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Conformation and collapse of a square-well chain in a square-well solvent PASSANG DORJI, MARK TAYLOR, Dept. of Physics, Hiram College — Interaction-site chains provide coarse-grained yet realistic models for polymers. Such models have long been used to study the collapse transition observed for polymers in dilute solution. In most of these studies, the variation in solvent quality (which drives the collapse) is treated implicitly through an effective polymer-polymer interaction and thus explicit polymer-solvent coupling is ignored. This coupling is expected to be important in the collapse transition due to the dramatic change in polymer conformation and exposure to solvent. Although a formally exact treatment of polymer-solvent coupling can be constructed, the required many-body solvation potential is not practical to compute. We have recently shown that for short 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 to construct approximate two-site solvation potentials for long square-well chains in solvent [2]. These solvation potentials are used to study the role of solvent in both driving and inhibiting chain collapse in square-well systems. [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).

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