PHY5410 FA22 HW04

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Problem 1 (6.3)**.** Using the relation that $u(r) = rR(r)$, $\varrho = \kappa r$ (more strictly, we should use the notation $v(\varrho) = u(r) = u(\varrho/\kappa)$ rather than $u(\varrho)$ to denote $u(\varrho/\kappa)$), define the following notation

$$\langle \varrho^k \rangle_u = 4\pi \int \mathrm{d}\varrho\, \varrho^k u(\varrho)^2$$

then one can verify

$$\langle \varrho^k \rangle_u = 4\pi \int \mathrm{d}\kappa r\, (\kappa r)^k r^2 R(r)^2 = 4\pi\kappa^{k+1} \int r^2\, \mathrm{d}r r^k R^r(r) = \kappa^{k+1} \langle r^k \rangle$$

Using the differential equation

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} - \frac{l(l+1)}{\rho^2} + \frac{2n}{\rho} - 1\right] u(\rho) = 0 \tag{1}$$

Multiply $\rho^{k+1} u'_{nl}(\rho)$ on the left, we get

$$\rho^{k+1} u' u'' - \rho^{k-1} l(l+1) u u' + 2n\rho^k u u' - \rho^{k+1} u u' = 0$$

Using the fact that

$$\begin{aligned}
4\pi \int \mathrm{d}\rho\, \rho^m u u' &= -\frac{m}{2} 4\pi \int \mathrm{d}\rho\, \rho^{m-1} u^2 = -\frac{m}{2} \langle \rho^{m-1} \rangle_u \\
4\pi \int \mathrm{d}\rho\, \rho^m u u' &= -2\pi(m-1) \int \mathrm{d}\rho\, \rho^{m-1} (u')^2 \\
4\pi \int \mathrm{d}\rho\, \rho^m u u'' &= -4\pi m \int \mathrm{d}\rho\, \rho^{m-1} u u' - 4\pi \int \mathrm{d}\rho\, \rho^m (u')^2
\end{aligned}$$

we can multiply the expression by 4π and integrate it

$$-2\pi(k+1) \int \mathrm{d}\rho\, \rho^k (u')^2 + \frac{1}{2}(k-1) l(l+1) \langle \rho^{k-2} \rangle_u - nk \langle \rho^{k-1} \rangle_u + \frac{1}{2}(k+1) \langle \rho^k \rangle_u = 0 \tag{2}$$

we can also multiply the equation by $\rho^k u_{nl}(\rho)$

$$\rho^k u u'' - l(l+1)\rho^{k-2} u^2 + 2n\rho^{k-1} u^2 - \rho^k u^2 = 0$$

multiply this equation by 4π and integrate it

$$\frac{1}{2} k(k-1) \langle \rho^{k-2} \rangle_u - 4\pi \int \mathrm{d}\rho\, \rho^k (u')^2 - l(l+1) \langle \rho^{k-2} \rangle_u + 2n \langle \rho^{k-1} \rangle_u - \langle \rho^k \rangle_u = 0 \tag{3}$$

Combing equation 2 and 3 to eliminate $(u')^2$ term, we can get

$$\begin{aligned}
[\frac{1}{2}(k-1) l(l+1) - \frac{1}{4} k(k^2-1) + \frac{1}{2} l(l+1)(k+1)] \langle \rho^{k-2} \rangle_u - [nk + n(k+1)] \langle \rho^{k-1} \rangle_u + (k+1) \langle \rho^k \rangle_u &= 0 \\
\frac{k}{4}[4l(l+1) - (k^2-1)] \langle \rho^{k-2} \rangle_u - n(2k+1) \langle \rho^{k-1} \rangle_u + (k+1) \langle \rho^k \rangle_u &= 0 \\
\frac{k}{4}[(2l+1)^2 - k^2] \langle \rho^{k-2} \rangle_u - n(2k+1) \langle \rho^{k-1} \rangle_u + (k+1) \langle \rho^k \rangle_u &= 0
\end{aligned}$$

Plugin $\kappa = 1/na$ and $\langle \rho^k \rangle_u = \kappa^{k+1} \langle r^k \rangle$, we obtain

$$\begin{aligned}
\frac{k}{4}[(2l+1)^2 - k^2] \langle r^{k-2} \rangle - n(2k+1)\kappa \langle r^{k-1} \rangle + (k+1)\kappa^2 \langle r^k \rangle &= 0 \\
\frac{k+1}{n^2} \langle r^k \rangle - (2k+1) a \langle r^{k-1} \rangle + \frac{k}{4}[(2l+1)^2 - k^2] a^2 \langle r^{k-2} \rangle &= 0
\end{aligned}$$

