Description of the dynamics of a random chain with rigid constraints in the path integral framework

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In this work we discuss the dynamics of a three dimensional chain. It turns out that the generalized nonlinear sigma model presented in Ref. 1 may be easily generalized to three dimensions. The formula of the probability distribution of two topologically entangled chain is provided. The interesting case of a chain which can form only discrete angles with respect to the $z$–axis is also presented.

Keywords: Statistical Field Theory; Brownian motion; Chain dynamics, Topological entanglement of two chains.

1. Introduction

In this brief report the dynamics of a chain fluctuating in some medium at fixed temperature $T$ is discussed. The three dimensional case is particularly interesting, because it allows to study the topological entanglement of two or more chains. The problem of the topological entanglement of two chains has been investigated for a long time in the statistical mechanics of polymers, see for instance Ref. 2 and references therein. If the topological constraints which limit the fluctuations of the chains are described by using the Gauss linking number, the probability distribution of the system turns out to be equivalent to the partition function of a zero-component Landau–Ginzburg model interacting with a pair of Chern–Simons fields. The analogous problem in polymer dynamics has not yet been solved. Here we show that the probability function of the system of two chains in the
presence of topological constraints may be simplified thanks to the introduction of a Chern–Simons field theory also in the case of dynamics. Finally, we provide a formula for the probability function of a chain which can form only discrete angles with respect to the \(z\)-axis.

2. A model of two topologically entangled chains

We would like to treat the dynamics of a chain fluctuating in some medium at constant temperature \(T\). In Ref. 1 (see also Ref. 3) the case of a two-dimensional chain has been discussed. The approach presented in those references can however be extended to any dimension. Let us consider the probability function \(\Psi\) which measures the probability that a \(D\)-dimensional continuous chain starting from a given spatial configuration \(\mathbf{R}_i(s)\) arrives after a time \(t_f - t_i\) to a final configuration \(\mathbf{R}_f(s)\). The chain is regarded as the continuous limit of a discrete chain consisting of particles connected together with segments of fixed length. In the continuous limit, the constraints arising due to the presence of the segments take the form: \(\left| \frac{\partial \mathbf{R}(t, s)}{\partial s} \right|^2 = 1\).

Then, an expression of \(\Psi\) in terms of path integrals may be written as follows:

\[
\Psi = \int_{\mathbf{R}(t_f, s) = \mathbf{R}_f(s)}^{\mathbf{R}(t_i, s) = \mathbf{R}_i(s)} D\mathbf{R}D\lambda \exp \left\{ -c \int_{t_i}^{t_f} dt \int_0^L ds \left( \frac{\partial \mathbf{R}}{\partial s} \right)^2 \right\} \times \exp \left\{ i \int_{t_i}^{t_f} dt \int_0^L ds \lambda \left( \left| \frac{\partial \mathbf{R}}{\partial s} \right|^2 - 1 \right) \right\}
\]

(1)

where the fields \(\mathbf{R}(t, s)\) represent \(D\)-dimensional vectors. Moreover \(c = \frac{M}{4kT\tau}\), \(M\) is the total mass of the chain, \(L\) is its length and \(k\) denotes the Boltzmann constant. Finally, the relaxation time \(\tau\) characterizes the rate of the decay of the drift velocity of the particles composing the chain. In Eq. (1) the Lagrange multiplier \(\lambda\) has been introduced in order to impose the constraints using the Fourier representation of the \(\delta\)-function \(\delta\left( \left| \frac{\partial \mathbf{R}}{\partial s} \right|^2 - 1 \right)\).

The model described by Eq. (1) will be called here the generalized nonlinear sigma model (GNLSM) due to its close resemblance to a two-dimensional nonlinear sigma model. Let us note that the holonomic constraint \(\mathbf{R}^2 = 1\) of the nonlinear sigma model has been replaced here by a nonholonomic constraint.

