A CHERN-SIMONS FIELD THEORY APPROACH TO THE POLYMER PHYSICS

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The problem of two or more entangled polymers is mapped to a topological (Ginzburg-Landau) model coupled to abelian Chern-Simons fields.

1 Introduction

Years ago it was discovered an intimate relationship between the statistical mechanics of long polymer molecules and certain field theories describing critical systems [1]. Later theoretical tools were deviced, able in principle to treat topological relations among the molecules in physical conditions when knotted configurations remain stable in time [2, 3]. The first Chern-Simons field theory approach to the subject was done in [4]. However, in spite of much work, a viable and satisfactory theoretical treatment of an ensemble of topologically linked polymers is still missing. The problem is in the way the topological states of the system are specified, because even by the use of the simplest topological invariant that explicitly refers to the polymer conformations, the Gauss linking number, effective analitic calculations remain mathematically difficult. Until now, field theoretical approaches have been confined to the case of a single test polymer immersed in a background of obstacles or Gaussian noise, which simulate the rest of the system; abelian Chern-Simons field theories have been successfully applied only to the study of DNA molecules [5, 6].
Some progress has recently been achieved in [7, 8] by mapping to a topological Ginzburg-Landau model the statistical mechanics of two fluctuating polymers subjected to the Gauss linking number constraint and applying Feynman diagram techniques to calculate the square average of the winding number. The formalism has been extended to the case of a system of N polymers [9]. However so far a drawback is that exluded volume forces, although physically important, have been ignored.
In the present paper we introduce the main steps building the formalism.

2 Path Integral Approach to Topological Polymers

Following the approach of Edwards [2, 4], we start from a path integral description of polymers in which they are viewed as self-avoiding Brownian trajectories. We introduce the probability of a configuration as a path integral over all possible trajectories $\mathbf{x}(s)$ with $0 \le s \le L$ and boundary conditions $\mathbf{x}(0) = \mathbf{y}$ and $\mathbf{x}(L) = \mathbf{x}$; namely

$$G(\mathbf{x}, \mathbf{y}, \mathbf{L}) = \int_{\mathbf{y}}^{\mathbf{x}} \mathcal{D}\mathbf{x}(s)\, e^{-(\mathcal{A}_0 + \mathcal{A}_{ev})} \qquad (1)$$

$$\mathcal{A}_0 = \frac{3}{2a} \int_0^L \dot{\mathbf{x}}^2 ds\ , \qquad (2)$$

$$\mathcal{A}_v = \frac{1}{2a^2} \int_0^L ds \int_0^L ds' \ \ v^0(\mathbf{x}(s) - \mathbf{x}(s'))\ . \qquad (3)$$

$\mathcal{A}_v$ takes into account the steric repulsion between the chain elements forming a polymer. The parameter a denotes the length of the chain elements.

It is obviously possible to rewrite the exponential of $-\mathcal{A}_v$ in (7) with the help of the following identity (see for instance [4]):

$$e^{-\mathcal{A}_v} = \int \mathcal{D}\phi\ e^{\mathcal{A}_\phi \exp\left[-i\int_0^L ds\ \phi(\mathbf{x}(s))\right]} \qquad (4)$$

after the introduction of a scalar field ϕ with euclidean action

$$\mathcal{A}_\phi = \frac{a^2}{2} \int d^3x\ \phi(\mathbf{x})[(v^0)^{-1}]\phi(\mathbf{x}). \qquad (5)$$

The passage to N entangled polymers is done introducing the *configurational probability* $G_{\{m\}}(\vec{\mathbf{x}}, \vec{\mathbf{y}}; \vec{L})$, which measures the probability to find the polymers P_i with end points at $\mathbf{x}^i, \mathbf{y}^i$ in a given topological configuration $\{m\}$. To compactify the notations, we collect the set of all end points in N-dimensional multi-vectors $\vec{\mathbf{x}} = (\mathbf{x^1}, \ldots, \mathbf{x^N})$, $\vec{\mathbf{y}} = (\mathbf{y^1}, \ldots \mathbf{y^N})$, with an analogous vector notation for the lenghts of the polymers: $\vec{L} = (L_1, \ldots, L_N)$. To distinguish different topological configurations, we use the Gauss link invariant:

$$\chi(P_i, P_j) = \frac{1}{4\pi} \int_0^{L_i} ds_i \int_0^{L_j} ds_j\ \ \dot{\mathbf{x}}(s_i) \cdot \left[\dot{\mathbf{x}}^j(s_j) \times \frac{\mathbf{x}^i(s_i) - \mathbf{x}^j(s_j)}{|\mathbf{x}^i(s_i) - \mathbf{x}^j(s_j)|^3}\right], \qquad (6)$$

defined for each pair P_i, P_j of polymers with $i \neq j$.

