SMR 1963

Conference on Knots and other Entanglements in Biopolymers:
Topological and Geometrical Aspects of DNA, RNA and Protein Structure

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POSTER ABSTRACTS

Conjugacy Classes of 3-Braid Group

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Abstract

In this article we describe the summit sets in 3-Braid Group B_3, the smallest element in a Summit set and we compute the Hilbert series corresponding to conjugacy

Classes. The Results will be related to Birman-Menesco classification of knots with braid index 3 or less than three.

The Energy Landscape of Coarse-Grained Hydrophobic-Polar Protein Model

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The protein folding problem has been attracting the attention of scientists from various disciplines for several decades. Although the physical principles are known, the complex energy profile of proteins and peptides makes the analysis of realistic proteins extremely difficult. Therefore, one of the most important questions in this field is how much detailed information can be neglected to establish effective, coarse-grained models yielding reasonable, at least qualitative, results that allow more global view an a funnel-like energy minimum in a rugged energy lansdcape [1]. One of the most known examples is the HP model of lattice proteins, which has been exhaustively investigated [2,3]. In this model, only two types of monomers are considered, with hydrophobic (H) and polar (P) character. Another off-lattice generalization of the HP model where the contact interaction is replaced by a more realistic distance-dependent Lennard-Jones type potential and an interaction accounts for the bending energy of any successive bonds [4].

In this study, we have performed multicanonical simulations [5] of hydrophobic-polar heteropolymers with a simple effective, corse-grained off-lattice HP protein model to study the structure and the topology of the energy lansdcape and enables one to better understand the critical behaviors and visualize the folding pathways of the considered protein model [6,7].

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Helical Conformations Of Biopolymers:
A White Noise Functional Approach

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Abstract

Using the white noise path integral approach [1], biopolymer conformations are viewed as Brownian paths [2] modulated by a specific choice of the drift coefficient [3]. In particular, the Fokker-Planck equation is solved to obtain the probability density function from which winding probabilities $W(n,L)$ are calculated. The $W(n,L)$ depends on the winding numbers n, the length of the polymer L, and a term of the form, $\int f(s)\, ds$, where $f(s)$ is a drift coefficient with $0 \leq s \leq L$. Different forms of the drift coefficient acting as a modulating function have been investigated where the resulting winding probabilities mimic experimentally observed biopolymer conformations [3-5]. In this work, we examine a drift coefficient of the form

$$f(s) = ks^2 J_1(\nu s)$$

where k is a constant and J_1 is a Bessel function. Its integral [6], given by,

$$\int_0^L ks^2 J_1(\nu s)\, ds = \frac{k}{\nu} L^2 J_2(\nu L)$$

leads to a winding probability for long polymers of the form,

$$W(n,L) = \sqrt{\frac{4\pi R^2}{lL}} \exp\left[-\frac{R^2}{lL} \left\{ 2\pi n + \frac{l}{2\nu R} \frac{k}{D} L^2 J_2(\nu L) \right\}^2 \right]$$

where D is the diffusion coefficient.

A graph of $W(n,L)$ versus L for different winding numbers n exhibits the experimentally observed overwinding of biopolymers when stretched [4,5], as well as a sequence of helix-turn-helix motif [3]. Note also that if we designate a clockwise winding ($n \leq -1$) as a right-handed biopolymer, and counterclockwise winding ($n \geq 0$) as left-handed, we could see that $W(-n,L) \neq W(n,L)$. The model, therefore, also incorporates the experimentally observed chirality of biopolymers [5].

