P1

$$L \equiv \alpha(x)\frac{\mathrm{d}^2}{\mathrm{d}^2 x} + \beta(x)\frac{\mathrm{d}}{\mathrm{d}x} + \gamma(x). \tag{1}$$

1. Conditions for self-adjointness

We calculate for $\langle f|Lg\rangle$ and $\langle Lf|g\rangle$ separately, and observe $\langle f|Lg\rangle - \langle Lf|g\rangle$.

- $\langle f|Lg\rangle$:

$$\begin{aligned}\langle f|Lg\rangle &= \int_{-\infty}^{\infty} \mathrm{d}x f^*(x)[\alpha g''(x) + \beta g'(x) + \gamma g(x)] \\ &= \underbrace{\int_{-\infty}^{\infty} f^*\alpha g''\,\mathrm{d}x}_{(1)} + \underbrace{\int_{-\infty}^{\infty} f^*\beta g'\,\mathrm{d}x}_{(2)} + \int_{-\infty}^{\infty} \gamma\,\mathrm{d}x\end{aligned} \tag{2}$$

Integrating by parts for each term, we have

$$\begin{aligned}(1) &= [f^*\alpha g' - f'^*\alpha g - f\alpha' g]_{-\infty}^{\infty} + \int_{-\infty}^{\infty}(f''^*\alpha + 2f'^*\alpha' + f^*\alpha'')g\,\mathrm{d}x; \\ (2) &= [f^*\beta g]_{-\infty}^{\infty} - \int_{-\infty}^{\infty}(\beta f'^* + \beta' f^*)g\,\mathrm{d}x.\end{aligned} \tag{3}$$

and thus

$$\langle f|Lg\rangle = [f^*\alpha g' - f'^*\alpha g - f^*\alpha' g + f^*\beta g]_{-\infty}^{\infty} + \int_{-\infty}^{\infty}[\alpha f''^* + (2\alpha' - \beta)f'^* + (\alpha'' - \beta' + \gamma)f^*]g\,\mathrm{d}x. \tag{4}$$

In an almost exact same way, we work out $\langle Lf|g\rangle$ using integration by parts, we have

$$\langle Lf|g\rangle = [\alpha g g'^* - \alpha g' f^* - \alpha' g f^* + \beta g f^*]_{-\infty}^{\infty} + \int_{-\infty}^{\infty} f^*[\alpha g'' + (2\alpha - \beta)g' + (\alpha'' - \beta' + c)g]\,\mathrm{d}x. \tag{5}$$

Subtracting the two, and using the fact that $f^*g'' - f''^*g = \frac{\mathrm{d}}{\mathrm{d}x}(f^*g' - (f')^*g)$, we arrive at

$$\langle f|Lg\rangle - \langle Lf|g\rangle = [\alpha(f'^*g - f^*g')]_{-\infty}^{\infty} + \int_{-\infty}^{\infty}(\alpha' - \beta)(f^*g' - f'^*g)\,\mathrm{d}x. \tag{6}$$

We observe that the condition for self-adjointness requires
1. $\beta(x) = \alpha'(x)$,
2. the boundary conditions $[\alpha(f'^*g - f^*g')]_{-\infty}^{\infty} = 0$.

2. The legendre operator is self adjoit on $[-1, 1\}$

We immediately read off that

$$\begin{aligned}\alpha(x) = -(1 - x^2),& \quad \alpha'(x) = 2x, \\ \beta(x) &= 2x, \\ \gamma(x) &= 0,\end{aligned} \tag{7}$$

and so

$$\begin{aligned}\alpha(\pm 1) = 0 \Rightarrow [\alpha(f'^*g - f^*g')]_{-\infty}^{\infty} &= 0, \\ \beta(x) &= \alpha'(x).\end{aligned} \tag{8}$$

This is suffice to show that the Legendre operator is self-adjoint on $[-1, 1]$, under the b.c. that f, g are finite at $x = \pm 1$.

P2

1. Show by induction that $[x_i, p_i^n] = ni\hbar p_i^{n-1}$, and $[p_i, x_i^n] = -ni\hbar x_i^{n-1}$

Recall that $\left[x_i, p_j\right] = i\hbar\delta_{ij}$.

