

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

1. Conditions for self-adjointness

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

• $\langle f|Lg \rangle$:

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

Integrating by parts for each term, we have

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

and thus

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

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

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

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

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

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 adjoint on $[-1, 1]$

We immediately read off that

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

and so

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

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 $[x_i, p_j] = i\hbar\delta_{ij}$.

- 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. $[x_i, p_i^k] = ki\hbar p_i^{k-1}$ and $[p_i, x_i^k] = -ki\hbar x_i^{k-1}$. We want to show true for $n = k + 1$.

Notice that

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

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 $G(\mathbf{p}) = \sum_m a_m \prod_r p_r^{m_r}$. Then

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

where

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

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

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

where

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

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

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

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

Then, we have

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

On the other hand,

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

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

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

then we can relate the poisson bracket to the commutator by

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

P3

Consider

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

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

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

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

Notice that

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

2.

From this, we see that

$$\langle x_{i'} \rangle = \langle \alpha | x_{i'} | \alpha \rangle = \langle \alpha | T^{\dagger}(\mathbf{l}) x_i T(\mathbf{l}) | \alpha \rangle = \langle \alpha | (x_i + l_i) | \alpha \rangle = \langle x_i \rangle + l_i. \quad (22)$$

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 $\psi_\alpha(x) = \langle x|\alpha\rangle$

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

1. Brute force using the Fourier transform relation

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

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

Noticing

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

we simplify (1) to

$$(1) = -i\hbar x \partial_x \int \delta(x-x') \psi_\alpha(x') dx' = -i\hbar x \psi'_\alpha(x). \quad (26)$$

Similarly,

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

Subtracting, we have

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

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

We simply make expansions and arrive at

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

The ground state position space wavefunction of the Hydrogen atom is

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

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

We first prove the following identity:

$$\begin{aligned} \int_{\mathbb{R}_3} e^{-i\mathbf{q}\cdot\mathbf{x}} f(r) d^3r &= \int_0^\infty r^2 f(r) dr \int_0^\pi \sin\theta e^{-iqr\cos\theta} d\theta \int_0^{2\pi} d\varphi \\ &\stackrel{u \equiv \cos\theta}{=} 2\pi \int_0^\infty r^2 f(r) dr \int_{-1}^1 e^{-iqr u} du \\ &= 4\pi \int_0^\infty r^2 f(r) \frac{\sin(qr)}{qr} dr \\ &= \frac{4\pi}{q} \int_0^\infty f(r) \sin(qr) r dr \end{aligned} \quad (31)$$

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

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

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:

$$\begin{aligned} \psi_{1s}(\mathbf{p}) &= \frac{1}{N} \frac{4\pi}{q} \int_0^\infty r \psi_{1s}(r) \sin(qr) dr \\ &= \frac{4\pi}{N} \frac{1}{\sqrt{\pi a_0^3}} \frac{1}{q} \int_0^\infty r e^{-\frac{r}{a_0}} \sin(qr) dr, \end{aligned} \quad (33)$$

where we use MATHEMATICA to find

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

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

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

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

Considering spherical symmetry, we have

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

While

$$\langle |\mathbf{p}| \rangle = \int_{\mathbb{R}} p |\psi_{1s}(p)|^2 d^3p = 4\pi \int_0^\infty p^2 |\psi_{1s}(p)|^2 dp. \quad (37)$$

Take $y = a_0 p / \hbar$, $dp = \hbar / a_0 dy$. Then

$$\langle |\mathbf{p}| \rangle = 4\pi \frac{8}{\pi^2} \left(\frac{a_0}{\hbar}\right)^3 \int_0^\infty \frac{p^3}{(1+y^2)^4} dp = \frac{8}{3\pi} \frac{\hbar}{a_0}. \quad (38)$$

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

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

and for even n , we have

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

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. $\langle x \rangle = \int_{-a}^a x |\psi_n(x)|^2 dx = 0$ 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

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

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

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

and so

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

Then, consider momentum:

$$\langle p \rangle = \int_{-a}^a \psi_n^* (-i\hbar \partial_x) \psi_n dx = -i\frac{\hbar}{2} [\psi_n^2(x)]_{-a}^a = 0; \quad (44)$$

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

Notice that

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

and so

$$\langle p^2 \rangle = \hbar^2 k_n^2 \int |\psi_n|^2 dx = \hbar^2 k_n^2 = \hbar^2 (n\pi/2a)^2. \quad (47)$$

and so

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

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