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Winding Probabilities

n1 = 3000
n2 = 5500
n3 = 10000

diffusion factor = 75000
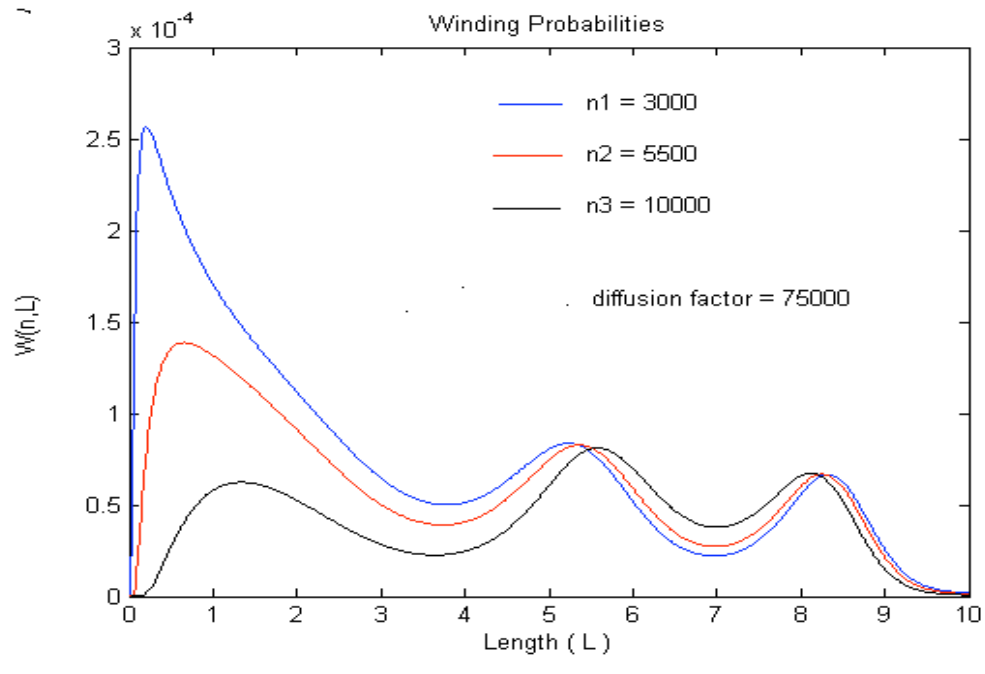
White Noise Path Integral Evaluation of the Probability Distribution for the Area Enclosed by a Polymer Loop

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In 1983, T. Hida and L. Streit introduced the use of white noise analysis in evaluating the Feynman path integral[1]. The method has been successfully applied to several quantum mechanical problems, e.g. [2, 3] and relativistic quantum systems [4]. In 2003, C.C. Bernido and M.V. Carpio-Bernido[5] consider the application of white noise analysis to statistical mechanics by treating entangled polymers. In addition to the work done in [5], we consider here the probability distribution in which a polymer loop in a gel encloses an algebraic area $A = \frac{1}{2}\int_0^N \left(x\frac{dx}{d\nu} - y\frac{dx}{d\nu} \right) d\nu$.

In obtaining the probability distribution in which a polymer will enclose an algebraic area, A, in the context of white noise analysis , we follow the model presented by Khandekar and Wiegel in [6, 7] that is: (1) represent a polymer by a continuous random walk;(2) approximate the steric and topological effects of other polymers in the system by a constraint that this walk encloses a fixed area.

In the framework of white noise analysis, the probability distribution can be obtained by first parametrizing the paths of the polymer in terms of the Brownian motion $B_x = \int_0^N \omega_x d\nu$ and $B_y = \int_0^N \omega_y d\nu$, that is

$$
\begin{aligned}
x(L) &= x_0 + lB_x(L), \qquad and \\
y(L) &= y_0 + lB_y(L)
\end{aligned}
$$

where ω_x and ω_y are the white noise variables and L is the length of the polymer loop. The end points of the polymer are then fixed by means of a Donsker delta function. With the parametrizations and expressing the Donsker delta function in its Fourrier representation , the probability distribution for the area enclosed by a polymer loop can then be written, in the language of white noise analysis, as

$$
\begin{aligned}
P(A, N) &= \frac{N}{8\pi^3} \int_{-\infty,p_x}^{+\infty} \int_{-\infty,p_x}^{+\infty} \int_{r_0}^{r_1} \exp\left\{ \int_N^{-N} \left(-\frac{1}{2}\omega_\nu^2 \right) d\nu \right\} \\
&\times \exp\left\{ \int_0^N \left(ip_x l\omega_\nu - \frac{1}{2}\lambda l y_0 \omega_\nu \right) d\nu + \int_{-N}^0 \left(ip_y l\omega_\nu + \frac{1}{2}\lambda l x_0 \omega_\nu \right) d\nu \right\} \\
&\times \exp\left\{ \lambda l^2 \int_{\bar{R}^2} \omega(\nu) F_S(\nu, \nu') \omega(\nu') d\nu d\nu' \right\} d\mu(\omega_\nu) dp_x dp_y,
\end{aligned}
\tag{1}
$$

