Equation of state in single-band Hubbard models in two- and three-dimensions[1] CHIA-CHEN CHANG, SHIWEI ZHANG, Department of Physics, College of William and Mary — We present results on ground-state energetics of the single-band Hubbard model in two- and three-dimensions with nearest-neighbor hopping and repulsive contact s-wave (on-site) interaction. Our calculations are done with the constrained-path auxiliary-field quantum Monte Carlo method. By incorporating generalized boundary conditions, we reduce finite-size effects due to open and closed shell filling and finite simulation cells. Results are obtained for the kinetic, interaction, and total energies and extrapolated to the thermodynamic limit for a range of interaction strengths (U/t) and electron densities.

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