Evaluating the convergence rate of the finite size effects in the thermodynamic limit of connectivity-twist-averaged coupled cluster calculations in the uniform electron gas

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We performed a numerical analysis on the thermodynamic limit (TDL) extrapolation power laws for the coupled cluster doubles correlation energy in the uniform electron gas using a new cost-reducing twist averaging method we recently developed.[1] The thermodynamic limit energies were found for a range of densities. The high-density limit, where exact TDL values are known, was then used to determine the convergence rate which showed a different convergence than the accepted 1/N rate.

[1] Mihm, T. N.; McIsaac, A. R.; Shepherd, J. J. J. Chem. Phys. 2019, 150 (19), 191101.