Multisliced Gausslet Bases for Electronic Structure

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A major driver of the cost of density matrix renormalization group, tensor network, and quantum computing algorithms for electronic structure scale is the number of terms in the Hamiltonian. A conventional basis, for which the number of two electron terms scales as N^4, where N is the number of basis functions, are not ideal for these methods. Gausslets[1] are a new type of basis set, based on wavelet technology, which allow strictly diagonal two electron Hamiltonians, with the number of terms equal to N^2. Gausslets are smooth, highly local, orthogonal, and integrate like delta functions, giving them the diagonal property. In our multisliced gausslet formulation[2], they also have variable resolution, and can be combined with ordinary Gaussian bases. Here we given an overview of this technology, with applications to hydrogen chains using DMRG, comparing results with standard bases in the full-CI, complete basis set limit. In this regime, for hydrogen chains, multisliced gausslets can surpass Gaussian basis sets in accuracy, without relying on extrapolation in the level of completeness. We also report on our progress in extending the approach to more general molecules.

References

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