量子力学作业-第六周

题目 1. (教材 3.12) 证明在离散的能量本征态下动量平均值为零.

(提示: 利用 $\left[\boldsymbol{r}, \hat{H}\right] = \left[\boldsymbol{r}, \frac{\hat{\boldsymbol{p}}^2}{2m}\right] = i\hbar\frac{\hat{\boldsymbol{p}}}{m}$)

解答. 对于离散的能量本征态

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

注意到

$$\left[\boldsymbol{r}, \hat{H}\right] = \left[\boldsymbol{r}, \frac{\hat{\boldsymbol{p}}^2}{2m}\right] = i\hbar\frac{\hat{\boldsymbol{p}}}{m}$$

因此

$$\begin{aligned}
\bar{\boldsymbol{p}} &= \int \psi^* \hat{\boldsymbol{p}}\psi d\tau = \frac{m}{i\hbar}\int \psi^* \left[\boldsymbol{r}, \hat{H}\right]\psi d\tau \\
&= \frac{m}{i\hbar}\int \psi^* \boldsymbol{r}\hat{H}\psi d\tau - \frac{m}{i\hbar}\int \psi^* \hat{H}\boldsymbol{r}\psi d\tau \\
&= \frac{m}{i\hbar}\int \psi^* \boldsymbol{r}\hat{H}\psi d\tau - \frac{m}{i\hbar}\int \left(\hat{H}\psi\right)^* \boldsymbol{r}\psi d\tau \\
&= \frac{m}{i\hbar}\int \psi^* \boldsymbol{r}E_n\psi d\tau - \frac{m}{i\hbar}\int \left(E_n\psi\right)^* \boldsymbol{r}\psi d\tau \\
&= \frac{mE_n}{i\hbar}\left[\int \psi^* \boldsymbol{r}\psi d\tau - \int \psi^* \boldsymbol{r}\psi d\tau\right] \\
&= 0
\end{aligned}$$

题目 2. (教材 3.14) 证明在 l_z 的本征态下, $\bar{l}_x = \bar{l}_y = 0$.

(提示: 利用 $l_y l_z - l_z l_y = \mathrm{i}\hbar l_x$, 求平均)

解答. 注意到

$$\begin{aligned}\left[\hat{L}_y, \hat{L}_z\right] &= [z\hat{p}_x - x\hat{p}_z, x\hat{p}_y - y\hat{p}_x] = [z\hat{p}_x, x\hat{p}_y] - [z\hat{p}_x, y\hat{p}_x] - [x\hat{p}_z, x\hat{p}_y] + [x\hat{p}_z, y\hat{p}_x] \\ &= [z\hat{p}_x, x\hat{p}_y] + [x\hat{p}_z, y\hat{p}_x] = x[z\hat{p}_x, \hat{p}_y] + [z\hat{p}_x, x]\hat{p}_y + [x, y\hat{p}_x]\hat{p}_z + x[\hat{p}_z, y\hat{p}_x] \\ &= -i\hbar z\hat{p}_y + i\hbar y\hat{p}_z = i\hbar\hat{L}_x\end{aligned}$$

同理可得

$$\left[\hat{L}_x, \hat{L}_y\right] = i\hbar\hat{L}_z, \left[\hat{L}_z, \hat{L}_x\right] = i\hbar\hat{L}_y$$

对于 l_z 的本征态，有

$$\hat{L}_z\psi = l_z\psi$$

因此

$$\begin{aligned}l_x &= \int \psi^*\hat{L}_x\psi d\tau = \frac{1}{i\hbar}\int \psi^*\left[\hat{L}_y, \hat{L}_z\right]\psi d\tau \\ &= \frac{1}{i\hbar}\left[\int \psi^*\hat{L}_y\hat{L}_z\psi d\tau - \int \psi^*\hat{L}_z\hat{L}_y\psi d\tau\right] \\ &= \frac{1}{i\hbar}\left[\int \psi^*\hat{L}_y\hat{L}_z\psi d\tau - \int \left(\hat{L}_z\psi\right)^*\hat{L}_y\psi d\tau\right] \\ &= \frac{1}{i\hbar}\left[\int \psi^*\hat{L}_y l_z\psi d\tau - \int (l_z\psi)^*\hat{L}_y\psi d\tau\right] \\ &= \frac{l_z}{i\hbar}\left[\int \psi^*\hat{L}_y\psi d\tau - \int \psi^*\hat{L}_y\psi d\tau\right] \\ &= 0\end{aligned}$$