where $d\mu(\omega_\nu)$ is a well defined white noise Gaussian measure, N is a normalization constant and $F_S(\nu, \nu') = \frac{1}{4}\left[X_{[-N,0]}^{(\nu)} X_{[0,-\nu]}^{(\nu')} + X_{[-N,0]}^{(\nu')} X_{[0,-\nu]}^{(\nu')} + X_{[0,N]}^{(\nu)} X_{[-\nu,0]}^{(\nu')} + X_{[0,N]}^{(\nu')} X_{[-\nu,0]}^{(\nu)} \right]$ with $X_{[a,b]}^{(c)}$ denotes an integration over c from a to b. Explicitly evlauting Eq.(1) and using the $T-$transform in white noise analysis in the integration over $d\mu(\omega)$, yields the result

$$
P(A, N) = \left[2Nl^2 \cosh^2\left(\frac{2\pi A}{Nl^2} \right) \right]^{-1},
\tag{2}
$$

which agrees with the result obtained by Khandekar and Wiegel [6].

One can also consider the application of white noise path integral method in doing analytical modeling of biopolymer conformation [8] and in determining how chirality can influence the three dimensional structure of a polymer [9].

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On braidings B^φ and link invariants

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Knot theory belongs to a branch of mathematics called topology. Topology deals with objects that can be continuously deformed from one to another; e.g. a torus (a donut) is equivalent to a mug. A knot is a single knotted circle, while a link is composed of two more entangled circles. In biology knots occur in the ribbon like structure DNA. This makes it possible for a molecule of DNA to knot. Molecules of DNA are large; this allows them to have the necessary stretching and bending abilities to form knots. Using knot theory, biologists are able to predict how more complex structures will look like. Researchers have tested such predictions and found they hold true. To experimentally verify results they examine knotted DNA using electron microscopes.

In this work I deal with knots from the abstract point of view. I present some examples of knot invariants, which arise from algebraic structures called "braids". These structures are important due to their relationship with links. It is very well known that each braid gives rise to an (oriented) link via closing. Now, according to a theorem of J. Alexander, any link is isotopic to the closure of some braid. A theorem of Markov asserts that the closure of two braids are isotopic if and only if these braids are equivalent with respect to the so called "Markov moves".

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Is robustness a funnel-like consequence of protein evolution?

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Minimalist models can provide important insights on protein evolution. In this work we propose a new approach using topological aspects. The model uses a 3x3x3 cubic lattice and a connection map between different conformations is found in the sequence and structural phase space. For each of 103,346 maximally compact conformations we designed the best unfrustrated sequence using an algorithm that maximizes the number for monomer types in the sequence. The maximum number of monomer types is 5. The desired properties for a protein are based on "protein-like"[1,2] concepts: the existence of a unique lowest energy conformation as well as high accessibility and robustness.

Out of all maximally compact conformations, only 4.75% generated protein-like sequences. This study focuses on these sequences and their corresponding conformations. Monte Carlo (MC) simulations are performed to probe for better sequence-structure relationships based on Z_{score}. The simulation first selects an initial conformation from a randomly selected sequence of 2 monomer types. Next, each MC step generates a new sequence by the following procedure: monomers at two positions are exchanged or a monomer is replaced at one position by anyone of 4 alternative types. If the Z_{score} of the new sequence increases, it is considered more stable than before, and the optimal sequence-conformation is chosen. This process is repeated until the sequence with the highest Z_{score} is reached. Keeping track of all MC trajectories, a map of connectivity of sequence-conformation is obtained. Different trajectories show connections between structures with low Z_{score}. A map of connections is presented for all trajectories obtained. The increase of Z_{score} along the simulation leads to a small group of preferred conformations with varying connection densities. The model suggests funnel-like structures for folding evolution, in which the structure or structures at the bottom of the funnel are associated with the "motif" of a protein. This result is a possible explanation for the restricted number of conformations despite of the large number of sequences in the Protein Data Bank (PDB).

