CHEM 1410 HW # 4 Due: Oct. 6
P6.5, P6.9, P6.18, P7.4, P7.8

P6.5

$$\left[\frac{d^2}{dx^2}, x\right] f(x) = \frac{d^2}{dx^2}\left(x f(x)\right) - x\left(\frac{d^2}{dx^2} f(x)\right)$$

$$= \left\{2\frac{df(x)}{dx} + x\frac{d^2 f(x)}{dx^2} - x\frac{d^2 f(x)}{dx^2}\right\} = \left(2\frac{d}{dx}\right) f(x)$$

$$\left[\frac{d^2}{dx^2}, x\right] = 2\frac{d}{dx}$$

P6.9

$$\left[\frac{d}{dr}, \frac{1}{r}\right] f(r) = \frac{d}{dr}\left(\frac{f(r)}{r}\right) - \frac{1}{r}\frac{df(r)}{dr}$$

$$= -\frac{1}{r^2} f(r) + \frac{1}{r}\frac{df(r)}{dr} - \frac{1}{r}\frac{df(r)}{dr} = -\frac{1}{r^2} f(r)$$

Therefore, $\left[\frac{d}{dr}, \frac{1}{r}\right] = -\frac{1}{r^2}$

6.18

As shown in Example Problem 6.1, the momentum and total energy operators only commute if $\frac{dV(x)}{dx} = 0$ over the whole range of x for the system of interest. However, $\frac{dV(x)}{dx} \neq 0$ at both ends of the box. Therefore, the total energy and momentum operators do not commute for this potential. Therefore the total energy eigenfunctions are not also eigenfunctions of the momentum operator.

7.4

We use the standard integrals $\int_0^\infty x^{2n}e^{-ax^2}\,dx = \frac{1\bullet 3\bullet 5\bullet\bullet\bullet(2n-1)}{2^{n+1}a^n}\sqrt{\frac{\pi}{a}}$ and

$$\int_0^\infty e^{-ax^2}dx = \left(\frac{\pi}{4a}\right)^{1/2}$$

$$\left\langle E_{potential}\right\rangle = \int \psi_0^*(x)\ \left(\frac{1}{2}kx^2\right)\psi_0(x)\,dx$$

$$= \frac{1}{2}k\left(\frac{\alpha}{\pi}\right)^{1/2}\int_{-\infty}^{\infty} x^2e^{-\alpha x^2}dx = k\left(\frac{\alpha}{\pi}\right)^{1/2}\int_0^\infty x^2e^{-\alpha x^2}dx$$

$$= k\left(\frac{\alpha}{\pi}\right)^{1/2}\frac{1}{4\alpha}\sqrt{\frac{\pi}{\alpha}} = k\frac{1}{4\alpha} = \frac{\hbar}{4}\sqrt{\frac{k}{\mu}}$$

$$\left\langle E_{kinetic}\right\rangle = \int \psi_0^*(x)\ \left(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2}\right)\psi_0(x)\,dx$$

$$= \int_{-\infty}^{\infty}\left(\frac{\alpha}{\pi}\right)^{1/4}e^{-\frac{1}{2}\alpha x^2}\left(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2}\right)\left(\frac{\alpha}{\pi}\right)^{1/4}e^{-\frac{1}{2}\alpha x^2}dx$$

$$= -\frac{\hbar^2}{\mu}\left(\frac{\alpha}{\pi}\right)^{1/2}\int_0^\infty e^{-\alpha x^2}\left(\alpha x^2-\alpha\right)dx$$

$$= -\frac{\hbar^2}{\mu}\left(\frac{\alpha}{\pi}\right)^{1/2}\left(\frac{\alpha}{4}\sqrt{\frac{\pi}{\alpha}} - \frac{\alpha}{2}\sqrt{\frac{\pi}{\alpha}}\right) = \frac{\hbar^2}{\mu}\frac{\alpha}{4}$$

$$= \frac{\hbar^2}{4\mu}\sqrt{\frac{k\mu}{\hbar^2}} = \frac{\hbar}{4}\sqrt{\frac{k}{\mu}}$$

