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A Brief Introduction to the Truncated Eigenfermion Decomposition[1] JONATHAN E. MOUSSA, JAMES R. CHELIKOWSKY, UT Austin — We present a computational formalism for the approximate unitary transformation of a many-body fermion Hamiltonian with two-body interactions. This work is a further development of the numerical canonical transformation approach of S. R. White [J. Chem. Phys. 117, 7472 (2002)]. The Hamiltonian can be diagonalized in a basis of *eigenfermion* operators, in which case the eigenstates are all single Slater determinants of eigenfermions. The transformation of two-body interactions generates higher-order interactions that can be approximated by effective two-body interactions using a novel generalization of normal ordering. The error in representating a target eigenstate is minimized by performing the generalized normal ordering with respect to that eigenstate. Numerical results are presented for several test cases, including Hubbard model clusters.

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