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Fractal Dimension and Localization of DNA Knots

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The scaling properties of homo- or heterogeneous mixture of DNA knot types were studied by Atomic Force Microscopy (AFM) [1]. DNA knots were deposited onto mica in regimes of (i) strong binding (deposition on 3-aminopropyltriethoxy silane vapors modified mica) that induces a kinetic trapping of the three-dimensional (3D) configuration, and of (ii) weak binding (deposition from a solution containing Mg^{2+} ions), that permits relaxation on the surface. The contour of each knotted molecule was analyzed by a box counting algorithm, giving the number of boxes containing a part of the molecule, $N(L)$, as a function of the box size, L, allowing to recover the relation $N(L) \approx L^{-d_f}$, where d_f is the fractal dimension and $\nu = 1/d_f$ is the scaling exponent. This relationship is complicated by the presence of a persistence length of DNA (about 50 nm) which introduces a crossover from a rigid rod behavior to a self-avoiding walk behavior. In (i) the radius of gyration of the adsorbed DNA knot scales with the 3D Flory exponent $\nu \approx 0.58$ within error. In (ii), the value $\nu \approx 0.66$, intermediate between the 3D and 2D ($\nu = 3/4$) exponents, was found, indicating an incomplete 2D relaxation or a different polymer universality class. A different analysis, where the fractal dimension was determined by a mass counting algorithm giving the knot mass as a function of the box size, yielded compatible results.
AFM images of weakly adsorbed simple knots show the localization behavior, which was predicted for 2D self avoiding chains [2].

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Statistical Properties of Intrinsically Curved Polymers

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Intrinsic curvature of biopolymers is emerging as an essential feature in various biological phenomena. They control the structure of the cell and play functional role in important cellular processes like cell division. Microtubule in animal cells and FtsZ filaments in Prokaryotic cells are important examples of intrinsically curved polymers. We study the general model for such polymers and report how intrinsic curvatures influence their statistical properties. We give exact results for the tangent-tangent spatial correlation function $C(r) = <\hat{t}(s) \cdot \hat{t}(s+r)>$ both in 2D and 3D, and numerically compute the distribution function P(R) of the end to end distance R using transfer matrix method and monte carlo techniques. Contrary to the mean field theory predictions, in three dimensions C(r) does not show any oscillatory behavior.

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Molecular Dynamics simulation of hepatitis C virus IRES IIId domain. Effects of mutations in electrostatic and structural properties.

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Abstract

Hepatitis C virus (HCV) translation initiation is mediated by an internal ribosome entry site (IRES) located in the 5′ unstranslated region (5′- UTR) of the viral mRNA. This sequence can functionally replace both the cap and also many of the proteins needed to recruit the ribosome to the start codon in a process that is RNA dependent. The HCV IRES region adopts a three dimensional folded structure composed by IV domains that has been characterized by cryo-electron microscopy, X-ray crystallography and NMR spectroscopy. In this study, the dynamic behavior of IRES domain IIId was analyzed by means of molecular dynamic (MD) simulations. The simulations were carried out in explicit water environment with mono- and divalent counterions using particle-mesh Ewald summation to account for the electrostatic interactions. The obtained results allow the characterization of IRES domain IIId dynamic behavior, the effects of counterions, hydrogen bond patterns and electrostatic properties. Within this context, IRES domain IIId mutations that hinder HCV IRES activity in both *in vitro* and *ex vivo* assays, identified in viral populations isolated from chronically infected patients, were analyzed through MD simulations and compared with the wild type reference structure. Comparative analysis showed the diverse effects of mutations and provided an explanation to the inhibition of HCV IRES activity.

Topological and geometrical features of supercoiled DNA

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The equilibrium configurations of the closed ring DNA molecule on the basis of elasticity theory are obtained: from the closed relaxed ring to the first supercoil. Distribution of bend and torsion energies and stress on length of the closed ring molecule are investigated.

Geometric features of the DNA double helix in the supercoiled state are considered. Influence of a strand corner on differential-geometric and topological characteristics of DNA molecule is investigated. The depending force characteristics on winding angle in DNA are calculated.

