psi_1\rangle\langle\psi_1| + 0|\psi_2\rangle\langle\psi_2| - \hbar|\psi_3\rangle\langle\psi_3| = \hbar|\psi_1\rangle\langle\psi_1| - \hbar|\psi_3\rangle\langle\psi_3|$. 根据第 11 次作业的599式可得

$$\exp\left(-i\beta\hat{l}_x/\hbar\right) = \exp(-i\beta)|\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2| + \exp(i\beta)|\psi_3\rangle\langle\psi_3| \tag{654}$$

(或者利用完备性关系 $|\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2| + |\psi_3\rangle\langle\psi_3| = \hat{I}$, 和 $\hat{I}\exp\left(-i\beta\hat{l}_x/\hbar\right)\hat{I}$ 也可以得到上式) 而 $|\psi_1\rangle\langle\psi_1|$, $|\psi_2\rangle\langle\psi_2|$, $|\psi_3\rangle\langle\psi_3|$ 对应的矩阵形式分别为

$$v_1 v_1^\dagger, \quad v_2 v_2^\dagger, \quad v_3 v_3^\dagger \tag{655}$$

所以 $\exp\left(-i\beta\hat{l}_x/\hbar\right)$ 的矩阵形式为

$$\exp(-i\beta)v_1v_1^\dagger + v_2v_2^\dagger + \exp(i\beta)v_3v_3^\dagger = \begin{pmatrix} \cos^2\frac{\beta}{2} & -\frac{i\sin\beta}{\sqrt{2}} & -\sin^2\frac{\beta}{2} \\ -\frac{i\sin\beta}{\sqrt{2}} & \cos\beta & -\frac{i\sin\beta}{\sqrt{2}} \\ -\sin^2\frac{\beta}{2} & -\frac{i\sin\beta}{\sqrt{2}} & \cos^2\frac{\beta}{2} \end{pmatrix} \tag{656}$$

5. 取 $\left(\hat{\boldsymbol{l}}^2, \hat{l}_z\right)$ 的共同本征态作为基矢 $\{|lm\rangle\}$, 一个量子体系处于已经归一化的态:

$$|\psi\rangle = \frac{1}{\sqrt{2}}|11\rangle + \frac{i}{4}|10\rangle + \frac{1}{4}|1-1\rangle - \frac{\sqrt{6}}{4}i|00\rangle$$

(1) 同时测量 $\hat{\boldsymbol{l}}^2$ 和 $\hat{l}_z$, 求得到结果为 $2\hbar^2$ 和 $\hbar$ 的概率;
(2) 求单独测量 $\hat{l}_z$ 时, 各种可能的结果及相应的概率;
(3) 求单独测量 $\hat{l}_z^2$ 时, 各种可能的结果及相应的概率;
(4) 求力学量 $\hat{l}_x$ 的平均值.
解:
(1) 若同时测量 $\hat{\boldsymbol{l}}^2$ 和 $\hat{l}_z$, 由于 $\hat{\boldsymbol{l}}^2 |11\rangle = 2\hbar^2 |11\rangle$, $\hat{l}_z |11\rangle = \hbar |11\rangle$, 得到结果为 $2\hbar^2$ 和 $\hbar$ 的概率为 $\frac{1}{2}$.
(2) 单独测量 $\hat{l}_z$, 测量值和对应概率为

$$\hbar, \frac{1}{2} \tag{657}$$
$$0, \left|\frac{i}{4}\right|^2 + \left|-\frac{\sqrt{6}}{4}i\right|^2 = \frac{7}{16} \tag{658}$$
$$-\hbar, \frac{1}{16} \tag{659}$$

(3) 单独测量 $\hat{l}_z^2$, 测量值和对应概率为

$$\hbar^2, \left|\frac{1}{\sqrt{2}}\right|^2 + \left|\frac{1}{4}\right|^2 = \frac{9}{16} \tag{660}$$
$$0, \left|\frac{i}{4}\right|^2 + \left|-\frac{\sqrt{6}}{4}i\right|^2 = \frac{7}{16} \tag{661}$$

(4) 体系处于态 $|\psi\rangle$, 利用 $\hat{l}_x = \frac{\hat{l}_+ + \hat{l}_-}{2}$ 可得:

$$\hat{l}_x |11\rangle = \frac{\hbar}{2}\sqrt{2} |1,0\rangle \tag{662}$$
$$\hat{l}_x |10\rangle = \frac{\hbar}{2}\sqrt{2} |1,1\rangle + \frac{\hbar}{2}\sqrt{2} |1,-1\rangle \tag{663}$$
$$\hat{l}_x |1-1\rangle = \frac{\hbar}{2}\sqrt{2} |1,0\rangle \tag{664}$$
$$\hat{l}_x |00\rangle = 0 \tag{665}$$

于是

$$\begin{aligned}\hat{l}_x |\psi\rangle &= \frac{1}{\sqrt{2}}\left(\frac{\hbar}{2}\sqrt{2} |1,0\rangle\right) + \frac{i}{4}\left(\frac{\hbar}{2}\sqrt{2} |1,1\rangle + \frac{\hbar}{2}\sqrt{2} |1,-1\rangle\right) + \frac{1}{4}\left(\frac{\hbar}{2}\sqrt{2} |1,0\rangle\right) \qquad (666)\\ &= \frac{\hbar}{8}\left(4+\sqrt{2}\right) |1,0\rangle + i\frac{\hbar}{8}\sqrt{2} |1,1\rangle + i\frac{\hbar}{8}\sqrt{2} |1,-1\rangle \qquad (667)\end{aligned}$$

所以

$$\langle\psi| \hat{l}_x |\psi\rangle = \frac{\hbar}{8}\left(4+\sqrt{2}\right)\frac{-i}{4} + i\frac{\hbar}{8}\sqrt{2}\frac{1}{\sqrt{2}} + i\frac{\hbar}{8}\sqrt{2}\frac{1}{4} = 0 \tag{668}$$

0.13 第十三次作业 2021.06.15

1. 课本第 80 页练习.

解:

$$\boldsymbol{r}\cdot\nabla V(x,y,z)=\boldsymbol{r}\cdot\nabla V(cx,cy,cz)\big|_{c=1} \tag{669}$$

$$=\frac{\partial cr_\alpha}{\partial c}\frac{\partial}{\partial cr_\alpha}V(cx,cy,cz)\bigg|_{c=1} \tag{670}$$

$$=\frac{\partial}{\partial c}V(cx,cy,cz)\bigg|_{c=1} \tag{671}$$

$$=nc^{n-1}V(cx,cy,cz)\big|_{c=1} \tag{672}$$

$$=nV(x,y,z) \tag{673}$$

由位力定理得: $2\left\langle\hat{T}\right\rangle=n\left\langle\hat{V}\right\rangle$.

谐振子势: $V(x,y,z)=\frac{1}{2}m\omega^2(x^2+y^2+z^2)$, 所以 $n=2$, 则 $\left\langle\hat{V}\right\rangle=\left\langle\hat{T}\right\rangle$.

Coulomb 势: $V(r)=-\frac{1}{r}$, 所以 $n=-1$, 则 $\left\langle\hat{V}\right\rangle=-2\left\langle\hat{T}\right\rangle$.

δ 势: $\delta(cx)=\frac{1}{|c|}\delta(x)$($c$ 为实数, $c\neq 0$), 所以 $n=-1$, 则 $\left\langle\hat{V}\right\rangle=-2\left\langle\hat{T}\right\rangle$.

2. 一维情形下的空间平移算符可以写为 $\hat{T}(a)=\exp\left[-\frac{ia}{\hbar}\hat{p}\right]$.

(1) 设动量算符 $\hat{p}$ 的本征态为 $|p'\rangle$, 满足 $\hat{p}|p'\rangle=p'|p'\rangle$, 证明空间平移算符可以写为

$$\hat{T}(a)=\int e^{-\frac{ia}{\hbar}p'}|p'\rangle\langle p'|\,dp';$$

(2) 已知 $\langle x|\psi\rangle=\sqrt{\lambda}e^{-\lambda|x|}$, 利用 (1) 中定义计算 $\langle x|\hat{T}(a)|\psi\rangle$.

解:

(1) 由 $\hat{p}|p'\rangle=p'|p'\rangle$ 可得 $\hat{T}(a)|p'\rangle=e^{-\frac{ia}{\hbar}p'}|p'\rangle$. 利用完备性关系 $\hat{I}=\int dp'|p'\rangle\langle p'|$ 可得:

$$\hat{T}(a)\hat{I}=\exp\left[-\frac{ia}{\hbar}\hat{p}\right]\int dp'|p'\rangle\langle p'| \tag{674}$$

$$=\int dp'\exp\left[-\frac{ia}{\hbar}\hat{p}\right]|p'\rangle\langle p'| \tag{675}$$

$$=\int e^{-\frac{ia}{\hbar}p'}|p'\rangle\langle p'|\,dp' \tag{676}$$

(2)

$$\langle x|\hat{T}(a)|\psi\rangle=\langle x|\hat{T}(a)\hat{I}|\psi\rangle \tag{677}$$

$$=\langle x|\int e^{-\frac{ia}{\hbar}p'}|p'\rangle\langle p'|\,dp'|\psi\rangle \tag{678}$$

$$=\frac{1}{2\pi\hbar}\int e^{-\frac{ia}{\hbar}p'}e^{i\frac{x}{\hbar}p'}\varphi(p')\,dp' \tag{679}$$

$$=\frac{1}{2\pi\hbar}\int e^{i\frac{x-a}{\hbar}p'}\varphi(p')\,dp' \tag{680}$$

$$=\psi(x-a) \tag{681}$$

$$=\sqrt{\lambda}e^{-\lambda|x|} \tag{682}$$

讨论: $\hat{T}(a)=\int e^{-\frac{ia}{\hbar}p'}|p'\rangle\langle p'|dp'$ 比 $\exp\left[-\frac{ia}{\hbar}\hat{p}\right]$ 具有更普遍的适用性. 后者并不适用于 $\langle x|\psi\rangle=\sqrt{\lambda}e^{-\lambda|x|}$, 因为它在 $x=0$ 处不可导.

