CYL110 2009-2010 Quantum Tutorial 2

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1. Discuss the source and nature of degeneracy for a particle in a 2−D and 3−D box.
2. A particle is confined to a two dimensional box of length L and $2L$. What are the allowed energy levels?
3. Many proteins contain metal porphyrin molecules. These molecules are planar and contain 26 π electrons. If the length of the molecule is $\sim$1000 pm, then what is the predicted lowest energy absorption of the porphyrin molecule?
4. The wave function of the first excited state of a harmonic oscillator is $Ax\exp(-ax^2)$. By substituting in the Schrödinger equation determine a. Determine A from the normalization condition.
5. The maximum potential energy that a diatomic molecule can store is $\frac{1}{2}kx^2$, where x is the amplitude of the vibration. If the force constant is 1.86 x 10^3 N m^{-1}, calculate the maximum amplitude of vibration for the CO molecule in the ground vibrational state.
6. It can be proved generally that for a harmonic oscillator
$$< x^2 >= (n + \frac{1}{2})\frac{\hbar}{\sqrt{\mu k}}$$
and that
$$< x^4 >= (n^2 + 2n + 1)\frac{3\hbar^2}{4\mu k}.$$
Verify these formulas for the first two states of the harmonic oscillator.
7. An analytic expression that is a good approximation to the potential energy curve of a diatomic molecule is $V(x) = D(1-\exp(-\beta x))^2$ where D and β are parameters that depend on the molecule. Derive a relation between the force constant and the parameters D and β. Now show that
$$\beta = 2\pi c\tilde{\nu}\left(\sqrt{\frac{\mu}{2D}}\right),$$
where $\tilde{\nu}$ is the vibrational frequency expressed in cm^{-1}.
8. Verify the recursion relation
$$H_{n+1}(z) - 2zH_n(z) + 2nH_{n-1}(z) = 0$$
using the first few Hermite polynomials.
9. In the infrared spectrum of H^{79}Br, there is an intense line at 2559 cm^{-1}. Calculate the force constant of H^{79}Br and the period of vibration of H^{79}Br.
10. In the vibrational motion of HI, the iodine atom remains stationary because of its large mass. Assume that the hydrogen atom undergoes harmonic motion and that the force constant is 317 N m^{-1}, what is the vibrational frequency ν_0? What is the zero point energy if H is replaced by D? Assume that there is no change in the force constant.