Ground State Energies of Coulomb Systems and One-Particle Reduced Density Matrices

Functionals of the one-particle reduced density matrix offer a tool for the computation of quantum ground state energies. Together with appropriate correlation inequalities they yield controlled approximations. We will discuss such functionals and will show, in particular, that the basic functional introduced by Müller (1984) and rediscovered and refined in quantum chemistry describes the ground state energy of atoms of nuclear charge Z correctly up to terms of order $o(Z^{5/3})$.