In the following, we will restrict ourselves to the physically relevant case \(D = 3\). The three-dimensional case is particularly interesting because it allows the introduction of topological relations. To this purpose, let us imagine two closed chains \(C_1\) and \(C_2\) of lengths \(L_1\) and \(L_2\) respectively. The trajectories of the two chains are described by the two vectors \(\mathbf{R}_1(t, s_1)\) and
\( \mathbf{R}_2(t, s_2) \) where \( 0 \leq s_1 \leq L_1 \) and \( 0 \leq s_2 \leq L_2 \). The simplest way to impose topological constraints on two closed trajectories is to use the Gauss linking number \( \chi \): 

\[
\chi(t, C_1, C_2) = \frac{1}{4\pi} \oint_{C_1} d\mathbf{R}_1 \cdot \oint_{C_2} d\mathbf{R}_2 \times [\mathbf{R}_1 - \mathbf{R}_2].
\]

If the trajectories of the chains were impenetrable, then \( \chi \) would not depend on time, since it is not possible to change the topological configuration of a system of knots if their trajectories are not allowed to cross themselves. However, since we are not going to introduce interactions between the two chains, we just require that, during the time \( t_f - t_i \), the average value of the Gauss linking number is an arbitrary constant \( m \), i.e.

\[
m = \frac{1}{t_f - t_i} \int_{t_i}^{t_f} \chi(t, C_1, C_2) dt.
\]

It is possible to show that the probability function of two chains whose trajectories satisfy the above topological constraint is given by:

\[
\Psi(C_1, C_2) = \int \mathcal{D}(fields)e^{-(S_1 + S_2)} e^{iS_{CS}} + \mathcal{F} \int_{+\infty}^{-\infty} d\xi f d^3x J^i A_i, \tag{2}
\]

where \( \mathcal{D}(fields) = \prod_{i=1}^{2} \mathcal{D}\mathbf{R}_i \mathcal{D}\lambda_i \mathcal{D}A_i \),

\[
S_i = \int_{t_i}^{t_f} dt \int_0^L ds_i \left[ c\dot{\mathbf{R}}^2_i + i\lambda_i \left( \left| \frac{\partial \mathbf{R}_i}{\partial s_i} \right|^2 - 1 \right) \right], \tag{3}
\]

\[
S_{CS} = \frac{1}{t_f - t_i} \int_{-\infty}^{+\infty} d\xi \int d^3x A_1(\xi, x) \cdot (\nabla_x \times A_2(\xi, x)), \tag{4}
\]

\[
J^i(\xi, x) = \int_{t_i}^{t_f} dt \int_0^L ds_i \delta(\xi - t) \frac{\partial \mathbf{R}_i(t, s_i)}{\partial s_i} \delta^{(3)}(x - \mathbf{R}_i(t, s_i)), \tag{5}
\]

3. Chain with constant angles of bending

To conclude, we would like to mention the interesting case in which the chain is forced to form with the \( z \)-axis only the two fixed angles \( \alpha \) and \( \pi - \alpha \). If there are no interactions depending on the \( z \) degree of freedom, it turns out that this problem can be reduced to a two dimensional one. Since in this work interactions are not considered, the probability function of the chain may be written as follows:

\[
\Psi^{3d}_{\alpha, \pi - \alpha} = \int Dx Dy \exp \left\{ -S_{\alpha, \pi - \alpha} \right\} \delta((\partial_x x)^2 + (\partial_y y)^2 - \tan^2 \alpha) \tag{6}
\]

where \( S_{\alpha, \pi - \alpha} = c \sin^2 \alpha \int_{t_i}^{t_f} dt \int_0^L ds [\dot{x}^2 + \dot{y}^2] \).

4. Conclusions

In this work the dynamics of a \( D \)-dimensional chain has been investigated. The probability function \( \Psi \) of this system is equivalent to the partition function of a generalized nonlinear sigma model. Next, the fluctuations of two
topologically entangled chains have been discussed. Analogously to what happens in the case of statistical mechanics, the complexities connected with the handling of the Gauss linking number may be partly eliminated with the introduction of Chern-Simons fields, which decouple the interactions of topological origin between the chains. Still, one has to perform a path integration over the trajectories of each chain separately. In statistical mechanics, this is equivalent to compute the path integral of a particle immersed in a magnetic field. In dynamics, the particle is replaced by a two dimensional field $R(t,s)$. To evaluate such path integral is a complicated task. Finally, the problem of a three dimensional chain admitting only fixed angles with respect to the $z-$axis is reduced to the problem of a two dimensional chain, in a way which is similar to the reduction of the statistical mechanics of a directed polymer to the random walk of a two dimensional particle.

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