

Semistochastic Heatbath Configuration Interaction Method and Orbital Optimization

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The Semistochastic Heatbath Configuration Interaction (SHCI) method [1, 2, 3, 4] is a variant of Selected Configuration Interaction plus Perturbation Theory (SCI+PT) methods that have been used for over 45 years, starting with the CIPSI method. Two key innovations make it faster than other SCI+PT methods:

1. It takes advantage of the fact that the Hamiltonian matrix elements for double excitations depend only on the four orbitals whose occupations change to make the determinant selection in both the variational and the perturbative steps much faster.
2. It overcomes the memory bottleneck of the perturbative step by evaluating the perturbative energy correction using a 3-step semistochastic approach.

The method has been applied to challenging molecular systems with more than 2 billion variational determinants and trillions of perturbative determinants, and to the homogeneous electron gas using more than 30,000 orbitals.

The efficiency of the method depends in part on the choice of orbitals. I will describe work in progress on improving the efficiency of the orbital optimization.

References

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