Local structure in hard-sphere chain-molecule fluids[1] SAMBID
WASTI, MARK TAYLOR, Dept. of Physics, Hiram College — The conforma-
tion of a polymer chain in solvent is coupled to the local structure of the solvent
environment. For hard-sphere systems, a monomeric solvent acts to compress a
flexible hard-sphere-solute chain and, for a dense system, the local solvent structure
is imprinted onto the chain. Here we use Monte Carlo simulation, including bond-
rebridging moves, to study the size and conformation of a hard sphere chain in a
hard-sphere solvent as a function of both solvent density and solvent diameter. We
also study the structure of a hard-sphere-chain solute in a hard-sphere-chain solvent.
In the case of a 5-mer chain in 5-mer solvent we show that the effects of solvent can
be mapped to a set of two-body solvation potentials. Following our previous work
on hard-sphere chains in monomeric solvent [1], we explore the application of these
short chain potentials to the study of longer chain-molecule fluids.

[1] M.P. Taylor and S. Ichida, J. Polym. Sci. B: Polym. Phys. 45, 3319 (2007).

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