Problem 2 (6.13). Let A_i denotes the ith component of $\mathbf{A}$, then

$$A_i = \frac{1}{2m}(\epsilon_{ijk}p_jL_k - \epsilon_{ijk}L_jp_k) - \frac{Ze^2}{r}x_i = \frac{1}{2m}\epsilon_{ijk}(p_jL_k + L_kp_j) - \frac{Ze^2}{r}x_i$$

where summation would be taken in place of j and k. Since $p_j^\dagger = p_j$, $L_k^\dagger = L_k$, then we can prove that A_i is hermitian

$$A_i^\dagger = \frac{1}{2m}\epsilon_{ijk}(L_k^\dagger p_j^\dagger + p_j^\dagger L_k^\dagger) - \frac{Ze^2}{r}x_i^\dagger = \frac{1}{2m}\epsilon_{ijk}(L_kp_j + p_jL_k) - \frac{Ze^2}{r}x_i = A_i$$

Therefore $\mathbf{A}$ is hermitian.

To prove that $[\mathbf{A}, H] = 0$, we can first prove $[A_i, H] = 0$. A_i could be simplified to the following expression by direct summation over j and k.

$$\begin{aligned}
A_i &= \frac{1}{2m}\epsilon_{ijk}\epsilon_{kmn}(p_jx_mp_n + x_mp_np_j) - \frac{Ze^2}{r}x_i \\
&= \frac{1}{2m}\epsilon_{ijk}\epsilon_{kmn}[(x_mp_j - i\hbar\delta_{jm}p_n + x_mp_np_j)] - \frac{Ze^2}{r}x_i \\
&= \frac{1}{2m}\epsilon_{kij}\epsilon_{kmn}(2x_mp_jp_n - i\hbar\delta_{jm}p_n) - \frac{Ze^2}{r}x_i \\
&= \frac{1}{2m}(\delta_{im}\delta_{jn} - \delta_{in}\delta_{jm})(2x_mp_jp_n - i\hbar\delta_{jm}p_n)
\end{aligned}$$

Since

$$\begin{aligned}
\delta_{im}\delta_{jn}x_mp_jp_n &= \delta_{jn}x_ip_jp_n = x_ip^2 \\
\delta_{in}\delta_{jm}x_mp_jp_n &= \delta_{jm}x_mp_ip_j = (x\cdot p)p_i \\
\delta_{im}\delta_{jm}\delta_{jn}i\hbar p_n &= \delta_{ij}\delta_{jn}i\hbar p_n = i\hbar p_i \\
\delta_{in}\delta_{jm}^2p_n &= \delta_{jm}^2 i\hbar p_i = 3i\hbar p_i
\end{aligned}$$

Then we have

$$A_i = \frac{1}{m}x_ip^2 - \frac{1}{m}(x\cdot p)p_i + \frac{1}{m}i\hbar p_i - \frac{Ze^2}{r}x_i$$

Using the fact that $H = p^2/2m - Ze^2/r$, we have

$$\begin{aligned}
A_iH &= \frac{1}{2m^2}[x_i(p^2)^2 - (x\cdot p)p^2p_i + i\hbar p^2p_i] - \frac{Ze^2}{2m}\frac{1}{r}x_ip^2 - \frac{Ze^2}{m}[x_ip^2\frac{1}{r} - (x\cdot p)p_i\frac{1}{r} + i\hbar p_i\frac{1}{r}] + \frac{Ze^4}{r^2}x_i \\
HA_i &= \frac{1}{2m^2}[p^2x_ip^2 - p^2(x\cdot p)p_i + i\hbar p^2p_i] - \frac{Ze^2}{2m}p^2\frac{1}{r}x_i - \frac{Ze^2}{m}[\frac{1}{r}x_ip^2 - \frac{1}{r}(x\cdot p)p_i + \frac{1}{r}i\hbar p_i] + \frac{Ze^4}{r^2}x_i
\end{aligned}$$

Using the commutation relationship

$$\begin{aligned}
p^2x_i &= x_ip^2 - 2i\hbar p_i \\
p^2(x\cdot p) &= \sum_j p^2x_jp_j = \sum_j x_jp^2p_j - 2i\hbar p_j^2 = (x\cdot p)p^2 - 2i\hbar p^2
\end{aligned}$$

Then it is easy to show that the blue parts are equal

$$p^2x_ip^2 - p^2(x\cdot p)p_i = x_i(p^2)^2 - 2i\hbar p^2p_i - (x\cdot p)p^2p_i + 2i\hbar p^2p_i = x_i(p^2)^2 - (x\cdot p)p^2p_i$$

