

STRONG CORRELATION IN ONE- AND TWO-DIMENSIONAL SYSTEMS

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DFT fails dramatically to describe strongly correlated electrons [1]. Natural Orbital Functional (NOF) theory is an ideal alternative to study strongly correlated electrons within one-particle theories. We show the ability of the PNOF7 approximation [2,3] to describe static correlation effects in two-dimensional systems. Correlation energies obtained by using PNOF7 are comparable to those of exact diagonalization, density matrix renormalization group, and auxiliary-field quantum Monte Carlo calculations for the two-dimensional Hubbard model up to 144 electrons, which is considered the prototype to study high-temperature superconductors [4]. For the latter, accurate results are obtained when particle-hole symmetry is broken away from half-filling. We report energies for different spin multiplicities of the Hubbard and the quantum mechanical Hamiltonians by means of an approximation exempt of spin contamination effects [5]. Dissociation processes are studied in one- and two-dimensional hydrogen lattices.

References

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Figures

