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Multi-determinant electron-nuclear quantum Monte Carlo method for ground state solution of molecular Hamiltonian ABHINANDEN SAMBASIVAM, JENNIFER ELWARD, ARINDAM CHAKRABORTY, Syracuse University — The focus of this work is to obtain the ground state energy of the non-relativistic spin-independent molecular Hamiltonian without making the Born-Oppenheimer (BO) approximation. In addition to avoiding the BO approximation, this approach avoids imposing separable-rotor and harmonic oscillator approximations. The ground state solution is obtained variationally using multi-determinant variational Monte Carlo method where all nuclei and electrons in the molecule are treated quantum mechanically. The multi-determinant VMC provides the right framework for including explicit correlation in a multi-determinant expansion. This talk will discuss the construction of the basis functions and optimization of the variational coefficient. The electron-nuclear VMC method will be applied to H_2, He_2 and H_2O and comparison of the VMC results with other methods will be presented. The results from these calculations will provide the necessary benchmark values that are needed in development of other multicomponent method such as electron-nuclear DFT and electron-nuclear FCIQMC.

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