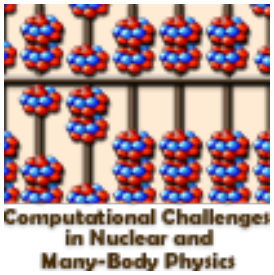

Contribution ID: **274** Type: **not specified**

New wavefunction forms for strong electron correlation inspired by the eigenvectors of exactly solveable model systems

Modeling strong correlation is so difficult that theorists often settle for qualitative descriptions of strongly-correlated substances (e.g. heavy-fermion materials, high-temperature superconductors). These qualitative approaches are typically based on model Hamiltonians for which the Schrödinger equation can be solved exactly via the Bethe ansatz. We recently realized that one can use the wavefunction-forms from exactly-solvable model Hamiltonians for calculations with the true Hamiltonian (with electrons and nuclei). Choosing a suitable model Hamiltonian ensures that the key qualitative features of the system are all captured, while the computational cost remains low because the exactly solvable model systems can be represented using independent quasiparticles. Our results from wavefunction-forms from the Richardson-Gaudin family of Hamiltonians have remarkable quantitative accuracy: the ground-state energies are typically within 0.001 eV of benchmark results from complete diagonalization in the exponentially big Hilbert space of paired electrons (i.e., doubly-occupied configuration interaction). Using symmetry-broken (unrestricted or general mixed-spin) orbitals to form the Richardson-pairs improves the results still further, and is especially important for spin-frustrated and non-singlet states. The models we present are highly effective for modelling strong correlation, but computationally efficient enough to be applied to large molecules.

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