3. 考虑处于二维无限深方势阱中的粒子, 分布在区间 $-\frac{L}{2}\leq x\leq\frac{L}{2}$ 和 $-\frac{L}{2}\leq y\leq\frac{L}{2}$. 其能量本征态和能量本征值分别为

$$\psi_{n_xn_y}(x,y)=\frac{2}{L}\sin\left[\frac{n_x\pi}{L}\left(x-\frac{L}{2}\right)\right]\sin\left[\frac{n_y\pi}{L}\left(y-\frac{L}{2}\right)\right]$$

$$E_{n_xn_y}=\frac{\pi^2\hbar^2}{2mL^2}\left(n_x^2+n_y^2\right)$$

这里 n_x,n_y 为正整数. 设想把该无限深方势阱绕着 z 轴顺时针旋转 $\frac{\pi}{2}$, 即 $\hat{R}\left(\hat{z},-\frac{\pi}{2}\right)\psi(r,\varphi)=\psi\left(r,\varphi+\frac{\pi}{2}\right)$.

(1) 证明 $\hat{R}\left(\hat{z},-\frac{\pi}{2}\right)\psi_{n_xn_y}(x,y)\propto\psi_{n_yn_x}(x,y)$, 即两者之差为一个常数因子.

(2) 证明当 n_x 和 n_y 都是偶数或奇数时, $\frac{1}{\sqrt{2}}\left(\psi_{n_xn_y}(x,y)\pm\psi_{n_yn_x}(x,y)\right)$ 是 $\hat{R}\left(\hat{z},-\frac{\pi}{2}\right)$ 的本征态.

证:

(1) 由 $\hat{R}\left(\hat{z},-\frac{\pi}{2}\right)\psi(r,\varphi)=\psi\left(r,\varphi+\frac{\pi}{2}\right)$ 得:

$$\begin{aligned}
\hat{R}\left(\hat{z},-\frac{\pi}{2}\right)\psi_{n_x,n_y}(x,y)&=\psi_{n_x,n_y}(-y,x) &(683)\\
&=\frac{2}{L}\sin\left[\frac{n_x\pi}{L}\left(-y-\frac{L}{2}\right)\right]\sin\left[\frac{n_y\pi}{L}\left(x-\frac{L}{2}\right)\right] &(684)\\
&=-\frac{2}{L}\sin\left[\frac{n_x\pi}{L}\left(y+\frac{L}{2}\right)\right]\sin\left[\frac{n_y\pi}{L}\left(x-\frac{L}{2}\right)\right] &(685)\\
&=-\frac{2}{L}\sin\left[\frac{n_x\pi}{L}\left(y-\frac{L}{2}\right)+n_x\pi\right]\sin\left[\frac{n_y\pi}{L}\left(x-\frac{L}{2}\right)\right] &(686)\\
&=-(-1)^{n_x}\sin\left[\frac{n_x\pi}{L}\left(y-\frac{L}{2}\right)\right]\sin\left[\frac{n_y\pi}{L}\left(x-\frac{L}{2}\right)\right] &(687)\\
&=-(-1)^{n_x}\psi_{n_yn_x}(x,y) &(688)
\end{aligned}$$

(2) 由 (1) 得:

$$\begin{aligned}
\hat{R}\left(\hat{z},-\frac{\pi}{2}\right)\psi_{n_x,n_y}(x,y)=-(-1)^{n_x}\psi_{n_yn_x}(x,y) &\qquad(689)\\
\hat{R}\left(\hat{z},-\frac{\pi}{2}\right)\psi_{n_y,n_x}(x,y)=-(-1)^{n_y}\psi_{n_xn_y}(x,y) &\qquad(690)
\end{aligned}$$

则

$$\begin{aligned}
&\hat{R}\left(\hat{z},-\frac{\pi}{2}\right)\frac{1}{\sqrt{2}}\left(\psi_{n_xn_y}(x,y)+\psi_{n_yn_x}(x,y)\right) &(691)\\
=&\frac{1}{\sqrt{2}}\left(-(-1)^{n_x}\psi_{n_yn_x}(x,y)-(-1)^{n_y}\psi_{n_xn_y}(x,y)\right) &(692)\\
=&-\frac{1}{\sqrt{2}}(-1)^{n_y}\left((-1)^{n_x-n_y}\psi_{n_yn_x}(x,y)+\psi_{n_xn_y}(x,y)\right) &(693)
\end{aligned}$$

当 n_x 和 n_y 都是偶数或者 n_x 和 n_y 都是奇数时 (原来的作业题中缺少这个条件),

$$\hat{R}\left(\hat{z},-\frac{\pi}{2}\right)\frac{1}{\sqrt{2}}\left(\psi_{n_xn_y}(x,y)+\psi_{n_yn_x}(x,y)\right)=-\frac{1}{\sqrt{2}}(-1)^{n_y}\left(\psi_{n_yn_x}(x,y)+\psi_{n_xn_y}(x,y)\right)\qquad(694)$$

类似的, 当 n_x 和 n_y 都是偶数或者 n_x 和 n_y 都是奇数时,

$$\hat{R}\left(\hat{z},-\frac{\pi}{2}\right)\frac{1}{\sqrt{2}}\left(\psi_{n_xn_y}(x,y)-\psi_{n_yn_x}(x,y)\right)=-\frac{1}{\sqrt{2}}(-1)^{n_y}\left(\psi_{n_yn_x}(x,y)-\psi_{n_xn_y}(x,y)\right) \tag{695}$$

3. 96 页 4.7

解: 体系的能量本征方程为

$$\hat{H}|n\rangle=E_n|n\rangle \tag{696}$$

两边对 λ 求导得

$$\frac{\partial\hat{H}}{\partial\lambda}|n\rangle+\hat{H}\frac{\partial|n\rangle}{\partial\lambda}=\frac{\partial E_n}{\partial\lambda}|n\rangle+E_n\frac{\partial|n\rangle}{\partial\lambda} \tag{697}$$

方程两边与 $|n\rangle$ 做内积得:

$$\langle n|\frac{\partial\hat{H}}{\partial\lambda}|n\rangle+\langle n|\hat{H}\frac{\partial|n\rangle}{\partial\lambda}=\langle n|\frac{\partial E_n}{\partial\lambda}|n\rangle+\langle n|E_n\frac{\partial|n\rangle}{\partial\lambda} \tag{698}$$

由能量本征方程两边取厄米共轭得

$$\langle n|\hat{H}=\langle n|E_n \tag{699}$$

并且由于 $|n\rangle$ 的归一性 $\langle n|n\rangle=1$, 所以方程 (698) 可化为:

$$\langle n|\frac{\partial\hat{H}}{\partial\lambda}|n\rangle+E_n\langle n|\frac{\partial|n\rangle}{\partial\lambda}=\frac{\partial E_n}{\partial\lambda}+E_n\langle n|\frac{\partial|n\rangle}{\partial\lambda} \tag{700}$$

所以

$$\frac{\partial E_n}{\partial\lambda}=\langle n|\frac{\partial\hat{H}}{\partial\lambda}|n\rangle \tag{701}$$

4. 一维谐振子势中的能量本征态为 $|n\rangle$, 能量本征值为 $E_n=\left(n+\frac{1}{2}\right)\hbar\omega$. 考虑处于该势阱中的三个无相互作用的全同粒子. 考虑三个粒子是玻色子或费米子两种情形.

(1) 分别写出基态的波函数和相应的能量;

(2) 分别写出第一激发态的波函数和相应的能量.

解:

(1) 对于玻色子, 基态波函数为

$$\psi_0(x_1)\psi_0(x_2)\psi_0(x_3), \tag{702}$$

相应的能量为 $3E_0=\frac{3}{2}\hbar\omega$; 对于费米子, 基态波函数为

$$\frac{1}{\sqrt{6}}\left(\psi_0(x_1)\psi_1(x_2)\psi_2(x_3)-\psi_1(x_1)\psi_0(x_2)\psi_2(x_3)-\psi_0(x_1)\psi_2(x_2)\psi_1(x_3)\right. \tag{703}$$

$$\left.-\psi_2(x_1)\psi_1(x_2)\psi_0(x_3)+\psi_2(x_1)\psi_0(x_2)\psi_1(x_3)+\psi_1(x_1)\psi_2(x_2)\psi_0(x_3)\right), \tag{704}$$

相应的能量为 $E_0+E_1+E_2=\left(3+\frac{3}{2}\right)\hbar\omega$;

(2) 对于玻色子, 第一激发态波函数为

$$\frac{1}{\sqrt{3}}\left(\psi_0(x_1)\psi_0(x_2)\psi_1(x_3)+\psi_0(x_1)\psi_0(x_3)\psi_1(x_2)+\psi_0(x_1)\psi_0(x_3)\psi_1(x_1)\right), \tag{705}$$

相应的能量为 $2E_0+E_1=\frac{3}{2}\hbar\omega$; 对于费米子, 第一激发态波函数为

$$\frac{1}{\sqrt{6}}\left(\psi_0\left(x_1\right)\psi_1\left(x_2\right)\psi_3\left(x_3\right)-\psi_1\left(x_1\right)\psi_0\left(x_2\right)\psi_3\left(x_3\right)-\psi_0\left(x_1\right)\psi_3\left(x_2\right)\psi_1\left(x_3\right)\right. \tag{706}$$

$$\left.-\psi_3\left(x_1\right)\psi_1\left(x_2\right)\psi_0\left(x_3\right)+\psi_3\left(x_1\right)\psi_0\left(x_2\right)\psi_1\left(x_3\right)+\psi_1\left(x_1\right)\psi_3\left(x_2\right)\psi_0\left(x_3\right)\right), \tag{707}$$

相应的能量为 $E_0+E_1+E_3=\left(4+\frac{3}{2}\right)\hbar\omega$.

5. 与玻色子类似, 定义费米子的梯算符 $\hat{c}$, $\hat{c}^\dagger$, 满足反对易关系:

$$\{\hat{c},\hat{c}\}=0 \tag{708}$$

$$\left\{\hat{c}^\dagger,\hat{c}^\dagger\right\}=0 \tag{709}$$

$$\left\{\hat{c},\hat{c}^\dagger\right\}=1 \tag{710}$$

这里对任意两个算符 $\hat{A}$, $\hat{B}$, 其反对易关系定义为 $\left\{\hat{A},\hat{B}\right\}\equiv\hat{A}\hat{B}+\hat{B}\hat{A}$. 定义算符 $\hat{N}\equiv\hat{c}^\dagger\hat{c}$.