The integral (6) is well-defined also for open trajectories, but it becomes a real topological invariant only for a pair of *closed* polymers in the limit $\mathbf{x}^i \to \mathbf{y}^i$, $\mathbf{x}^i \to \mathbf{y}^i$. In the latter case it counts how many times P_i winds up around P_j. Thus we have

$$\begin{aligned} G_{\{m\}}\left(\vec{\mathbf{x}}, \vec{\mathbf{y}}, \vec{L}\right) \; &= \; \int_{\mathbf{y}^1}^{\mathbf{x}^1} \mathcal{D}\mathbf{x}'(s_1) \cdots \int_{\mathbf{y}^N}^{\mathbf{x}^N} \mathcal{D}\mathbf{x}^N(s_N)\; e^{-(\mathcal{A}_0 + \mathcal{A}_{ev})} \\ &\times \prod_{i=1}^{N-1} \prod_{\substack{j=2 \\ j>i}}^{N} \delta\left(\chi(P_i, P_j) - m_{ij}\right), \end{aligned} \tag{7}$$

where $\mathcal{A}_0$ is the euclidean action of a random-chain

$$\mathcal{A}_0 = \frac{3}{2a} \sum_{i=1}^{N} \int_0^{L_i} \dot{\mathbf{x}}^{i\,2} ds_i \quad ; \tag{8}$$

$$\mathcal{A}_v = \frac{1}{2a^2} \sum_{i,j=1}^{N} \int_0^{L_i} ds_i \int_0^{L_i} ds_j \; v_{ij}^0 \; \delta^{(3)}\left(\mathbf{x}^i(s_i) - \mathbf{x}^j(s_j)\right) \; . \tag{9}$$

By Fourier transform (7) with respect to the topological numbers $\{m\}$ we can go on with the expression

$$G_{\{\lambda\}}\left(\vec{\mathbf{x}}, \vec{\mathbf{y}}; \vec{L}\right) = \int_{\mathbf{y}^1}^{\mathbf{x}^1} \mathcal{D}\mathbf{x}^1(s_1) \cdots \int_{\mathbf{y}^N}^{\mathbf{x}^N} \mathcal{D}\mathbf{x}^N(s_N) \times e^{-(\mathcal{A}_0 + \mathcal{A}_v + \mathcal{A}_{\text{top}})} \; , \tag{10}$$

$$\mathcal{A}_{\text{top}} = i \sum_{i=1}^{N-1} \sum_{\substack{j=2 \\ j>i}}^{N} \chi(P_i, P_j) \lambda_{ij} \tag{11}$$

The topological term (11) is non-Markoffian and rather complicated. We solve the difficulty by introducing auxiliary fields like in (4), namely writing

$$e^{-\mathcal{A}_v} = \int \mathcal{D}\phi_i \cdots \mathcal{D}\phi_N \; e^{\mathcal{A}_\phi} \prod_{i=1}^{N} \times \exp\left[-i \int_0^{L_i} ds_i \phi_i\left(\mathbf{x}^i(s_i)\right)\right]. \tag{12}$$

with the additional advantage of getting a precious disentanglement of the interactions.

