Abstract Submitted
for the OSS08 Meeting of
The American Physical Society

Conformation and collapse of a polymer chain in explicit solvent: A solvation potential approach MARK TAYLOR, Dept. of Physics, Hiram College — The conformation of a polymer chain in solution is intrinsically coupled to the chain's local solvent environment. In much of the theoretical work on polymers in solution solvent effects are treated implicitly and explicit chain-solvent coupling is ignored. Although a formally exact treatment of chain-solvent coupling can be constructed, the required many-body solvation potential is not practical to compute. We have recently shown that for short hard-sphere and square-well chain-in-solvent systems this many-body solvation potential can be made tractable via an "exact" decomposition into a *set* of two-site potentials [1]. Here we use these exact short chain results, combined with the pure solvent potential of mean force, to construct approximate two-site solvation potentials for long chains under a range of solvent conditions [2]. Monte Carlo simulations for full chain-in-solvent systems verify the accuracy of our solvation potential mapping. We use this approach to study the role of solvent in both driving and inhibiting chain collapse in square-well systems and discuss the possibility of solvent driven chain collapse in the symmetric hard-sphere chain-in-solvent system. [1] M. P. Taylor and G. M. Petersen, J. Chem. Phys. **127**, 184901 (2007). [2] M. P. Taylor and S. Ichida, J. Polym. Sci., Part B: Polym. Phys. **45**, 3319 (2007).

Mark Taylor
Dept. of Physics, Hiram College

Date submitted: 03 Mar 2008 Electronic form version 1.4