

TITLE: Electron correlation from the adiabatic-connection-fluctuation-dissipation-theorem approach for a multireference wavefunction.

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ABSTRACT:

In the first part of the talk I will present a general formalism that employs adiabatic connection formula and the fluctuation dissipation theorem that leads to a correlation functional if single-reference and some multireference wavefunctions are used. Then the formalism will be employed in connection with the strongly orthogonal geminal model to describe subtle correlation effects in weakly interacting multireference systems. Such systems require proper description of the long-range dynamic correlation together with the long-range static effects. They pose a serious challenge for a coupled cluster CCSD(T) method and a multireference CASPT2 approach.