3 Topological Interactions

The goal now is to express the topological interactions term by suitable fields in order to simplify $\mathcal{A}_{\rm top}$ in the path integral (10). Such fields are provided by Chern-Simons theories [4]. Let A_μ^α, with $\alpha = 1, \ldots, N'$, be a set of N' Chern-Simons fields with euclidean spatial indices $\mu = 1, 2, 3$. They allow us to write the identity

$$e^{-\mathcal{A}_{\rm top}} = \frac{\int \mathcal{D}\mathbf{A} e^{-i\mathcal{A}_{\rm CS} + i\Sigma_{i=1}^N \Sigma_{\beta=1}^{N'} \int d^3x\, h_{i\beta} \mathbf{J}^i \cdot \mathbf{A}^\beta}}{\int \mathcal{D}\mathbf{A}\ e^{-i\mathcal{A}_{\rm CS}}} \tag{13}$$

where $\mathcal{A}_{\rm cs}$ is a the Chern-Simons action

$$\mathcal{A}_{\rm CS} = \sum_{\alpha,\beta=1}^{N'} \int d^3x \mathbf{A}^\alpha \cdot \left(\nabla \times \mathbf{A}^\beta\right) g_{\alpha\beta} \tag{14}$$

and $\mathbf{J}^i$ are currents

$$\mathbf{J}^i(\mathbf{x}) = \int_0^{L_i} ds_i\, \dot{\mathbf{x}}^i(s_i)\, \delta^{(3)}\left(\mathbf{x} - \mathbf{x}^i(s_i)\right). \tag{15}$$

The measure of functional integration $\mathcal{D}\mathbf{A}$ is short for the product $\prod_{\alpha=1}^{N'} \mathcal{D}\mathbf{A}^\alpha$. We assume $g_{\alpha\beta}$ to be a suitable $N' \times N'$ symmetric matrix to be specified later, which possesses an inverse $(g^{-1})^{\alpha\beta}$, while $h_{i\alpha}$ is a $N \times N'$ matrix.

The right-hand side of Eq. (13) has the desired Markoffian form. To calculate it explicitly, we quantize the Chern-Simons fields A_μ^α in the Lorentz gauge, where they are completely transverse and have the following two-point correlation functions

$$G_{\mu\nu}^{\alpha\beta}(\mathbf{x}, \mathbf{y}) \equiv \langle A_\mu^\alpha(\mathbf{x}) A_\nu^\beta(\mathbf{y})\rangle = \frac{(g^{-1})^{\alpha\beta}}{4\pi} \varepsilon_{p\nu\rho} \frac{(x-y)^\rho}{|\mathbf{x}-\mathbf{y}|^3}. \tag{16}$$

After some calculations we find

$$\frac{\int \mathcal{D}\mathbf{A} e^{-i\mathcal{A}_{\rm CS} + i\Sigma_{i=1}^N \Sigma_{\alpha=1}^{N'} \int d^3x\, h_{i\alpha} \cdot \mathbf{J}^i \mathbf{A}^\alpha}}{\int \mathcal{D}\mathbf{A} e^{-i\mathcal{A}_{\rm CS}}} = \exp\left[-\frac{i}{4} \sum_{i,j=1}^N h_{i\alpha} (g^{-1})^{\alpha\beta} h_{j\beta} \chi(P_i, P_j)\right] \tag{17}$$

The right-hand side coincides with the term $e^{-\mathcal{A}_{\rm top}}$ of Eq. (13), where the topological action $\mathcal{A}_{\rm top}$ is given in (11) only if the equation

$$h_{i\alpha}(g^{-1})^{\alpha\beta} h_{j\beta} = 2\lambda_{ij}. \tag{18}$$

is satisfied. Since the matrix λ_{ij} has vanishing diagonal elements, this condition automatically eliminates the appearance of non-topological terms of the form $\chi(P_i, P_i)$ with $i = 1, \ldots, N$. At this point, it is convenient to introduce the linear combinations of the Chern-Simons fields

$$\mathbf{C}^i = \sum_{\alpha=1}^{N'} h_{i\alpha} \mathbf{A}^\alpha, \tag{19}$$

such that Eq. (13) becomes

$$e^{-\mathcal{A}_{\rm top}} = \frac{\int \mathcal{D}\mathbf{A} e^{-i\mathcal{A}_{\rm CS} + i\sum_{i=1}^{N} \int d^3x\, \mathbf{J}^i \cdot \mathbf{C}^i}}{\int \mathcal{D}\mathbf{A} e^{-i\mathcal{A}_{\rm CS}}} \tag{20}$$

All the correlation functions of the new fields $C^i_\mu(\mathbf{x})$ can be evaluated starting from the old correlation functions in Eq. (16). In this way it is easy to see that:

$$\langle C^i_\mu(\mathbf{x}) C^i_\nu(\mathbf{y}) \rangle = 0, \quad i = 1, \ldots, N. \tag{21}$$

Thus, the $C^i_\mu(\mathbf{x})$ have purely off-diagonal correlation functions.
It is important to notice (see [9]) that the number of Chern-Simons fields which are necessary to describe the topological entanglements of the system should be at least equal to N. Indeed in the sequel it will be convenient to set a theory with $N' > N$, which however can be shown to be equivalent to one having N Chern-Simons fields only.

