Applications of a generalization of the nonlinear sigma model with 
$O(d)$ group of symmetry to the dynamics of a constrained chain

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Subject of this work are the applications of a field theoretical model, called here 
generalized nonlinear sigma model or simply GNLσM, to the dynamics of a chain subjected to constraints. Chains with similar properties and constraints have been discussed in a seminal paper of Edwards and Goodyear using an approach based on the Langevin equation.

The GNLσM has been proposed in a previous publication in order to describe 
the dynamics of a two dimensional chain. In this paper the model is extended to $d$ dimensions and a bending energy term is added to its action. As an application, two observables are computed in the case of a very stiff chain. The first observable is the dynamical form factor of a ring shaped chain. The second observable is a straightforward generalization to dynamics of the static form factor. This observable is relevant in order to estimate the average distance between two arbitrary points of the chain.

Finally, a variant of the GNLσM is presented, in which the topological conditions which constrain the motion of two linked chains are imposed with the help of the Gauss linking invariant.

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I. INTRODUCTION

Subject of this work is the dynamics of a chain obtained by taking the continuous limit of a freely jointed chain consisting of \( N - 1 \) segments of length \( a \) and \( N \) beads of mass \( m \) attached at the joints between two consecutive segments. This problem has been addressed in the seminal paper of [1] using an approach based on the Langevin equation [31]. It was shown in [1] that the condition of fixed length segments becomes in the continuous limit a constraint which is similar to that of incompressible fluids in hydrodynamics. The authors of Ref. [1] have also described several interesting regimes in which their model of a constrained chain can be applied, like for instance an isolated cold chain or a hot polymer in the vapor phase. The statistical mechanics of a freely jointed chain in the continuous limit has been later investigated exploiting different methods, see for example [4, 5]. Interesting related results may be found also in Ref. [6]. Up to recent times, however, most of the developments in the dynamics of a chain with rigid constraints have been confined to numerical simulations, see for example Refs. [7, 8, 9].

To overcome at least in part the complications of the dynamical case, it has been proposed in Ref. [10] a path integral framework for the dynamics of the constrained chain discussed in [1]. The resulting model, which describes the fluctuations of a two dimensional chain, is a generalization of the \( O(2) \) nonlinear sigma model. For this reason, it has been called generalized nonlinear sigma model or simply GNL\( \sigma \)M. The relation of the GNL\( \sigma \)M with the Rouse model [11] has been studied in details in Ref. [10]. A difference between the two models concerns the scales of time and length at which the chain is observed. In the Rouse model only the long time-scale behavior of the chain is considered [12]. On the other side, the GNL\( \sigma \)M takes into account the short time-scale behavior and the finest details of the chain. These facts make the GNL\( \sigma \)M suitable to study the response of a chain to mechanical stresses in micromanipulations, for instance when it is stretched under a constant force [13, 14]. Indeed, some experiments point out that the freely jointed chain model is able to capture the behavior of DNA in the limit of low applied forces [15].

The GNL\( \sigma \)M does not take into account the hydrodynamic and self-avoiding interactions. The lack of hydrodynamic interactions limits its validity to the cases in which the motion of the beads is slow. This happens for instance when the viscosity of the fluid is large or the temperature is low. The conformations of the chain change slowly also in the presence
of stiffness. The treatment of chain stiffness, a feature which was missing in the formulation of the GNLσM of Ref. [10], will be included in this work. A concrete application of the GNLσM could be polymers in a very dilute solutions at the so-called Θ point, in which self-avoiding interactions play no role. The assumption that the chain is phantom, i.e., it can cross itself, is however dangerous at the Θ point because in that case it is very likely that the chain is knotted [16] and one should take into account the resulting topological constraints. In general, the fixing of constraints in (stochastic) dynamics requires some mathematical effort [7, 12, 17, 18]. The field theoretical formulation of the chain dynamics provided by the GNLσM has the advantage that it is relatively easy to add further constraints, like for instance those which are necessary to impose topological conditions in the case of ring-shaped chains.

