

Assignment 1 – Newton Raphson Method

Oves Badami

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Note: This Assignment is for 10 Marks Due: 1 week

Using the techniques/methods discussed in the class solve the following problems

1. The inter-atomic potential energy of a diatomic molecule is modelled by Lenard-Jones potential, $U(r)$

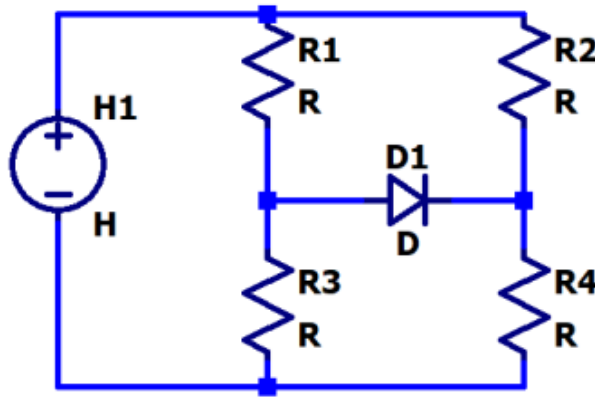
$$U(r) = 4\epsilon \left[\left(\frac{\sigma}{d} \right)^{12} - \left(\frac{\sigma}{d} \right)^6 \right]$$

Here the σ and ϵ are parameters $\sigma = 0.31589$ nm, $\epsilon = 775$ Joules/mol. (5)

- (a) Plot the Lenard Jones Potential. Please mark the x and y axis label clearly
- (b) Calculate the bond length of an a molecule with parameters specified.
- (c) Verify that your solution is correct.

Note: The net force acting on an atom is given by ($F = -\nabla U(r)$)

2. Consider a circuit shown below: Calculate the current through the diode for the following parameters (5)



The current through diode is $I_D = I_0 \left[\exp \left(\frac{V_D}{\eta V_T} \right) - 1 \right]$ $R1 = 1k \Omega$ $R2 = 3k \Omega$ $R3 = 4k \Omega$ $R4 = 2k \Omega$ $I_0 = 3nA$ $\eta = 2$. Assume that the supply of 5 V