类似地

$$\begin{aligned}l_y &= \int \psi^*\hat{L}_y\psi d\tau = \frac{1}{i\hbar}\int \psi^*\left[\hat{L}_z, \hat{L}_x\right]\psi d\tau \\ &= \frac{1}{i\hbar}\left[\int \psi^*\hat{L}_z\hat{L}_x\psi d\tau - \int \psi^*\hat{L}_x\hat{L}_z\psi d\tau\right] \\ &= \frac{1}{i\hbar}\left[\int \left(\hat{L}_z\psi\right)^*\hat{L}_x\psi d\tau - \int \psi^*\hat{L}_x\hat{L}_z\psi d\tau\right] \\ &= \frac{1}{i\hbar}\left[\int (l_z\psi)^*\hat{L}_x\psi d\tau - \int \psi^*\hat{L}_x l_z\psi d\tau\right] \\ &= \frac{l_z}{i\hbar}\left[\int \psi^*\hat{L}_x\psi d\tau - \int \psi^*\hat{L}_x\psi d\tau\right] \\ &= 0\end{aligned}$$

题目 3. (教材 3.16) 设体系处于 $\psi = c_1 Y_{11} + c_2 Y_{20}$ 状态 (已归一化, 即 $|c_1|^2 + |c_2|^2 = 1$). 求:

(a) l_z 的可能测值及平均值;

(b) l^2 的可能测值及相应的概率;

(c) l_x 的可能测值及相应的概率.

解答. 由球谐函数的性质可知，Y_{11} 和 Y_{20} 即是 $\hat{L}^2$ 的本征函数，也是 $\hat{L}_z$ 的本征函数，满足

$$\hat{L}^2 Y_{11} = 2\hbar^2 Y_{11}, \hat{L}^2 Y_{20} = 6\hbar^2 Y_{20}$$

$$\hat{L}_z Y_{11} = \hbar Y_{11}, \hat{L}_z Y_{20} = 0$$

(a)l_z 的可能测值有 0 和 $\hbar$, 平均值

$$\bar{l}_z = |c_1|^2 \hbar + |c_2|^2 \cdot 0 = \hbar \, |c_1|^2$$

(b)l^2 的可能测值有 $\sqrt{2}\hbar$ 和 $\sqrt{6}\hbar$, 相应的概率

$$P_{\sqrt{2}\hbar} = |c_1|^2 , P_{\sqrt{6}\hbar} = |c_2|^2$$

(c) 要确定 l_x 的可能测值及相应的概率，只需将波函数展开为 l_x 的本征函数的线性叠加，考虑到 $\hat{L}^2$ 和 $\hat{L}_z$ 的共同本征函数为球谐函数

$$Y_{lm} = (-1)^m \sqrt{\frac{(2l+1)}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m (\cos\theta) \, e^{im\varphi}$$

具体地

$$Y_{00} = \frac{1}{\sqrt{4\pi}}, Y_{10} = \sqrt{\frac{3}{4\pi}} \cos\theta = \sqrt{\frac{3}{4\pi}} \frac{z}{r}$$

$$Y_{1\pm1} = \mp\sqrt{\frac{3}{8\pi}} \sin\theta e^{\pm i\varphi} = \mp\sqrt{\frac{3}{8\pi}} \frac{x \pm iy}{r}$$

$$Y_{20} = \sqrt{\frac{5}{16\pi}} \left(3\cos^2\theta - 1\right) = \sqrt{\frac{5}{16\pi}} \left(3\frac{z^2}{r^2} - 1\right)$$

$$Y_{2\pm1} = \mp\sqrt{\frac{15}{8\pi}} \sin\theta\cos\theta e^{\pm i\varphi} = \mp\sqrt{\frac{15}{8\pi}} \frac{z}{r} \frac{x \pm iy}{r}$$

$$Y_{2\pm2} = \sqrt{\frac{15}{32\pi}} \sin^2\theta e^{\pm 2i\varphi} = \sqrt{\frac{15}{32\pi}} \frac{(x \pm iy)^2}{r^2}$$