- Base case ($n=1$): Trivially true, as $[x_i, p_i] = i\hbar$ and $[p_i, x_i] = -i\hbar$.
- Inductive case: Assume true for $n = k$, i.e. $\left[x_i, p_i^k\right] = ki\hbar p_i^{k-1}$ and $\left[p_i, x_i^k\right] = -ki\hbar x_i^{k-1}$. We want to show true for $n = k+1$.

Notice that

$$\begin{aligned}
\left[x_i, p_i^{k+1}\right] &= \left[x_i, p_i^k p_i\right] = \left[x_i, p_i^k\right]p_i + p_i^k[x_i, p_i] = ki\hbar p_i^{k-1}p_i + p_i^k i\hbar = (k+1)i\hbar p_i^k, \\
\left[p_i, x_i^{k+1}\right] &= \left[p_i, x_i^k x_i\right] = \left[p_i, x_i^k\right]x_i + x_i^k[p_i, x_i] = -ki\hbar x_i^{k-1}x_i + x_i^k(-i\hbar) = -(k+1)i\hbar x_i^k.
\end{aligned} \tag{9}$$

Then by induction, we have $[x_i, p_i^n] = ni\hbar p_i^{n-1}$ and $[p_i, x_i^n] = -ni\hbar x_i^{n-1}$ for all positive integers n.

2. Use the result in (1) to show that $[x_i, G(p_i)] = i\hbar\frac{\partial G}{\partial p_i}$ and $[p_i, F(x_i)] = -i\hbar\frac{\partial F}{\partial x_i}$ for any analytic functions F and G.

Proof: Expand $G(\boldsymbol{p}) = \sum_m a_m \prod_r p_r^{m_r}$. Then

$$[x_i, G(\boldsymbol{p}] = \sum_m a_m \left[x_i, \prod_r p_r^{m_r}\right], \tag{10}$$

where

$$\begin{aligned}
\left[x_i, \prod_r p_r^{m_r}\right] &= \prod_{r\neq i} p_r^{m_r}\left[x_i, p_i^{m_i-1}\right] \\
&= \prod_{r\neq i} p_r^{m_r} m_i i\hbar p_i^{m_i-1} \\
\Rightarrow [x_i, G(\boldsymbol{p})] &= i\hbar\sum_m m_i p_i^{m_i-1}\prod_{r\neq i} p_r^{m_r} \\
&= i\hbar\sum_m a_m \frac{\partial}{\partial p_i}\left(\prod_r p_r^{m_r}\right) = i\hbar\frac{\partial G(\boldsymbol{p})}{\partial p_i}.
\end{aligned} \tag{11}$$

■

Similarly, expanding $F(\boldsymbol{x}) = \sum_m a_m \prod_r x_r^{m_r}$, we can show that

$$[p_i, F(\boldsymbol{x})] = \sum_m a_m \left[p_i, \prod_r x_r^{m_r}\right] \tag{12}$$

where

$$\begin{aligned}
\left[p_i, \prod_r x_r^{m_r}\right] &= \prod_{r\neq i} x_r^{m_r}\left[p_i, x_i^{m_i}\right] \\
&= \prod_{r\neq i} x_r^{m_r}\left(-m_i i\hbar x_i^{m_i-1}\right) \\
\Rightarrow [p_i, F(\boldsymbol{x})] &= -i\hbar\sum_m a_m m_i x_i^{m_i-1}\prod_{r\neq i} x_r^{m_r} \\
&= -i\hbar\sum_m a_m \frac{\partial}{\partial x_i}\left(\prod_r x_r^{m_r}\right) = -i\hbar\frac{\partial F(\boldsymbol{x})}{\partial x_i}.
\end{aligned} \tag{13}$$

■

3. Comparing $[x^2, p^2]$ with $\{x^2, p^2\}$.

We first work out $[x_i, p^2]$, with $p^2 = \sum_j p_j^2$:

$$[x_i, p^2] \sum_j (p_j [x_i, p_j] + [x_i, p_j] p_j) = \sum_j (p_j i\hbar\delta_{ij} + i\hbar\delta_{ij} p_j) = 2i\hbar p_i. \tag{14}$$

