《量子力学教程》课后习题——第三章 量子力学中的力学量

物理（4+4）1801　胡喜平　学号 U201811966

网站 https://hxp.plus/　邮件 hxp201406@gmail.com

2020 年 11 月 4 日

3.1

$$\overline{U}=\frac{1}{2}m\omega\overline{x^2}=\frac{1}{2}m\omega^2\frac{\alpha}{\sqrt{\pi}}\int_{-\infty}^{+\infty}\mathrm{e}^{-\frac{1}{2}\alpha^2x^2}x^2\mathrm{e}^{-\frac{1}{2}\alpha^2x^2}\,\mathrm{d}x=\frac{1}{2}m\omega^2\frac{\alpha}{\sqrt{\pi}}\cdot\frac{\sqrt{\pi}}{\alpha}\frac{1}{2\alpha^2}=\frac{1}{4}\frac{m\omega^2}{\alpha^2}$$

其中用到高斯积分公式

$$\int_{-\infty}^{+\infty}x^{2n}\mathrm{e}^{-\alpha x^2}\,\mathrm{d}x=\sqrt{\frac{\pi}{\alpha}}\frac{(2n-1)!!}{(2\alpha)^n}$$

同理

$$\begin{aligned}\overline{T}&=\frac{\alpha}{\sqrt{\pi}}\int_{-\infty}^{+\infty}\mathrm{e}^{-\frac{1}{2}\alpha^2x^2}\frac{-\hbar}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\mathrm{e}^{-\frac{1}{2}\alpha^2x^2}\,\mathrm{d}x=-\frac{\alpha\hbar}{2m\sqrt{\pi}}\int_{-\infty}^{+\infty}\mathrm{e}^{-\frac{1}{2}\alpha x^2}\cdot\alpha^2\left(\alpha^2x^2-1\right)\cdot\mathrm{e}^{-\frac{1}{2}\alpha^2x^2}\,\mathrm{d}x\\&=-\frac{\alpha^3\hbar}{2m\sqrt{\pi}}\int_{-\infty}^{+\infty}\left(\alpha^2x^2-1\right)\mathrm{e}^{-\alpha^2x^2}\,\mathrm{d}x=-\frac{\alpha^2\hbar}{2m\sqrt{\pi}}\int_{-\infty}^{+\infty}\left(\alpha^2x^2-1\right)\mathrm{e}^{-\alpha^2x^2}\,\mathrm{d}\left(\alpha x\right)\\&=-\frac{\alpha^2\hbar}{2m\sqrt{\pi}}\left[\frac{\sqrt{\pi}}{2}-\sqrt{\pi}\right]=\frac{1}{4}\frac{\hbar\alpha^2}{m}=\frac{\hbar\omega}{4}\end{aligned}$$

动量的概率密度为

$$c\left(p\right)=\int_{-\infty}^{+\infty}\frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{ipx/h}\sqrt{\frac{\alpha}{\pi^{1/2}}}\mathrm{e}^{-\frac{1}{2}\alpha^2x^2}\,\mathrm{d}x=\sqrt{\frac{1}{\alpha\hbar\sqrt{\pi}}}\mathrm{e}^{-\frac{p^2}{2\alpha^2\hbar^2}}$$

动量概率的分布函数为

$$w\left(p\right)=\left|c\left(p\right)\right|^2=\frac{1}{\alpha\hbar\sqrt{\pi}}\mathrm{e}^{-\frac{p^2}{\alpha^2\hbar^2}}$$

3.2　r 的期望值为

$$\overline{r}=\iiint\psi\left(r\right)r\psi\left(r\right)\sin\theta r^2\,\mathrm{d}\theta\,\mathrm{d}r\,\mathrm{d}\phi=\frac{3}{2}a_0$$

势能 U 的期望值为

$$\overline{U}=\iint\mathrm{d}\Omega\int_0^{\infty}\psi\left(r\right)-\frac{e_s^2}{r}\psi\left(r\right)r^2\,\mathrm{d}r=-\frac{e_s^2}{a_0}$$

