《量子力学教程》课后习题——第三章 量子力学中的力学量

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3.1

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

其中用到高斯积分公式

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

同理

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

动量的概率密度为

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

动量概率的分布函数为

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

3.2 r 的期望值为

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

势能 U 的期望值为

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

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

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

动量的概率密度为

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

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

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

因此

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

即

$$J_{er} = 0$$

$$J_{e\varphi} = \frac{\hbar m}{m_e r \sin \theta} \left| \psi_{nlm} \right|^2 e_{\varphi}$$

3.4

$$dM = J_e r dr d\theta \cdot \pi r^2 \sin^2 \theta = -\frac{\pi e \hbar m}{m_e} w_{nl} r^2 \sin \theta dr d\varphi d\theta$$

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

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

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

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

$$A^{2} = \frac{1}{\int_{0}^{\pi/k} |\psi(x)|^{2} dx} = \frac{2k}{\pi}$$

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

$$\overline{T} = \frac{\overline{p^{2}}}{2m} = \int_{0}^{\pi/k} \psi^{*}(x) \frac{-\hbar^{2}}{2m} \frac{\mathrm{d}^{2}}{\mathrm{d}x^{2}} \psi(x) dx = \frac{5\pi\hbar^{2}k}{16m} A^{2} = \frac{5\hbar^{2}k^{2}}{8m}$$