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Inhomogeneous ground state in the Hubbard model: a mean-field study[1] JIE XU, CHIA-CHEN CHANG, ERIC J. WALTER, SHIWEI ZHANG, The College of William snd Mary — We report unrestricted Hartree-Fock (UHF) results for the ground state of the single-band Hubbard model in two- and three-dimensions with repulsive onsite interaction and nearest-neighbor hopping. At half-filling, the Hartree-Fock (HF) approach is sufficient to capture the basic physics of long-range antiferromagnetic order. Away from half-filling, many earlier HF calculations have been performed in the 2-D Hubbard model, which indicated the formation of domain walls and stripes. We numerically solve the self-consistent UHF equations for a range of densities at weak and intermediate interaction strengths. An annealing scheme coupled with multiple initial configurations is adopted to reach the global minimum. Our goal is to contrast the UHF ground state in the Hubbard model and the HF spin-density wave states in the continuum (jellium) [1]. A second goal is to obtain quantitative information of the UHF ground state for examination by accurate many-body methods such as quantum Monte Carlo. [1] A. W. Overhauser, Phys. Rev. 128, 1437 (1962); Shiwei Zhang and D.M.Ceperley, Phys. Rev. Lett. 100, 236404 (2008).

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