Then, we have

$$\begin{aligned}
[x^2, p^2] &= \left[\sum_i x_i^2, p^2\right] \\
&= \sum_i (x_i [x_i, p^2] + [x_i, p^2] x_i \\
&= \sum_i (x_i 2hi\hbar p_i + 2i\hbar p_i x_i) \\
&= 2i\hbar \sum_i (x_i p_i + p_i x_i) \\
&= 2i\hbar(\boldsymbol{x} \cdot \boldsymbol{p} + \boldsymbol{p} \cdot \boldsymbol{x}).
\end{aligned} \tag{15}$$

On the other hand,

$$\{x^2, p^2\} = \sum_i \left(\partial_{x_i} x^2 \cdot \partial_{p_i} p^2 - \partial_{p_i} x^2 \cdot \partial_{x_i} p^2\right) = \sum_i (2x_i \cdot 2p_i - 0) = 4\boldsymbol{x} \cdot \boldsymbol{p}. \tag{16}$$

Now, notice that if we define a mapping s.t.

$$\boldsymbol{x} \cdot \boldsymbol{p} \mapsto \frac{1}{2}(\boldsymbol{x} \cdot \boldsymbol{p} + \boldsymbol{p} \cdot \boldsymbol{x}), \tag{17}$$

then we can relate the poisson bracket to the commutator by

$$i\hbar\{x^2, p^2\} \mapsto 1\hbar \cdot 4 \cdot \frac{1}{2}(\boldsymbol{x} \cdot \boldsymbol{p} + \boldsymbol{p} \cdot \boldsymbol{x}) = [x^2, p^2]. \tag{18}$$

P3

Consider

$$T(\boldsymbol{l}) = \exp\left(\frac{-i\boldsymbol{p}\cdot\boldsymbol{l}}{\hbar}\right), \tag{19}$$

1. Find $[x_i, T(\boldsymbol{l})]$ **.**

Using the result in P2(2), taking $G(\boldsymbol{p}) = \exp\left(\frac{-i\boldsymbol{p}\cdot\boldsymbol{l}}{\hbar}\right)$, we have

$$[x_i, T(\boldsymbol{l})] = i\hbar\frac{\partial}{\partial p_i}\left(\exp\left(\frac{-i\boldsymbol{p}\cdot\boldsymbol{l}}{\hbar}\right)\right) = i\hbar\exp\left(\frac{-i\boldsymbol{p}\cdot\boldsymbol{l}}{\hbar}\right)\frac{-il_i}{\hbar} = l_i T(\boldsymbol{l}). \tag{20}$$

Notice that

$$\begin{aligned} [x_i, T(\boldsymbol{l})] &= x_i T(\boldsymbol{l}) - T(\boldsymbol{l}) x_i = l_i T(\boldsymbol{l}) \\ \Rightarrow T^{\dagger(\boldsymbol{l})} x_i T(\boldsymbol{l}) &= x_i + l_i. \end{aligned} \tag{21}$$

2.

From this, we see that

$$\langle x_{i'}\rangle = \langle\alpha|x_{i'}|\alpha\rangle = \left\langle\alpha\middle|T^{\dagger(\boldsymbol{l})} x_i T(\boldsymbol{l})\middle|\alpha\right\rangle = \langle\alpha|(x_i + l_i)\alpha\rangle = \langle x_i\rangle + l_i. \tag{22}$$

P4

Using identity below and $x|x'\rangle = x'|x'\rangle$, $p|p'\rangle = p'|p\rangle$; find $\langle x|[x,p]|\alpha\rangle$ in terms of $\psi_\alpha(x) = \langle x|\alpha\rangle$

$$\langle x|p\rangle = \frac{1}{2\pi\hbar}\exp\left(\frac{ipx}{\hbar}\right). \tag{23}$$

1. Brute force using the Fourier transform relation

$\langle x|[\hat{x},\hat{p}]|\alpha\rangle = \underbrace{\langle x|\hat{x}\hat{p}|\alpha\rangle}_{(1)} - \underbrace{(x,\hat{p}\hat{x},\alpha)}_{(2)}$. We denote $N = 2\pi\hbar$.