(1) 证明: $\left[\hat{c},\hat{N}\right]=\hat{c}$, $\left[\hat{c}^\dagger,\hat{N}\right]=-\hat{c}^\dagger$.

(2) 证明: $\hat{N}^2=\hat{N}$. 由此判断 $\hat{N}$ 的本征值为多少?

(3) 证明: 真空态 $|0\rangle$ (满足 $\hat{c}\,|0\rangle=0$) 和 $\hat{c}^\dagger\,|0\rangle$ 是 $\hat{N}$ 的本征态.

(4) 在表象 $\left\{|0\rangle\,,\hat{c}^\dagger\,|0\rangle\right\}$ 中, 分别求 $\hat{c}$,$\hat{c}^\dagger$ 和 $\hat{N}$ 的矩阵表示.

解:

(1)

$$\left[\hat{c},\hat{N}\right]=\left[\hat{c},\hat{c}^\dagger\hat{c}\right]=\left\{\hat{c},\hat{c}^\dagger\right\}\hat{c}-\hat{c}^\dagger\left\{\hat{c},\hat{c}\right\}=\hat{c}, \tag{711}$$

$$\left[\hat{c}^\dagger,\hat{N}\right]=\left[\hat{c}^\dagger,\hat{c}^\dagger\hat{c}\right]=\left\{\hat{c}^\dagger,\hat{c}^\dagger\right\}\hat{c}-\hat{c}^\dagger\left\{\hat{c}^\dagger,\hat{c}\right\}=-\hat{c}^\dagger, \tag{712}$$

(2) 由 $\{\hat{c},\hat{c}\}=0$ 得, $\hat{c}\hat{c}=0$; 类似的, $\hat{c}^\dagger\hat{c}^\dagger=0$; 由 $\left\{\hat{c},\hat{c}^\dagger\right\}=1$ 得: $\hat{c}\hat{c}^\dagger=1-\hat{c}^\dagger\hat{c}$; 所以

$$\hat{N}^2=\hat{c}^\dagger\hat{c}\hat{c}^\dagger\hat{c}=\hat{c}^\dagger\left(1-\hat{c}^\dagger\hat{c}\right)\hat{c}=\hat{c}^\dagger\hat{c}-\hat{c}^\dagger\hat{c}^\dagger\hat{c}\hat{c}=\hat{N} \tag{713}$$

令 ψ 为 $\hat{N}$ 的本征态, $\hat{N}\psi=\lambda\psi$, 于是 $\hat{N}^2\psi=\hat{N}\psi$, $\lambda^2\psi=\lambda\psi$, 可得 $\lambda=0$ 或 1.

(3) 由于 $\hat{c}\,|0\rangle=0$, 于是 $\hat{N}\,|0\rangle=\hat{c}^\dagger\hat{c}\,|0\rangle=0$, $\hat{N}\hat{c}^\dagger\,|0\rangle=\hat{c}^\dagger\hat{c}\hat{c}^\dagger\,|0\rangle=\hat{c}^\dagger\left(1-\hat{c}^\dagger\hat{c}\right)|0\rangle=\hat{c}^\dagger\,|0\rangle$.

(4) 可以验证 $|0\rangle$ 与 $\hat{c}^\dagger\,|0\rangle$ 是正交的. 由于 $\hat{c}\,|0\rangle=0$, 故 $\hat{c}$ 的矩阵表示的第 1 列为 $(0,0)^T$; $\hat{c}\hat{c}^\dagger\,|0\rangle=\left(1-\hat{c}^\dagger\hat{c}\right)|0\rangle=|0\rangle$, 故 $\hat{c}$ 的矩阵表示的第 2 列为 $(1,0)^T$; 所以 $\hat{c}^\dagger$ 的矩阵表示为 $\begin{pmatrix}0&1\\0&0\end{pmatrix}$.

由于 $\hat{c}^\dagger\,|0\rangle=\hat{c}^\dagger\,|0\rangle$, 故 $\hat{c}^\dagger$ 的矩阵表示的第 1 列为 $(0,1)^T$; $\hat{c}^\dagger\hat{c}^\dagger\,|0\rangle=0$, 故 $\hat{c}$ 的矩阵表示的第 2 列为 $(0,0)^T$; 所以 $\hat{c}$ 的矩阵表示为 $\begin{pmatrix}1&0\\0&0\end{pmatrix}$.

由于 $\hat{N}\,|0\rangle=0\,|0\rangle$, 故 $\hat{N}$ 的矩阵表示的第 1 列为 $(0,0)^T$; $\hat{N}\hat{c}^\dagger\,|0\rangle=\hat{c}^\dagger\hat{c}\hat{c}^\dagger\,|0\rangle=\hat{c}^\dagger\left(1-\hat{c}^\dagger\hat{c}\right)|0\rangle=\hat{c}^\dagger\,|0\rangle$, 故 $\hat{c}$ 的矩阵表示的第 2 列为 $(0,1)^T$; 所以 $\hat{N}$ 的矩阵表示为 $\begin{pmatrix}0&0\\0&1\end{pmatrix}$. 可以看出 $\begin{pmatrix}0&0\\0&1\end{pmatrix}=\begin{pmatrix}1&0\\0&0\end{pmatrix}\begin{pmatrix}0&1\\0&0\end{pmatrix}$

讨论:

(1) 对于任意线性算符 $\left[\hat{A},\hat{B}\hat{C}\right]=\hat{B}\left[\hat{A},\hat{C}\right]+\left[\hat{A},\hat{B}\right]\hat{C}=\left\{\hat{A},\hat{B}\right\}\hat{C}-\hat{B}\left\{\hat{A},\hat{C}\right\}$.

(2) 本题的结论对于费米型算符具有普适性.

0.14 第十四次作业

1. 中心力场问题的径向方程 $\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\frac{l(l+1)\hbar^2}{2\mu r^2}+V(r)\right]u(r)=Eu(r)$ 可以等效的当作一维能量本征方程, $u(r)$ 相当于波函数, 等效能量算符 $H_l(r)=-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\frac{l(l+1)\hbar^2}{2\mu r^2}+V(r)$, 能量本征值记为 E_{ln_r}, 试用 Fyenman-Hellman 定理 (见 96 页习题 4.7) 证明: l 越大, E_{ln_r} 越高 (n_r 固定).

解: 根据 Feynman-Hellman 定理,

$$\frac{\partial E_{ln_r}}{\partial l}=\langle ln_r|\frac{\partial \hat{H}_l}{\partial l}|ln_r\rangle \tag{714}$$
$$=\langle ln_r|\frac{(2l+1)\hbar^2}{2\mu r^2}|ln_r\rangle \tag{715}$$
$$=\frac{(2l+1)\hbar^2}{2\mu r^2}\langle ln_r|\frac{1}{r^2}|ln_r\rangle>0 \tag{716}$$

所以 l 越大, E_{ln_r} 越高.

2. 令 $\hat{H}$ 为氢原子的哈密顿量,

(1) 计算 $\left[\left[\hat{H},\hat{x}\right],\hat{x}\right]$, 这里 $\hat{x}$ 是坐标算符的 x 分量;

(2) 利用 (1) 的结果, 在氢原子的基态上计算 $\langle\psi_{100}|\hat{x}\hat{H}\hat{x}|\psi_{100}\rangle$.

解:

(1) 由于 $\left[\hat{x},\hat{H}\right]=i\hbar\frac{\hat{p}}{\mu}$, $[\hat{x},\hat{p}]=i\hbar$, 则 $\left[\left[\hat{H},\hat{x}\right],\hat{x}\right]=-\frac{\hbar^2}{\mu}$.

(2) 利用 $\left[\hat{x},\left[\hat{x},\hat{H}\right]\right]=2\hat{x}\hat{H}\hat{x}-\hat{H}\hat{x}^2-\hat{x}^2\hat{H}$ 得:

$$\langle\psi_{100}|\left[\left[\hat{H},\hat{x}\right],\hat{x}\right]|\psi_{100}\rangle=\langle\psi_{100}|-2\hat{x}\hat{H}\hat{x}+\hat{H}\hat{x}^2+\hat{x}^2\hat{H}|\psi_{100}\rangle=-\frac{\hbar^2}{\mu} \tag{717}$$

需要计算积分

$$\langle\psi_{100}|\hat{x}^2|\psi_{100}\rangle=\int\psi^*_{100}(r)\,\hat{x}^2\psi_{100}(r)\,dV \tag{718}$$
$$=\frac{1}{3}\int_0^\infty\frac{1}{\sqrt{\pi}a^{3/2}}e^{-r/a}r^2\frac{1}{\sqrt{\pi}a^{3/2}}e^{-r/a}4\pi r^2dr \tag{719}$$

这里, 得到方程719时用到了对称性, 即 $\langle\psi_{100}|\hat{x}^2|\psi_{100}\rangle=\langle\psi_{100}|\hat{y}^2|\psi_{100}\rangle=\langle\psi_{100}|\hat{z}^2|\psi_{100}\rangle$. 于是,

$$\langle\psi_{100}|\hat{x}^2|\psi_{100}\rangle=\frac{4}{3a^3}\int_0^\infty e^{-2r/a}r^4dr \tag{720}$$
$$=\frac{4}{3a^3}\left(\frac{e^{-2r/a}}{\left(-\frac{2}{a}\right)}r^4\Bigg|_0^\infty-\int_0^\infty\frac{e^{-2r/a}}{\left(-\frac{2}{a}\right)}4r^3dr\right) \tag{721}$$

可见 $\int_0^\infty e^{-2r/a}r^ndr=\frac{na}{2}\int_0^\infty e^{-2r/a}r^{n-1}dr=n!\left(\frac{a}{2}\right)^n\int_0^\infty e^{-2r/a}dr=n!\left(\frac{a}{2}\right)^{n+1}$, 于是 $\int_0^\infty e^{-2r/a}r^4dr=4!\left(\frac{a}{2}\right)^5$. 所以

$$\langle\psi_{100}|\hat{x}^2|\psi_{100}\rangle=\frac{4}{3a^3}4!\left(\frac{a}{2}\right)^5=a^2 \tag{722}$$

由此可得:

$$\langle\psi_{100}|\hat{x}\hat{H}\hat{x}|\psi_{100}\rangle=\frac{1}{2}\left(\frac{\hbar^2}{\mu}+\langle\psi_{100}|\hat{H}\hat{x}^2+\hat{x}^2\hat{H}|\psi_{100}\rangle\right) \tag{723}$$
$$=\frac{1}{2}\left(\frac{\hbar^2}{\mu}+2E_1a^2\right) \tag{724}$$

这里, $E_1=-\frac{\hbar^2}{2\mu a^2}$, 于是

$$\langle\psi_{100}|\,\hat{x}\hat{H}\hat{x}\,|\psi_{100}\rangle=0 \tag{725}$$

3. 粒子处于状态 $\psi\left(x,y,z\right)=A\left(x+y+2z\right)e^{-\lambda r}$, ($\lambda>0$):

(1) $\psi\left(x,y,z\right)$ 是否 $\hat{\boldsymbol{l}}^2$ 的本征态?

