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Visualizing Molecular Wavefunctions Using Monte Carlo Methods STEVE ALEXANDER, Southwestern University, R.L. COLDWELL, University of Florida — Using explicitly correlated wavefunctions and variational Monte Carlo we calculate the electron density, the electron density difference, the intracule density, the extracule density, two forms of the kinetic energy density, the Laplacian of the electron density, the Laplacian of the intracule density and the Laplacian of the extracule density on a dense grid of points for the ground state of the hydrogen molecule at three internuclear distances (0.6,1.4,8.0). With these values we construct a series of contour plots and describe how each function can be used to visualize the distribution of electrons in this molecule. We also examine the effect of electron correlation on each expectation value by calculating each function with a Hartree-Fock wavefunction and then comparing these values with our explicitly correlated values.

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