Tensor Product Multiscale Many-Particle Spaces with Finite-Order Weights for the Electronic Schrödinger Equation

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We study tensor product multiscale many-particle spaces with finite-order weights and their application for the electronic Schrdinger equation. Any numerical solution of the electronic Schrdinger equation using conventional discretization schemes is impossible due to its high dimensionality. Therefore, typically Monte Carlo methods (VMC/DMC) or nonlinear model approximations like Hartree-Fock (HF), coupled cluster (CC) or density functional theory (DFT) are used. We present a new numerical method which combines the favorable properties of efficient Gaussian type orbitals basis sets, which are applied with good success in conventional electronic structure methods, and tensor product multiscale bases, which provide guaranteed convergence rates and allow for adaptive resolution. To this end, the approach is based on a modified adaptive sparse grid technique and a certain particle-wise decomposition with respect to one-particle functions obtained by a nonlinear rank-1 approximation. Sparse grids allow to overcome the exponential complexity exhibited by conventional discretization procedures. Here, we employ a multiscale Gaussian frame for the sparse grid spaces and we use Gaussian type orbitals to represent the rank-1 approximation. With this approach we are able to treat small atoms and molecules with up to six electrons.

Literature:

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