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Pfaffian wave functions and topology of fermion nodes

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Pfaffian is defined as a signed sum of all pair partitions of even number of elements and it can be viewed as a nontrivial generalization of determinant. Pfaffian enables to define the simplest possible antisymmetric wave function based on pair spinorbital(s) and therefore represents a pairing generalization of the Slater determinant of one-particle orbitals. Pfaffians actually accomodate several types of pairing wave functions, for example, one special case is the Bardeen-Cooper- Schrieffer wave function. Using this platform we propose pfaffian wave functions with simultaneous pairings both in singlet and triplet channels and we benchmark their performance in fixed-node quantum Monte Carlo. We implement Gaussian elimination-like algorithm which enables to calculate pfaffians with efficiency similar to calculation of determinants. For a testing set of first row atoms and molecules we show that single pfaffians provide correlation energies systematically at the level of about 95%. Linear combinations of small number of pfaffians recover another fraction of the missing correlation energy comparable to significantly larger determinantal expansions. In addition, we show that pfaffians possess an important property of fermionic wave functions, namely, the minimal number of two nodal domains defined by fermion nodes. This is related to the proof that under rather general conditions closed-shell ground state wave functions of fermionic systems in $d>1$ have two nodal domains for arbitrary system size. The explicit proofs cover a number of paradigmatic models such as fermions on a sphere surface, in a periodic box, atomic states, etc, and we discuss the implications of this on efficient construction of wave functions and on several types of many-body effects. Supported by NSF and done in collaboration with M. Bajdich, L.K. Wagner, G. Drobny, and K.E Schmidt.
Refs: L. Mitas, PRL 96, 240402 (2006); L. Mitas, cond-mat/0605550; M. Bajdich et al, PRL 96, 130201 (2006); cond-mat/0610850.