Enhanced screening in polymer melts with periodic boundary conditions

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We study polymer melts via high precision Monte Carlo simulations of Hamiltonian paths of up to $N = 100$ million steps on the simple cubic lattice with periodic boundary conditions. The Monte Carlo simulations are performed using a novel and especially fast $O(\log N)$ implementation of the so-called backbite algorithm. We characterise the crossover scaling behaviour of within-chain correlations, confirming to unprecedented precision predictions of short-chain power-law decay, and discovering novel long-chain correlation behaviour.

The long-chain behaviour is especially interesting as the periodic boundary condition results in rapid decay of correlations, more so than if the polymer were in an actual melt. We argue that the boundary conditions force the chain to "regress to the mean" and forget its past structure, and this phenomenom explains the observed enhanced screening.