Uva Wellassa University of Sri Lanka
Faculty of Science and Technology
Science and Technology Degree Programme
End Semester Examination – August/September 2014

SCT 333-2 Computational Chemistry

PART C – (50 Marks)
Answer all questions

1. a. Derive the quantum mechanical operators for the three components of angular momentum in Cartesian coordinates, starting from the classical definition of angular momentum, $\vec{l} = \vec{r} \times \vec{p}$.

b. If a hydrogen atom is in a state with a total angular momentum $\sqrt{6}\hbar$, (10 marks)

(i). find the value of l.

(ii). what orbital is represented by this l value?

(iii). what are the possible m values for this state?

(iv). Draw an angular momentum vector diagram to show the magnitude of the total angular momentum and the magnitudes and relative directions of the angular momenta for the states specified by different m values.

(v). Deduce the angular momentum along the z-axis for the orbitals A and B whose $\Theta(\theta)$ and $\Phi(\phi)$ functions are given below $\left(\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}\right)$

	$\Theta(\theta)$	$\Phi(\phi)$
A	$\frac{1}{2}\sqrt{\frac{15}{2}}(3\cos^2\theta - 1)$	$\frac{1}{\sqrt{2\pi}}$
B	$\sqrt{\frac{15}{2}}\sin\theta\cos\theta$	$\frac{1}{\sqrt{2\pi}}e^{i\phi}$

2. Answer <u>all</u> parts. (15 marks)

a. i. Describe the variation method used in quantum mechanics.

(5 marks)

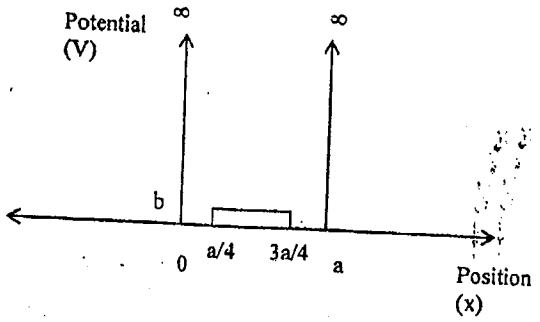
ii. Show that $\psi = x(x-a)$ is a suitable variation function for a particle in one-dimensional infinite potential box in which potential is zero for $0 \leq x \leq a$ and it is infinite elsewhere. Also show that $\psi = k(x-a)^2$ is not suitable for a trial function for the same problem.

(5 marks)

iii. Apply the variation function, $\psi = x(x-a)$ for a particle in the potential box described in part (i) above and calculate an upper bound to the ground state energy.

(7.5 marks)

b. An electron is in a one-dimensional system whose potential varies with position as given below.



If b is small, find the lowest allowed energy using first order perturbation theory.

(7.5 marks)