Fluctuating Stiff Polymers[1]

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Abstract

This work is intended to systematically develop the perturbative path integral approach to the statistical mechanics of a single semiflexible polymer. The approach is essentially based on a unified formulation of the wormlike chain model with bending degrees of freedom as a standard nonlinear sigma model in one spacetime dimension. By a field-theoretic treatment of this model, we set up a nontrivial perturbation theory to higher orders capable of yielding both large-stiffness and large-d expansions. We find a variational interpolation between two regimes in order to describe a single chain properties for the entire parameter range from rigid-rod to random-coil behavior.

Recently, the study of biopolymers has become a subject of increasing interest in the research of biological materials. Forming networks as a constituent filaments, such macromolecules play an important role in the structure and function of living cells and other biological entities. Considerable motivation stems from the crucial importance of the elasticity of biopolymers and, in particular DNA, for the mechanical properties of cells. Because of this property most constituent filamentary biopolymers are semiflexible with intermediate values of the flexibility L/ξ, where L is the length and ξ the persistence length of the polymer. An appropriate model for a theoretical description of a single semiflexible polymer with arbitrary stiffness is the wormlike chain model. A central feature of this model is the local inextensibility of filaments which is mathematically accounted for by constraining the length of all tangent vectors to unity. Because of this condition the wormlike chain model of stiff polymer is a nonlinear σ-model in one spacetime dimension in which the ends are fluctuating freely. This causes important differences with respect to the presently available theory which exists only for periodic and Dirichlet boundary conditions.

In the recent paper [1], we modify this theory appropriately and show how to perform a systematic large-stiffness expansions of all physically interesting quantities in powers of L/ξ. This requires special procedures for regularizing highly divergent Feynman integrals. We show that by adding to the unperturbed action a correction term $\mathcal{A}^{\rm corr}$, we can calculate all Feynman diagrams with Green functions satisfying Neumann boundary conditions. Our expansions yield, order by order, properly normalized end-to-end distribution function in arbitrary dimensions d, its even and odd moments, and all correlation functions.

In the paper [2], we calculate the polymer properties near the random-coil limit by developing the powerful approximation scheme from a formulation of the wormlike chain model in an arbitrary dimension d and an expansion of the path integrals in powers of $1/d$. The virtue of this expansion is that it is valid for *any* stiffness. In $1/d$-approximation, the leading contributions are obtained from the path integrals at the uniform saddle point $(\lambda(s) = \omega^2, b, a)$. They describe a simple Gaussian behavior of a polymer properties in the random-chain limit. The leading corrections are derived by expanding the resulting effective actions in powers of ω^2 around the extremum up to ω^4 and performing the

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ordinary Gaussian integrals over ω^2 along the imaginary direction. Depending on the reduced length ξ_*, they are counted by powers of $1/d$ and also accompanied by inverse powers of L. Expansions in higher powers of ω^2 yield the sub-leading corrections. In this way, we obtain the Daniels-type fluctuation corrections to the end-to-end distribution function, all even moments and other rotationally invariant quantities of stiff polymers near the random-chain limit up to order L^{-3} in inverse powers of L for L large.

References

[1] H. Kleinert and A. Chervyakov, *Perturbation Theory for Path Integrals of Stiff Polymers*, J. Phys. **A39**, 8231-8255 (2006).

[2] H. Kleinert and A. Chervyakov, *Path Integral for Wormlike Chain Model: Large-d Approximation*, preprint-FUB, Berlin, 2007.