Physics Colloquium Mainz

May 21, 2024 at 16 c.t.

Lecture room KPH,
Johann-Joachim-Becher-Weg 45, JGU

Polymer Physics by Quantum Computing

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Sampling equilibrium ensembles of dense polymer mixtures is a paradigmatically hard problem in computational physics, even in lattice-based models. For instance, using real-space Monte Carlo to sample polymer systems becomes impractical for increasing size, rigidity, and density of the chains. In response to these challenges, we introduce and apply a formalism to recast polymer sampling as a quadratic unconstrained binary optimization (QUBO) problem [1].
Thanks to this mapping, dense systems of stiff polymers on a lattice can be efficiently sampled with classical QUBO solvers, resulting in more favourable performance scaling compared to real-space Monte Carlo [2]. Tackling the same problems with the D-Wave quantum annealer leads to further performance improvements [2]. As an application, we discuss the use of the quantum-inspired encoding on a hitherto untackled problem, namely the linking probability of equilibrated melts of ring polymers, for which we unveil counterintuitive topological effects.

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