Physics 731: Assignment #2, Solutions

1. (a) The operator L is self-adjoint if $\langle f|Lg\rangle = \langle Lf|g\rangle$. To derive the conditions for which this holds, we begin with

$$\langle f|Lg\rangle = \int_{-\infty}^{\infty} f^*\alpha g'' dx + \int_{-\infty}^{\infty} f^*\beta g' dx + \int_{-\infty}^{\infty} f^*\gamma g\, dx.$$

Integrating the first two terms by parts once, we have

$$\begin{aligned}\langle f|Lg\rangle &= \alpha f^* g'|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} (\alpha' f^* g' + \alpha f^{*\prime} g')dx + \beta f^* g|_{-\infty}^{\infty} \\ &- \int_{-\infty}^{\infty} (\beta' f^* g + \beta f^{*\prime} g)dx + \int_{-\infty}^{\infty} f^*\gamma g\, dx.\end{aligned}$$

The quantity $\langle Lf|g\rangle$ is given by

$$\langle Lf|g\rangle = \int_{-\infty}^{\infty} f^{*\prime\prime}\alpha g dx + \int_{-\infty}^{\infty} f^{*\prime}\beta g dx + \int_{-\infty}^{\infty} f^*\gamma g\, dx.$$

Again integrating the first two terms by parts once,

$$\begin{aligned}\langle Lf|g\rangle &= \alpha f^{*\prime} g|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} (\alpha' f^{*\prime} g + \alpha f^{*\prime} g')dx + \beta f^* g|_{-\infty}^{\infty} \\ &- \int_{-\infty}^{\infty} (\beta' f^* g + \beta f^{*\prime} g)dx + \int_{-\infty}^{\infty} f^*\gamma g\, dx.\end{aligned}$$

Hence,

$$\langle f|Lg\rangle - \langle Lf|g\rangle = (\alpha f^* g' - \alpha f^{*\prime} g)|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} (\beta - \alpha') f^{*\prime} g\, dx - \int_{-\infty}^{\infty} (\alpha' - \beta) f^* g' dx.$$

Since this quantity must vanish for all f and g in the space for L to be self-adjoint, this results in the conditions that

$$\alpha(f^* g' - f^{*\prime} g)|_{-\infty}^{\infty} = 0, \qquad \alpha' = \beta.$$

(b) From the above, we see that since $\alpha(x) = -(1-x^2)$ and $\beta(x) = 2x$, the condition $\alpha' = \beta$ holds. Furthermore, the condition on the boundary terms, which takes the form

$$-(1-x^2)(f^* g' - f^{*\prime} g)|_{-1}^{1} = 0,$$

is also satisfied if the functions f and g are finite and well-behaved at $x = \pm 1$. Hence, the Legendre operator satisfies the requirement for Hermiticity.

2. (a) Consider $[x_i, p_i^2]$, which is given by

$$[x_i, p_i^2] = p_i[x_i, p_i] + [x_i, p_i]p_i = 2i\hbar p_i.$$

Similarly, for $[x_i, p_i^3]$, we have

$$[x_i, p_i^3] = p_i[x_i, p_i^2] + [x_i, p_i]p_i^2 = 2i\hbar p_i^2 + i\hbar p_i^2 = 3i\hbar p_i^2.$$

Now suppose it is true for $[x_i, p_i^{n-1}]$. We can then show it is true for $[x_i, p_i^n]$:

$$\begin{aligned}
[x_i, p_i^n] &= p_i[x_i, p_i^{n-1}] + [x_i, p_i]p_i^{n-1} \\
&= (n-1)i\hbar p_i^{n-1} + i\hbar p_i^{n-1} = ni\hbar p_i^{n-1},
\end{aligned}$$

which is what we wanted to show. For $[p_i, x_i^n]$, there are analogous calculations: starting first with $[p_i, x_i^2] = x_i[p_i, x_i] + [p_i, x_i]x_i = -2i\hbar x_i$, etc., then showing that if the relation holds for $[p_i, x_i^{n-1}]$, it holds for $[p_i, x_i^n]$:

$$[p_i, x_i^n] = x_i[p_i, x_i^{n-1}] + [p_i, x_i]x_i^{n-1} = (n-1)(-i\hbar)x_i^{n-1} - i\hbar x_i^{n-1} = -ni\hbar x_i^{n-1}.$$

(b) Now, let $G(\mathbf{p})$ have the following expansion: $G(\mathbf{p}) = \sum_{nm\ell} c_{nm\ell} p_i^n p_j^m p_k^\ell$, where the sums on the indices n, m, and ℓ run from zero to infinity. Then we have

$$[x_i, G(\mathbf{p})] = \sum_{nm\ell} i\hbar n c_{nm\ell} p_i^{n-1} p_j^m p_k^\ell = i\hbar \frac{\partial G}{\partial p_i}.$$