The main goal of this work is the development of possible applications of the GNLσM model. The most important result is indeed the calculation of the expectation values of two observables in a semiclassical approximation, which is valid if the changes in the chain conformation due to the fluctuations are small. This may happen when the chain is relatively rigid or in the following two cases: The temperature is low or the chain is moving in a very viscous solution. All these situations are compatible with the conditions of validity of the GNLσM mentioned before. The first observable which we consider is the dynamical form factor of the chain [12]. The second observable is a straightforward generalization to dynamics of the static form factor. It is shown that this observable is related to the average distance between two points of the chain. The calculation of both observables is complicated by the presence of ultraviolet divergences, which are regulated with the help of the zeta function regularization [19]. Let us note that divergences of this kind do not appear in analogous computations of the dynamical form factor performed using the Rouse model [20].

Another purpose of the present work is to improve the formulation of the GNLσM given in [10], making it more suitable for concrete applications. For this reason, we consider here the dynamics of a chain in $d$ spatial dimensions. This case leads to a GNLσM with $O(d)$ group of symmetry, which is a straightforward generalization of the two dimensional model already discussed in [10]. With respect to Ref. [10], we have also included in our approach the bending energy of the chain. In order to make the description of the chain dynamics closer to realistic situations, a method to take into account the topological entanglement of two
closed chains is proposed. The topological constraints are imposed using the Gauss linking invariant. Unfortunately, it is not possible to apply to dynamics in a straightforward way the strategy based on Chern-Simons field theory which is used in the statistical mechanics of polymers, see for example Refs. [21, 22, 23, 24, 25, 26]. The main difference from statics is that in dynamics one has to take into account the motion in time of the chain. This implies that, rather than with the one dimensional trajectory of the chain, one has to deal with the two dimensional surface that the chain spans during its motion. To cope with this situation, we have generalized the multi-component Chern-Simons field theory of statistical mechanics to four dimensions. Mathematically, it is not possible to do that while keeping the topological invariance of the theory with respect to diffeomorphisms which depend both on time and on the spatial dimensions. However, the condition of invariance under diffeomorphism depending on time is not strictly necessary in the case of a non-relativistic chain and has been relaxed.

The presented results are organized as follows. In Section II the problem of the dynamics of a chain in \( d \) dimensions is mapped into an \( O(d) \) GNL\( \sigma \)M. The generating functional of the correlation functions of the bond vectors is expressed in the path integral form. In Section III the background field method is applied to the computation of the generating functional. Particular care is dedicated to the boundary conditions imposed on the fields to allow the freedom of performing integrations by part in the action without producing unwanted and cumbersome boundary terms. The action of the GNL\( \sigma \)M is modified in order to take into account the bending energy of the chain. In Section IV the dynamical form factor and another related observable are computed. In Section V a model of two entangled chain is presented. Finally, our Conclusions are drawn in Section VI.

## II. FORMULATION OF THE MODEL

In this section a path integral formulation of the dynamics of a freely jointed chain of length \( L \) is provided. The chain is regarded as a set of \( N \) beads connected together by \( N - 1 \) segments of fixed length \( a \). In addition, \( N \), \( L \) and \( a \) satisfy the relation \( L = Na \). Denoting with \( \mathbf{R}_n(t), n = 1, \ldots, N \) the positions of \( N \) beads, it is possible to describe the fluctuations of the chain as a random walk of the beads constrained by the conditions:

\[
|\mathbf{R}_n(t) - \mathbf{R}_{n-1}(t)|^2 = a^2 \quad n = 2, \ldots, N
\]
These conditions are required by the fact that the length of the $N-1$ segments connecting the beads is equal to $a$. We also demand that at the initial and final instants $t = 0$ and $t = t_f$ the $n$-th bead is located respectively at the positions $R_n(0) = R_{0,n}$ and $R_n(t_f) = R_{f,n}$. At this point, following Ref. [10], we introduce the probability function $\psi_N$ which measures the probability that the chain after a given time $t_f$ passes from an initial configuration $R_{0,n}$ to a final configuration $R_{f,n}$. Using an approach which is widespread in the statistical mechanics of polymers subjected to constraints, we define $\psi_N$ as follows:

$$\psi_N = \int_{R_1(t_f)=R_{f,1}}^{R_1(0)=R_{0,1}} \mathcal{D}R_1(t) \ldots \int_{R_N(t_f)=R_{f,n}}^{R_N(0)=R_{0,n}} \mathcal{D}R_N(t) \exp \left\{ - \sum_{n=1}^{N} \int_{0}^{t_f} dt \frac{\dot{R}_n^2(t)}{4D} \right\} \times \prod_{n=2}^{N} \delta \left( \frac{|R_n(t) - R_{n-1}(t)|^2}{a^2} - 1 \right)$$

(2)

where $D$ denotes the diffusion constant.

