

Abstract for the ISTCP-X Conference

Ali Alavi, Aron Cohen, Hongjun Luo, Kai Guther, Werner Dobrautz, David Tew

Max Planck Institute for Solid State Research, Stuttgart
Office-alavi@fkf.mpg.de

We investigate the utility of non-unitary similarity transformations, based on Jastrow or Gutzwiller factorisation of the electronic wavefunction. Such factorisations generally lead to non-Hermitian effective Hamiltonians which contain three-body interactions. Such Hamiltonians are treatable via the projective FCIQMC technique, which does not suffer from the non-Hermitian characteristic of the Hamiltonian, nor do the 3-body terms present an insuperable obstacle. In this formalism, there is no need for projection operators that are essential in R12/F12 type of explicit correlation methods, and highly flexible Jastrow factors can be used. We show that these are effective in delivering highly accurate total energies even with modest basis sets. In the case of Gutzwiller factorisation, we apply this method to the 2D Hubbard model in the strong correlation off-half-filling regime, which is an extremely challenging problem. We show that the similarity transformation results in compact right eigenvectors, which can be sampled accurately by the i-FCIQMC method, even for systems containing 50 sites and ~ 50 electrons. The methodology opens up the prospect to study strongly correlated molecular systems, where much of the dynamical correlation can be captured by the correlation factor, and the strong correlation aspects via the multi-configurational reference function.