Moreover, using the fact that

$$\begin{aligned}
p_i\frac{1}{r} &= i\hbar\frac{1}{r^3}x_i + \frac{1}{r}p_i \\
p_ip_j\frac{1}{r} &= i\hbar\frac{1}{r^3}x_ip_j + i\hbar\frac{1}{r^3}x_jp_i + \frac{1}{r}p_ip_j + \hbar^2\frac{\delta_{ij}r^2-3x_ix_j}{r^5} \\
p^2\frac{1}{r} &= 2i\hbar\frac{1}{r^3}(x\cdot p) + \frac{1}{r}p^2 \\
p^2x_i\frac{1}{r} &= x_ip^2\frac{1}{r} - 2i\hbar p_i\frac{1}{r} = 2i\hbar\frac{1}{r^3}x_i(x\cdot p) + \frac{1}{r}x_ip^2 + 2\hbar^2\frac{1}{r^3}x_i - 2i\hbar\frac{1}{r}p_i
\end{aligned}$$

we have

$$\begin{aligned}
-\frac{Ze^2}{2m}\frac{1}{r}x_ip^2 - \frac{Ze^2}{m}[x_ip^2\frac{1}{r} - (x\cdot p)p_i\frac{1}{r} + i\hbar p_i\frac{1}{r}] &= -\frac{Ze^2}{2m}\frac{1}{r}x_ip^2 - \frac{Ze^2}{m}\Big[2i\hbar\frac{1}{r^3}x_i(x\cdot p) + \frac{1}{r}x_ip^2 \\
&- i\hbar\frac{1}{r^3}x_i(x\cdot p) - i\hbar\frac{1}{r}p_i - \frac{1}{r}(x\cdot p)p_i + 2\hbar^2\frac{1}{r^3}x_i \\
&- \hbar^2\frac{1}{r^3}x_i + i\hbar\frac{1}{r}p_i\Big] \\
&= -\frac{Ze^2}{2m}\frac{1}{r}x_ip_i - \frac{Ze^2}{m}\Big[\frac{1}{r}x_ip^2 - \frac{1}{r}(x\cdot p)p_i \\
&+ i\hbar\frac{1}{r^3}x_i(x\cdot p) + \hbar^2\frac{1}{r^3}x_i\Big] \\
-\frac{Ze^2}{2m}p^2\frac{1}{r}x_i - \frac{Ze^2}{m}[\frac{1}{r}x_ip^2 - \frac{1}{r}(x\cdot p)p_i + \frac{1}{r}i\hbar p_i] &= -\frac{Ze^2}{2m}\frac{1}{r}x_ip^2 - \frac{Ze^2}{m}i\hbar\frac{1}{r^3}x_i(x\cdot p) - \frac{Ze^2}{m}\hbar^2\frac{1}{r^3}x_i \\
&+ \frac{Ze^2}{m}i\hbar\frac{1}{r}p_i - \frac{Ze^2}{m}\Big[\frac{1}{r}x_ip^2 - \frac{1}{r}(x\cdot p)p_i + i\hbar\frac{1}{r}p_i\Big] \\
&= -\frac{Ze^2}{2m}\frac{1}{r}x_ip^2 - \frac{Ze^2}{m}\Big[\frac{1}{r}x_ip^2 - \frac{1}{r}(x\cdot p)p_i \\
&+ i\hbar\frac{1}{r^3}x_i(x\cdot p) + \hbar^2\frac{1}{r^3}x_i\Big]
\end{aligned}$$

Hence the red part is also equal. Therefore $[A_i, H] = 0$, we have $[\mathbf{A}, H] = 0$.

The proof of $\mathbf{A}\cdot\mathbf{L} = \mathbf{L}\cdot\mathbf{A} = 0$ begins from the following claims.

Claim. $\mathbf{L}\cdot x = x\cdot\mathbf{L} = 0$.

Proof. Note that

$$\begin{aligned}
x\cdot\mathbf{L} &= \sum_{ijk}\epsilon_{ijk}x_ix_jp_k = \sum_k\left(\sum_{ij}\epsilon_{ijk}x_ix_j\right)p_k = \sum_k 0p_k = 0 \\
\mathbf{L}\cdot x &= \sum_{ijk}\epsilon_{ijk}x_jp_kx_i = \sum_{ijk}\epsilon_{ijk}x_j(x_ip_k - i\hbar\delta_{ik}) = \sum_{ijk}\epsilon_{ijk}x_ix_jp_k - i\hbar\epsilon_{ijk}\delta_{ik} = 0
\end{aligned}$$

□

Claim. $\mathbf{L}\cdot(p\times\mathbf{L} - \mathbf{L}\times p) = (p\times\mathbf{L} - \mathbf{L}\times p)\cdot\mathbf{L} = 0$.

