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A benchmark study of the two-dimensional Hubbard model with auxiliary-field quantum Monte Carlo[1] MINGPU QIN, HAO SHI, SHIWEI ZHANG, College of William and Mary — The ground state properties of the two-dimensional Hubbard model are calculated with the auxiliary-field quantum Monte Carlo (AFQMC) method. With general twist boundary conditions, the shell effect is eliminated. We use large lattice sizes ($L \times L$ lattices with L up to 24) and average over many twist angles to extrapolate to the thermodynamic limit and ensure convergence of the calculated physical quantities. At half filling, we obtain accurate results for the ground-state energy, sublattice magnetization and double occupancy, and other correlation functions for interactions ranging from $U/t = 2$ to 8. We then study the doped cases with a constraint to control the "minus sign" problem. We apply the latest development [2] in the constrained path AFQMC technique to benchmark the effect of different trial wave functions, and study ground-state properties in the thermodynamic limit. The different competing phases close to half filling are investigated.

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[2]Hao Shi, Shiwei Zhang, Phys. Rev. B. **88**, 125132 (2013); Hao Shi, Carlos A. Jiménez-Hoyos, R. Rodríguez-Guzmán, Gustavo E. Scuseria, and Shiwei Zhang, Phys. Rev. B. **89**, 125129 (2014)

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