(2) $\hat{l}_z$ 在 $\psi\left(x,y,z\right)$ 上的平均值;

(3) $\hat{l}_z$ 的测量值为 $\hbar$ 的概率;

(4) $\hat{l}_y$ 的可能取值和相应的概率.

提示: 把 $\psi\left(x,y,z\right)$ 的角度部分表示为球谐函数.

解:

(1) 利用球坐标,

$$\begin{aligned}\psi\left(x,y,z\right)&=Ar\left(\sin\theta\cos\varphi+\sin\theta\sin\varphi+2\cos\theta\right)e^{-\lambda r} &(726)\\ &=Ar\left(\sqrt{\frac{8\pi}{3}}\left(\frac{1}{2}\left(-Y_{11}+Y_{1-1}\right)+\frac{1}{2i}\left(-Y_{11}-Y_{1-1}\right)\right)+2\sqrt{\frac{4\pi}{3}}Y_{10}\right)e^{-\lambda r} &(727)\\ &=A\sqrt{\frac{2\pi}{3}}r\left(\left(-1+i\right)Y_{11}+\left(1+i\right)Y_{1-1}+2\sqrt{2}Y_{10}\right)e^{-\lambda r} &(728)\end{aligned}$$

由于 $\hat{\boldsymbol{l}}^2Y_{lm}=l\left(l+1\right)\hbar^2Y_{lm}$, 所以 $\psi\left(x,y,z\right)$ 是 $\hat{\boldsymbol{l}}^2$ 的本征态.

(2) 首先归一化的角向波函数可以表示为

$$|\phi\rangle=\frac{1}{2\sqrt{3}}\left(\left(-1+i\right)|11\rangle+\left(1+i\right)|1,-1\rangle+2\sqrt{2}\,|10\rangle\right) \tag{729}$$

于是

$$\begin{aligned}\langle\phi|\,\hat{l}_z\,|\phi\rangle=&\frac{1}{12}\left(\left(-1-i\right)\langle 11|+\left(1-i\right)\langle 1,-1|+2\sqrt{2}\,\langle 10|\right)\hat{l}_z\left(\left(-1+i\right)|11\rangle+\left(1+i\right)|1,-1\rangle+2\sqrt{2}\,|10\rangle\right) &(730)\\ =&\frac{1}{12}\left(\left(-1-i\right)\langle 11|+\left(1-i\right)\langle 1,-1|+2\sqrt{2}\,\langle 10|\right)\left(\hbar\left(-1+i\right)|11\rangle-\hbar\left(1+i\right)|1,-1\rangle\right) &(731)\\ =&0 &(732)\end{aligned}$$

(3) 归一化的角向波函数可以表示为

$$\langle 11\,|\phi\rangle=\frac{|-1+i|}{2\sqrt{3}} \tag{733}$$

所以 $\hat{l}_z$ 的测量值为 $\hbar$ 的概率为 $\frac{1}{6}$.

(4) $\hat{l}_y\,|11\rangle=\frac{\hat{l}_+-\hat{l}_-}{2i}\,|11\rangle=\frac{i\hbar}{\sqrt{2}}\,|10\rangle$; $\hat{l}_y\,|10\rangle=\frac{\hat{l}_+-\hat{l}_-}{2i}\,|10\rangle=\frac{-i\hbar}{\sqrt{2}}\,|11\rangle+\frac{i\hbar}{\sqrt{2}}\,|1-1\rangle$; $\hat{l}_y\,|1-1\rangle=\frac{\hat{l}_+-\hat{l}_-}{2i}\,|1-1\rangle=\frac{-i\hbar}{\sqrt{2}}\,|10\rangle$; 故在基 $\{|11\rangle, |10\rangle, |1-1\rangle\}$ 下, $\hat{l}_y$ 的矩阵表示为: $\frac{\hbar}{\sqrt{2}}\begin{pmatrix}0&-i&0\\ i&0&-i\\ 0&i&0\end{pmatrix}$. 其本征值为 $\hbar$, 0, $-\hbar$. 对应的本征向量为 $|11\rangle_y=\frac{1}{2}(-|11\rangle-i\sqrt{2}\,|10\rangle+|1-1\rangle)$, $|10\rangle_y=\frac{1}{\sqrt{2}}(|11\rangle+|1-1\rangle)$, $|1-1\rangle_y=\frac{1}{2}(-|11\rangle+i\sqrt{2}\,|10\rangle+|1-1\rangle)$. $\hat{l}_y$ 的测量值为 $\hbar$ 的概率幅

$$\langle 11|_y\,|\phi\rangle=\frac{1}{4\sqrt{3}}\left(\left(1-i\right)-i\sqrt{2}\cdot 2\sqrt{2}+\left(1+i\right)\right)=\frac{1-2i}{2\sqrt{3}} \tag{734}$$

相应的概率为 $\frac{5}{12}$. 类似的, 可得 $\hat{l}_y$ 的测量值为 0 的概率为 $\frac{1}{6}$, $\hat{l}_y$ 的测量值为 $-\hbar$ 的概率为 $\frac{5}{12}$.

4. 对于氢原子体系, 定义算符 $\hat{\boldsymbol{M}}=\frac{1}{2m}\left(\hat{\boldsymbol{p}}\times\hat{\boldsymbol{l}}-\hat{\boldsymbol{l}}\times\hat{\boldsymbol{p}}\right)-\frac{e^2\boldsymbol{r}}{4\pi\epsilon_0 r}$, 证明 $\hat{\boldsymbol{M}}$ 是守恒量.

解: 由方程522得: $\hat{\boldsymbol{p}}\times\hat{\boldsymbol{l}}-\hat{\boldsymbol{l}}\times\hat{\boldsymbol{p}}=\frac{1}{i\hbar}\left[\hat{\boldsymbol{l}}^2,\hat{\boldsymbol{p}}\right]$. 体系的 Hamiltonian $\hat{H}=\frac{\hat{\boldsymbol{p}}^2}{2m}-\frac{e^2}{4\pi\epsilon_0 r}$. 则

$$\begin{aligned}\left[\hat{\boldsymbol{M}},\hat{H}\right]&=\left[\frac{1}{i\hbar}\frac{1}{2m}\left[\hat{\boldsymbol{l}}^2,\hat{\boldsymbol{p}}\right]-\frac{e^2\boldsymbol{r}}{4\pi\epsilon_0 r},\hat{H}\right] &(735)\\
&=\frac{1}{i\hbar}\frac{1}{2m}\left[\left[\hat{\boldsymbol{l}}^2,\hat{\boldsymbol{p}}\right],\hat{H}\right]-\left[\frac{e^2\boldsymbol{r}}{4\pi\epsilon_0 r},\hat{H}\right] &(736)\\
&=-\frac{1}{i\hbar}\frac{1}{2m}\left[\left[\hat{H},\hat{\boldsymbol{l}}^2\right],\hat{\boldsymbol{p}}\right]+\frac{1}{i\hbar}\frac{1}{2m}\left[\left[\hat{\boldsymbol{p}},\hat{H}\right],\hat{\boldsymbol{l}}^2\right]-\left[\frac{e^2\boldsymbol{r}}{4\pi\epsilon_0 r},\frac{\hat{\boldsymbol{p}}^2}{2m}\right] &(737)\end{aligned}$$

由于 $\left[\hat{H},\hat{\boldsymbol{l}}^2\right]=0$, $\left[\hat{\boldsymbol{p}},\hat{H}\right]=\left[\hat{\boldsymbol{p}},-\frac{e^2}{4\pi\epsilon_0 r}\right]=i\hbar\frac{e^2}{4\pi\epsilon_0}\frac{\boldsymbol{r}}{r^3}$, 于是

$$\begin{aligned}\left[\hat{\boldsymbol{M}},\hat{H}\right]&=\frac{1}{2m}\left[\frac{e^2}{4\pi\epsilon_0}\frac{\boldsymbol{r}}{r^3},\hat{\boldsymbol{l}}^2\right]-\left[\frac{e^2\boldsymbol{r}}{4\pi\epsilon_0 r},\frac{\hat{\boldsymbol{p}}^2}{2m}\right] &(738)\\
&=\frac{1}{2m}\frac{e^2}{4\pi\epsilon_0}\left(\left[\frac{\boldsymbol{r}}{r^3},\hat{\boldsymbol{l}}^2\right]-\left[\frac{\boldsymbol{r}}{r},\hat{\boldsymbol{p}}^2\right]\right) &(739)\\
&=\frac{1}{2m}\frac{e^2}{4\pi\epsilon_0}\left(\left[\frac{\boldsymbol{r}}{r},\frac{\hat{\boldsymbol{l}}^2}{r^2}\right]-\left[\frac{\boldsymbol{r}}{r},\hat{\boldsymbol{p}}^2\right]\right) &(740)\end{aligned}$$

由方程556得, $\frac{\hat{\boldsymbol{l}}^2}{r^2}=\hat{\boldsymbol{p}}^2-\hat{p}_r^2$, 那么

$$\left[\hat{\boldsymbol{M}},\hat{H}\right]=-\frac{1}{2m}\frac{e^2}{4\pi\epsilon_0}\left(\left[\frac{\boldsymbol{r}}{r},\hat{p}_r^2\right]\right) \tag{741}$$

而 $\hat{p}_r=\frac{\hbar}{i}\frac{1}{r}+\frac{\hbar}{i}\frac{\partial}{\partial r}$, 所以

$$\left[\frac{\boldsymbol{r}}{r},\hat{p}_r^2\right]=\hat{p}_r\left[\frac{\boldsymbol{r}}{r},\hat{p}_r\right]+\left[\frac{\boldsymbol{r}}{r},\hat{p}_r\right]\hat{p}_r \tag{742}$$

这里 $\frac{\boldsymbol{r}}{r}=(\sin\theta\cos\varphi,\sin\theta\sin\varphi,\cos\theta)$ 只是角向的函数, 于是 $\left[\frac{\boldsymbol{r}}{r},\hat{p}_r\right]=0$, 所以 $\left[\hat{\boldsymbol{M}},\hat{H}\right]=0$.