$$\begin{aligned}
(1) &= \int \langle x|\hat{x}\hat{p}|p'\rangle\langle p'|\alpha\rangle\,\mathrm{d}p' \\
&= \int \langle x|\hat{x}p'|p'\rangle\langle p'|\alpha\rangle\,\mathrm{d}p' \\
&= \int \langle x|\hat{x}p'|p'\rangle\langle p'|x'\rangle\langle x'|\alpha\rangle\,\mathrm{d}p'\,\mathrm{d}x' \\
&= p'x\int \langle x|p'\rangle\langle p'|x'\rangle\langle x'|\alpha\rangle\,\mathrm{d}p'\,\mathrm{d}x' \\
&= xp'\int \frac{1}{N}\exp(ip'x/\hbar)\frac{1}{N}\exp(-ip'x'/\hbar)\psi_\alpha(x')\,\mathrm{d}p'\,\mathrm{d}x' \\
&= xp'\int \frac{1}{N^2}\exp(ip'(x-x')/\hbar)\psi_\alpha(x')\,\mathrm{d}p'\,\mathrm{d}x'.
\end{aligned} \tag{24}$$

Noticing

$$\frac{1}{N}\int \exp\left(\frac{ip(x-x')}{\hbar}\right)p\,\mathrm{d}p = -i\hbar\partial_x\delta(x-x'), \tag{25}$$

we simplify (1) to

$$(1) = -i\hbar x\partial_x\int \delta(x-x')\psi_\alpha(x')\,\mathrm{d}x' = -i\hbar x\psi'_\alpha(x). \tag{26}$$

Similarly,

$$\begin{aligned}
(2) = \int \langle x|\hat{p}|p'\rangle\langle p'|\hat{x}|\alpha\rangle\,\mathrm{d}p' \\
&= p'\int \langle x|p'\rangle\langle p'|\hat{x}|\alpha\rangle\,\mathrm{d}p' \\
&= p'\int \langle x|p'\rangle\langle p'|\hat{x}|x'\rangle\langle x'|\alpha\rangle\,\mathrm{d}p'\,\mathrm{d}x' \\
&= p'x'\int \langle x|p'\rangle\langle p'|x'\rangle\psi_\alpha(x')\,\mathrm{d}p'\,\mathrm{d}x' \\
&= p'x'\int \frac{1}{N}e^{ip'x/\hbar}\frac{1}{N}e^{-ip'x'\hbar}\psi_\alpha(x')\,\mathrm{d}p'\,\mathrm{d}x' \\
&= x'p'\int \frac{1}{N^2}e^{ip'(x-x')/\hbar}\,\mathrm{d}p'\,\mathrm{d}x' \\
&= -i\hbar\partial_x\int \delta(x-x')x'\psi_\alpha(x')\,\mathrm{d}x' \\
&= -i\hbar(\psi(\alpha) + x\psi'(\alpha))
\end{aligned} \tag{27}$$

Subtracting, we have

$$\langle x|[\hat{x},\hat{p}]|\alpha\rangle = (1) - (2) = -i\hbar x\psi'_\alpha(x) + i\hbar(\psi_\alpha(x) + x\psi'_\alpha(x)) = i\hbar\psi_\alpha(x). \tag{28}$$

2. Using the fact that in $|x\rangle$ representation, $p = -i\hbar\partial_x$.

We simply make expansions and arrive at

$$
\begin{aligned}
\langle x|[x,p]|\alpha\rangle &= \langle x|x\; i\hbar\partial_x - i\hbar\partial_x\; x|\alpha\rangle = x(-i\hbar\partial_x\psi_\alpha(x)) - (-i\hbar\partial_x(x\psi_\alpha(x))) \\
&= -i\hbar x\partial_x\psi_\alpha(x) + i\hbar\psi_\alpha(x) + i\hbar x\partial_x\psi_{\alpha(x)} = i\hbar\psi_\alpha(x).
\end{aligned} \tag{29}
$$

P5

The ground state positiion space wavefunction of the Hydrogen atom is

$$\psi_{1s}(\boldsymbol{x}) = \langle \boldsymbol{x}|1s\rangle = \frac{1}{\sqrt{\pi a_0^3}} \exp(-r/a_0). \tag{30}$$