The path integral (2) describes the random walks of the $N$ beads composing the chain. The insertion of the Dirac delta functions is needed to enforce the conditions (1), which describe the rigid constraints due to the non extensibility of the individual segments. We remember that the diffusion constant $D$ satisfies the relation $D = \mu k_B T$, where $\mu$ is the mobility of a bead, $k_B$ is the Boltzmann constant and $T$ is the temperature. Moreover, $\mu = \frac{\tau}{m}$, where $m$ is the mass of the bead and $\tau$ is the relaxation time which characterizes the ratio of the decay of the drift velocity of the beads. Supposing that the total mass of the chain is $M$, we have of course that $m = \frac{M}{N} = \frac{M}{L} a$. Thus, Eq. (2) becomes:

$$\psi_N = \prod_{n=1}^{N} \int_{R_n(t_f)=R_{f,n}}^{R_n(0)=R_{0,n}} \mathcal{D}R_n(t) \exp \left\{ - \frac{M}{4k_B T \tau L} \sum_{n=1}^{N} a \int_{0}^{t_f} dt \dot{R}_n^2(t) \right\} \times \prod_{n=2}^{N} \delta \left( \frac{|R_n(t) - R_{n-1}(t)|^2}{a^2} - 1 \right)$$

(3)

The limit $N \rightarrow \infty$, $a \rightarrow 0$ in which the continuous chain is rigorously recovered has been already discussed in Ref. [10] in the two dimensional case. The extension to $d$ dimensions is straightforward. Basically, the continuous limit consists in the following replacements of the basic ingredients appearing in the path integral of Eq. (3):

$$\prod_{n=1}^{N} \int_{R_n(t_f)=R_{f,n}}^{R_n(0)=R_{0,n}} \mathcal{D}R_n(t) \rightarrow \int \mathcal{D}R(t,s)$$

$$\sum_{n=1}^{N} a \int_{0}^{t_f} dt \dot{R}_n^2(t) \rightarrow \int_{0}^{t_f} dt \int_{0}^{L} ds \dot{R}_n^2(t,s)$$
where \(s\) is the arc-length of the chain and \(0 \leq s \leq L\). We have also introduced the notation \(R' \equiv \frac{\partial R}{\partial s}\). Applying Eqs. \((4)\) to Eq. \((3)\), the probability function \(\psi_N\) becomes:

\[
\Psi(R_f(s), R_0(s)) = \int_{R(t_f, s) = R_f(s)} \mathcal{D}R(t, s) \mathcal{D}\lambda(t, s) \exp \left\{ -c \int_0^{t_f} dt \int_0^L ds \dot{R}^2 \right\} \times \exp \left\{ i \int_0^{t_f} dt \int_0^L ds \lambda(R'^2 - 1) \right\}
\]

with \(c = \frac{M}{4k_B T \tau L}\). In the above equation the Lagrange multiplier \(\lambda = \lambda(t, s)\) has been introduced in order to represent conveniently the functional Dirac delta function appearing in the right hand side of Eq. \((4)\).

Formally, the path integral in the right hand side of Eq. \((5)\) resembles the partition function of a quantum mechanical chain with constant density mass \(\frac{M}{L}\) after the analytical continuation to purely imaginary times:

\[
S_0 = \frac{M}{2L} \int_0^{t_f} dt \int_0^L ds \dot{R}^2
\]

To stress the close analogy with quantum mechanics, we remark that in Eq. \((5)\) the action \(S_0\) is multiplied by the inverse of the factor \(\kappa = 2k_B T \tau\). It is known that \(\kappa\) plays in the Brownian motion the same role of the Planck constant, due to the well known duality between quantum mechanics and Brownian motion \([27]\). One may show that the action \(S_0\) originates from the continuous limit of the kinetic energy of a free chain, see Ref. \([10]\) in the two dimensional case and Ref. \([28]\) in three dimensions. As we see from Eq. \((5)\), the presence of rigid constraints is responsible for the appearance besides the action \(S_0\) of an additional nonlinear term given by

\[
S_1 = -i \int_0^{t_f} dt \int_0^L ds \lambda(R'^2 - 1)
\]

The Lagrange multiplier \(\lambda(s, t)\) in \(S_1\) closely resembles the pressure in incompressible hydrodynamics, as it has been noticed in \([1]\). It expresses the fact that the segments composing the chain have a fixed length and thus they may not be compressed.

