CYL100 2013–14 II semester Homework 2

Handed out: January 17, 2014 Due in: January 24, 2014
Note: Any data you require will be found in the back pages of Atkins's book

1. (a) Evaluate the probability of locating a particle in the middle third of 1-D box. (b) Find the probability that a particle in a box L wide can be found between $x = 0$ and $x = L/n$ when it is in the nth state.

2. Consider two wave functions which describe any two different states of a particle in a box. Show that these satisfy the relation $\int_0^L \psi_i^* \psi_j dx = \delta_{ij}$, where $\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ if $i \neq j$.

3. Verify the uncertainty principle for the particle in a box.

4. Below are some general statements about wave functions for stationary states of unique energy for a particle bound in a one-dimensional potential well $V(x)$. Decide whether each statement is true or false. Name one or more counterexamples for false statements. Be careful: except where noted, these are meant to be general statements, true, for example, even if there is a classically forbidden region *inside* the well. The phrase "outside the well" for any given energy E means a continuous classically forbidden region ($E < V(x)$) extending to infinity.

   (a) There are no nodes in the wave function outside the well.

   (b) There are no nodes in classically forbidden regions.

   (c) If the potential has only one relative minimum, the ground state probability function $|\psi|^2$ has only one maximum.

   (d) The ground state probability function has no nodes.

   (e) The ground state probability function has only one maximum.

   (f) The probability function for any state is greater at positions of higher potential than at positions of lower potential.

   (g) For a given region outside the well, the probability function is smaller as one goes farther from the well.

5. Many proteins contain metal porphyrin molecules. These molecules are planar and contain 26 π electrons. If the length of the molecule is ∼1000 pm, then what is the predicted lowest energy absorption of the porphyrin molecule?

6. For a hydrogen atom in the ground state find the classically forbidden region and calculate the probability of finding the electron in this region.

7. Compute the average value of r, the most probable value of r, and the root-mean-square value of r for the $1s$ and $2p$ levels of the hydrogen atom. Compare the three kinds of values and explain the origin of their differences.

8. Show that the hydrogenlike atomic wave function ψ_{210} is normalized and that it is orthogonal to ψ_{200}.

9. Calculate the probability that an electron described by a hydrogen $1s$ wave function will be found within one Bohr radius of the nucleus.

10. Prove that $< V >= 2 < E >$ and, consequently, that $< K > = - < E >$, for a $2s$ electron.

11. Compute $< r >$ in the $2s$, $2p$ states of the hydrogen atom. Compare your result with the general formula
$$< r_{nl} >= \frac{a_0}{2} \left[3n^2 - l(l+1)\right].$$

12. Where do the maxima in $r^2\psi_{2s}^2(r)$ occur?

13. What combinations of the d ($l = 2$) atomic orbitals will produce the Cartesian function $d_{xz} = xzR_{nl}(r)$ and $d_{xy} = xyR_{nl}(r)$.