5. 已知氢原子的能量本征态为 $|nlm\rangle$,

(1) 利用位力定理证明 $\langle nlm|\frac{1}{r}|nlm\rangle=\frac{1}{n^2a}$, 这里 a 是玻尔半径, $r=|\boldsymbol{r}|$.

(2) 判断 $\langle nlm|\frac{1}{r}|nlm\rangle=\frac{1}{\langle nlm|r|nlm\rangle}$ 是否成立? 给出判断根据.

解:

(1) 由位力定理得: $\langle nlm|\boldsymbol{r}\cdot\nabla V|nlm\rangle=2\langle nlm|\hat{T}|nlm\rangle=-\frac{e^2}{4\pi\epsilon_0}\langle nlm|\boldsymbol{r}\cdot\nabla\frac{1}{r}|nlm\rangle=\frac{e^2}{4\pi\epsilon_0}\langle nlm|\frac{1}{r}|nlm\rangle$. 而 $\langle nlm|\boldsymbol{r}\cdot\nabla V|nlm\rangle=-\frac{e^2}{4\pi\epsilon_0}\langle nlm|\boldsymbol{r}\cdot\nabla\frac{1}{r}|nlm\rangle=\frac{e^2}{4\pi\epsilon_0}\langle nlm|\frac{1}{r}|nlm\rangle$. 于是

$$2\langle nlm|\hat{T}|nlm\rangle=\frac{e^2}{4\pi\epsilon_0}\langle nlm|\frac{1}{r}|nlm\rangle \tag{743}$$

另外 $\langle nlm|\hat{T}|nlm\rangle-\frac{e^2}{4\pi\epsilon_0}\langle nlm|\frac{1}{r}|nlm\rangle=E_n$, 所以

$$\begin{aligned}\langle nlm|\frac{1}{r}|nlm\rangle&=-\frac{8\pi\epsilon_0}{e^2}E_n &(744)\\
&=-\frac{8\pi\epsilon_0}{e^2}\left(-\frac{e^2}{8\pi\epsilon_0 an^2}\right)=\frac{1}{n^2a} &(745)\end{aligned}$$

(2) 若 $\langle nlm|\frac{1}{r}|nlm\rangle = \frac{1}{\langle nlm|r|nlm\rangle}$, 则 $\langle nlm|r|nlm\rangle = \frac{1}{n^2a}$ 应该成立. 下面计算 $\langle nlm|r|nlm\rangle = \int_0^\infty dr\chi_n r\chi_n$, 这里, χ_n 是实的, 且 $\chi_n = rR_n$. χ_n 满足方程

$$\chi_n'' = \left[\frac{l(l+1)}{r^2} - \frac{2mE_n}{\hbar^2} - \frac{2m}{\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)\frac{1}{r}\right]\chi_n \tag{746}$$

利用 $-\frac{2mE_n}{\hbar^2} = \frac{1}{a^2n^2}$, $\frac{me^2}{4\pi\epsilon_0\hbar^2} = \frac{1}{a}$ 得:

$$\chi_n'' = \left[\frac{l(l+1)}{r^2} + \frac{1}{a^2n^2} - \frac{2}{a}\frac{1}{r}\right]\chi_n \tag{747}$$

$$\int dr\chi_n' r\chi_n' = \chi_n' r\chi_n\big|_0^\infty - \int dr\frac{d}{dr}(\chi_n' r)\chi_n \tag{748}$$

$$= -\int dr\chi_n'' r\chi_n - \int dr\chi_n'\chi_n \tag{749}$$

这里, $\int dr\chi_n'\chi_n = -\int dr\chi_n\chi_n'$, 故 $\int dr\chi_n'\chi_n = 0$. 方程747代入方程749得:

$$\int dr\chi_n' r\chi_n' = -\int dr\left[\frac{l(l+1)}{r^2} + \frac{1}{a^2n^2} - \frac{2}{a}\frac{1}{r}\right]\chi_n r\chi_n \tag{750}$$

$$= -l(l+1)\left\langle\frac{1}{r}\right\rangle - \frac{1}{a^2n^2}\langle r\rangle + \frac{2}{a} \tag{751}$$

另一方面,

$$\int dr\chi_n' r\chi_n' = \chi_n'\frac{r^2}{2}\chi_n'\Big|_0^\infty - \int dr\chi_n''\frac{r^2}{2}\chi_n' - \int dr\chi_n'\frac{r^2}{2}\chi_n'' = -\int dr\chi_n' r^2\chi_n'' \tag{752}$$

$$= -\int dr\chi_n' r^2\left[\frac{l(l+1)}{r^2} + \frac{1}{a^2n^2} - \frac{2}{a}\frac{1}{r}\right]\chi_n \tag{753}$$

$$= 0 - \frac{1}{a^2n^2}\int dr\chi_n' r^2\chi_n + \frac{2}{a}\int dr\chi_n' r\chi_n \tag{754}$$

这里, $\int dr\chi_n' r^2\chi_n = -2\int dr\chi_n r\chi_n - \int dr\chi_n r^2\chi_n'$, 即 $\int dr\chi_n r^2\chi_n' = -\langle r\rangle$, 类似的, $\int dr\chi_n' r\chi_n = -\frac{1}{2}$. 代入方程754得:

$$\int dr\chi_n' r\chi_n' = \frac{1}{a^2n^2}\langle r\rangle - \frac{1}{a} \tag{755}$$

式751与755相等得:

$$-l(l+1)\left\langle\frac{1}{r}\right\rangle - \frac{1}{a^2n^2}\langle r\rangle + \frac{2}{a} = \frac{1}{a^2n^2}\langle r\rangle - \frac{1}{a} \tag{756}$$

(这是一个简化的 Kramer 关系的推导) 故

$$\langle r\rangle = n^2a\left(\frac{3}{2} - \frac{l(l+1)a}{2}\left\langle\frac{1}{r}\right\rangle\right) \tag{757}$$

$$= \frac{3}{2}n^2a - \frac{l(l+1)a}{2} \neq n^2a \tag{758}$$

故 $\langle nlm|\frac{1}{r}|nlm\rangle$ 不成立.

6. $t=0$ 时, 氢原子的波函数为: $|\psi(0)\rangle = A\left[2|100\rangle + |210\rangle + \sqrt{2}|211\rangle + \sqrt{3}|21-1\rangle\right]$. 不考虑自旋.

(1) 求该体系能量的平均值;

(2) 求 $t>0$ 时刻体系的状态 $|\psi(t)\rangle$;

(3) 任意 $t>0$ 时刻体系处于 $l=1$, $m=1$ 的概率;

(4) 一次测量发现 $l=1$, $l_x=1$, 求测量后瞬间体系的波函数.

解: 确定归一化因子 A, $\langle\psi(0)|\psi(0)\rangle=|A|^2(4+1+2+3)=1$, 故 A 可以取为 $\frac{1}{\sqrt{10}}$.

(1) 对于氢原子体系, $\hat{H}|\psi(0)\rangle=A\left[2E_1|100\rangle+E_2|210\rangle+\sqrt{2}E_2|211\rangle+\sqrt{3}E_2|21-1\rangle\right]$, 则

$$\begin{aligned}\langle\psi(0)|\hat{H}|\psi(0)\rangle=&|A|^2(4E_1+E_2+2E_2+3E_2) &(759)\\ =&\frac{1}{5}(2E_1+3E_2) &(760)\\ =&-\frac{e^2}{40\pi\epsilon_0 a}\left(2+\frac{3}{4}\right)=-\frac{11e^2}{160\pi\epsilon_0 a} &(761)\end{aligned}$$

(2) $|\psi(0)\rangle$ 为非本征态. 由非定态含时演化的一般公式得:

$$|\psi(t)\rangle=\frac{1}{\sqrt{10}}\left[2|100\rangle e^{-iE_1t/\hbar}+\left(|210\rangle+\sqrt{2}|211\rangle+\sqrt{3}|21-1\rangle\right)e^{-iE_2t/\hbar}\right] \tag{762}$$

这里 $E_n=-\frac{e^2}{8\pi\epsilon_0 an^2}$.

(3) 只有 $|211\rangle$ 的角向 $l=1$, $m=1$, 故体系处于 $l=1$, $m=1$ 的概率为 $\langle 211|\psi(t)\rangle=\frac{1}{\sqrt{5}}$, 即处于 $l=1$, $m=1$ 的概率为 $\frac{1}{5}$.

(4) 在 $l=1$ 的子空间, $\left(\hat{\boldsymbol{l}}^2,\hat{l}_z\right)$ 的共同本征态作为基矢, 我们在前面已经得到 $\hat{l}_x$ 的本征值和相应的本征向量为: $l'_{x1}=\hbar$, $v_1=\frac{1}{2}\left(|11\rangle+\sqrt{2}|10\rangle+|1-1\rangle\right)$; $l'_{x2}=0$, $v_2=\frac{1}{\sqrt{2}}\left(|11\rangle-|1-1\rangle\right)$; $l'_{x3}=\hbar$, $v_3=\frac{1}{2}\left(|11\rangle-\sqrt{2}|10\rangle+|1-1\rangle\right)$. 测量发现 $l=1$, $l_x=1$, 即体系坍缩到 $l'_{x1}=\hbar$ 对应的本征态, 故测量后瞬间体系的波函数为 $|\psi\rangle=\frac{1}{2}\left(|211\rangle+\sqrt{2}|210\rangle+|2,1-1\rangle\right)$.

