Multi-pfaffian pairing wave functions for quantum Monte Carlo
MICHAL BAJDICH, LUBOS MITAS, CHIPS, Department of Physics, North Carolina State University, Raleigh, NC 27695, KEVIN E. SCHMIDT, Department of Physics, Arizona State University, Tempe, AZ 85287 — We investigate the limits of accuracy of trial wave function for quantum Monte Carlo based on pfaffian functional form with singlet and triplet pairing. Using a set of first row atoms and molecules we find that this wave function provides very consistent and systematic behaviour in recovering the correlation energies on the level of 95% . In order to get beyond this limit we have explored the possibilities of multi-pfaffian pairing wave functions. We show that small number of pfaffians recovers another large fraction of the missing correlation energy comparable to the larger-scale configuration iteraction wave functions. The trade-offs between the size of the underlying optimization problem and amounts correlation energy recovered will be discussed.

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