We compute the denominator in the right hand side of (20) first noticing that since $g_{\alpha\beta}$ is a $N' \times N'$ symmetric matrix, it can always be expressed as follows:

$$g_{\alpha\beta} = \sum_{\beta=1}^{N'} \eta_{\alpha\gamma} \eta_{\beta\beta} \tag{22}$$

where $\eta_{\alpha\beta}$ is again a $N' \times N'$ symmetric matrix. Performing in Eq. (14) the substitution

$$\mathbf{a}_\alpha = \sum_{\beta=1}^{N'} \eta_{\alpha\beta} \mathbf{A}^\beta\,, \tag{23}$$

the Chern-Simons action becomes

$$\mathcal{A}_{\rm CS} = \sum_{\alpha=1}^{N'} \int d^3x\, \varepsilon^{\mu\nu\rho} a^\alpha_\mu \partial_\nu a^\alpha_\rho \tag{24}$$

i.e., the dependence on $g_{\alpha\beta}$ disappears. Thus, apart from an irrelevant constant factor, we have:

$$\int \mathcal{D}\mathbf{A} e^{-i\mathcal{A}_{\mathrm{CS}}(\mathbf{A}^{\alpha})} = [\det(g_{\alpha\beta})]^{1/2} \tag{25}$$

4 Field Theory

To compute the numerator in the right hand side of (20) we exploit the freedom of enlarging the number of topological vector fields. The simplest Chern-Simons field theory for our purpose contains $N' = 2(N-1)$ fields $\mathbf{A}^1, \ldots \mathbf{A}^{N-1}$ and $\mathbf{B}^1, \ldots, \mathbf{B}^{N-1}$. The action $\mathcal{A}_{\mathrm{CS}}$ is given by

$$\mathcal{A}_{\mathrm{CS}} = \kappa \sum_{i=1}^{N-1} \varepsilon^{\mu\nu\rho} \int d^3x \; A^i_\mu \partial_\nu B^i_\rho \,. \tag{26}$$

Equation (20) becomes

$$e^{-\mathcal{A}_{\mathrm{top}}} = c^{-1} \int \mathcal{D}\mathbf{A}\mathcal{D}\mathbf{B} \; e^{-i\mathcal{A}_{\mathrm{CS}}} \exp\left\{\sum_{i=1}^{N} \int d^3x \; \mathbf{C}^i \cdot \mathbf{J}^i\right\}, \tag{27}$$

where the currents $J^i_\mu(\mathbf{x})$ have been already defined in Eq. (15) and the fields $\mathbf{C}^i$ of Eq. (19) have the following explicit expressions ($i = 2, \ldots, N-1$):

$$\mathbf{C}^1 = \mathbf{B}^1, \quad \mathbf{C}^N = \kappa \sum_{i=1}^{N-1} \lambda_{Ni} \mathbf{A}^i, \quad \mathbf{C}^i = \kappa \sum_{j=i}^{i-1} \lambda_{ij} \mathbf{A}^j + \mathbf{B}^i \tag{28}$$

Using Eq. (12) and (27) in expression (10) we obtain the path integral representation

$$G_{\{\lambda\}}\left(\vec{\mathbf{x}}, \vec{\mathbf{y}}; \vec{L}\right) = \left\langle \prod_{i=1}^{N} G\left(\mathbf{x}^i, \mathbf{y}^i; L_i | \phi_i, \mathbf{C}^i\right) \right\rangle , \tag{29}$$

$$G\left(\mathbf{x}^i, \mathbf{y}^i; L_i | \phi_i, \mathbf{C}^i\right) = \int_{\mathbf{y}^i}^{\mathbf{x}^i} \mathcal{D}\mathbf{x}^i(s_i) \, e^{-\left[\int_0^{L_i} ds_i \, \mathcal{L}_{\phi_i}(\mathbf{x}^i(s_i)) + \int_0^{L_i} ds_i \, \dot{\mathbf{x}}^i(s_i) \cdot \mathbf{C}^i(\mathbf{x}^i(s_i))\right]} , \tag{30}$$

$$\mathcal{L}_{\phi_i}(\mathbf{x}^i(s_i)) = \frac{3}{2a} \dot{\mathbf{x}}^{i\,2}(s_i) + i\phi_i(\mathbf{x}^i(s_i)) \,. \tag{31}$$

