A study of the entanglement in systems of curves with Periodic Boundary Conditions

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Abstract

Periodic Boundary Conditions (PBC) are often used for the simulation of complex physical systems of open and closed curve models, such as polymer melts or vortex fields. In such dense systems the conformational freedom and motion of a chain is significantly affected by entanglement with other chains which generates obstacles of topological origin to its movement. In this talk we will discuss methods by which one may quantify and extract entanglement information from a physical system using tools from knot theory. Using a classical measure of entanglement, the Gauss linking number, we define the periodic linking number as a measure of entanglement for two oriented curves in a system employing PBC. We apply this measure of linking to assess the extend of entanglement in a polymer melt and we study the effect of CReTA (Contour Reduction Topological Analysis) algorithm on the entanglement of polyethylene chains. Our results show that the new linking measure is consistent for the original and reduced systems.

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