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Identifying Entanglement States of Ring Polymers Using Knot Polynomials JIAN QIN, SCOTT MILNER, ChE at Penn State University — Melts of ring polymers have fixed topologies in the absence of ring opening or reconnecting operations. We identify the topological states by recognizing how rings are knotted with each other, which can be achieved by computing knot invariant polynomials. We used this idea to count the entanglement states of ring polymers, prepared with off-lattice Monte Carlo simulations, in which the system topology is allowed to change by various ring rebridging moves. We project polymer configurations to obtain crossing diagrams, and use algorithms based on knot theory to compute the Jones invariant polynomial. We studied both aperiodic and periodic systems, to estimate the surface effects on entanglements. For the periodic case, we extended the algorithm for aperiodic knots to deal with periodic patterns. These tools enable us to accumulate the probability distribution of topological states for rings of different lengths, from which we determined the entanglement length by identifying the topological entropy as k_B per entanglement strand.

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