Smith College
*Department of Chemistry*ψ

Chm 331 Fall, 2010

Problems: Special Set One: Preparation for Practical Exam One

51.0.1. You have a pole with a potential of infinity at $x < 0$, a potential of 0 from $x = 0$ to $x = 1$, after which the potential increases linearly with x with a slope of 3. Use numerical techniques to find the energy of the ground state wave function.

51.0.2. Plot the result from 51.0.1.

51.0.3. For the same pole as in problem 51.0.1., find the energy of the first excited state and plot the wave function.

51.0.4. For the ground state wave function of problem 51.0.1., find the probability that the parve will be between 0 and 1.

51.0.5. For the first excited wave function (see 51.0.3.) find the expectation value of x.

51.0.6. For the ground state of 51.0.1., find the most probable value of x.

51.0.7. Find the probability that the parve will be in the non-classical region for problem 51.0.1.

51.0.8. Show that two eigenfunctions of the harmonic oscillator are orthogonal.

51.0.9. Take the $n = 4$ level of the harmonic oscillator (in q notation; from HermiteH[4,q]) and show that it satisfies S.E. in the form:

$$d^2\psi/dq^2 \; -(q^2 - K)\psi = 0$$

51.0.10. What is the energy of your answer to 51.0.9.? HINT: You need to recall what K is.

51.0.11. Manually find the coefficients a_0 to a_{10} from the recursion formula for $n_{max} = 10$.

51.0.12. The ladder operator, a_+, in q notation is

$$\text{Sqrt}[2] \, (q - d/dq)$$

Show, using this operator, that $a_+ \, a_+ \, |2\rangle \; = \; |4\rangle$, where the wavefunctions are for the harmonic oscillator levels $n = 2$ and $n = 4$, respectively.

51.0.13. Use M. to find the $n = 6$ level for a harmonic osciallator. Use the Hamiltonian for the harmonic oscillator written in q notation to determine the eigenfunction of this level.

51.0.14. Determine the commutator for the Hamiltonian for the harmonic oscillator with p_x.

51.0.15. Does the kinetic energy operator commute with momentum?

51.0.16. A wave function for a parve in a certain one-dimensional potential energy is found to be

$$(4x^3 - 7x^2 - 2x)\mathrm{Exp}[-2*x]$$

over the range of x from 0 to 2. What is the probability the particle will be found between x = 0 and x = 1?

51.0.17. What is the expectation value of x for the wave function of 51.0.16.?

51.0.18. At what x is it most probable to find the parve for the wave function of 51.0.16.?

51.0.19. Find the expansion coefficients when this wave function is expressed in terms of the eigenfunctions of a parve on a pole of length 2 (with zero potential energy) for the wave function of 51.0.16.

51.0.20. Give a verbal justification about the reasonableness of the answer to 51.0.19.

51.0.21. If a parve on a pole of length two is prepared in the state described by the wave function of 51.0.16., what is the probability that an energy measurement will give the answer 4.9348 $hbar^2/m^2$.

51.0.22. This problem concerns a harmonic oscillator. Plot the wave function for a harmonic oscillator in the level n = 9 using the q parameter, q = Sqrt[m w/hbar] x.

51.0.23. How do you express the momentum operator in terms of the parameter q for the wave function of 51.0.22.?

51.0.24. Find the expectation value of the momentum for the wave function of 51.0.22.

51.0.25. Justify your answer to 51.0.24.

51.0.26. Show that the answer to 51.0.22. is orthogonal to the level with n = 1.

51.0.27. Show *by working with the actual functions* that the lowering operator, a_-, takes the n = 9 function for a harmonic oscillator and produces n = 8, i.e., show that $(a_-)|9\rangle = n\,|8\rangle$ where n is a number.

51.0.28. What is the value of the number n in 51.0.28.?

51.0.29. Find the commutator of the harmonic oscillator raising operator with q (defined in 51.0.22.). That is, find

$$[a_+ , q]$$

51.0.30. Is the harmonic oscillator raising operator, a_+, a Hermitian operator? Show your work. HINT: There are two ways to show this.