动能 T 的期望值为

$$\overline{T}=\iint \mathrm{d}\Omega\int_0^\infty\left[\psi\left(r\right)\frac{-\hbar}{2mr}\frac{\partial^2}{\partial r^2}r\psi\left(r\right)\right]r^2\,\mathrm{d}r=\frac{e_s^2}{2a_0}$$

在最概然半径处，径向概率取级值

$$\frac{\mathrm{d}}{\mathrm{d}r}\left[w\left(r\right)\right]=\frac{\mathrm{d}}{\mathrm{d}r}\left[R^2\left(r\right)r^2\right]=\frac{\mathrm{d}}{\mathrm{d}r}\left[\frac{4\mathrm{e}^{-2r/a_0}}{a_0^3}r^2\right]=0\Rightarrow r=a_0$$

动量分布的概率幅为

$$c\left(p\right)=\iiint\frac{1}{\left(\sqrt{2\pi\hbar}\right)^3}\mathrm{e}^{-i\frac{p\cdot r}{\hbar}}\psi\left(r\right)\mathrm{d}r$$

动量的概率密度为

$$w\left(p\right)=\left|c\left(p\right)\right|^2=\frac{8a_0^3\hbar^5}{\pi^2\left(\hbar^2+a_0^2p^2\right)^4}$$

3.3 概率流密度公式为

$$\vec{J}=\frac{i\hbar}{2m}\left(\psi\nabla\psi^*-\psi^*\nabla\psi\right)$$

其中

$$\nabla\psi_{nlm}=\left(-1\right)^m N_{lm}\left[e_rP_l^m\mathrm{e}^{im\phi}\frac{\partial R_{nl}}{\partial r}+e_\theta\frac{R_{nl}\mathrm{e}^{im\phi}}{r}\frac{\partial P_l^m}{r\sin\theta}+e_\phi\frac{R_{nl}P_l^m}{r\sin\theta}\frac{\partial\mathrm{e}^{im\phi}}{\partial\phi}\right]$$

因此

$$\vec{J}\left(\vec{r},t\right)=\frac{i\hbar}{2m_e}\left[\left(N_{lm}R_{nl}P_l^m\right)^2\left(\frac{-2im}{r\sin\theta}\right)e_\varphi\right]=\frac{\hbar m}{m_er\sin\theta}\left|\psi_{nlm}\right|^2e_\varphi$$

即

$$\begin{aligned}&J_{er}=0\\&J_{e\varphi}=\frac{\hbar m}{m_er\sin\theta}\left|\psi_{nlm}\right|^2e_\varphi\end{aligned}$$

3.4

$$\mathrm{d}M=J_er\,\mathrm{d}r\,\mathrm{d}\theta\cdot\pi r^2\sin^2\theta=-\frac{\pi e\hbar m}{m_e}w_{nl}r^2\sin\theta\,\mathrm{d}r\,\mathrm{d}\varphi\,\mathrm{d}\theta$$

$$M=\iint\mathrm{d}M=-\frac{e\hbar m}{2m_e}$$

3.5 转子的哈密顿算符为

$$H=L^2/\left(2I\right)$$

定轴转动，薛定谔方程为

$$\frac{\hat{L}^2}{2I}\psi = -\frac{\hbar^2}{2I}\frac{\mathrm{d}^2\psi}{\mathrm{d}\varphi^2} = E\left(\varphi\right)$$