利用坐标轮换，$\hat{L}^2$ 和 $\hat{L}_x$ 的共同本征函数为

$$Y_{00}^x = \frac{1}{\sqrt{4\pi}}, Y_{10}^x = \sqrt{\frac{3}{4\pi}} \cos\theta = \sqrt{\frac{3}{4\pi}} \frac{x}{r}$$

$$Y^x_{1\pm1}=\mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\varphi}=\mp\sqrt{\frac{3}{8\pi}}\frac{y\pm iz}{r}$$
$$Y^x_{20}=\sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta-1\right)=\sqrt{\frac{5}{16\pi}}\left(3\frac{x^2}{r^2}-1\right)$$
$$Y^x_{2\pm1}=\mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{\pm i\varphi}=\mp\sqrt{\frac{15}{8\pi}}\frac{x}{r}\frac{y\pm iz}{r}$$
$$Y^x_{2\pm2}=\sqrt{\frac{15}{32\pi}}\sin^2\theta e^{\pm2i\varphi}=\sqrt{\frac{15}{32\pi}}\frac{\left(y\pm iz\right)^2}{r^2}$$

因此，对于题目中的 Y_11 和 Y_20，可以利用上述本征函数展开

$$\begin{aligned}Y_{11}&=-\sqrt{\frac{3}{8\pi}}\frac{x+iy}{r}\\&=-\sqrt{\frac{3}{8\pi}}\left[\sqrt{\frac{4\pi}{3}}Y^x_{00}-i\frac{1}{2}\sqrt{\frac{8\pi}{3}}\left(Y^x_{11}+Y^x_{1-1}\right)\right]\\&=-\frac{1}{\sqrt{2}}Y^x_{00}+\frac{i}{2}Y^x_{11}+\frac{i}{2}Y^x_{1-1}\end{aligned}$$

注意到

$$Y^x_{2+2}+Y^x_{2-2}=\sqrt{\frac{15}{32\pi}}\frac{2\left(y^2-z^2\right)}{r^2}=\sqrt{\frac{15}{32\pi}}\frac{2r^2-2x^2-4z^2}{r^2}$$

因此

$$\begin{aligned}\frac{3z^2}{r^2}&=\frac{3}{4}\left[\frac{2r^2-2x^2}{r^2}-\sqrt{\frac{32\pi}{15}}\left(Y^x_{2+2}+Y^x_{2-2}\right)\right]\\&=\frac{3}{2}-\frac{1}{2}\left(\sqrt{\frac{16\pi}{5}}Y^x_{20}+1\right)-\frac{3}{4}\sqrt{\frac{32\pi}{15}}\left(Y^x_{2+2}+Y^x_{2-2}\right)\\&=1-\sqrt{\frac{4\pi}{5}}Y^x_{20}-\sqrt{\frac{6\pi}{5}}\left(Y^x_{2+2}+Y^x_{2-2}\right)\end{aligned}$$

从而

$$\begin{aligned}Y_{20}&=\sqrt{\frac{5}{16\pi}}\left(3\frac{z^2}{r^2}-1\right)\\&=\sqrt{\frac{5}{16\pi}}\left[-\sqrt{\frac{4\pi}{5}}Y^x_{20}-\sqrt{\frac{6\pi}{5}}\left(Y^x_{2+2}+Y^x_{2-2}\right)\right]\\&=-\frac{1}{2}Y^x_{20}-\sqrt{\frac{3}{8}}Y^x_{2+2}-\sqrt{\frac{3}{8}}Y^x_{2-2}\end{aligned}$$

