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Conformation of a Lennard-Jones polymer in explicit solvent[1]
YUTING YE, Dept. of Physics, Hiram College, Hiram OH, MARK TAYLOR, Dept. of Physics, Hiram College, Hiram, OH — The conformation of a polymer chain is solution is coupled to the local structure of the surrounding solvent and can undergo large changes in response to variations in solvent density and temperature. The many-body effects of solvent on the structure of an n-mer chain can be formally mapped to an exact n-body solvation potential. These potentials map the chain-solvent system to a single chain, thereby dramatically reducing the computational complexity of the polymer chain-in-solvent problem. We have recently shown that a pair-decomposition of this n-body potential is valid for short Lennard-Jones (LJ) chains in explicit LJ solvent [1]. Here we use these short chain results to construct solvation potentials for long chains. We present results for the size and intramolecular structure of LJ chains up to length n=400 in LJ solvent at state points spanning the solvent phase diagram (including vapor, liquid, and super-critical regions). In comparison with simulation results for the corresponding full chain-in-solvent system, our solvation potential approach is found to be quantitatively accurate for a wide range of solvent conditions and chain lengths.

[1] M.P. Taylor and S.R. Adhikari, J. Chem. Phys. 135, 044903 (2011).

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