和一维粒子相同可以解出

$$E_m = \frac{m^2\hbar^2}{2I}$$

定点转动时

$$-\frac{\hbar^2}{2I}\nabla^2\psi = E\psi$$

边界条件为

$$\psi\left(\theta, \varphi + 2\pi\right) = \psi\left(\theta, \varphi\right)$$

且在无穷远处有界，因此

$$E_l = \frac{l\left(l+1\right)\hbar^2}{2I}$$

3.6 函数是周期函数，只需要在一个周期内求动能和动量的期望

$$A^2 = \frac{1}{\int_0^{\pi/k}\left|\psi\left(x\right)\right|^2\mathrm{d}x} = \frac{2k}{\pi}$$

$$\overline{p} = \int_0^{\pi/k}\psi^*\left(x\right)\left(-i\hbar\right)\frac{\mathrm{d}}{\mathrm{d}x}\psi\left(x\right)\mathrm{d}x = 0$$

$$\overline{T} = \overline{\frac{p^2}{2m}} = \int_0^{\pi/k}\psi^*\left(x\right)\frac{-\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi\left(x\right)\mathrm{d}x = \frac{5\pi\hbar^2k}{16m}A^2 = \frac{5\hbar^2k^2}{8m}$$

3.7 归一化因子

$$A^2 = \frac{1}{\int_{-\infty}^{+\infty}\left|\psi\left(x\right)\right|^2\mathrm{d}x} = 4\lambda^3$$

动量分布概率幅为

$$c\left(p\right) = \int_{-\infty}^{+\infty}\frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{i\frac{px}{\hbar}}\psi\left(x\right)\mathrm{d}x = \frac{2\lambda^{3/2}}{\sqrt{2\pi\hbar}}\cdot\frac{1}{\left(\lambda + ip/\hbar\right)^2}$$

动量概率的分布函数为

$$w\left(p\right) = \left|c\left(p\right)\right|^2 = \frac{2\lambda^3\hbar^3}{\pi}\frac{1}{\left(\hbar^2\lambda^2 + p^2\right)^2}$$

动量的期望值为

$$\overline{p} = \int p w\left(p\right)\mathrm{d}p = 0$$

3.8 归一化因子

$$A^2=\frac{1}{\int_0^a x^2\left(a-x\right)^2}\,\mathrm{d}x=\frac{30}{a^5}$$

能量的概率幅度为

$$c_n=\int_0^a\sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}Ax\left(a-x\right)\mathrm{d}x=\frac{4\sqrt{15}}{n^3\pi^3}\left[1-\left(-1\right)^n\right]$$

能量的概率分布为

$$w_n=\left|c_n\right|^2=\begin{cases}\dfrac{960}{n^6\pi^6} & n=2k+1\\ 0 & n=2k\end{cases}$$

能量的期望值为

$$\overline{E}=\sum_{n=2k+1}w_nE_n=\frac{480\hbar^2}{ma^2\pi^4}\sum_{n=2k+1}\frac{1}{n^4}=\frac{5\hbar^2}{ma^2}$$

3.9 氢原子处在 $\psi_{2,1,0}$ 和 $\psi_{2,1,-1}$ 两种状态，其中 $c_{2,1,0}=\frac{1}{2}$，$c_{2,1,-1}=-\frac{\sqrt{3}}{2}$。能量的期望值为

$$E=\sum\left|c_{nlm}^2\right|E_1/n^2=-\frac{me_s^4}{8\hbar^2}$$

角动量平方期望值为

$$\overline{L^2}=\sum\left(c_{nlm}^2\right)l\left(l+1\right)\hbar^2=2\hbar^2$$

角动量 z 分量的期望值为

$$\overline{L_z}=\sum\left(c_{nlm}^2\right)m\hbar=-\frac{3}{4}\hbar$$

3.10 将势能代入径向方程，考虑无穷远处势能为零，以及球对称性（$l=0$）

$$\begin{cases}\dfrac{\mathrm{d}^2}{\mathrm{d}r^2}R+\dfrac{2}{r}\dfrac{\mathrm{d}}{\mathrm{d}r}R+k^2R=0 & r<a\\ R=0 & r>a\end{cases}$$