Similarly, $F(\mathbf{x}) = \sum_{n=0}^{\infty} d_{nm\ell} x_i^n x_j^m x_k^\ell$, and

$$[p_i, F(\mathbf{x})] = \sum_{nm\ell} n d_{nm\ell} x_i^{n-1} x_j^m x_k^\ell = -i\hbar \frac{\partial F}{\partial x_i}.$$

(b) Here $[x^2, p^2] = \sum_{i,j}[x_i^2, p_j^2]$, which evaluates to

$$\sum_{i,j}[x_i^2, p_j^2] = \sum_{i,j} x_i[x_i, p_j^2] + [x_i, p_j^2]x_i = \sum_i 2i\hbar(x_i p_i + p_i x_i) = 2i\hbar(\mathbf{x}\cdot\mathbf{p} + \mathbf{p}\cdot\mathbf{x}).$$

The Poisson bracket is given by

$$i\hbar\{x^2, p^2\}_{\text{classical}} = \sum_i \left(\frac{\partial x^2}{\partial x_i}\frac{\partial p^2}{\partial p_i} - \frac{\partial x^2}{\partial p_i}\frac{\partial p^2}{\partial x_i}\right) = 4\sum_j x_j p_j = 4\mathbf{x}\cdot\mathbf{p},$$

or equivalently $2(\mathbf{x}\cdot\mathbf{p} + \mathbf{p}\cdot\mathbf{x})$. Therefore, the Poisson bracket multiplied by the quantity $(i\hbar)$ gives the result obtained for the commutator, with the important caveat that in quantum mechanics we have to be careful about operator ordering. The general lesson is that non-commuting variables must be symmetrized when passing from classical mechanics to quantum mechanics. (This is an example of what is known as *Weyl ordering*.)

3. (a) The commutator $[x_i, T(\mathbf{l})]$ is given by

$$[x_i, T(\mathbf{l})] = [x_i, e^{-i\mathbf{p}\cdot\mathbf{l}/\hbar}] = i\hbar\frac{\partial}{\partial p_i}e^{-i\mathbf{p}\cdot\mathbf{l}/\hbar} = l_i T(\mathbf{l}).$$

(b) The expectation value of $\mathbf{x}$ in the translated state $|T\alpha\rangle = T(\mathbf{l})|\alpha\rangle$ is

$$\begin{aligned}
\langle\mathbf{x}\rangle_{\mathbf{l}} &\equiv \langle T\alpha|\mathbf{x}|T\alpha\rangle = \langle\alpha|T^\dagger\mathbf{x}T|\alpha\rangle = \langle\alpha|T^\dagger T\mathbf{x}|\alpha\rangle + \langle\alpha|T^\dagger[\mathbf{x}, T]|\alpha\rangle \\
&= \langle\alpha|\mathbf{x}|\alpha\rangle + \mathbf{l}\langle\alpha|\alpha\rangle = \langle\mathbf{x}\rangle + \mathbf{l}.
\end{aligned}$$

4. We are to evaluate the two terms in $\langle x|[x,p]|\alpha\rangle = \langle x|xp|\alpha\rangle - \langle x|px|\alpha\rangle$. The first term is

$$\begin{aligned}
\langle x|xp|\alpha\rangle &= \int dx'\,dp\,dp'\,dx''\langle x|x|x'\rangle\langle x'|p\rangle\langle p|p|p'\rangle\langle p'|x''\rangle\langle x''|\alpha\rangle \\
&= \int dx'\,dp\,dp'\,dx''\,x'\delta(x-x')\langle x'|p\rangle p'\delta(p-p')\langle p'|x''\rangle\psi_\alpha(x'') \\
&= \int dp\,dx''\,x\,p\,\langle x|p\rangle\langle p|x''\rangle\psi_\alpha(x'') = \frac{1}{2\pi\hbar}\int dp\,dx''\,x\,p\,e^{ipx/\hbar}e^{-ipx''/\hbar}\psi_\alpha(x'') \\
&= \frac{1}{2\pi\hbar}\int dp\,dx''\,x(-i\hbar\frac{d}{dx}e^{ipx/\hbar})e^{-ipx''/\hbar}\psi_\alpha(x'') = -i\hbar\frac{x}{2\pi\hbar}\frac{d}{dx}\int dp\,dx''\,e^{ip(x-x'')/\hbar}\psi_\alpha(x'') \\
&= -i\hbar\frac{x}{2\pi\hbar}\frac{d}{dx}\int dx''(2\pi\hbar)\delta(x-x'')\psi_\alpha(x'') = -i\hbar x\frac{d}{dx}\psi_\alpha(x).
\end{aligned}$$

