Spectroscopy

Assignment 1

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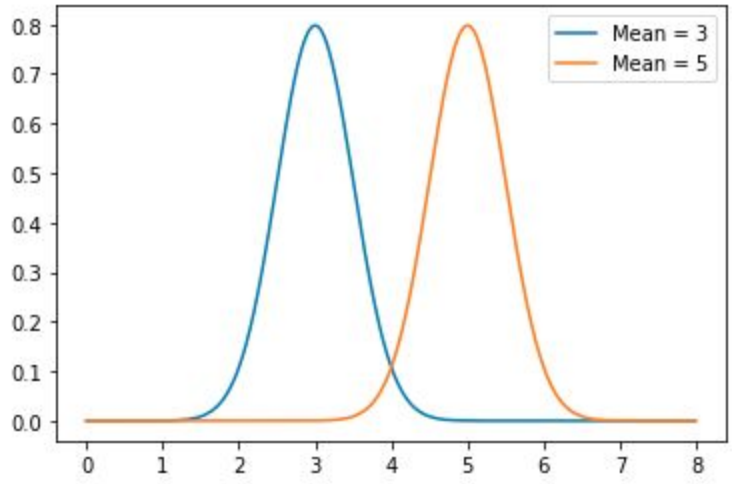
Wavefunctions visualised

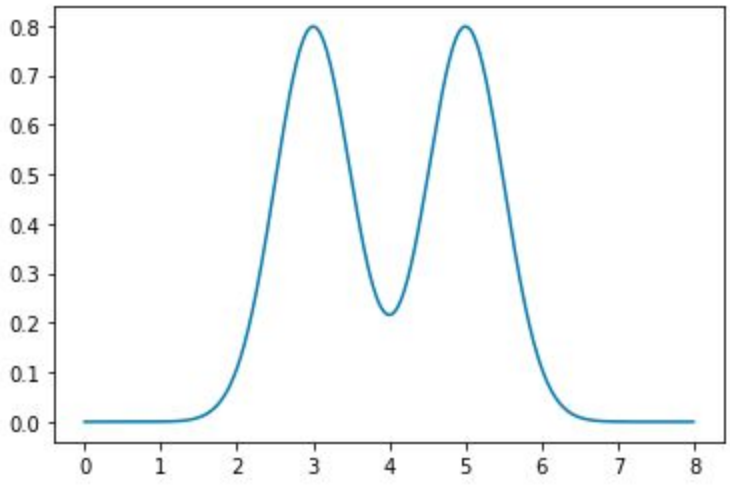


The blue curve corresponds to the Gaussian Distribution with mean = 3.0 and standard deviation = 0.5

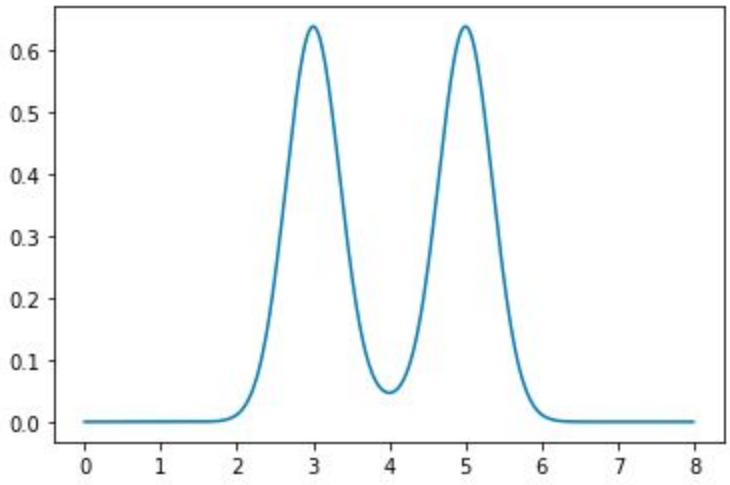
The orange curve corresponds to the Gaussian Distribution with mean = 5.0 and standard deviation = 0.5

Q1) Plotting the resulting wavefunctions

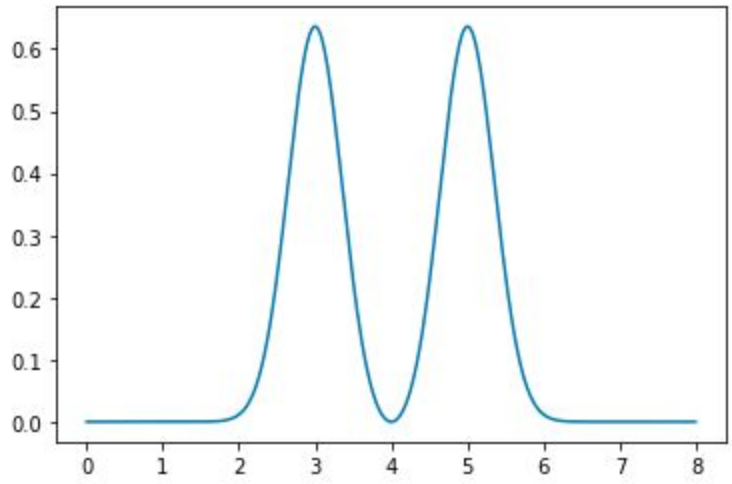
A) Psi(A) + Psi(B)



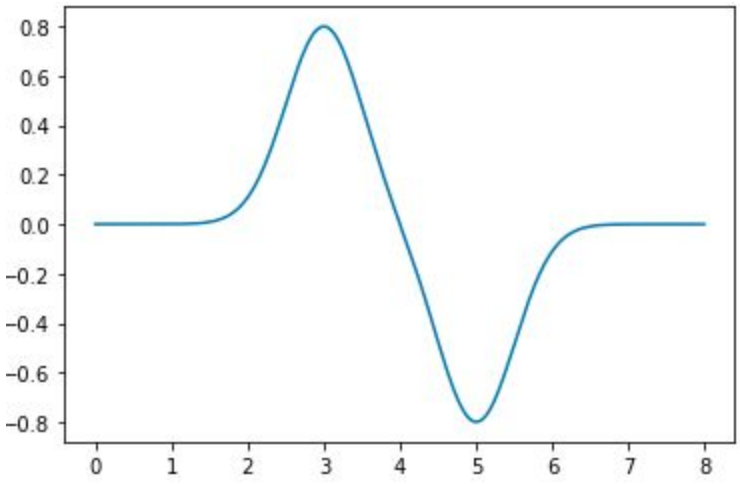
B) $(Psi(A) + Psi(B))^2$



C) $(Psi(A) - Psi(B))^2$



D) Psi(A) - Psi(B)



Q2) Comparing Plots B and C

Given that the atoms are placed at positions x_A (3) and x_B (5), and their corresponding wavefunctions are Psi(A) and Psi(B).

The plot C has a value of 0 for x = 4, while in plot B: the value for x =4 (though very small) is non zero. This occurs due to the difference in phases between the two wavefunctions. In part B the two wavefunctions interfere constructively whereas in part C the two wavefunctions interfere destructively. The square of wave functions gives us the probability, therefore we can say that the Probability of finding an electron at x=4 is 0 for part C as the two wavefunctions are 180 degrees out of phase. x=4 forms a node in part C. A bonding orbital is formed when the wave functions add (in phase) and an antibonding orbital is formed when they subtract (out of phase).