得 ψ 在新球谐函数下的展开式

$$\begin{aligned}\psi&=c_1Y_{11}+c_2Y_{20}\\&=c_1\left(-\frac{1}{\sqrt{2}}Y^x_{00}+\frac{i}{2}Y^x_{11}+\frac{i}{2}Y^x_{1-1}\right)+c_2\left(-\frac{1}{2}Y^x_{20}-\sqrt{\frac{3}{8}}Y^x_{2+2}-\sqrt{\frac{3}{8}}Y^x_{2-2}\right)\\&=-\frac{1}{\sqrt{2}}c_1Y^x_{00}+\frac{i}{2}c_1Y^x_{11}+\frac{i}{2}c_1Y^x_{1-1}-\frac{1}{2}c_2Y^x_{20}-\sqrt{\frac{3}{8}}c_2Y^x_{2+2}-\sqrt{\frac{3}{8}}c_2Y^x_{2-2}\end{aligned}$$

因此，l_x 的可能测量值有 $0, \hbar, -\hbar, 2\hbar, -2\hbar$，相应的概率分别为

$$
\begin{aligned}
P_0 &= \left(-\frac{1}{\sqrt{2}}c_1\right)^* \left(-\frac{1}{\sqrt{2}}c_1\right) + \left(-\frac{1}{2}c_2\right)^* \left(-\frac{1}{2}c_2\right) = \frac{1}{2}\left|c_1\right|^2 + \frac{1}{4}\left|c_2\right|^2 \\
P_\hbar &= \left(\frac{i}{2}c_1\right)^* \left(\frac{i}{2}c_1\right) = \frac{1}{4}\left|c_1\right|^2 \\
P_{-\hbar} &= \left(\frac{i}{2}c_1\right)^* \left(\frac{i}{2}c_1\right) = \frac{1}{4}\left|c_1\right|^2 \\
P_{2\hbar} &= \left(-\sqrt{\frac{3}{8}}c_2\right)^* \left(-\sqrt{\frac{3}{8}}c_2\right) = \frac{3}{8}\left|c_2\right|^2 \\
P_{-2\hbar} &= \left(-\sqrt{\frac{3}{8}}c_2\right)^* \left(-\sqrt{\frac{3}{8}}c_2\right) = \frac{3}{8}\left|c_2\right|^2
\end{aligned}
$$

容易验证

$$
\sum_i P_i = P_0 + P_\hbar + P_{-\hbar} + P_{2\hbar} + P_{-2\hbar} = \left|c_1\right|^2 + \left|c_2\right|^2 = 1
$$

题目 4. (教材 4.1) 判断下列说法的正误, 并给出每一问的证明:

(a) 在非定态下, 力学量的平均值随时间变化;

(b) 设体系处于定态, 则不含时力学量的测值的概率分布不随时间变化;

(c) 设 Hamilton 量为守恒量, 则体系处于定态;

(d) 中心力场中的粒子, 处于定态, 则角动量取确定值;

(e) 自由粒子处于定态, 则动量取确定值;

(f) 一维粒子的能量本征态无简并;

（g）中心力场中粒子能级的简并度至少为 $(2l+1), l = 0, 1, 2, \cdots$.

解答. (a) 错误，如果某力学量 F 不显含时间，并且与哈密顿算符对易，则

$$
\begin{aligned}
\frac{\mathrm{d}\overline{F}(t)}{\mathrm{d}t} &= \frac{1}{\mathrm{i}\hbar}\left[-\int (\hat{H}\Psi(\boldsymbol{r},t))^*\hat{F}\Psi(\boldsymbol{r},t)\mathrm{d}\tau + \int \Psi^*(\boldsymbol{r},\mathrm{t})\hat{F}\hat{H}\Psi(\boldsymbol{r},t)\mathrm{d}\tau\right] \\
&= -\frac{i}{\hbar}\left(-\int \Psi^*(\boldsymbol{r},t)\hat{H}\hat{F}\Psi(\boldsymbol{r},t)\mathrm{d}\tau + \int \Psi^*(\boldsymbol{r},t)\hat{F}\hat{H}\Psi(\boldsymbol{r},t)\mathrm{d}\tau\right) \\
&= -\frac{i}{\hbar}\left(\int \Psi^*(\boldsymbol{r},t)(\hat{F}\hat{H} - \hat{H}\hat{F})\Psi(\boldsymbol{v},t)\mathrm{d}\tau\right) \\
&= 0
\end{aligned}
$$

