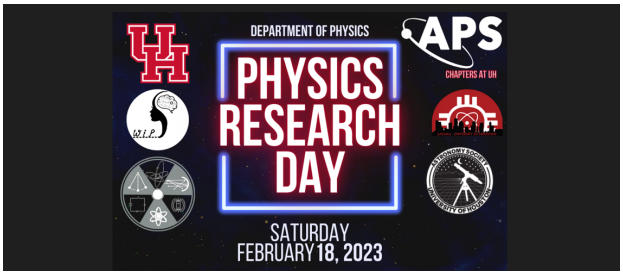

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Effects of Curvature on the Conformational Properties of Confined Semi-Flexible Polymers

Saturday 18 February 2023 12:50 (5 minutes)

Biomolecules experience confined conditions during many biological processes in vivo. The behavior of these biomolecules depends strongly on the local curvature of the confining geometry, inducing conformational changes which may affect binding activity in vitro and in vivo. An effective coarse-grained approach consists of modeling biomolecules as semi-flexible polymers, facilitating the formulation of tractable computational methods and theoretical predictions. Here, the relationship between confined semi-flexible polymers and the one-dimensional telegraph is detailed. The telegraph model's characteristic global parameters (the global persistence length) are shown to be directly related to average configurational properties such as the number of turns and the distance between turns of a semi-flexible polymer. This motivates a formal definition of a hairpin backfold for three-dimensional worm-like chains under cylindrical and toroidal confinement geometries. Simple theoretical models are proposed to account for the change in global properties of the chain due to the difference in curvature of these geometries. Analytic results are compared to data obtained from Monte-Carlo simulations which agree with established theory.

Academic year

5th year and/or beyond

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