Two Exciton States In Continuum Alpha Helical Proteins

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ABSTRACT

Nonlinear molecular excitations in alpha helical proteins are governed by soliton modes as proposed by Davydov [1,2]. He suggested that nonlinear self-trapping could serve as a method of energy transport along quasi-one dimensional chains of protein molecules through the formation of solitons moving without loss of energy. A soliton along the hydrogen bonding spines in alpha helical proteins is formed as a result of the dynamical balance between the dispersion due to the resonant interaction of intrapeptide dipole vibrations and the nonlinearity provided by the interaction of these vibrations with the local displacements of the equilibrium positions of the peptide groups. Davydov's method is to guess a functional form for the trial wave function which has a number of parameters [1,2]. By identifying these parameters and momenta conjugate to other co-ordinates in the problem, he was able to write the equations of motion for the parameters in the form of the classical Hamiltonian equations.

Recently it was observed a N-H stretching mode self-trapping in the poly-γ-benzyl-L-glutamate helix by applying ultra fast infrared pump-probe spectroscopy [3]. Two positive bands in the transient absorption spectrum have been assigned to self-trapped two exciton states [3]. Motivated by this, the two exciton states in alpha helical proteins is studied in this paper. For this purpose the Davydov Hamiltonian is modified by including higher order excitations and interactions using the second quantized operators. A suitable two-exciton trial wave function is used to construct the equations of motion. Under coherent representation, in the continuum limit, the collective molecular excitations are found to be governed by a perturbed Nonlinear Schrödinger equation. A multiple scaling perturbation analysis is used to construct the soliton solution to the resulting equation which shows the that the velocity and amplitude of the soliton do not change. The perturbed soliton is also constructed.

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Modeling filament kinematics
for proteic coding and viral spooling

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ABSTRACT

In this paper we study different time-dependent evolutions of filament coiling for modeling DNA proteic coding, viral spooling and chromosome packing. For this, we introduce the concept of *hierarchical kinematics* to describe the super-position of curve evolutions of increasing complexity, starting from a base (primary) curve and evolving towards secondary and tertiary structures, to capture higher-order coiling. Preliminary work [1, 2] has been gradually extended to model mechanisms of proteic coding and viral spooling [3], and here we extend these results further to investigate the role of geometric quantities such as writhing, curvature and torsion localization, and relative rates, in relation to elastic deformation energy, filament compaction and packing efficiency.

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Velocity selection of B-Z transition of DNA on carbon nanotube.

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August 8, 2008

Abstract:

In a recent experiment (D. A. Heller et. al. SCIENCE, 311, 508, (2006)) a conformational transition from the B form to the Z form of DNA on a carbon nanotube has been monitored as a function of time. This transition is thermodynamically identical for DNA on and off the nanotube. We propose a theory for the selected uniform velocity of this propagation.

A molecular Dynamics Study of DNA Topology

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DNA circles of sizes ranging 90-356 base pairs with various levels of over and
under winding have been simulated using atomistic molecular dynamics. These
computer simulations have shown that writhing depends on salt concentration,
circle size, and superhelical density.   Sequence dependence effects, including
denaturation, have also been analysed in an attempt to discover their role. In
addition a mesoscopic model has been developed to investigate supercoiling on
a much larger scale.

Topological Methods for Measuring the Entanglement of Polymers

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August 8, 2008

Abstract

Linear polymer chains are long flexible molecules that impose topological constraints, called entanglements, that affect the conformation and motion of the chains in a polymer melt. In this research, we extend the notions of self-linking and linking from closed chains to open chains. We study the scaling of the average writhe, self-linking and linking number of uniform and equilateral random walks and polygons as their length increases. We prove that the mean squared writhe of an oriented uniform random polygon of length n in a confined space is of the form $O(n^2)$. For a fixed simple closed curve in the confined space, we rigorously show that the mean absolute value of the linking number between this curve and a uniform random polygon of n vertices is of the form $O(n)$. Our numerical study confirms those results and indicates that the mean absolute value of the linking number between two oriented uniform random polygons of length n each is of the form $O(n)$. In the case of equilateral random walks and polygons our numerical simulations suggest that the mean absolute value of the linking number between two oriented equilateral random walks whose starting points coincide shows the scaling exponent of ~ 0.44, and the self-linking number for an oriented equilateral random walk shows the scaling exponent of ~ 0.5. We introduce a new measure of entanglement for collections of open chains that can be used to measure the entanglement of polymer melts, the linking matrix. We demonstrate that the self-linking of the chains is the most important factor of entanglement of the collection of polymer chains.

