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Entanglement elasticity in polymer chain melts: microscopic calculation of the rubbery plateau modulus via intermolecular correlations
DANIEL SUSSMAN, University of Pennsylvania, KEN SCHWEIZER, University of Illinois at Urbana-Champaign — Textbook models of stress relaxation in melts of entangled polymer chains are built on the assumption that intra-molecular or backbone stresses are the dominant contribution to the system's total stress. Numerous simulations over the last two decades have challenged this assumption, but calculating the intermolecular or non-bonded contribution to the stress has proven a daunting theoretical task. Building on our recent progress in microscopically constructing the transverse confinement field of entangled rods (PRL 107, 078102 (2011)) and ideal coils (PRL 109, 168306 (2012)), we explicitly separate stress correlations into intra- and inter-molecular terms, and calculate the contribution of intermolecular stress correlations in the "plateau" region of stress relaxation. We derive, with no adjustable parameters, the characteristic relation $G_e \sim k_B T/p^3$ (where p is the packing length) with a prefactor that agrees within a factor of two with experiment and simulation. This theoretical advance has major implications for the effect of nonlinear deformation, confinement, and chain orientational ordering on entanglement elasticity.

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