Chem 2430 - Answers Exam #1.

1. Yes, e^{-ax^2} is reasonable as it $\to 0$ as $x \to \pm\infty$, and it is symmetric about $x=0$

$$\langle E\rangle = 2\int_0^\infty e^{-ax^2} H e^{-ax^2} dx \Big/ 2\int_0^\infty e^{-2ax^2} dx$$

$$\langle E\rangle = \frac{2\int_0^\infty e^{-ax^2}\left(-\frac{1}{2}\frac{d^2}{dx^2}\right) e^{-ax^2} dx + 2V_0 \int_{b/2}^\infty e^{-2ax^2} dx}{\sqrt{\frac{\pi}{2}}\frac{1}{\sqrt{a}}}$$

$$\langle E\rangle = \frac{2\int_0^\infty (a-2a^2x^2) e^{-2ax^2} dx + 2V_0 \int_{b/2}^\infty e^{-2ax^2} dx}{\sqrt{\frac{\pi}{2}}\frac{1}{\sqrt{a}}}$$

$$= \frac{\frac{1}{2}\sqrt{a}\sqrt{\pi/2} + \sqrt{\frac{\pi}{2}}\frac{V_0}{\sqrt{a}}\,\mathrm{erfc}\left(\sqrt{\frac{a}{2}}b\right)}{\sqrt{\frac{\pi}{2}}\frac{1}{\sqrt{a}}}$$

$$= a/2 + V_0\,\mathrm{erfc}\left(\sqrt{\frac{a}{2}}b\right)$$

A good approximate wavefunction for the first excited state is $x e^{-ax^2}$.

2. $H = \hbar\omega\left(a^+a + \frac{1}{2}\right)$

$$[a, [1/2, a^+]] = a\tfrac{1}{2}a^+ - aa^+ 1/2 - 1/2 a^+a + a^+ 1/2 a = 0$$

$$[a, [a^+a, a^+]] = a a^+ a a^+ - a a^+ a^+ a - a^+ a a^+ a + a^+ a^+ a a$$

$$= a a^+ [aa^+ - a^+a] - a^+[aa^+ - a^+a] a$$

but $aa^+ - a^+a = 1$

So $[a, [a^+a, a^+]] = aa^+ - a^+a = 1$

So $[a, [H, a^+]] = \hbar\omega$ which is no longer an operator

3. I, $Ae^{ik_1x} + Be^{-ik_1x}$, $k_1 = \sqrt{2mE}/\hbar$

II. $Ce^{ik_2x} + De^{-ik_2x}$, $k_2 = \sqrt{2m(E-V_1)}/\hbar$

III Ee^{-Kx} $K = \sqrt{2m(V_2-E)}/\hbar$

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4. In Cartesian coordinates

$$E = \frac{\hbar\omega}{2} + n_x\hbar\omega + \frac{\hbar\omega}{2} + n_y\hbar\omega = \hbar\omega(1+n_x+n_y)$$

$$E(0,0) = \hbar\omega, \quad E(10) = E(0,1) = 2\hbar\omega$$

$$E(2,0) = E(0,2) = E(1,1) = 3\hbar\omega$$

In polar coordinates

$$-\frac{1}{2\mu}\left[\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\phi^2}\right]\psi + \frac{1}{2}kr^2\psi = E\psi$$

$$\psi = f(r)g(\phi) = f(r)e^{im\phi}$$

$$-\frac{1}{2\mu}\left[\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} - \frac{m^2}{r^2}\right]\psi + \frac{1}{2}kr^2\psi = E\psi$$

Lets try $f(r) = e^{-ar^2}$, for the case $m=0$

This gives $E = 2a/\mu$, $a = \frac{1}{2}\sqrt{k\mu}$

$E = \sqrt{k/\mu} \rightarrow \hbar\omega$ same as in cartesian coord.

For $m = \pm 1$, try $f(r) = re^{-ar^2}$

This gives $E = 2\hbar\omega$, again the same as above