Chem 2430 HW #2

1. Consider a 2-dimensional particle-in-the-box problem. Suppose the box starts off as square with sides of length a. Now distort the square so that one side increases by δ and the other decreases by δ.

a. Show that through terms linear in δ that the energy of the (1,1) ground state level is not altered upon this distortion.

b. Through terms quadratic in δ does the energy of the (1,1) state go up or down upon distortion from the square box. Explain your result.

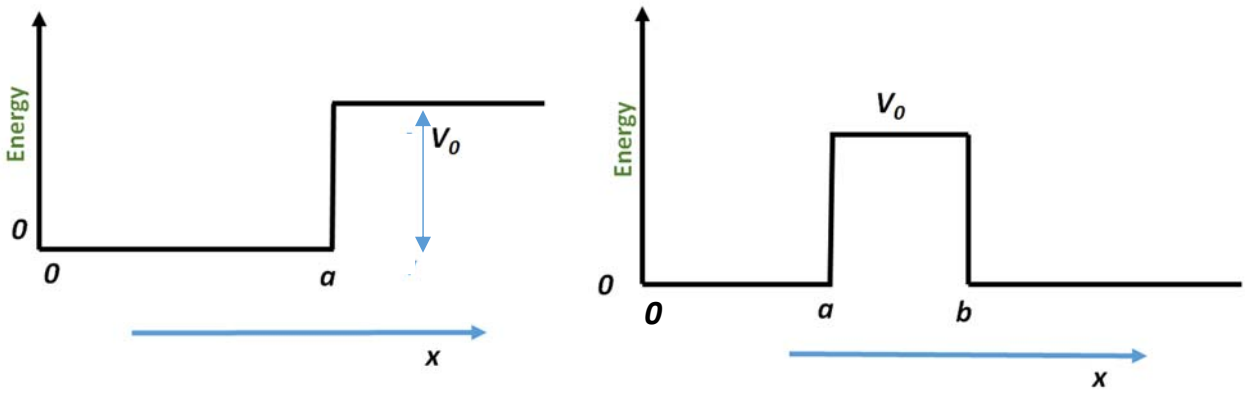
c. Now consider the (2,1) and (1,2) levels. Describe how their energies vary through terms linear in δ upon distortion.

2. Evaluate the integrals

a. $\langle 1 \mid \hat{x}^2 \mid 1 \rangle$ and $\langle 2 \mid \hat{x}^2 \mid 2 \rangle$ for the one-dimensional particle in the box problem.

b) Evaluate the integrals $\langle 1 \mid \hat{x}\hat{p}_x \mid 1 \rangle$ and $\langle 1 \mid \hat{p}_x\hat{x} \mid 1 \rangle$ for the particle in the box problem. Discuss your result.

3.



a) Consider the two potentials depicted above. (Assume $V = \infty$ for $x < 0$. Sketch the ground state wave function assuming $E < V_0$. For the right hand potential choose an E that corresponds to a resonance.

b) Work out as far as you can the solution (energy, wave function) of the Schrödinger equation of the right hand potential. (Please refrain from looking this up.)

c) For the potential shown on the left what is the change in ψ'' as one moves across the discontinuity at $x = a$?