SAIP2012

Contribution ID : 332

Topological equivalence of polymers: regular isotopy in a projection geometry

Thursday 12 Jul 2012 at 16:40 (00h20')

Abstract :

Entanglements occur naturally in polymers and pose many mathematical difficulties for dynamical and equilibrium descriptions of polymer systems. Historically, matters of topological equivalence have been commonly dealt with through topological knot invariants; due to the nature of the constraints most of these are almost impossible to implement except in simple cases [1], [2]. We present here an approach based in a projection geometry, which maintains topology (regular isotopy) through Reidemeister moves [3] without the explicit construction of invariants. Permissible conformational changes of polymers are reduced to microscopic dynamics of crossings of knots, as governed by said Reidemeister moves. Crossings are modelled here as particles that move in a space derived from the polymer arc, with specific creation and annihilation operators. This, in turn, opens doors to a host of mathematical techniques from other well-explored fields in physics, although a full microscopic dynamical theory remains difficult to handle analytically. In principle, this problem lends itself well to Monte Carlo-type simulations. We discuss some analytical statistical physics results for knotted closed polymer loops, obtained for a reduced picture using this framework as a basis, and propose strategies to address further questions.[1] S. F. Edwards, Proc. Phys. Soc. 91 513 (1967)[2] A. L. Kholodenko and T. A. Vilgis, Physics Reports 298 251 (1998)[3] K. Reidemeister, Knotentheorie, Chelsea Pub. Co., New York (1948)

Award :

Yes

Level :

PhD

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Paper :

No

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Session classification : Theoretical

Track classification : Track G - Theoretical and Computational Physics

Type : Oral Presentation