Chem 2430 HW #3 Answers

2. $\langle 0|x^3|1\rangle$

$\langle 0|(a^+ + a)^3|1\rangle = \langle 0|aaa^+|1\rangle + \langle 0|aa^+a|1\rangle$

$= \sqrt{2}\sqrt{2}\sqrt{1} + \sqrt{1}\sqrt{1}\sqrt{1} = 3$

$\langle 0|x^3|1\rangle = 3\left(\frac{\hbar}{2m\omega}\right)^{3/2}$

$\langle 0|x^3|3\rangle$

$\langle 0|(a^+ + a)^3|3\rangle = \langle 0|aaa|3\rangle = \sqrt{1}\sqrt{2}\sqrt{3} = \sqrt{6}$

$\langle 0|x^3|3\rangle = \sqrt{6}\left(\frac{\hbar}{2m\omega}\right)^{3/2}$

$\langle 0|x^4|0\rangle$

$\langle 0|(a^+ + a)^4|0\rangle = \langle 0|aaa^+a^+|0\rangle + \langle 0|aa^+aa^+|0\rangle$

$= 2 + 1 = 3$

$\langle 0|x^4|0\rangle = 3\left(\frac{\hbar}{2m\omega}\right)^2$

$\langle 0|\hat{p}_x^2|0\rangle$

$\langle 0|(a^+ - a)^2|0\rangle = \langle 0|(-aa^+|0\rangle = -1$

$\langle 0|\hat{p}_x^2|0\rangle = \frac{\hbar m\omega}{2}$

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1. $U = A/R^{12} - B/R^6$, $R_e = (2A/B)^{1/6}$

Series expansion about $R_e = -\frac{B^2}{4A} + 9B^3\left(\frac{A}{B}\right)^{2/3}\left(R - \left(\frac{2A}{B}\right)^{1/6}\right)^2 +$

$k = 18B^3\left(\frac{A}{B}\right)^{2/3}$

$\omega = \sqrt{k/m}$