0.15 第十五次作业 2021.06.29

1. (1) 证明 $e^{i\boldsymbol{\alpha}\cdot\boldsymbol{\sigma}} = \sigma_0 \cos\alpha + i\left(\boldsymbol{e}_\alpha \cdot \boldsymbol{\sigma}\right)\sin\alpha$. 这里 $\boldsymbol{e}_\alpha = \frac{\boldsymbol{\alpha}}{\alpha}$ 为 $\boldsymbol{\alpha}$ 方向的单位矢量, $\alpha = |\boldsymbol{\alpha}|$;

(2) 证明 $e^{-i\frac{\alpha}{2}\sigma_x}\sigma_y e^{i\frac{\alpha}{2}\sigma_x} = \sigma_y \cos\alpha + \sigma_z \sin\alpha$.

证: (1) $\boldsymbol{\alpha}\cdot\boldsymbol{\sigma} = \alpha\boldsymbol{e}_\alpha\cdot\boldsymbol{\sigma}$, $\left(\boldsymbol{e}_\alpha\cdot\boldsymbol{\sigma}\right)^2 = e_{\alpha,i}\sigma_i e_{\alpha,j}\sigma_j = e_{\alpha,i}e_{\alpha,j}\sigma_i\sigma_j = e_{\alpha,i}e_{\alpha,j}\left(\delta_{ij}\sigma_0 + \mathrm{i}\epsilon_{ijk}\sigma_k\right) = \boldsymbol{e}_\alpha\cdot\boldsymbol{e}_\alpha\sigma_0 + \mathrm{i}\boldsymbol{e}_\alpha\times\boldsymbol{e}_\alpha\cdot\boldsymbol{\sigma} = \sigma_0$. 于是,

$$
\begin{aligned}
e^{i\boldsymbol{\alpha}\cdot\boldsymbol{\sigma}} &= e^{i\alpha\boldsymbol{e}_\alpha\cdot\boldsymbol{\sigma}} = \sum_{n=0}^{\infty}\frac{\left(i\alpha\boldsymbol{e}_\alpha\cdot\boldsymbol{\sigma}\right)^n}{n!} && (763)\\
&= \sum_{k=0}^{\infty}\frac{\left(i\alpha\boldsymbol{e}_\alpha\cdot\boldsymbol{\sigma}\right)^{2k}}{(2k)!} + \sum_{k=0}^{\infty}\frac{\left(i\alpha\boldsymbol{e}_\alpha\cdot\boldsymbol{\sigma}\right)^{2k+1}}{(2k+1)!} && (764)\\
&= \sum_{k=0}^{\infty}\frac{(-1)^k\alpha^k}{(2k)!}\sigma_0 + i\boldsymbol{e}_\alpha\cdot\boldsymbol{\sigma}\sum_{k=0}^{\infty}\frac{(-1)^k\alpha^{2k+1}}{(2k+1)!} && (765)\\
&= \sigma_0\cos\alpha + i\left(\boldsymbol{e}_\alpha\cdot\boldsymbol{\sigma}\right)\sin\alpha && (766)
\end{aligned}
$$

(2) 由 (1) 得:

$$
\begin{aligned}
e^{-i\frac{\alpha}{2}\sigma_x}\sigma_y e^{i\frac{\alpha}{2}\sigma_x} &= \left(\sigma_0\cos\frac{\alpha}{2} - i\sigma_x\sin\frac{\alpha}{2}\right)\sigma_y\left(\sigma_0\cos\frac{\alpha}{2} + i\sigma_x\sin\frac{\alpha}{2}\right) && (767)\\
&= \left(\sigma_0\cos\frac{\alpha}{2} - i\sigma_x\sin\frac{\alpha}{2}\right)\left(\sigma_y\cos\frac{\alpha}{2} + i\sigma_y\sigma_x\sin\frac{\alpha}{2}\right) && (768)\\
&= \left(\sigma_0\cos\frac{\alpha}{2} - i\sigma_x\sin\frac{\alpha}{2}\right)\left(\sigma_y\cos\frac{\alpha}{2} + \sigma_z\sin\frac{\alpha}{2}\right) && (769)\\
&= \sigma_y\cos^2\frac{\alpha}{2} - i\sigma_x\sin\frac{\alpha}{2}\sigma_y\cos\frac{\alpha}{2} + \sigma_z\cos\frac{\alpha}{2}\sin\frac{\alpha}{2} - i\sigma_x\sin\frac{\alpha}{2}\sigma_z\sin\frac{\alpha}{2} && (770)\\
&= \sigma_y\cos\frac{\alpha}{2}^2 + \sigma_z\sin\frac{\alpha}{2}\cos\frac{\alpha}{2} + \sigma_z\cos\frac{\alpha}{2}\sin\frac{\alpha}{2} - \sigma_y\sin^2\frac{\alpha}{2} && (771)\\
&= \sigma_y\cos\alpha + \sigma_z\sin\alpha && (772)
\end{aligned}
$$

2. 已知 Pauli 矩阵 σ_α $(\alpha = x, y, z)$

(1) 求 σ_y 的本征值和本征态;

(2) 若取 σ_y 的本征态作为基矢 (即在 σ_y 的表象里), 求 σ_y, σ_x 和 σ_z.

解: (1) $\det\left(\sigma_y - \lambda\sigma_0\right) = 0$, 得 $\lambda = \pm 1$. 当 $\lambda = 1$ 时, $\begin{pmatrix} -1 & -i \\ i & -1 \end{pmatrix} \to \begin{pmatrix} 1 & i \\ 0 & 0 \end{pmatrix}$, 于是 $v_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}$. 类似的, $\lambda = -1$ 时的本征向量为 $v_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$.

(2) v_1 和 v_2 对应的基矢分别表示为 $|y,+\rangle = \frac{1}{\sqrt{2}}\left(|z,+\rangle + i\,|z,-\rangle\right)$, $|y,-\rangle = \frac{1}{\sqrt{2}}\left(|z,+\rangle - i\,|z,-\rangle\right)$. 令 $\hat{I} = |y,+\rangle\langle y,+| + |y,-\rangle\langle y,-|$. 在 σ_y 的表象里, $\sigma_y = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

$$
\begin{aligned}
\hat{\sigma}_z\,|y,+\rangle &= \left(|z,+\rangle\langle z,+| - |z,-\rangle\langle z,-|\right)|y,+\rangle && (773)\\
&= |z,+\rangle\frac{1}{\sqrt{2}} - |z,-\rangle\frac{i}{\sqrt{2}} && (774)\\
&= |y,-\rangle && (775)
\end{aligned}
$$

$$\hat{\sigma}_z\left|y,-\right\rangle = \left(\left|z,+\right\rangle\left\langle z,+\right| - \left|z,-\right\rangle\left\langle z,-\right|\right)\left|y,-\right\rangle \tag{776}$$

$$= \left|z,+\right\rangle\frac{1}{\sqrt{2}} + \left|z,-\right\rangle\frac{i}{\sqrt{2}} \tag{777}$$

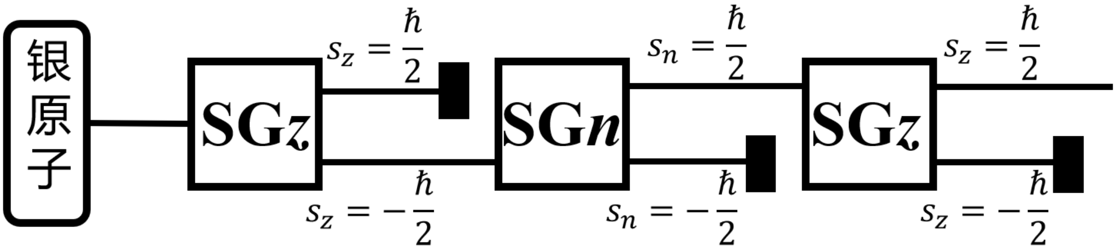
$$= \left|y,+\right\rangle \tag{778}$$

于是 $\sigma_z = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. 同理可得 $\sigma_x = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$.

3. 考虑一个电子在均匀沿 z 方向的均匀磁场中运动, $\hat{H} = -\hat{s}_z B$. 在 $t = 0$ 时刻测量到电子自旋沿 $+y$ 方向. 求在 $t > 0$ 时自旋的波函数, 及沿 x 方向的平均极化率 (正比于 $\hat{s}_x$ 的平均值).

解: 已知 $\hat{H} = -\frac{\hbar B}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. $t = 0$ 时刻测量到电子自旋沿 $+y$ 方向, 即 $\left|\chi(t=0)\right\rangle = \frac{1}{\sqrt{2}}\left(\left|z,+\right\rangle + i\left|z,-\right\rangle\right)$. 于是在 $t > 0$ 时, $\left|\chi(t)\right\rangle = \frac{1}{\sqrt{2}}\left(\left|z,+\right\rangle e^{i\frac{B}{2}t} + i\left|z,-\right\rangle e^{-i\frac{B}{2}t}\right)$. 用旋量表示 $\chi(t) = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{i\frac{B}{2}t} \\ ie^{-i\frac{B}{2}t} \end{pmatrix}$, 则平均极化率 $\chi^{\dagger}(t)\sigma_x\chi(t) = \sin(Bt)$.

4. 一束自旋 $\frac{1}{2}$ 的基态银原子 (不考虑轨道角动量) 如下穿过一系列斯特恩 -盖拉赫装置 (如图: SG):



- 第一个斯特恩 -盖拉赫装置 (如图: SGz) 的磁场方向为 z, 并且只能让自旋为 $s_z = -\frac{\hbar}{2}$ 的银原子通过, 挡住了自旋为 $s_z = \frac{\hbar}{2}$ 的银原子;
- 第二个斯特恩 -盖拉赫装置 (如图: SGn) 的磁场方向为 $\boldsymbol{n}$, 并且只能让自旋为 $s_n = \frac{\hbar}{2}$ 的银原子通过, 挡住了自旋为 $s_n = -\frac{\hbar}{2}$ 的银原子. s_n 是 $\hat{\boldsymbol{s}}\cdot\boldsymbol{n}$ 的本征值, $\hat{\boldsymbol{s}}$ 是自旋算符, $\boldsymbol{n} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$, $0 \le \theta < \pi$, $0 \le \varphi < 2\pi$.
- 第三个斯特恩 -盖拉赫装置的磁场方向为 z(如图: SGz), 并且只能让自旋为 $s_z = \frac{\hbar}{2}$ 的银原子通过, 挡住了自旋为 $s_z = -\frac{\hbar}{2}$ 的银原子.