7.8

We use the standard integrals $\int_0^\infty x^{2n} e^{-ax^2} dx = \frac{1 \cdot 3 \cdot 5 \cdots (2n-1)}{2^{n+1} a^n} \sqrt{\frac{\pi}{a}}$ and

$$\int_0^\infty e^{-\alpha x^2} dx = \left(\frac{\pi}{4a}\right)^{1/2}$$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \psi_n^*(x)(x^2)\psi_n dx$$

for $n = 0$, $\langle x^2 \rangle = \int_{-\infty}^{\infty} \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha x^2} (x^2) \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{1}{2}\alpha x^2} dx$

$$\langle x^2 \rangle = \left(\frac{\alpha}{\pi}\right)^{1/2} \int_{-\infty}^{\infty} x^2 e^{-\alpha x^2} dx = 2\left(\frac{\alpha}{\pi}\right)^{1/2} \int_0^\infty x^2 e^{-\alpha x^2} dx$$

$$\langle x^2 \rangle = 2\left(\frac{\alpha}{\pi}\right)^{1/2} \frac{1}{2^2 \alpha} \sqrt{\frac{\pi}{\alpha}} = \frac{1}{2\alpha} = \frac{\hbar}{2\sqrt{k\mu}}$$

for $n = 1$, $\langle x^2 \rangle = \int_{-\infty}^{\infty} \left(\frac{4\alpha^3}{\pi}\right)^{1/4} x e^{-\frac{1}{2}\alpha x^2} (x^2) \left(\frac{4\alpha^3}{\pi}\right)^{1/4} x e^{-\frac{1}{2}\alpha x^2} dx$

$$\langle x^2 \rangle = \left(\frac{4\alpha^3}{\pi}\right)^{1/2} \int_{-\infty}^{\infty} x^4 e^{-\alpha x^2} dx = 2\left(\frac{4\alpha^3}{\pi}\right)^{1/2} \int_0^\infty x^4 e^{-\alpha x^2} dx$$

$$\langle x^2 \rangle = 2\left(\frac{4\alpha^3}{\pi}\right)^{1/2} \frac{3}{2^3 \alpha^2} \sqrt{\frac{\pi}{\alpha}} = \frac{3}{2\alpha} = \frac{3\hbar}{2\sqrt{k\mu}}$$

for $n = 2$, $\langle x^2 \rangle = \int_{-\infty}^{\infty} \left(\frac{\alpha}{4\pi}\right)^{1/4} (2\alpha x^2 - 1) e^{-\frac{1}{2}\alpha x^2} (x^2) \left(\frac{\alpha}{4\pi}\right)^{1/4} (2\alpha x^2 - 1) e^{-\frac{1}{2}\alpha x^2} dx$

$$\langle x^2 \rangle = \left(\frac{\alpha}{4\pi}\right)^{1/2} \int_{-\infty}^{\infty} (4\alpha^2 x^6 - 4\alpha x^4 + x^2) e^{-\alpha x^2} dx = 2\left(\frac{\alpha}{4\pi}\right)^{1/2} \int_0^\infty (4\alpha^2 x^6 - 4\alpha x^4 + x^2) e^{-\alpha x^2} dx$$

$$\langle x^2 \rangle = 2\left(\frac{\alpha}{4\pi}\right)^{1/2} \left(4\alpha^2 \frac{15}{2^4 \alpha^3} \sqrt{\frac{\pi}{\alpha}} - 4\alpha \frac{3}{2^3 \alpha^2} \sqrt{\frac{\pi}{\alpha}} + \frac{1}{2^2} \sqrt{\frac{\pi}{\alpha}}\right) = \frac{5}{2\alpha} = \frac{5\hbar}{2\sqrt{k\mu}}$$