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Ropelength of Knots

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Abstract

The ropelength of a knot is the minimal length of rope we need to tie a knot subject to maintaining an embedded normal tube of fixed radius around the knot.

An interesting question is to find a lower bound for the ropelength of a nontrivial knot in general position. The best known lower bound for the ropelength of a nontrivial knot is 31.32 proved by Elizabeth Denne, Yuanan Diao and John Sullivan. This work presents some of the ideas used to get this lower bound and a new technique that shows that a lower bound for the ropelength of a trefoil knot is more than 31.32.

We expect to extend this result for any nontrivial knot using the fact that any knot has an essential arc.

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FKA & Differential geometry of polymer models

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We developed an algorithm -Fourier Knot Algorithm (FKA)- in order to study statistical properties of knots (closed curves)[1]. The FKA is a purely mathematical algorithm that generates infinitely-smooth curves. We show that unlike the FKA, common physical models such as Worm-Like-Chain (WLC) yield curves with limited smoothness and therefore one can expect that FKA and WLC generate ensembles of curves with different statistical properties [2]. We found that despite the difference in smoothness, many of the properties of the two ensembles coincide. However, we also found a striking difference: while a single correlation length describes the properties of WLC, two different lengths are needed to describe the ensemble of loops generated by FKA. We show that the appearance of two correlation lengths occurs due to the smoothness of the model. In order to generate ensemble of higher smoothness we used a Hamiltonian which is the classic WLC with torsion rigidity (WLCT).

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Conformation of Circular DNA in 2 Dimensions

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The conformation of circular DNA molecules of various lengths adsorbed in a 2D conformation on a mica surface is studied using Atomic Force Micoscopy (AFM) [1].

The results for the radius-of-gyration, the end-to-end distance, and the bond correlation function are compared to theoretical findings [2,3], and confirm the conjecture that the critical exponent ν is topologically invariant and equal to the self-avoiding walk (SAW) value (in the present case $\nu = 3/4$). It is also found that the topology and dimensionality of the system strongly influences the cross-over between the rigid regime and the self-avoiding regime at a length $L \approx 9l_p$, l_p being the persistence length. In accord with theoretical predictions [2] we do not observe a Gaussian behaviour of the chain between the rigid-rod and SAW regimes, the reason being that for circular molecules confined in 2D, self-avoidance is a strong constraint, and will thus influence the molecular conformation at relatively short scales compared to the finding for linear DNA molecules in 3D.

The bond correlation function scales with the molecular length L as predicted; in the case of long and intermediate molecular lengths we find good agreement with the scaling theory from Ref. [3], while for short molecular lengths, $L \leq 5l_p$, circular DNA behaves like a stiff molecule with approximately elliptic shape.

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Dodging the crisis of folding proteins with knots

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We prove that proteins with nontrivial topology, containing knots and slipknots, have the ability to fold to their native states without any additional external forces invoked. Our studies are based on a simple coarse-grained model with interactions modeled only by the native contacts. We demonstrate that folding of knotted proteins YibK and YbeA proceeds through an intermediate configuration with a slipknot. Analysis of topological barriers and backtracking associated to these trajectories reveals to which extent various native contacts are responsible for a folding process. From this we conclude how to modify their strength to get more realistic model, with a higher ratio of properly folded structures. We also discuss dependence of folding properties on temperature, presence of side groups, and the extension of protein chain.

Base Flipping in DNA induced by Protein

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Abstract

Protein-DNA interaction plays an important role in a large number of cellular processes such as gene expression, suppression, replication, transcription, recombination, repair and few others. DNA participation in the above processes are mediated or catalyzed by DNA-binding proteins like polymerases, helicases, nucleases, isomerases, ligases and histones. During this process most of the proteins are known to change the conformation of DNA when it binds to DNA [1, 2]. Therefore, it is important to investigate the conformational changes in DNA through nonlinear excitations when protein binds to DNA. We carry out the analysis by considering DNA as a two coupled linear chain [3] and protein as a single chain [4] interacting of DNA through linear harmonic coupling. The equation of motion is derived from the Hamiltonian through a semi-classical approach using Glauber's coherent state method combined with Holstain-Primakoff (H-P) bosonic representation in the continuum limit. The dynamics of the DNA-Protein system is found to be governed by the completely integrable nonlinear Schrodinger equation which admits N-soliton solutions. Thus, the results indicate that the base pair opening in DNA that appears in the form of a bubble is induced by the protein molecule and thus acts as a zip runner.

