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Solvation potentials for polymer chains in solution MARK TAYLOR, Physics Dept., 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 system and a corresponding isolated 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 first demonstrate that the two-site approximation for flexible interaction-site chain-in-solvent systems is rigorously valid for short chains by computing "exact" solvation potentials for these chains. We then combine these exact short chain results with the potential of mean force of the pure solvent to construct approximate two-site solvation potentials for long chains. Monte Carlo simulations have been performed for both the isolated effective-potential chains and the full chain-in- solvent systems. These simulations show that our solvation potentials provide a quantitatively accurate description of the conformation of a chain in explicit solvent.

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