1. Find $\psi_{1s}(\boldsymbol{p})$.

We first prove the following identity:

$$\begin{aligned}
\int_{\mathbb{R}_3} e^{-i\boldsymbol{q}\cdot\boldsymbol{x}} f(r) \mathrm{d}^3 r &= \int_0^\infty r^2 f(r)\,\mathrm{d}r \int_0^\pi \sin\theta e^{-iqr\cos\theta}\,\mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\varphi \\
&\underset{u\equiv\cos\theta}{=} 2\pi \int_0^\infty r^2 f(r)\,\mathrm{d}r \int_{-1}^1 e^{-iqru}\,\mathrm{d}u \\
&= 4\pi \int_0^\infty r^2 f(r) \frac{\sin(qr)}{qr}\,\mathrm{d}r \\
&= \frac{4\pi}{q} \int_0^\infty f(r)\sin(qr) r\,\mathrm{d}r
\end{aligned} \tag{31}$$

We then consider $\psi(\boldsymbol{p})$ using fourier transform:

$$\psi(\boldsymbol{p}) = \langle \boldsymbol{p}|1s\rangle = \int \langle \boldsymbol{p}|\boldsymbol{x}\rangle\langle \boldsymbol{x}|1s\rangle \mathrm{d}^3 x = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}} \int e^{-i\boldsymbol{p}\cdot\boldsymbol{x}/\hbar} \psi_{1s}(\boldsymbol{x}) \mathrm{d}^3 x. \tag{32}$$

Taking $f(r) = \psi_{1s}(r), q = \frac{p}{\hbar}, N = (2\pi\hbar)^{\frac{3}{2}}$ we can use the identity above to yield:

$$\begin{aligned}
\psi_{1s}(\boldsymbol{p}) &= \frac{1}{N}\frac{4\pi}{q} \int_0^\infty r\psi_{1s}(r)\sin(qr)\,\mathrm{d}r \\
&= \frac{4\pi}{N}\frac{1}{\sqrt{\pi a_0^3}}\frac{1}{q} \int_0^\infty re^{-\frac{r}{a_0}}\sin(qr)\,\mathrm{d}r,
\end{aligned} \tag{33}$$

where we use Mathematica to find

$$\int_0^\infty re^{-\alpha r}\sin(\beta r)\,\mathrm{d}r = \frac{2\alpha\beta}{(\alpha^2+\beta^2)^2}, \quad \alpha,\beta\in\mathbb{R} \tag{34}$$

Having $\alpha = \frac{1}{a_0}, \beta = q = \frac{p}{\hbar}$, we have

$$\begin{aligned}
\psi_{1s}(\boldsymbol{p}) &= \frac{4\pi}{N}\frac{1}{\sqrt{\pi a_0^3}}\frac{1}{q}\frac{2\left(\frac{1}{a_0}\right)q}{\left(\left(\frac{1}{a_0}\right)^2+q^2\right)^2} \\
&= \frac{8\pi}{N}\frac{1}{\sqrt{\pi(a_0)^3}}\frac{1/a_0}{\left((1/a_0)^2+(p/\hbar)^2\right)^2}.
\end{aligned} \tag{35}$$

2. find $\langle \boldsymbol{p}\rangle, \langle|\boldsymbol{p}|\rangle$.

Considering spherical symmetry, we have

$$\langle \boldsymbol{p}\rangle = \int_{\mathbb{R}_3} \boldsymbol{p}\ |\psi_{1s}(\boldsymbol{p})|^2\ \mathrm{d}^3 p = 0. \tag{36}$$

While

$$\langle|\boldsymbol{p}|\rangle = \int_{\mathbb{R}}^3 p|\psi_{1s}(p)|^2 \mathrm{d}^3 p = 4\pi\int_0^\infty p^2|\psi_{1s}(p)|^2\,\mathrm{d}p. \tag{37}$$

Take $y = a_0 p/\hbar, \mathrm{d}p = \hbar/a_0\,\mathrm{d}y$. Then

$$\langle|\boldsymbol{p}|\rangle = 4\pi\frac{8}{\pi^2}\left(\frac{a_0}{\hbar}\right)^3 \int_0^\infty \frac{p^3}{(1+y^2)^4}\,\mathrm{d}p = \frac{8}{3\pi}\frac{\hbar}{a_0}. \tag{38}$$

P6

> Find $\langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle$ for a particle in a 1d infinite square well for the n-th eigenstate of potential, and find numerical result for ground and first state.

