Explicitly Correlated Coupled-Cluster in Real Space

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A first-quantized formulation of Coupled-Cluster is presented and used to implement Coupled-Cluster in real-space methods. All terms that are usually derived in diagrammatic form and are then transferred to second quantization, can be expressed in first quantization. The full regularization of all singularities using explicit correlation makes the method feasible. An implementation of CC2 using multi-resolution analysis (MRA) in the `Madness` program packages shows its applicability for small molecules, and correlation energies close to the basis set limit are obtained. Furthermore, CC2 excitation energies are computed using the same regularization procedure as for the ground state.

References

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