因此，不管系统处于定态与否，该力学量都不会随时间变化;

(b) 正确，系统波函数可以展开为力学量 F 本征波函数的线性叠加

$$
\psi\left(t\right) = \sum_n a_n\left(t\right)\psi_n
$$

其中

$$a_n = \int \psi_n^* \psi\left(t\right) d\tau$$

对于定态

$$\hat{H}\psi\left(t\right) = E\psi\left(t\right)$$

因此

$$\begin{aligned}\frac{da_n}{dt} &= \frac{d}{dt}\int \psi_n^* \psi\left(t\right) d\tau = \int \psi_n^* \frac{\partial \psi\left(t\right)}{\partial t} d\tau \\ &= \frac{1}{i\hbar}\int \psi_n^* \hat{H}\psi\left(t\right) d\tau = \frac{E}{i\hbar}\int \psi_n^* \psi d\tau = \frac{E}{i\hbar} a_n\end{aligned}$$

同理可得 $\frac{da_n^*}{dt} = -\frac{E}{i\hbar} a_n^*$, 从而概率幅随时间的变化

$$\frac{d}{dt}\left[a_n^*\left(t\right) a_n\left(t\right)\right] = \frac{da_n^*\left(t\right)}{dt} a_n\left(t\right) + a_n^*\left(t\right)\frac{da_n\left(t\right)}{dt} = -\frac{E}{i\hbar} a_n^* a_n\left(t\right) + a_n^*\left(t\right)\frac{E}{i\hbar} a_n = 0$$

另一方面，由于 F 不显含时间，因此可以和 $\frac{\partial}{\partial t}$ 对易, 因此

$$\begin{aligned}\frac{d\bar{F}}{dt} &= \int \psi^* \hat{F}\psi d\tau = \int \frac{d\psi^*}{dt}\hat{F}\psi d\tau + \int \psi^* \hat{F}\frac{d\psi}{dt} d\tau \\ &= \int \left(\frac{1}{i\hbar}\hat{H}\psi\right)^* \hat{F}\psi d\tau + \int \psi^* \hat{F}\left(\frac{1}{i\hbar}\hat{H}\psi\right) d\tau \\ &= \frac{1}{i\hbar}\int \left(E_n\psi\right)^* \hat{F}\psi d\tau - \int \psi^* \hat{F} E_n \psi d\tau \\ &= \frac{E_n}{i\hbar}\left[\int \psi^* \hat{F}\psi d\tau - \int \psi^* \hat{F}\psi d\tau\right] \\ &= 0\end{aligned}$$

于是体系处于定态时，不含时力学量 F 的测值的概率分布不随时间变化;

(c) 错误，只要 Hamilton 量不显含时间，由于其与自身对易，因此始终为守恒量，与系统是否处于定态无关;

(d) 错误，中心力场中的粒子的角动量算符为 $\hat{\boldsymbol{l}} = \hat{\boldsymbol{r}} \times \hat{\boldsymbol{p}}$，哈密顿算符为

$$\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} + \hat{V}\left(r\right)$$

注意到

$$\begin{aligned}\left[\hat{l}_x, \boldsymbol{p}^2\right] &= \left[y\hat{p}_z - z\hat{p}_y, \hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2\right] = \left[y\hat{p}_z, \hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2\right] - \left[z\hat{p}_y, \hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2\right] \\ &= \left[y\hat{p}_z, \hat{p}_y^2\right] - \left[z\hat{p}_y, \hat{p}_z^2\right] = \left[y, \hat{p}_y^2\right]\hat{p}_z - \left[z, \hat{p}_z^2\right]\hat{p}_y = 2i\hbar\hat{p}_y\hat{p}_z - 2i\hbar\hat{p}_z\hat{p}_y = 0\end{aligned}$$

