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Correction of finite-size errors in many-body electronic structure[1]
HENDRA KWEE, SHIWEI ZHANG, HENRY KRAKAUER, College of William and Mary — Quantum Monte Carlo (QMC) calculations using simulation cells with periodic boundary conditions are subject to finite-size errors. Often, such errors are corrected or reduced by extrapolation using increasingly larger simulation cells, combined with size corrections from less accurate calculations, such as from Hartree Fock (HF) or density functional theory (DFT). Direct extrapolation is computationally costly. Size-corrections from standard HF and DFT calculations introduce additional errors and are less reliable. This has led to several recent attempts at improved methods to correct for finite-size errors. Here we develop a scheme which uses modified density functionals to estimate the finite size errors. Tests on simple solids and molecules using plane-wave auxiliary-field QMC calculations show encouraging results.

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