A Trial Wave Function for Electrons in Molecular and Atomic Hydrogen

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The potential energy is an essential ingredient to investigate the phase diagram of hydrogen with numerical methods (molecular dynamic or Monte Carlo methods). Here we propose a novel Shadow Wave Function for disordered fermionic systems in the context of variational quantum Monte Carlo. The accuracy of this trial wavefunction is demonstrated on solid molecular and atomic hydrogen at very high pressure and compared to the standard Jastrow-Slater Determinant approach.