Homework11 答案

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1.定义径向动量算符$p_r=\frac{1}{2}(\vec{e_r}\cdot\vec{p}+\vec{p}\cdot\vec{e_r})$，证明:
(1)p_r是厄米的
(2)$p_r=-i\hbar(\frac{\partial}{\partial r}+\frac{1}{r})$
(3)$[r,p_r]=i\hbar$
(4)$p_r^2=-\hbar^2\frac{1}{r}\frac{\partial^2}{\partial r^2}r=-\hbar^2\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}$
证明：(1)

因为$(ABC)^\dagger=C^\dagger B^\dagger A^\dagger$
所以

$$\begin{aligned}
p_r^\dagger &= \frac{1}{2}(\frac{1}{r}\vec{r}\cdot\vec{p}+\vec{p}\cdot\vec{r}\frac{1}{r})^\dagger \\
&= \frac{1}{2}(\vec{p}^\dagger\cdot\vec{r}^\dagger(\frac{1}{r})^\dagger+(\frac{1}{r})^+\vec{r}^+\vec{p}^+) \\
&= \frac{1}{2}(\vec{p}\cdot\vec{r}\frac{1}{r}+\frac{1}{r}\vec{r}\cdot\vec{p}) \\
&= p_r
\end{aligned}$$

故p_r是厄米的.
(2)

$$\begin{aligned}
p_r\psi &= \frac{1}{2}(\frac{\vec{r}}{r}\cdot\vec{p}+\vec{p}\cdot\frac{\vec{r}}{r})\psi \\
&= \frac{1}{2}(\frac{\vec{r}}{r}\cdot\vec{p}\psi+\vec{p}\cdot(\frac{\vec{r}}{r}\psi)) \\
&= -\frac{i\hbar}{2}(2\frac{\vec{r}}{r}\cdot\nabla\psi+\psi\nabla\cdot\frac{\vec{r}}{r}) \\
&= -\frac{i\hbar}{2}\{2\frac{\vec{r}}{r}\cdot\nabla\psi+\psi[(\nabla\frac{1}{r})\cdot\vec{r}+\frac{1}{r}\nabla\cdot\vec{r}]\} \\
&= -\frac{i\hbar}{2}\{2\frac{\vec{r}}{r}\cdot\nabla\psi+\psi[\frac{-\vec{r}}{r^3}\cdot\vec{r}+\frac{3}{r}]\} \\
&= -i\hbar(\frac{\partial}{\partial r}+\frac{1}{r})\psi \qquad (1)
\end{aligned}$$

故$p_r=-i\hbar(\frac{\partial}{\partial r}+\frac{1}{r})$.
(3)

$$[r,p_r]\psi = -i\hbar[r,\frac{\partial}{\partial r}+\frac{1}{r}]\psi$$

$$
\begin{aligned}
&= -i\hbar[r(\frac{\partial}{\partial r}+\frac{1}{r})-(\frac{\partial}{\partial r}+\frac{1}{r})r]\psi \\
&= -i\hbar[r\frac{\partial\psi}{\partial r}-\frac{\partial}{\partial r}(r\psi)] \\
&= i\hbar\psi \qquad (2)
\end{aligned}
$$

故$[r,p_r]=i\hbar$.

(4)

$$
\begin{aligned}
p_r^2\psi &= -\hbar^2[(\frac{\partial}{\partial r}+\frac{1}{r})(\frac{\partial}{\partial r}+\frac{1}{r})]\psi \\
&= -\hbar^2[\frac{\partial^2}{\partial r^2}+\frac{\partial}{\partial r}\frac{1}{r}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}]\psi \\
&= -\hbar^2[\frac{\partial^2\psi}{\partial r^2}+(-\frac{1}{r^2}\psi)+\frac{2}{r}\frac{\partial\psi}{\partial r}+\frac{\psi}{r^2}] \\
&= -\hbar^2[\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}]\psi \qquad (3)
\end{aligned}
$$

