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Solvation potentials for polymer chains in solution MARK TAYLOR, Dept. of Physics, Hiram College — The conformation of a polymer chain in solution is intrinsically coupled to properties of the solvent. In much of the theoretical work on polymers in dilute solution the effects of solvent are treated in an implicit fashion: thus one studies an isolated chain interacting via an effective site-site potential. Although a formally exact mapping is possible between the chain-in-solvent and corresponding effective- potential-chain, this mapping involves a many-site solvation potential which is not practical to compute. Thus, one generally resorts to a two-site potential approximation. Here we examine the validity of this two-site approximation for short hard-sphere and square-well chain-in-solvent systems. We demonstrate that at least for some systems, the two site approach is rigorously valid, however a set of two-site potentials (rather than a single effective potential) is required.

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