Similarly, the second term is

$$\begin{aligned}
\langle x|px|\alpha\rangle &= \int dx'\,dx''\,dp\,dp'\,\langle x|p\rangle\langle p|p|p'\rangle\langle p'|x''\rangle\langle x''|x|x'\rangle\langle x'|\alpha\rangle \\
&= \int dx'\,dx''\,dp\,dp'\,\langle x|p\rangle p'\delta(p-p')\langle p'|x'\rangle x'\delta(x'-x'')\psi_\alpha(x'') \\
&= \int dx'\,dp\,p\,x'\langle x|p\rangle\langle p|x'\rangle\psi_\alpha(x') = \frac{1}{2\pi\hbar}\int dx'\,dp\,p\,x'e^{ip(x-x')/\hbar}\psi_\alpha(x') \\
&= \frac{-i\hbar}{2\pi\hbar}\frac{d}{dx}\int dx'\,dp\,x'e^{ip(x-x')/\hbar}\psi_\alpha(x') \\
&= \frac{-i\hbar}{2\pi\hbar}\frac{d}{dx}\int dx'\,x'(2\pi\hbar)\delta(x-x')\psi_\alpha(x') = -i\hbar\frac{d}{dx}\left[x\psi_\alpha(x)\right].
\end{aligned}$$

Hence,

$$\langle x|xp|\alpha\rangle - \langle x|px|\alpha\rangle = -i\hbar x\frac{d}{dx}\psi_\alpha(x) + i\hbar\frac{d}{dx}\left[x\psi_\alpha(x)\right] = i\hbar\psi_\alpha(x),$$

as expected. This can also be done by replacing $p = -i\hbar d/dx$ (as an operator statement) at the onset:

$$\begin{aligned}
\langle x|xp|\alpha\rangle &= -i\hbar\langle x|x\frac{d}{dx}|\alpha\rangle = -i\hbar\int dx'\,dx''\langle x|x|x'\rangle\langle x'|\frac{d}{dx}|x''\rangle\langle x''|\alpha\rangle \\
&= -i\hbar\int dx'\,dx''\,x'\delta(x-x')\frac{d}{dx'}\langle x'|x''\rangle\langle x''|\alpha\rangle = i\hbar\int dx'\,dx''\frac{d}{dx'}(x'\delta(x-x'))\delta(x'-x'')\psi_\alpha(x'') \\
&= -i\hbar\int dx'\,x'\delta(x-x')\frac{d}{dx'}\psi_\alpha(x') = -i\hbar x\frac{d\psi_\alpha(x)}{dx}. \\
\langle x|px|\alpha\rangle &= -i\hbar\langle x|\frac{d}{dx}x|\alpha\rangle \\
&= -i\hbar\int dx'\,dx''\langle x|\frac{d}{dx}|x'\rangle\langle x'|x|x''\rangle\langle x''|\alpha\rangle = -i\hbar\int dx'\,dx''\frac{d}{dx}\delta(x-x')x''\delta(x'-x'')\langle x''|\alpha\rangle \\
&= i\hbar\int dx'\,\delta'(x-x')x'\psi_\alpha(x') = -i\hbar\frac{d}{dx}\left[x\psi_\alpha(x)\right].
\end{aligned}$$

5. (a) The momentum space wavefunction $\varphi_{1s}(\mathbf{p})$ is given by

$$\varphi_{1s}(\mathbf{p}) = \frac{1}{(2\pi\hbar)^{3/2}}\int d^3x\,e^{-i(\mathbf{p}\cdot\mathbf{x})/\hbar}\psi_{1s}(\mathbf{x}).$$

First, note that for $f(\mathbf{x}) = f(r)$,

$$F(\mathbf{q}) = \int e^{-i\mathbf{q}\cdot\mathbf{x}}f(\mathbf{x})d^3x = \frac{4\pi}{q}\int r f(r)\sin(qr)dr.$$

To show this, we note that due to the spherical symmetry, without loss of generality we can choose the $\hat{z}$ axis along $\mathbf{q}$, such that the angular part of the integrations is given by $\int d\Omega = 2\pi \int_{-1}^{1} d(\cos\theta)$, and $F(\mathbf{q})$ becomes

$$F(\mathbf{q}) = 2\pi \int_0^\infty r^2 dr f(r) \int_{-1}^{1} e^{-iqr\cos\theta} d(\cos\theta) = \frac{4\pi}{q} \int_0^\infty r f(r) \sin(qr) dr.$$