Proof. Note that

$$\mathbf{L}\cdot(p\times\mathbf{L} - \mathbf{L}\times p) = \sum_{ijk}\epsilon_{ijk}L_ip_jL_k - \epsilon_{ijk}L_iL_jp_k = \sum_{ijk}\epsilon_{ijk}L_i(p_jL_k + L_kp_j)$$

$$
\begin{aligned}
&= \sum_{ijk} \epsilon_{ijk}(2L_i L_k p_j + i\hbar \sum_l \epsilon_{kjl} p_l) \\
&= \sum_{ijk} 2\epsilon_{ijk} L_i L_k p_j - i\hbar \epsilon_{ijk}\epsilon_{kjl} L_i p_l \\
&= -\sum_j 2i\hbar L_j p_j - \sum_k i\hbar L_k p_k + \sum_i 3i\hbar L_i p_i \\
&= 0 \\
(p \times \mathbf{L} - \mathbf{L} \times p) \cdot \mathbf{L} &= \sum_{ijk} \epsilon_{ijk}(p_j L_k + L_k p_j) L_i \\
&= \sum_{ijk} \epsilon_{ijk}(2p_j L_k + i\hbar \sum_l \epsilon_{kjl} p_l) L_i \\
&= \sum_j 2i\hbar p_j L_j + \sum_k i\hbar p_k L_k - 3\sum_i p_i L_i \\
&= 0
\end{aligned}
\qquad \square
$$

Therefore, it is easy to show that

$$
\begin{aligned}
\mathbf{L} \cdot \mathbf{A} &= \frac{1}{2m} \mathbf{L} \cdot (p \times \mathbf{L} - \mathbf{L} \times p) - (\mathbf{L} \times x) \frac{Ze^2}{r} = 0 \\
\mathbf{A} \cdot \mathbf{L} &= \frac{1}{2m} (p \times \mathbf{L} - \mathbf{L} \times p) - \frac{Ze^2}{r} (r \times \mathbf{L}) = 0
\end{aligned}
$$

Problem 3 (7.1). Since

$$
\begin{aligned}
\nabla \cdot \mathbf{j} &= \frac{1}{2m} \left[\psi^*(-i\hbar \nabla^2 \psi - \frac{e}{c} A \cdot \nabla \psi - \frac{e}{c} (\nabla \cdot \mathbf{A}) \psi) + (\nabla \psi^*) \cdot (-i\hbar \nabla \psi - \frac{e}{c} \mathbf{A} \psi) \right] + \text{c.c.} \\
&= \frac{1}{2m} \left(-i\hbar \psi^* \nabla^2 \psi - \frac{e}{c} \psi^* \mathbf{A} \cdot \nabla \psi - \frac{e}{c} (\nabla \cdot \mathbf{A}) \psi^* \psi - i\hbar \nabla \psi^* \cdot \nabla \psi - \frac{e}{c} \nabla \psi^* \cdot \mathbf{A} \psi \right) + \text{c.c.} \\
&= \frac{1}{2m} \left(-i\hbar \psi^* \nabla^2 \psi - \frac{e}{c} \psi^* \mathbf{A} \cdot \nabla \psi - \frac{e}{c} (\nabla \cdot \mathbf{A}) \psi^* \psi - \frac{e}{c} \nabla \psi^* \cdot \mathbf{A} \psi \right) + \text{c.c.} \\
&= \frac{1}{2m} \left(-i\hbar \psi^* \nabla^2 \psi - \frac{2e}{c} \psi^* \mathbf{A} \cdot \nabla \psi - \frac{e}{c} (\nabla \cdot \mathbf{A}) \psi^* \psi \right) + \text{c.c.}
\end{aligned}
$$

and

$$
\begin{aligned}
\frac{\partial}{\partial t} \psi^* \psi &= \psi^* \frac{\partial}{\partial t} \psi + \text{c.c.} \\
&= \frac{1}{i\hbar} \psi^* H \psi + \text{c.c.} \\
&= \frac{1}{i\hbar} \psi^* \left(-\frac{\hbar^2}{2m} \nabla^2 \psi + \frac{i\hbar e}{mc} \mathbf{A} \cdot \nabla \psi + \frac{i\hbar e}{2mc} (\nabla \cdot \mathbf{A}) \psi + \frac{e^2}{2mc} \mathbf{A}^2 \psi + e\Phi \psi \right) + \text{c.c.} \\
&= \frac{1}{2m} \left(i\hbar \psi^* \nabla^2 \psi + \frac{2e}{c} \psi^* \mathbf{A} \cdot \nabla \psi + \frac{e}{c} (\nabla \cdot \mathbf{A}) \psi^* \psi \right) + \text{c.c.}
\end{aligned}
$$

Hence $\partial_t \psi^* \psi + \nabla \cdot \mathbf{j} = 0$.

Problem 4 (7.3).