

Oberseminar der AG Numerik am 04.12.13:

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TITLE: The method of configuration interaction in computational quantum chemistry

ABSTRACT: We will discuss the linear algebra of N-fermion systems and introduce the configuration interaction (CI) expansion of N-electron wave functions. All features of electronic structure are reflected in the full CI expansion of a state's wave function. The electronic structure software program GAMESS, which computes approximate solutions of the N-electron Schrödinger equation, often specifies the approximate solution in terms of CI data. From such CI data, Rada Weishäupl and I [1] have confirmed that the two core electrons in small atoms or molecules (e.g., B or LiH) appear to form a "strongly separated" pair of electrons in a pure quantum state, statistically independent of the other N-2 electrons.