设能够通过第一个斯特恩 -盖拉赫装置的银原子的总数为 N,

(1) 计算通过第三个斯特恩 -盖拉赫装置的银原子总数.

(2) 通过计算判断如何设定第二个斯特恩 -盖拉赫装置的磁场方向, 才能使通过第三个斯特恩 -盖拉赫装置的原子数最多.

解: (1) 第一个斯特恩 -盖拉赫装置的银原子的总数为 N, 处于状态 $\left|z,-\right\rangle \to \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, 即进入到第二个斯特恩 -盖拉赫装置的银原子的量子态.

对于第二个斯特恩 -盖拉赫装置, 由 $\det(\boldsymbol{\sigma}\cdot\boldsymbol{n}-\lambda I)=0$ 得

$$\det\begin{pmatrix}\cos\theta-\lambda & \sin\theta e^{-i\varphi}\\ \sin\theta e^{i\varphi} & -\cos\theta-\lambda\end{pmatrix}=0 \tag{779}$$

所以 $\lambda=\pm1$. 当 $\lambda_1=1$ 时,

$$\begin{pmatrix}\cos\theta-1 & \sin\theta e^{-i\varphi}\\ \sin\theta e^{i\varphi} & -\cos\theta-1\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix}=0 \tag{780}$$

所以 $\frac{a}{b}=-\frac{\sin\theta e^{-i\varphi}}{\cos\theta-1}=\frac{\cos\frac{\theta}{2}e^{-\varphi}}{\sin\frac{\theta}{2}}$, 此时本征态为 $\begin{pmatrix}\cos\frac{\theta}{2}e^{-i\varphi}\\ \sin\frac{\theta}{2}\end{pmatrix}$. 因此通过第二个斯特恩 -盖拉赫装置原子的量子态为 $\begin{pmatrix}\cos\frac{\theta}{2}e^{-i\varphi}\\ \sin\frac{\theta}{2}\end{pmatrix}$. 处于该量子态的原子的概率为:

$$\left|\begin{pmatrix}\cos\frac{\theta}{2}e^{-i\varphi}\\ \sin\frac{\theta}{2}\end{pmatrix}^{\dagger}\begin{pmatrix}0\\ 1\end{pmatrix}\right|=\sin^2\frac{\theta}{2} \tag{781}$$

能通过第三个斯特恩 -盖拉赫装置的原子的量子态为 $|z,+\rangle\to\begin{pmatrix}1\\ 0\end{pmatrix}$,

$$\left|\begin{pmatrix}1\\ 0\end{pmatrix}^{\dagger}\begin{pmatrix}\cos\frac{\theta}{2}e^{-i\varphi}\\ \sin\frac{\theta}{2}\end{pmatrix}\right|^2=\cos^2\frac{\theta}{2} \tag{782}$$

所以通过第三个斯特恩 -盖拉赫装置的原子总数为 $N\sin^2\frac{\theta}{2}\cos^2\frac{\theta}{2}=\frac{N}{4}\sin^2\theta$.

(2) 为使通过第三个斯特恩 -盖拉赫装置的原子数最多, 需要使 $\theta=\frac{\pi}{2}$, φ 任意.

5. 考虑轨道角动量 $\hbar$ 与自旋角动量 $\frac{\hbar}{2}$ 的合成. 令 $\hat{\boldsymbol{j}}=\hat{\boldsymbol{l}}+\hat{\boldsymbol{s}}$, 取基矢为

$$\{|11\rangle\left|\frac{1}{2}\frac{1}{2}\right\rangle,|1,-1\rangle\left|\frac{1}{2},-\frac{1}{2}\right\rangle,|1,-1\rangle\left|\frac{1}{2}\frac{1}{2}\right\rangle,|10\rangle\left|\frac{1}{2},-\frac{1}{2}\right\rangle,|10\rangle\left|\frac{1}{2}\frac{1}{2}\right\rangle,|11\rangle\left|\frac{1}{2},-\frac{1}{2}\right\rangle\}.$$

在此表象下, 求 $\hat{\boldsymbol{j}}^2$ 和 $\hat{j}_z$ 的矩阵表示.

解:

对于 $\hat{\boldsymbol{j}}^2 = \hat{\boldsymbol{l}}^2 + \hat{\boldsymbol{s}}^2 + 2\hat{\boldsymbol{l}} \cdot \hat{\boldsymbol{s}} = \hat{\boldsymbol{l}}^2 + \hat{\boldsymbol{s}}^2 + \hat{l}_+\hat{s}_- + \hat{l}_-\hat{s}_+ + 2\hat{l}_z\hat{s}_z$, 则

$$\hat{\boldsymbol{j}}^2 \left|1m\right\rangle \left|\frac{1}{2}m_s\right\rangle = \left(\hat{\boldsymbol{l}}^2 + \hat{\boldsymbol{s}}^2 + \hat{l}_+\hat{s}_- + \hat{l}_-\hat{s}_+ + 2\hat{l}_z\hat{s}_z\right)\left|1m\right\rangle \left|\frac{1}{2}m_s\right\rangle \tag{783}$$

$$= \left(1\left(1+1\right)\hbar^2 + \frac{1}{2}\left(\frac{1}{2}+1\right)\hbar^2 + 2\hbar^2 m m_s\right)\left|1m\right\rangle \left|\frac{1}{2}m_s\right\rangle \tag{784}$$

$$+ \hbar^2\sqrt{1\left(1+1\right) - m\left(m+1\right)}\sqrt{\frac{1}{2}\left(\frac{1}{2}+1\right) - m_s\left(m_s-1\right)}\left|1, m+1\right\rangle \left|\frac{1}{2}, m_s - \frac{1}{2}\right\rangle \tag{785}$$

$$+ \hbar^2\sqrt{1\left(1+1\right) - m\left(m-1\right)}\sqrt{\frac{1}{2}\left(\frac{1}{2}+1\right) - m_s\left(m_s+1\right)}\left|1, m-1\right\rangle \left|\frac{1}{2}, m_s + \frac{1}{2}\right\rangle \tag{786}$$

$$= \left(2\hbar^2 + \frac{3}{4}\hbar^2 + 2\hbar^2 m m_s\right)\left|1m\right\rangle \left|\frac{1}{2}m_s\right\rangle \tag{787}$$

$$+ \hbar^2\sqrt{2 - m\left(m+1\right)}\sqrt{\frac{3}{4} - m_s\left(m_s-1\right)}\left|1, m+1\right\rangle \left|\frac{1}{2}, m_s - \frac{1}{2}\right\rangle \tag{788}$$

$$+ \hbar^2\sqrt{2 - m\left(m-1\right)}\sqrt{\frac{3}{4} - m_s\left(m_s+1\right)}\left|1, m-1\right\rangle \left|\frac{1}{2}, m_s + \frac{1}{2}\right\rangle \tag{789}$$

于是,

$$\hat{\boldsymbol{j}}^2 \left|11\right\rangle \left|\frac{1}{2}\frac{1}{2}\right\rangle = \frac{15\hbar^2}{4}\left|11\right\rangle \left|\frac{1}{2}\frac{1}{2}\right\rangle \tag{790}$$

$$\hat{\boldsymbol{j}}^2 \left|1,-1\right\rangle \left|\frac{1}{2},-\frac{1}{2}\right\rangle = \frac{15\hbar^2}{4}\left|1,-1\right\rangle \left|\frac{1}{2},-\frac{1}{2}\right\rangle \tag{791}$$

$$\hat{\boldsymbol{j}}^2 \left|1,-1\right\rangle \left|\frac{1}{2}\frac{1}{2}\right\rangle = \frac{7\hbar^2}{4}\left|1,-1\right\rangle \left|\frac{1}{2}\frac{1}{2}\right\rangle + \sqrt{2}\hbar^2\left|1,0\right\rangle \left|\frac{1}{2} - \frac{1}{2}\right\rangle \tag{792}$$

$$\hat{\boldsymbol{j}}^2 \left|10\right\rangle \left|\frac{1}{2},-\frac{1}{2}\right\rangle = \frac{11\hbar^2}{4}\left|10\right\rangle \left|\frac{1}{2},-\frac{1}{2}\right\rangle + \sqrt{2}\hbar^2\left|1,-1\right\rangle \left|\frac{1}{2}\frac{1}{2}\right\rangle \tag{793}$$

$$\hat{\boldsymbol{j}}^2 \left|10\right\rangle \left|\frac{1}{2}\frac{1}{2}\right\rangle = \frac{11\hbar^2}{4}\left|10\right\rangle \left|\frac{1}{2}\frac{1}{2}\right\rangle + \sqrt{2}\hbar^2\left|11\right\rangle \left|\frac{1}{2},-\frac{1}{2}\right\rangle \tag{794}$$

$$\hat{\boldsymbol{j}}^2 \left|11\right\rangle \left|\frac{1}{2},-\frac{1}{2}\right\rangle = \frac{7\hbar^2}{4}\left|11\right\rangle \left|\frac{1}{2},-\frac{1}{2}\right\rangle + \sqrt{2}\hbar^2\left|10\right\rangle \left|\frac{1}{2}\frac{1}{2}\right\rangle \tag{795}$$

所以 $\hat{\boldsymbol{j}}^2$ 的矩阵表示为:

$$\hat{\boldsymbol{j}}^2 \to \hbar^2 \begin{pmatrix} \frac{15}{4} & & & & & \\ & \frac{15}{4} & & & & \\ & & \frac{7}{4} & \sqrt{2} & & \\ & & \sqrt{2} & \frac{11}{4} & & \\ & & & & \frac{11}{4} & \sqrt{2} \\ & & & & \sqrt{2} & \frac{7}{4} \end{pmatrix} \tag{796}$$

$$\hat{j}_z\left|1m\right\rangle \left|\frac{1}{2}m_s\right\rangle = \left(\hat{l}_z + \hat{s}_z\right)\left|1m\right\rangle \left|\frac{1}{2}m_s\right\rangle = \left(m + m_s\right)\hbar\left|1m\right\rangle \left|\frac{1}{2}m_s\right\rangle \tag{797}$$

所以 $\hat{j}_z$ 的矩阵表示为:

$$\hat{j}_z \to \hbar \begin{pmatrix} \frac{3}{2} & & & & & \\ & -\frac{3}{2} & & & & \\ & & -\frac{1}{2} & & & \\ & & & -\frac{1}{2} & & \\ & & & & \frac{1}{2} & \\ & & & & & \frac{1}{2} \end{pmatrix} \tag{798}$$

6. 两个自旋为 $\frac{1}{2}$ 的粒子组成一个复合体系. 自旋 A 在 $S_z = \frac{1}{2}$ 的本征态, 自旋 B 在 $S_x = \frac{1}{2}$ 的本征态. 求发现体系总自旋为 0 的概率.

