## **CHM102** Assignment **April 9, 2017**

- 1. Calculate the first order correction to the ground state energy for a particle in a box, whose potential is of the form  $V = -\varepsilon \sin(\pi x/L)$ .
- 2. Use the trial function  $\varphi(x) = (1 + c\alpha x^2) \exp(-\alpha x^2/2)$ , where  $\alpha = (k\mu/\hbar^2)^{1/2}$ . In this function, 'c' is a variational parameter. If you use this function for calculation of the ground state energy of the harmonic oscillator, what would the value of 'c' and E<sub>min</sub> be? Why?
- 3. Use the trial function  $\varphi(x) = c_1 \exp(-\alpha r) + c_2 \exp(-\alpha r^2)$  to carry out a variational calculation for the ground state of the hydrogen atom, what would be the value of the variational parameters  $c_1$  and  $c_2$ ? What would be the value of  $\alpha$  and  $E_{min}$ ?
- 4. Derive term states for the following electronic configurations and identify the gound state among the states you have derived.

A) He:  $1s^{1}2p^{1}$ 

B)  $B:1s^22s^22p^1$ 

C)  $C:1s^22s^22p^13p^1$ 

D) F:1s<sup>2</sup>2s<sup>2</sup>2p<sup>5</sup>
E) Ne: B:1s<sup>2</sup>2s<sup>2</sup>2p<sup>6</sup>
F) C: B:1s<sup>2</sup>2s<sup>2</sup>2p<sup>2</sup>