In Eq. (29), the expression in the expectation symbol $\langle \; \rangle$ must be averaged with respect to the fields ϕ_i with $i = 1, \ldots, N$ and the Chern-Simons fields $\mathbf{A}^j$, $\mathbf{B}^j$ with $j = 1, \ldots, N-1$.

The path integral in Eq. (30) describes a Markoffian random walk of a particle immersed in an electromagnetic field $(\mathbf{C}^i, i\phi_i)$. In analogy with the evolution kernel of a particle in quantum mechanics, $G\left(\mathbf{x}^i, \mathbf{y}^i, L_i|\phi_i, \mathbf{C}^i\right)$ satisfies a Schrödinger-like equation

$$\left[\frac{\partial}{\partial L_i} - \frac{a}{6}\mathbf{D_i}^2 + i\phi_i\right] G\left(\mathbf{x}^i, \mathbf{y}^i; L_i \middle| \phi_i, \mathbf{C}^i\right) = \delta(L_i)\delta(\mathbf{x}^i - \mathbf{y}^i)\,, \tag{32}$$

$$\mathbf{D}_i = \nabla + i\mathbf{C}^i. \tag{33}$$

It is convenient to consider the Laplace-transform in the length parameter L_i:

$$G_{\{\lambda\}}(\vec{\mathbf{x}}, \vec{\mathbf{y}}; \vec{\mu}) = \int_0^{+\infty} dL_1 \cdots dL_N \; e^{-\sum_{i=1}^N \mu_i L_i} G_{\{\lambda\}}\left(\vec{\mathbf{x}}, \vec{\mathbf{y}}; \vec{L}\right). \tag{34}$$

Applying such transformations to both sides of Eq. (29), we find

$$G_{\{\lambda\}}(\vec{\mathbf{x}}, \vec{\mathbf{y}}; \vec{\mu}) = \left\langle \prod_{i=1}^N G\left(\mathbf{x}^i, \mathbf{y}^i; \mu^i \middle| \phi_i, \mathbf{C}^i\right) \right\rangle, \tag{35}$$

where $G\left(\mathbf{x}^i, \mathbf{y}^i; \mu_i|\phi_i, \mathbf{C}^i\right)$ is the Laplace transformed correlation function (30), obeying the stationary equation

$$\left[\mu_i - \frac{a}{6}\mathbf{D}_i^2 + i\phi_i\right] G\left(\mathbf{x}^i, \mathbf{y}^i; \mu_i|\phi_i, \mathbf{C}^i\right) = \delta(\mathbf{x}^i - \mathbf{y}^i). \tag{36}$$

Equation (36) can be solved (see [4]) in terms of fluctuating polymer fields ψ_i^*, ψ_i as

$$G\left(\mathbf{x}^i, \mathbf{y}^i; \mu_i|\phi_i, \mathbf{C}^i\right) = \frac{1}{Z_i}\int \mathcal{D}\psi_i\mathcal{D}\psi_i^* \times \psi_i(\mathbf{x}^i)\psi_i^*(\mathbf{y}^i)e^{-\mathcal{A}_{\rm pol}[\psi_i^*, \psi_i]} \tag{37}$$

where $\mathcal{A}_{\rm pol}$ is the polymer action

$$\mathcal{A}_{\rm pol}[\psi_i^*, \psi_i] = \int d^3x \left[\frac{a}{6}|\mathbf{D}^i\psi_i|^2 + (\mu_i + i\phi_i)|\psi_i|^2\right] \tag{38}$$

and Z_i is the associated partition function

$$Z_i = \int \mathcal{D}\psi_i\mathcal{D}\psi_i^* e^{-\mathcal{A}_{\rm pol}[\psi_i^*, \psi_i]}\,. \tag{39}$$

The integrations over the auxiliary fields ϕ_i is complicated by the presence of the factor Z_i^{-1} in Eq. (37), which makes them non-gaussian. This problem can be solved exploiting the method or field replicas.