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Physical Pseudo-knots: a new type of Entanglement

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It is generally accepted that Entanglements, as described by the reptation model, explain some mechanical properties of polymers, like viscoelasticity. According to the reptation model entanglements behave as dynamic links that are destroyed and created in time. Whether entanglements could alternatively produce local and stable links, with similar effects to chemical bonds, remains unclear. In this presentation I will discuss how a new type of entanglement produces local and stable links. We call these bonds physical pseudo-knots. They are formed with high probability in helical structures, and the energies required to create and destroy them can differ by at least one order of magnitude. Furthermore, they remain localized. As a result they are controllable and a wide range of potential applications could emerge in many fields: material science, nano- and biotechnology. Their implication in living systems should also be studied as they could be used for their normal functioning or instead be implicated in diseases.

Numerical simulations of DNA catenanes: Energetical and topological influence of supercoiling

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DNA offers the possibility to study a great variety of topological problems. Until now, DNA knots attracted most of the attention in numerical simulations [1, 2]. But another class of topological entanglement involving DNA exists and was much less studied: DNA catenanes. These are produced during replication and are generally formed by two multiply linked chains. Simulations of catenanes [3] were, until now, limited to the case of nicked molecules (without torsional stress). We extend here the simulations to the case of covalently closed rings and try then to apply to catenanes the type of analysis already used for knots. First, we show how the topological constraint limits the extend of supercoiling. Second, we address topological mechanisms involving local geometry. As was shown for knots [2], local geometry properties, like chirality, are an important factor explaining the activity of topoisomerases. We try to show that these properties also have a central role in the decatenation process and that they are influenced by supercoiling.

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Semiflexible Interacting Growing Walk

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The configurational properties of RNA-like polymers may be investigated using simplified models such as self-avoiding walk on a lattice [1]. In such cases each segment (step) of the walk represents a monomer and the set of all segments represents the chain configuration. Standard models of interacting self-avoiding walks describe the Θ-transition from a swollen coil at high temperature to a compact globule at low temperature by introducing short range interactions between monomers that are nonconsecutive along the chain. Additional energy contributions have been introduced aiming to describe specific properties of the polymer chains [1-5]. The main Monte Carlo algorithms applied to lattice SAW are the PERM [1] and the flat PERM [2] methods. However the application of such algorithms to study phase transition between different dense phases is a hard task since require the relaxation of some constraints [1-2]. The Interacting Growth Walk algorithm (IGW) introduced by Narasimhan *et al* [6] grows self-avoiding configuration chains at any given temperature $T \geq 0$ and could be especially useful to investigate polymers systems at low temperatures where phase transition between dense phases could occur. The IGW works like a "kinetic algorithm" which performs a walk based on local Boltzmann weights calculated taking into account the local energy associated to each available growth site, generating long walks at low temperature because sample attrition is less severe than that observed in the standard algorithms for SAW chains. Moreover, it describes the universal behavior of SAW above, at, and below the Θ-point. In this work we introduce a bending energy contribution to the interacting growing walk model and investigate the resulting semiflexible polymer model by means of Monte Carlo simulation on a square lattice. The role of chain stiffness is computed assigning an energy cost to a corner formation, that is, a bending energy is added for each change of direction of the growing tip. We found that the model reproduces the qualitative behavior observed in standard semiflexible polymers models based on the SAW. Depending on the stiffness strength two qualitative regimes are observed. In the low stiffness regime, upon decreasing the temperature the polymer undergoes two different phase transitions: a transition from a coil state to a compact globule and then a first order transition to an anisotropic ordered crystalline-like state. In the high stiffness regime the system jumps directly from the coil state to the crystalline-like phase undergoing a first order transition. For low stiffness strength and in the dilute solution (single molecule) limit, the phase diagram exhibits three qualitatively different behaviors: a swollen (coil) state at high temperatures, a collapsed (molten) state at intermediate temperatures, and an anisotropic crystalline-like state at low temperatures. Upon increasing the stiffness strength the collapsed phase is suppressed and the system undergoes a phase transition from the coil directly to the anisotropic crystalline state.

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