In our case, $\mathbf{q} = \mathbf{p}/\hbar$ and $f(r) = (\pi a_0^3)^{1/2} e^{-r/a_0}$, such that

$$\varphi_{1s}(\mathbf{p}) = \frac{4\pi}{q} \frac{1}{(2\pi\hbar)^{3/2}} \frac{1}{\sqrt{\pi a_0^3}} \int_0^\infty r e^{-r/a_0} \sin(qr) dr.$$

The integral is easily evaluated, for example by recalling that $\sin(qr)$ is the imaginary part of e^{iqr}, and that for $\mathrm{Re}(\lambda) > 0$, $\int_0^\infty r e^{-\lambda r} dr = -\frac{d}{d\lambda}(1/\lambda) = 1/\lambda^2$. Putting it together, we obtain

$$\varphi_{1s}(\mathbf{p}) = \frac{8\sqrt{\pi}}{a_0(2\pi\hbar a_0)^{3/2}} \frac{1}{\left[\frac{1}{a_0^2} + \frac{p^2}{\hbar^2}\right]^2}.$$

(b) (i) The expectation value of the magnitude of the momentum is

$$\langle p \rangle = \int d^3p\, p |\varphi_{1s}(\mathbf{p})|^2 = \frac{32}{\pi a_0^5 \hbar^3} \int_0^\infty \frac{p^3 dp}{\left[\frac{1}{a_0^2} + \frac{p^2}{\hbar^2}\right]^4}.$$

Writing $\lambda = 1/a_0^2$, the integral can be expressed as

$$\int_0^\infty \frac{p^3 dp}{\left[\frac{1}{a_0^2} + \frac{p^2}{\hbar^2}\right]^4} = \int_0^\infty \frac{q^3 dq}{(\lambda + q^2)^4} = \frac{1}{2} \int_0^\infty \frac{x dx}{(\lambda + x)^4} = \frac{1}{12\lambda^2} = \frac{a_0^4}{12}.$$

Therefore,

$$\langle p \rangle = \frac{8\hbar}{3\pi a_0}.$$

(ii) The expectation value of $\mathbf{p}$ is trivially zero:

$$\langle \mathbf{p} \rangle = \int d^3p\, \mathbf{p} |\varphi_{1s}(\mathbf{p})|^2 = 0,$$

since $\varphi_{1s}(\mathbf{p})$ only depends on $|\mathbf{p}|$ (*i.e*, there is no preferred direction).

6. The even and odd parity eigenfunctions of the infinite square well of width $2a$ can be summarized as follows:

$$\psi_n(x) = \sqrt{\frac{1}{a}} \sin\left(\frac{n\pi(x+a)}{2a}\right), \quad n = 1, 2, 3, \ldots$$

Therefore,

$$\begin{aligned} \langle x \rangle &= \frac{1}{a} \int_{-a}^{a} x \sin^2\left(\frac{n\pi(x+a)}{2a}\right) dx = 0 \\ \langle x^2 \rangle &= \frac{1}{a} \int_{-a}^{a} x^2 \sin^2\left(\frac{n\pi(x+a)}{2a}\right) dx = a^2 \left[\frac{1}{3} - \frac{2}{n^2\pi^2}\right], \end{aligned}$$

and

$$\begin{aligned}
\langle p \rangle &= \frac{-i\hbar}{a} \int_{-a}^{a} \sin\left(\frac{n\pi(x+a)}{2a}\right) \frac{d}{dx} \sin\left(\frac{n\pi(x+a)}{2a}\right) dx = 0 \\
\langle p^2 \rangle &= \frac{-\hbar^2}{a} \int_{-a}^{a} \sin\left(\frac{n\pi(x+a)}{2a}\right) \frac{d^2}{dx^2} \sin\left(\frac{n\pi(x+a)}{2a}\right) dx = \frac{\hbar^2 n^2 \pi^2}{4a^2}.
\end{aligned}$$

Thus, the $x - p$ uncertainty product and the generalized uncertainty principle take the form

$$\langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle = \frac{\hbar^2}{4}\left(\frac{\pi^2 n^2}{3} - 2\right) \geq \frac{1}{4}|\langle[x,p]\rangle|^2 = \frac{\hbar^2}{4}.$$

Note that this product is smallest for $n = 1$, in which case the LHS is $\sim 1.29\hbar^2/4$. For $n = 2$, the LHS is $\sim 11.16\hbar^2/4$.