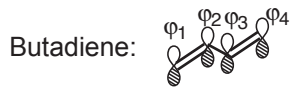
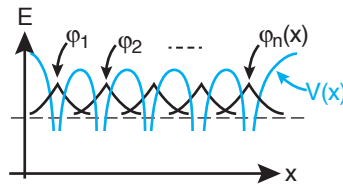
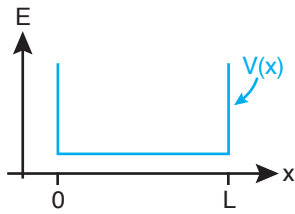
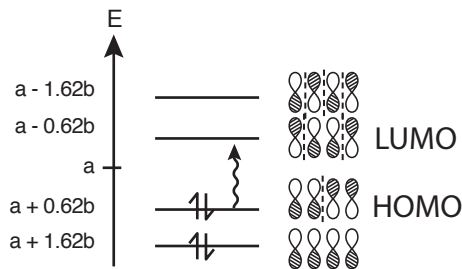


The Hückel model: Particle in a box with tunneling between atoms

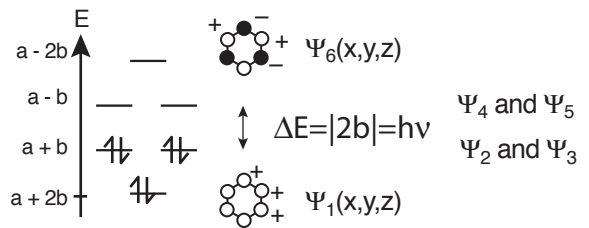
Hückel model: PIB with tunneling



Solving,



Solving,



Note on nodes in benzene:

The Ψ_1 function has no nodal plane, the Ψ_6 function has 3 nodal planes.

In the numbering scheme used here, Ψ_2 and Ψ_3 are degenerate, and Ψ_4 and Ψ_5 are also degenerate.

Ψ_2 and Ψ_3 each have 1 nodal plane. Of course, you can draw 3 different functions with one nodal plane,



but only 2 are linearly independent; people usually like to pick the following 2 linear combos:



It's like p_x , p_y vs. $Y_{1,-1}$, $Y_{1,1}$ rotational basis functions: different linear combinations can be made, they all have the same degenerate energy.

$$\Psi \approx \alpha_1 \Psi_1(x_1, y_1, z_1) + \alpha_2 \Psi_2(x_2, y_2, z_2) + \alpha_3 \Psi_3(x_3, y_3, z_3) + \alpha_4 \Psi_4(x_4, y_4, z_4) + \alpha_5 \Psi_5(x_5, y_5, z_5) + \alpha_6 \Psi_6(x_6, y_6, z_6)$$



Comparison of benzene to particle in a ring:

