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**Effective potentials for multiscale representations of polymer melts**[1] MARINA GUENZA, JAMES MCCARTY, JEREMY COPPERMAN , ANTHONY CLARK, University of Oregon — Numerically optimized reduced descriptions of macromolecular liquids often present thermodynamic inconsistency with atomistic level descriptions even if the total correlation function, i.e. the structure, appears to be in agreement. We present an analytical expression for the effective potential between a pair of coarse-grained units, for a polymer liquid where each chain is represented as a collection of interpenetrating soft coarse-grained units, with a variable number of units, $n_b$, of size $N_b$. The potential is characterized by a long tail, slowly decaying with characteristic scaling exponent of $N_b^{1/4}$. This general result applies to any coarse-grained model of polymer melts with units larger than the persistence length. It is our contention that with a reasonable molecular model along with the correct parameters, both structural and thermodynamic properties can be simultaneously preserved in coarse-graining, at variable length of the unit size, without the need of recurring to any numerical re-optimization scheme. The effect of the potential on the structural and dynamical properties of polymer melts will be illustrated.

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