于是 $\left[\hat{\boldsymbol{l}},\hat{\boldsymbol{p}}^2\right]=0$，另一方面

$$\begin{aligned}\left[\hat{l}_x,\hat{V}\left(r\right)\right]&=\left[y\hat{p}_z-z\hat{p}_y,\hat{V}\left(r\right)\right]=y\left[\hat{p}_z,\hat{V}\left(r\right)\right]-z\left[\hat{p}_y,\hat{V}\left(r\right)\right]\\&=y\hat{V}'\left(r\right)\frac{z}{r}-z\hat{V}'\left(r\right)\frac{y}{r}=0\end{aligned}$$

故 $\left[\hat{\boldsymbol{l}},\hat{V}\left(r\right)\right]=0$，因此 $\left[\hat{\boldsymbol{l}},\hat{H}\right]=0$，即系统角动量是守恒量，但这并不意味着角动量取确定值;

(e) 与 (d) 原理相同，只能说明动量 $\boldsymbol{p}$ 是守恒量，不能说明动量取确定值；

(f) 错误，对于某些不规则势阱，如一维氢原子 $V(x)\propto-\frac{1}{|x|}$, 除基态外，其他束缚态二重简并；

(g) 正确, 中心力场中的能量本征方程为

$$\left[-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2}r+\frac{l^2}{2\mu r^2}+V(r)\right]\psi=E\psi$$

体系的一组 CSCO 可以选择为 $(\hat{H},\hat{\boldsymbol{l}}^2,l_z)$, 因此能量本征函数为

$$\phi(r,\theta,\varphi)=R_l(r)Y_{lm}(\theta,\varphi),\quad m=l,l-1,\cdots,-l,l=0,1,2,\cdots$$

代入能量本征方程，有

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2}R_l(r)+\frac{2}{r}\frac{\mathrm{d}}{\mathrm{d}r}R_l(r)+\left[\frac{2\mu}{\hbar^2}(E-V(r))-\frac{l(l+1)}{r^2}\right]R_l(r)=0$$

作变量代换 $R_l(r)=\chi_l(r)/r$, 则有

$$\chi_l''(r)+\left[\frac{2\mu}{\hbar^2}(E-V(r))-\frac{l(l+1)}{r^2}\right]\chi_l(r)=0$$

可见 E 的本征值与 l 有关，与 m 无关, 因此有 m 简并，而 $m=l,l-1,\cdots,-l$ 有 $(2l+1)$ 个取值，从而中心力场中粒子能级的简并度至少为 $(2l+1),l=0,1,2,\cdots$

题目 5. (教材 4.5) 设力学量 A 不显含 t, 证明在束缚定态下 $\frac{\mathrm{d}\bar{A}}{\mathrm{d}t}=0$.

解答. 由于 A 不显含时间，因此可以和 $\frac{\partial}{\partial t}$ 对易，对于束缚态，ψ 可以归一化，在定态下

$$\hat{A}\psi=E_n\psi$$

因此

$$\begin{aligned}\frac{d\bar{A}}{dt}&=\int\psi^*\hat{A}\psi d\tau=\int\frac{d\psi^*}{dt}\hat{A}\psi d\tau+\int\psi^*\hat{A}\frac{d\psi}{dt}d\tau\\&=\int\left(\frac{1}{i\hbar}\hat{H}\psi\right)^*\hat{A}\psi d\tau+\int\psi^*\hat{A}\left(\frac{1}{i\hbar}\hat{H}\psi\right)d\tau\\&=\frac{1}{i\hbar}\int\left(E_n\psi\right)^*\hat{A}\psi d\tau-\int\psi^*\hat{A}E_n\psi d\tau\\&=\frac{E_n}{i\hbar}\left[\int\psi^*\hat{A}\psi d\tau-\int\psi^*\hat{A}\psi d\tau\right]\\&=0\end{aligned}$$