Abstract Submitted
for the OSS13 Meeting of
The American Physical Society

Solvation Potentials & Partition Function Zeros for a Polymer Chain[1] MARK TAYLOR, YUTING YE, PYIE PHYO AUNG, Dept. of Physics, Hiram College — In this poster we present results for model interaction-site polymers built from either Lennard-Jones (LJ) or square-well (SW) sphere monomers. First, we study the conformation of LJ chain polymers in explicit LJ solvent. We compute numerically exact sets of solvation potentials for chains of length five across the LJ solvent phase diagram. We use these exact short chain results to construct accurate solvation potentials for long LJ chains in solvent. These solvation potentials map the many-body chain-in-solvent problem onto a few-body single-chain problem, thereby greatly reducing the computational complexity of studying long chains in explicit solvent. Second, we study phase transitions of an isolated SW polymer chain by examining the zeros of the single-chain partition function. These partition functions are obtained either through exact calculation for short chains ($n \leq 6$) or via Wang-Landau simulation for long chains (up to length $n = 256$). Maps of the partition function zeros provide insight into the location and nature of the single-chain collapse and freezing transitions. Of particular interest is the disappearance of the collapse transition for a sufficiently short SW interaction range, analogous to the disappearance of the liquid phase in a SW monomer fluid.

[1]Funded by: National Science Foundation, Division of Materials Research (DMR-1204747)

Mark Taylor
Dept. of Physics, Hiram College

Date submitted: 28 Feb 2013 Electronic form version 1.4