For odd n, we have

$$\psi_n(x) = \frac{1}{\sqrt{a}}\cos\left(\frac{n\pi}{2a}x\right). \tag{39}$$

and for even n, we have

$$\psi_n(x) = \frac{1}{\sqrt{a}}\sin\left(\frac{n\pi}{2a}x\right). \tag{40}$$

We work out each term in $(\Delta x))^2 = \langle x^2\rangle - \langle x\rangle^2, (\Delta p)^2 = \langle p^2\rangle - \langle p\rangle^2$ separately.
1. $\langle x\rangle = \int_{-a}^{a} x\left|\psi_n(x)^2\right| \mathrm{d}x = 0$ as the integrand is odd.
2. For $\langle x^2\rangle$: odd n: $\psi_n = \frac{1}{\sqrt{a}}\cos(n\pi x/2a.)$; even n: $\psi_n = \frac{1}{\sqrt{a}}\sin(n\pi x/2a)$.

Notice $|\psi_n|$ is same for both cases, and so

$$\int_{-a}^{a} x^2|\psi_n(x)|^2\,\mathrm{d}x = \int_{-a}^{a} x^2\left|\cos^2\left(\frac{n\pi}{2a}x\right)\right| \mathrm{d}x = \underbrace{\frac{1}{2}\int_{-a}^{a} x^2\,\mathrm{d}x}_{2a^3/3.} + \underbrace{\frac{1}{2}\int_{-a}^{a} x^2\left|\cos\left(\frac{n\pi}{a}x\right)\right| \mathrm{d}x.}_{\star} \tag{41}$$

where taking $\beta = n\pi/a$,

$$\star = \frac{4a\cos(\beta a)}{\beta^2} = \left|\frac{4a^3(-1)^n}{n^2\pi^2}\right| \tag{42}$$

and so

$$\langle x^2\rangle = \frac{1}{a}\left(\frac{a^3}{3} - \frac{2a^3}{n^2\pi^2}\right) = a^2\left(\frac{1}{3} - \frac{2}{\pi^2 n^2}\right). \tag{43}$$

Then , consider momemtum:

$$\langle p\rangle = \int_{-a}^{a} \psi_n^*(-i\hbar\partial_x)\psi_n\,\mathrm{d}x = -i\frac{\hbar}{2}\left[\psi_n^2(x)\right]_{-a}^{a} = 0; \tag{44}$$

$$\begin{aligned}\langle p^2\rangle &= \int_{-a}^{a} \psi_n^*(x)\hat{p}^2\psi_n(x)\,\mathrm{d}x \\ &= \int_{-a}^{a} \psi_n^*(x)\left(-\hbar^2\frac{\mathrm{d}^2}{\mathrm{d}^2}\psi_n(x)\right)\mathrm{d}x \\ &= -\hbar^2\int_{-a}^{a} \psi_n^*\psi_n''(x)\,\mathrm{d}x\end{aligned} \tag{45}$$

Notice that

$$-\frac{\hbar^2}{2m}\psi_n''(x) = E_n\psi_n(x) \Rightarrow \psi_n''(x) = -k_n^2\psi_n(x), \quad k_n = n\pi/2a \tag{46}$$

and so

$$\langle p^2\rangle = \hbar^2 k_n^2\int|\psi_n|^2\,\mathrm{d}x = \hbar^2 k_n^2 = \hbar^2(n\pi/2a)^2. \tag{47}$$

and so

$$\langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle = \frac{\hbar^2}{4}\left(\frac{\pi^2 n^2}{3} - 2\right). \tag{48}$$

$$n = 1 : 1.28987\frac{\hbar^2}{4}; \quad n = 2 : 11.1595\frac{\hbar^2}{4}. \tag{49}$$