$$
\begin{aligned}
-\hbar^2\frac{1}{r}\frac{\partial^2}{\partial r^2}(r\psi) &= -\hbar^2\frac{1}{r}\frac{\partial}{\partial r}\frac{\partial}{\partial r}(r\psi) \\
&= -\hbar^2\frac{1}{r}\frac{\partial}{\partial r}(\psi+r\frac{\partial\psi}{\partial r}) \\
&= -\hbar^2\frac{1}{r}(2\frac{\partial\psi}{\partial r}+r\frac{\partial^2\psi}{\partial r^2}) \\
&= -\hbar^2[\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}]\psi \qquad (4)
\end{aligned}
$$

$$
\begin{aligned}
-\hbar^2\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}\psi &= -\hbar^2\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial\psi}{\partial r}) \\
&= -\hbar^2\frac{1}{r^2}(2r\frac{\partial\psi}{\partial r}+r^2\frac{\partial^2\psi}{\partial r^2}) \\
&= -\hbar^2[\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}]\psi \qquad (5)
\end{aligned}
$$

故$p_r^2=-\hbar^2\frac{1}{r}\frac{\partial^2}{\partial r^2}r=-\hbar^2\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}$.

2. 根据中心力场问题的径向波函数χ本征方程，利用Hellmann定理证明：l越大，能量E越大。

证明：$\chi(r)$满足径向方程

$$(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V(r)+\frac{l(l+1)\hbar^2}{2\mu r^2})\chi(r)=E\chi(r) \qquad (6)$$

其H相当于

$$H=-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V(r)+\frac{l(l+1)\hbar^2}{2\mu r^2} \qquad (7)$$

将l视为参数，根据Hellmann定理有

$$\frac{\partial E}{\partial l} = \langle \frac{\partial H}{\partial l} \rangle = (2l+1)\frac{\hbar^2}{2\mu}\langle \frac{1}{r^2} \rangle > 0 \tag{8}$$

因此，能量E随l的增大而增大。

3. 粒子在对数形式中心力场$V(r) = -V_0 ln(r/r_0), V_0 < 0$中运动。利用Hellman和维里定理证明：（a）各束缚本征态的动能期望值相同；（b）能级间距不随粒子质量变。
解：（a）由维里定理得

$$\begin{aligned} 2\langle T \rangle_n &= \langle \vec{r} \cdot \nabla V \rangle_n \\ &= -V_0 \langle \vec{r} \cdot (\frac{\vec{r}}{r^2}) \rangle_n \\ &= -V_0 \end{aligned} \tag{9}$$

即各束缚态动能期望值相同。
(b) 由于$\langle T \rangle_n = \langle \frac{p^2}{2m} \rangle_n$, 由Hellman定理

$$\begin{aligned} \langle \frac{\partial H}{\partial m} \rangle_n = -\frac{1}{m}\langle \frac{p^2}{2m} \rangle_n = \frac{\partial E_n}{\partial m} = \frac{V_0}{2m} \\ E_n = \frac{V_0}{2}\ln(m/m_0) + e_n \end{aligned} \tag{10}$$

其中e_n是和m无关的量，m_0 是一个质量量纲的常数。当$m = m_0$时，能级完全又e_n决定。表明质量的变化只移动能级一个常数。因此能级间隔$\Delta E = \Delta e$和m无关。

一个相反的例子是氢原子的能级。根据维里定理，$T_n = -E_n$. 再根据Hellmann定理.

$$\frac{\partial E_n}{\partial m} = \frac{E_n}{m} \tag{11}$$

积分之后, $\ln(E_n/E_0) = \ln(m/m_0)$. 推出$E_n = E_0 m/m_0$ 说明E_n正比与m.
4. 计算基态氢原子的Δx，Δp_x，验证测不准关系。
解：氢原子基态波函数为$\psi(r) = \frac{1}{\sqrt{\pi a^3}}e^{-r/a}$, 利用基态波函数我们可以解得

$$\langle x \rangle = \int d^3\vec{r}\psi^* x \psi = 0 \tag{12}$$

$$\langle p_x \rangle = \int d^3\vec{r}\psi^* (-i\hbar\frac{\partial}{\partial x})\psi = 0 \tag{13}$$

