

Copy of a printed graph referenced as "Density at points along the nuclear axis for the attractive and repulsive states of H+2"

Contributors

Fuller, Watson, 1935-

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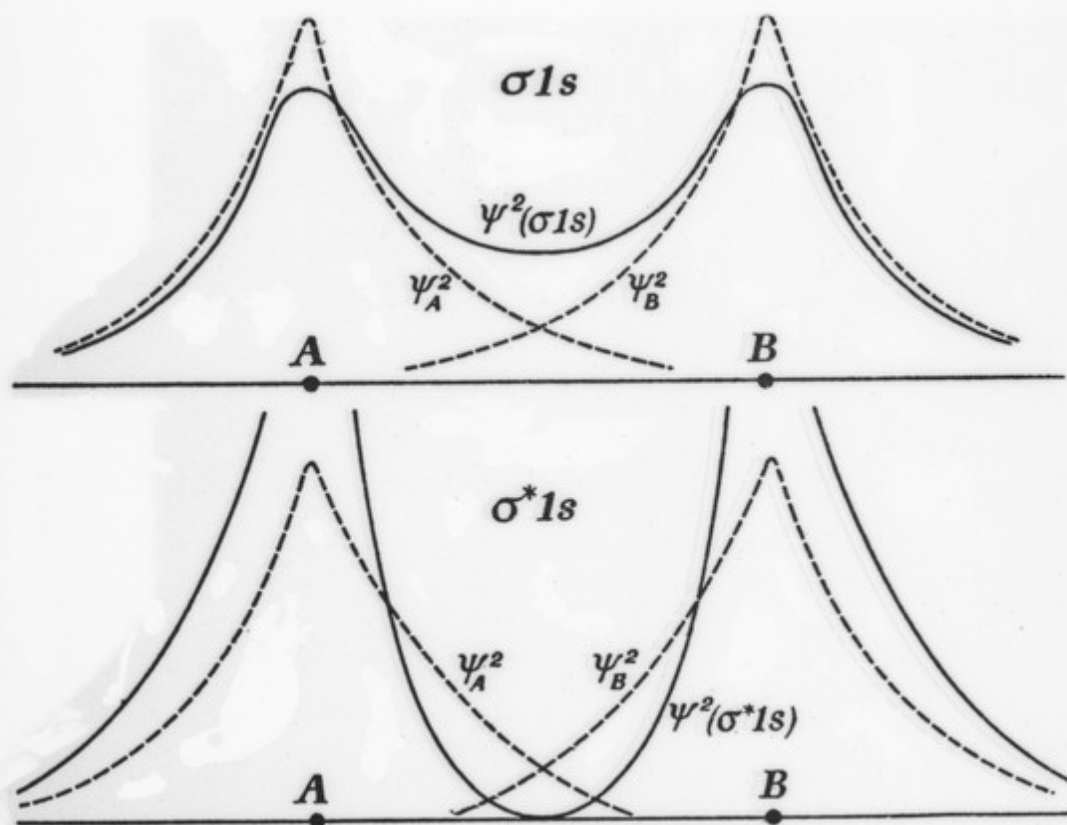
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Fig. 4 shows contours of constant ψ^2 , i.e. charge-cloud density, or probability. The plane of the paper is any plane through the nuclei A and B . Even though more accurate wave functions would change the shapes of these contours slightly, these diagrams are substantially correct. Fig. 5 shows the value of ψ^2 at points along the nuclear axis, and also the values of ψ_A^2 and ψ_B^2 for com-



The density ψ^2 at points along the nuclear axis for the attractive $\sigma 1s$ and the repulsive $\sigma^* 1s$ states of H_2^+ . [No screening constant introduced here.]

parison, though these latter are drawn to half scale. This is to enable us to compare the 'true' density ψ^2 with the sum of the atomic densities $\psi_A^2 + \psi_B^2$ that

- (i) in a bonding orbital the charge is concentrated rather more between the nuclei than would be expected by superposition of the component a.o. densities;
- (ii) in a bonding orbital the lateral spread is not very great and the charge-cloud is less