解: 两自旋的量子态为 $|\psi\rangle = |\uparrow\rangle_1 \otimes \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_2 + |\downarrow\rangle_2\right) = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1 |\uparrow\rangle_2 + |\uparrow\rangle_1 |\downarrow\rangle_2\right)$. 总自旋为 0 的量子态为 $|00\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2)$. 体系总自旋为 0 的概率为 $|\langle 00|\, \psi\rangle|^2 = \frac{1}{4}$.

7. 考虑处于一维量子谐振子势中的粒子, 谐振子是 $V(x) = \frac{1}{2}kx^2$, $k = \mu\omega^2$. μ 为粒子质量, 其能量本征值为 $E_n^{(0)} = \left(n + \frac{1}{2}\right)\hbar\omega$, $n = 0, 1, 2, \cdots$. 如果质量 μ 有一个微小的变化 $\mu \to (1-\epsilon)\mu$, ϵ 是小量, 并且 $\epsilon > 0$.

(a) 计算新的谐振子势中, 粒子的精确能量本征值; 并把它展开到 ϵ 的两阶.

(b) 利用定态微扰论, 计算基态能量本征值的一阶修正, 并与 (a) 中的结果相比较.

解: (a) 令 $\tilde{\mu} = (1-\epsilon)\mu$. 变化后一维量子谐振子的 Hamiltonian 为

$$\hat{H} = \frac{\hat{p}^2}{2\tilde{\mu}} + \frac{1}{2}\tilde{\mu}\omega^2 x^2 \tag{799}$$

由变化前谐振子势中粒子的能量本征值为 $E_n^{(0)} = \left(n + \frac{1}{2}\right)\hbar\omega$, 可知变化后能量本征值为

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \tag{800}$$

(b) 变化后体系的 Hamiltonian:

$$\hat{H} = \frac{\hat{p}^2}{2\mu} + \frac{1}{2}\mu\tilde{\omega}^2 x^2 = \hat{H}_0 + \epsilon\left(\frac{\hat{p}^2}{2\mu} - \frac{1}{2}\mu\omega^2\hat{x}^2\right) \tag{801}$$

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$$\hat{H}' = \epsilon\left(\frac{\hat{p}^2}{2\mu} - \frac{1}{2}\mu\omega^2\hat{x}^2\right) \tag{802}$$

能量本征值的一阶修正为

$$\left\langle\psi_n^{(0)}\right|\hat{H}'\left|\psi_n^{(0)}\right\rangle = \epsilon\left\langle\psi_n^{(0)}\right|\frac{\hat{p}^2}{2\mu} - \frac{1}{2}\mu\omega^2\hat{x}^2\left|\psi_n^{(0)}\right\rangle \tag{803}$$

由于 $\hat{x} = \sqrt{\frac{\hbar}{2\mu\omega}}\left(\hat{a}^\dagger + \hat{a}\right)$, 首先计算

$$\left\langle\psi_n^{(0)}\right|\frac{1}{2}\mu\omega^2\hat{x}^2\left|\psi_n^{(0)}\right\rangle = \frac{1}{2}\mu\omega^2\frac{\hbar}{2\mu\omega}\left\langle\psi_n^{(0)}\right|\left(\hat{a}^{\dagger 2} + \hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger + \hat{a}\hat{a}\right)\left|\psi_n^{(0)}\right\rangle \tag{804}$$

利用 $\hat{a}\left|\psi_n^{(0)}\right\rangle = \sqrt{n}\left|\psi_{n-1}^{(0)}\right\rangle$ 和 $\hat{a}^\dagger\left|\psi_n^{(0)}\right\rangle = \sqrt{n+1}\left|\psi_{n+1}^{(0)}\right\rangle$ 得到:

$$\begin{aligned}\left\langle\psi_n^{(0)}\right|\frac{1}{2}k\hat{x}^2\left|\psi_n^{(0)}\right\rangle &= \frac{\hbar\omega}{4}\left\langle\psi_n^{(0)}\right|\left(\hat{a}^{\dagger 2}+\hat{a}^\dagger\hat{a}+\hat{a}\hat{a}^\dagger+\hat{a}\hat{a}\right)\left|\psi_n^{(0)}\right\rangle \quad (805)\\ &= \frac{\hbar\omega}{4}(2n+1) \quad (806)\\ &= \left(n+\frac{1}{2}\right)\hbar\omega\frac{1}{2} \quad (807)\end{aligned}$$

类似的, 可得 $\left\langle\psi_n^{(0)}\right|\frac{\hat{p}^2}{2\mu}\left|\psi_n^{(0)}\right\rangle = \left(n+\frac{1}{2}\right)\hbar\omega\frac{1}{2}$, 所以 $\left\langle\psi_n^{(0)}\right|\hat{H}'\left|\psi_n^{(0)}\right\rangle = 0$.

0.16 第十六次作业

1. 考虑一个量子体系, 它具有 3 个正交归一的态, 其 Hamiltonian 的形式为

$$H_0 = V_0\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 2\end{pmatrix}$$

这里, V_0 是实常数. 引入微扰 $H' = V_0\begin{pmatrix}-\epsilon & 0 & 0\\ 0 & 0 & \epsilon\\ 0 & \epsilon & 0\end{pmatrix}$, ϵ 是小量 ($\epsilon > 0$, $\epsilon \ll 1$).

(a) 求 H_0 的本征值和本征矢量;

(b) 求 $H = H_0 + H'$ 的精确本征值, 并展开到 ϵ 的两阶;

(c) 利用简并微扰论, 计算微扰项对 H_0 的简并能量本征值的一阶修正.

解: (1) H_0 的本征方程为:

$$H_0\psi^{(0)} = \lambda^{(0)}\psi^{(0)} \quad (808)$$

$$\begin{pmatrix}V_0-\lambda & 0 & 0\\ 0 & V_0-\lambda & 0\\ 0 & 0 & 2V_0-\lambda\end{pmatrix}\psi^{(0)} = 0 \quad (809)$$

由于 H_0 是对角矩阵, 本征值和相应的本征矢量为

$$\lambda_1^{(0)} = V_0, \qquad \psi_1^{(0)} = \begin{pmatrix}1\\0\\0\end{pmatrix} \quad (810)$$

$$\lambda_2^{(0)} = V_0, \qquad \psi_2^{(0)} = \begin{pmatrix}0\\1\\0\end{pmatrix} \quad (811)$$

$$\lambda_3^{(0)} = 2V_0, \qquad \psi_3^{(0)} = \begin{pmatrix}0\\0\\1\end{pmatrix} \quad (812)$$

(b) H 的本征方程为

$$H\psi = \lambda\psi \tag{813}$$

$$\begin{pmatrix} V_0(1-\epsilon)-\lambda & 0 & 0 \\ 0 & V_0-\lambda & V_0\epsilon \\ 0 & V_0\epsilon & 2V_0-\lambda \end{pmatrix}\psi = 0 \tag{814}$$

本征值可如下确定,

$$\det\begin{pmatrix} V_0(1-\epsilon)-\lambda & 0 & 0 \\ 0 & V_0-\lambda & V_0\epsilon \\ 0 & V_0\epsilon & 2V_0-\lambda \end{pmatrix} = 0 \tag{815}$$

$$(V_0(1-\epsilon)-\lambda)\left[(V_0-\lambda)(2V_0-\lambda)-V_0^2\epsilon^2\right] = 0 \tag{816}$$

解得:

$$\lambda_1 = V_0(1-\epsilon) \tag{817}$$

$$\lambda_2 = \frac{3-\sqrt{1+4\epsilon^2}}{2}V_0 \tag{818}$$

$$\lambda_3 = \frac{3+\sqrt{1+4\epsilon^2}}{2}V_0 \tag{819}$$

这里, λ_2 和 λ_3 展开到 ϵ 的两阶为

$$\lambda_2 = \left(1-\epsilon^2\right)V_0 \tag{820}$$

$$\lambda_3 = \left(2+\epsilon^2\right)V_0 \tag{821}$$

(3) 在 $\psi_1^{(0)}$ 和 $\psi_2^{(0)}$ 张开的子空间中, H' 的矩阵表示为

$$H' \to \begin{pmatrix} \psi_1^{(0)\dagger}H'\psi_1^{(0)} & \psi_1^{(0)\dagger}H'\psi_2^{(0)} \\ \psi_2^{(0)\dagger}H'\psi_1^{(0)} & \psi_2^{(0)\dagger}H'\psi_2^{(0)} \end{pmatrix} = \begin{pmatrix} -V_0\epsilon & 0 \\ 0 & 0 \end{pmatrix} \tag{822}$$

计算 $\begin{pmatrix} -V_0\epsilon & 0 \\ 0 & 0 \end{pmatrix}$ 的本征值:

$$\det\begin{pmatrix} -V_0\epsilon-\lambda' & 0 \\ 0 & -\lambda' \end{pmatrix} = 0 \tag{823}$$

所以

$$\lambda_1' = -V_0\epsilon, \qquad \lambda_2' = 0 \tag{824}$$

即 H_0 的简并能量本征值的一阶修正分别为 $-V_0\epsilon$ 和 0, 与方程817, 820的结果一致.