另 $x=kr$

$$R''+\frac{2}{x}R'+R=0$$
$$R\left(ka\right)=0$$

另 $u=xR$

$$\begin{cases}u''+u=0\\ u\left(0\right)=u\left(ka\right)=0\end{cases}$$

通解为

$$u = A\sin x + B\cos x = A\sin kr + B\cos kr$$

代入边界条件

$$\sin ka = 0 \Rightarrow k_n = n\pi/a$$

本征函数和能量为

$$E_n = \frac{\hbar^2\pi^2 n^2}{2ma^2}$$
$$R_n = A\frac{u}{x} = A\frac{\sin k_n r}{k_n r}$$

归一化因子为

$$A = \frac{1}{\sqrt{\int_0^a |R_n|^2 r^2\,\mathrm{d}r}} = k_n\sqrt{2/a}$$

波函数为

$$\psi_{n,0,0} = R_{n,0}(r)\,Y_{00}(\theta,\varphi) = A\frac{\sin k_n r}{k_n r}\cdot\frac{1}{\sqrt{4\pi}} = \frac{1}{\sqrt{2\pi a}}\frac{\sin k_n r}{r}$$

3.11 由于 $\overline{p} = 0$，$\overline{p^2} = \frac{5}{4}\hbar^2 k^2$

$$\overline{(\Delta p)^2} = \overline{p^2} - \overline{p}^2 = \frac{5}{4}\hbar^2 k^2$$

$$\overline{x} = \int_{-\infty}^{+\infty}\psi^* x\psi\,\mathrm{d}x = A^2\int_{-\infty}^{+\infty} x\left[\sin^2 kx + \frac{1}{2}\cos kx\right]^2\mathrm{d}x = 0$$
$$\overline{x^2} = \int_{-\infty}^{+\infty}\psi^* x^2\psi\,\mathrm{d}x = A^2\int_{-\infty}^{+\infty} x^2\left[\sin^2 kx + \frac{1}{2}\cos kx\right]^2\mathrm{d}x = \infty$$

$$\overline{(\Delta x)^2} = \overline{x^2} - \overline{x}^2 = \infty$$

所以

$$\overline{(\Delta x)^2}\cdot\overline{(\Delta p)^2} = \infty$$

3.12

$$\overline{x} = \int_{-\infty}^{+\infty}\psi^* x\psi\,\mathrm{d}x = \frac{1}{\sqrt{2\pi\xi^2}}\int_{-\infty}^{+\infty} x\mathrm{e}^{-x^2/\left(2\xi^2\right)}\,\mathrm{d}x = 0$$
$$\overline{x^2} = \int_{-\infty}^{+\infty}\psi^* x^2\psi\,\mathrm{d}x = \frac{1}{\sqrt{2\pi\xi^2}}\int_{-\infty}^{+\infty} x^2\mathrm{e}^{-x^2/\left(2\xi^2\right)}\,\mathrm{d}x = \xi^2$$
$$\overline{p} = \int_{-\infty}^{+\infty}\psi^*\frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x}\psi\,\mathrm{d}x = p_0$$
$$\overline{p^2} = \int_{-\infty}^{+\infty}\psi^*\left(\frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x}\right)\psi\,\mathrm{d}x = p_0^2 + \frac{\hbar^2}{4\xi^2}$$

不确定性关系为

$$\overline{(\Delta x)^2} \cdot \overline{(\Delta p)^2} = \left(\overline{x^2} - \overline{x}^2\right) \cdot \left(\overline{p^2} - \overline{p}^2\right) = \frac{\hbar^2}{4}$$

3.13 不确定性关系为

$$p \cdot r = \hbar$$

氢原子的能量为

$$E = \frac{p^2}{2m} - \frac{e_s^2}{r} = \frac{\hbar^2}{2mr^2} - \frac{e_s^2}{r}$$

当

$$r = \frac{\hbar^2}{me_s^2}$$

时，能量取得最小值

$$E_{min} = -\frac{me_s^4}{2\hbar^2} = -13.6 \text{ eV}$$