Chem 2430 HW #3

1. $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} Ax(L-x) = -2A \neq \text{const } Ax(L-x)$

So $Ax(L-x)$ is not an eigenfunction of H.

The energy associated with this wavefunction is

$$\frac{A^2\int_0^L (xL-x^2)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)(xL-x^2)\,dx}{A^2\int_0^L (xL-x^2)^2\,dx}$$

$$= \frac{\frac{\hbar^2}{2m}\int_0^L (xL-x^2)(2)\,dx}{\int_0^L (x^4-2Lx^3+x^2L^2)\,dx} = \frac{\frac{2\hbar^2}{2m}\left(\frac{xL^2}{2}-\frac{x^3}{3}\right)\Big|_0^L}{\left(\frac{x^5}{5}-\frac{2Lx^4}{4}+\frac{x^3L^2}{3}\right)\Big|_0^L}$$

$$= \frac{\frac{\hbar^2}{m}\left(\frac{L^3}{2}-\frac{L^3}{3}\right)}{\frac{L^5}{5}-\frac{L^5}{2}+\frac{L^5}{3}} = \frac{\frac{\hbar^2}{m}\frac{L^3}{6}}{L^5/30} = \frac{5\hbar^2}{mL^2}$$

The ground state energy for the exact ψ_1 is $\sim \frac{4.53\hbar^2}{mL^2}$

So $x(L-x)$ is a reasonable approximation to the true wavefunction.

Express this approximate wavefunction in terms of ϕ_1, ϕ_2, and ϕ_3, the first three eigenfunctions for this problem.

$$\sqrt{\frac{30}{L^5}}\,x(L-x) \approx c_1\sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right) + c_2\sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right) + c_3\sqrt{\frac{2}{L}}\sin\left(\frac{3\pi x}{L}\right) + \cdots$$

$c_2 = 0$ by symmetry

$$c_1 = \sqrt{\frac{30}{L^5}}\sqrt{\frac{2}{L}}\int_0^L x(L-x)\sin\left(\frac{\pi x}{L}\right)dx$$

$$c_3 = \sqrt{\frac{30}{L^5}}\sqrt{\frac{2}{L}}\int_0^L x(L-x)\sin\left(\frac{3\pi x}{L}\right)dx$$

$$c_1 = \frac{\sqrt{60}}{L^3}\int_0^L (xL - x^2)\sin\left(\frac{\pi x}{L}\right)dx = \sqrt{60}\,\frac{4}{\pi^3}$$

$$\boxed{C3} = \frac{\sqrt{60}}{L^3}\int_0^L (xL - x^2)\sin\left(\frac{3\pi x}{L}\right)dx = \sqrt{60}\,\frac{4}{27\pi^3}$$

$$\psi_{trial} \sim \frac{\sqrt{60}\cdot 4}{\pi^3}\left\{\sin\left(\frac{\pi x}{a}\right) + \frac{1}{27}\sin\left(\frac{3\pi x}{a}\right)\right\}$$

2. Is $(\hat{A} + \hat{B})^2 = \hat{A}^2 + \hat{B}^2 + 2\hat{A}\hat{B}$?

This would be true only if $\hat{A}$ and $\hat{B}$ commute.

3. $e^{d/dx} = 1 + d/dx + \frac{1}{2} d^2/dx^2 + \ldots$

$$e^{d/dx} f = f(x) + f'(x) + \frac{1}{2}f''(x) + \ldots$$

recall the Taylor series for expanding $f(x)$ about x_0

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2}f''(x_0)(x - x_0)^2 + \ldots$$

$$f(x_0 + 1) = f(x_0) + f'(x_0) + \frac{1}{2}f''(x_0) + \ldots$$

which proves the identity.