For each pair of fields ψ_i, ψ_i^* we introduce a set of n_i replica fields $\psi_i^{a_i}, \psi_i^{*a_i}$ with $a_i = 1, \ldots, n_i$. It is convenient to group such replica fields in $n_i$tuplets

$$\Psi_i = (\psi_i^1, \ldots, \psi_i^{n_i}), \quad \Psi_i^* = \left(\psi_i^{*1}, \ldots, \psi_i^{*n_i}\right).$$

With these fields the correlation function (37) can be rewritten as follows:

$$G\left(\mathbf{x}^i, \mathbf{y}^i; \mu_i | \phi_i, \mathbf{C}^i\right) = \lim_{n_i \to 0} \int \mathcal{D}\Psi_i \mathcal{D}\Psi_i^* \psi_i^{\bar{a}_i}(\mathbf{x}^i) \psi_i^{*\bar{a}_i}(\mathbf{y}^i)\ e^{-\mathcal{A}_{\mathrm{rep}}[\Psi_i, \Psi_i^*]}, \tag{40}$$

$$\int \mathcal{D}\Psi_i \mathcal{D}\Psi_i^* = \int \prod_{a_i=1}^{n_i} \mathcal{D}\psi_i^{a_i} \mathcal{D}\psi_i^{*a_i}, \tag{41}$$

$$\mathcal{A}_{\mathrm{rep}}[\Psi_i, \Psi_i^*] = \sum_{a_i=1}^{n_i} \left[\frac{a}{6} |\mathbf{D}_i \psi_i^{a_i}|^2 + (\mu_i + i\phi_i) |\psi_i^{a_i}|^2\right] \tag{42}$$

The index $\bar{a}_i$ in (40) is a fixed replica index chosen arbitrarily in the range $1 \leq a_i \leq n_i$. The limit of zero replica number in (40) is performed by an analytic extrapolation; namely the path integral on the right hand side is calculated for integer values of n_i and the result is then extrapolated analytically to the point $n_i = 0$. The final formal result (see [9]) is

$$G_{\{\lambda\}}(\vec{\mathbf{x}}, \vec{\mathbf{y}}; \vec{\mu}) = \lim_{n_1, \ldots n_N \to 0} \int \mathcal{D}\mathbf{A} \mathcal{D}\mathbf{B} \left[\prod_{i=1}^{N} \mathcal{D}\Psi_i \mathcal{D}\Psi_i^* \psi_i^{\bar{a}_i}(\mathbf{x})^i \psi_i^{*\bar{a}_i}(\mathbf{y}^i)\right] e^{-\mathcal{A}_{\mathrm{tot}}} \tag{43}$$

where

$$\mathcal{A}_{\mathrm{tot}} = i\mathcal{A}_{\mathrm{CS}} + \sum_{i=1}^{N} \int d^3x \left[\Psi_i^* \left(-\mathbf{D}_i^2 + m_i^2\right) \Psi_i + \sum_{i,j=1}^{N} \frac{2M^2 v_{ij}^0}{a^2} |\Psi_i|^2 |\Psi_j|^2\right.$$

$$m_i^2 = 2M\mu_i \tag{44}$$

Following [4], we have introduced a mass parameter M and a parameter playing a similar role as the Planck constant in quantum mechanical path integrals, that is $\hbar = \mu_a/3$. The value of M is taken fixed with respect to the step length a by requiring the condition $\hbar = 1$.

In this way, the action (44) becomes that of a standard field theory with unit Planck constant. Moreover, $\mathcal{A}_{\rm tot}$ is a quadratic form with respect to the parameters λ_{ij}, so that the inverse Fourier transformations leading to the original configurational probability can be performed after a diagrammatic evaluation of the correlation functions (43).

We mention that actual calculation are in progress using the formalism we have depicted. However it is worth citing that results have already been obtained for the two entangled polymers case, namely the "exact" computation of the second topological moment $< m^2 >$ in [8]. Such result is used to estimate approximately the mean square average of the linking number of a single polymer in a dilute solution of meny others.

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