$$\begin{aligned} \langle x^2 \rangle &= \int d^3\vec{r}\psi^* x^2 \psi \\ &= \frac{1}{\pi a^3}\int\int\int e^{-2r/a}x^2 r^2 sin\theta d\theta d\phi dr \\ &= \frac{1}{\pi a^3}\int_0^\infty e^{-2r/a}r^4 dr \int_0^\pi sin^3\theta d\theta \int_0^{2\pi} cos^2\phi d\phi \\ &= a^2 \end{aligned} \tag{14}$$

$$\begin{aligned}
\langle p_x^2\rangle &= -\frac{\hbar^2}{\pi a^3}\int\int\int e^{-r/a}(\frac{\partial^2}{\partial x^2}e^{-r/a})r^2 sin\theta d\theta d\phi dr \\
&= \frac{\hbar^2}{\pi a^4}\int\int\int e^{-2r/a}[\frac{1}{r}-(\frac{1}{r}+\frac{1}{a})(\frac{x}{r})^2]r^2 sin\theta d\theta d\phi dr \\
&= \frac{\hbar^2}{\pi a^4}\int\int\int e^{-2r/a}[\frac{1}{r}-(\frac{1}{r}+\frac{1}{a})sin^2\theta cos^2\phi]r^2 sin\theta d\theta d\phi dr \\
&= \frac{\hbar^2}{\pi a^4}[4\pi\int_0^\infty e^{-2r/a}dr-\int_0^\infty e^{-2r/a}(r+\frac{r^2}{a})dr\int_0^\pi sin^3\theta d\theta\int_0^{2\pi}cos^2\phi d\phi] \\
&= \frac{\hbar^2}{3a^2} \qquad (15)
\end{aligned}$$

另外，我们也可以通过计算动能的平均值，来计算$\langle p_x^2\rangle$. 由维里定理

$$\langle T\rangle = -\frac{1}{2}\langle V\rangle \qquad (16)$$

代入氢原子基态能量

$$-\frac{e^2}{2a} = \langle T\rangle+\langle V\rangle = -\langle T\rangle \qquad (17)$$

得$\langle T\rangle = e^2/2a$,因此

$$\langle p^2\rangle = 2m\langle T\rangle = \frac{\hbar^2}{a^2} \qquad (18)$$

考虑到对称性

$$\langle p_x^2\rangle = \langle p_y^2\rangle = \langle p_z^2\rangle \qquad (19)$$

我们得到

$$\langle p_x^2\rangle = \frac{\hbar^2}{3a^2} \qquad (20)$$

利用对称性，我们也可以通过计算$\langle r^2\rangle$得到$\langle x^2\rangle = \frac{1}{3}\langle r^2\rangle$。由以上计算结果，可得

$$\begin{aligned}
\Delta x &= \sqrt{\langle x^2\rangle-\langle x\rangle^2} = a \qquad (21) \\
\Delta p_x &= \sqrt{\langle p_x^2\rangle-\langle p_x\rangle^2} = \frac{\hbar}{\sqrt{3}a} \qquad (22) \\
\Delta x\Delta p_x &= \frac{\hbar}{\sqrt{3}} \geq \frac{\hbar}{2} \qquad (23)
\end{aligned}$$

5. （1）一个粒子在半径为R的刚球内自由运动（无限深球势阱）。请计算s态能级和波函数，球壁受的压力为多大？（压力可根据粒子对球壁作功等于能量变化来计算）；（2）如果粒子在半径R_1到R_2球壳内自由运动，请计算s波能级和波函数。

解：(1) 刚球势为

$$V(r) = \begin{cases} 0, & r < R \\ \infty, & r \geq R \end{cases} \tag{24}$$

s波为$l=0$的最低能量态，波函数为$\psi(r,\theta,\phi) = R(r)Y_{00} = \frac{1}{\sqrt{4\pi}}R(r)$.
令$R(r) = u(r)/r$, $u(r)$ 在球内$r < R$满足方程

$$\frac{d^2u(r)}{dr^2} + k^2u(r) \quad = \quad 0, \quad (k = \sqrt{2mE/\hbar^2}, E > 0) \tag{25}$$

其解为

$$u(r) = Asinkr + Bcoskr \tag{26}$$

因为$r \to 0$, $\psi = \frac{1}{\sqrt{4\pi}}u(r)/r \to C$, C为常数。那么

$$\lim_{r\to 0} u(r) = 0 \tag{27}$$

即B=0.又因为$r \geq R$, $u(r) = 0$.波函数在$r = R$处连续，因此

$$kR = n\pi \quad \to \quad k = \frac{n\pi}{R}, n = 1, 2, 3\cdots \tag{28}$$

则

$$E_n \quad = \quad \frac{n^2\pi^2\hbar^2}{2mR^2} \tag{29}$$

$$\psi \quad = \quad \frac{1}{\sqrt{4\pi}r}Asin\frac{n\pi}{R}r \tag{30}$$

进行归一化，

$$\frac{1}{4\pi}|A|^2\int\frac{1}{r^2}sin^2\frac{n\pi r}{R}r^2 sin\theta dr d\theta d\phi = 1 \qquad \to A = \sqrt{\frac{2}{R}} \tag{31}$$

故s波波函数和能级为

$$\psi_{100} = \begin{cases} \frac{1}{r\sqrt{2\pi R}}sin\frac{\pi r}{R}, & r < R \\ 0, & r \geq R \end{cases} \tag{32}$$

$$E_1 \quad = \quad \frac{\pi^2\hbar^2}{2mR^2} \tag{33}$$

设粒子对球壁的平均作用力为$\langle F\rangle$。假定球壁的半径在此力的作用下增大了ΔR,则粒子对外做功$\langle F\rangle\Delta R$,它等于粒子能量的减小$-(dE/dR)\Delta R$, 故有$\langle F\rangle = -\frac{dE}{dR}$。将基态能量$E = \frac{\pi^2\hbar^2}{2mR^2}$代入上式，得平均作用力$\langle F\rangle$

$$\langle F\rangle = -\frac{dE}{dR} = \frac{n^2\pi^2\hbar^2}{mR^3} \tag{34}$$

(2) 如果粒子在半径R_1到R_2球壳内自由运动, 则刚球势变为

$$V(r)=\begin{cases}0, & R_1<r<R_2\\ \infty, & r\le R_1, r\ge R_2\end{cases}$$

对于$r\le R_1, r\ge R_2$, $u(r)=0$. 根据式(25),再结合连续性边界条件$u(R_1)=0$,$u(R_2)=0$,有

$$Asin(kR_1)+Bcos(kR_1)=0 \qquad Asin(kR_2)+Bcos(kR_2)=0 \tag{35}$$

解得

$$k = \frac{n\pi}{R_2-R_1} \tag{36}$$

$$E_n = \frac{n^2\pi^2\hbar^2}{2m(R_1-R_2)^2} \qquad n=1,2,3,\cdots \tag{37}$$

$$\psi = \frac{1}{\sqrt{4\pi}r}Asin(\frac{n\pi}{R_2-R_1}(r-R_1)) \tag{38}$$

归一化可得$A=\sqrt{\frac{2}{R_2-R_1}}$.则,

$$\psi=\begin{cases}\frac{1}{\sqrt{2\pi(R_2-R_1)}}sin(\frac{n\pi}{R_2-R_1}(r-R_1)) & R_1<r<R_2\\ 0, \quad others\end{cases} \tag{39}$$

所以s波波函数和能级为

$$\psi_{100}=\begin{cases}\frac{1}{r\sqrt{2\pi(R_2-R_1)}}sin\frac{\pi(r-R_1)}{R_2-R_1}, & R_1<r<R_2\\ 0, \quad others\end{cases} \tag{40}$$

$$E_1=\frac{\pi^2\hbar^2}{2m(R_2-R_1)^2} \tag{41}$$

6 参见讲义