To conclude this introductory Section, we specify the set of boundary conditions satisfied by the bond vector \(R(t, s)\) in the probability function \((5)\). First of all, the boundary conditions are

\[
\prod_{n=2}^N \delta \left( \frac{\left| R_n(t) - R_{n-1}(t) \right|^2}{a^2} - 1 \right) \rightarrow \delta(R'^2(t, s) - 1)
\]

\[
R_{f,n} \rightarrow R_f(s)
\]

\[
R_{0,n} \rightarrow R_0(s)
\]
conditions at the initial and final instants 0 and $t_f$ are given by

$$R(0, s) = R_0(s) \quad R(t_f, s) = R_f(s)$$

(8)

where $R_0(s)$ and $R_f(s)$ are static chain conformations. Additionally, it will be convenient to choose boundary conditions with respect to the arc-length $s$ which allow integrations by parts in this variable without generating cumbersome boundary terms in the actions $S_0$ and $S_1$. To this purpose, we will limit ourselves to the following two choices:

1. periodic boundary conditions in the case of a ring-shaped chain

$$R(t, s + L) = R(t, s)$$

(9)

2. fixed end boundary conditions in the case of an open chain

$$R(t, 0) = r_1 \quad R(t, L) = r_2$$

(10)

where $r_1$ and $r_2$ are constant vectors. For the Lagrange multiplier $\lambda$ one may impose trivial boundary conditions in time

$$\lambda(0, s) = \lambda(t_f, s) = 0$$

(11)

and boundary conditions analogous to Eq. (9) in the case of a ring-shaped chain. For an open chain it is sufficient to require that:

$$\lambda(t, 0) = 0 \quad \lambda(t, L) = 0$$

(12)

III. THE GENERATING FUNCTIONAL $\Psi[J]$ AND THE BENDING ENERGY

To the probability function $\Psi(R_f(s), R_0(s))$ of Eq. (5) we associate the following generating functional $\Psi[J]$:

$$\Psi[J] = \int_{b.c.} DRD\lambda e^{-\frac{1}{2} T^t S_0 - S_1} e^{\int_0^{t_f} dt \int_0^L ds J \cdot R}$$

(13)

where $S_0$ and $S_1$ have been defined in Eqs. (6) and (7) and $J$ is an external current. The subscript $b.c.$ near the integration symbol means that an appropriate set of boundary conditions among those of Eqs. (8)–(12) should be chosen. If $J = 0$, one obtains back the probability
function $\Psi(R_f(s), R_0(s))$ of Eq. (5). In the right hand side of Eq. (13) we perform the following shift of variables

$$R(t, s) = R_b(t, s) + R_q(t, s)$$ (14)

The field $R_q(t, s)$ describes the fluctuations around a fixed background chain conformation $R_b(t, s)$. We require that $R_b(t, s)$ satisfies the boundary conditions

$$\begin{align*}
R_b(t_f, s) &= R_f(s) \\
R_b(0, s) &= R_0(s)
\end{align*}$$ (15)

with respect to the time $t$. The boundary conditions in the variable $s$ corresponding to Eqs. (9) and (10) are:

1. ring-shaped chain conformations

$$R_b(t, s + L) = R_b(s)$$ (16)

2. open chain conformations

$$R_b(t, 0) = r_1 \quad R_b(t, L) = r_2$$ (17)

Finally, we demand that the background conformation fulfills the constraint

$$R_b'^2 = 1$$ (18)

The fluctuations $R_q(t, s)$ obey instead the following boundary conditions with respect to the time variable $t$:

$$R_q(t_f, s) = 0 \quad R_q(0, s) = 0$$ (19)

In the case of the variable $s$, the analogs of Eqs. (16) and (17) are respectively:

1. ring-shaped chain conformations

$$R_q(t, s + L) = R_q(t, s)$$ (20)

2. open chain conformations

$$R_q(t, 0) = 0 \quad R_q(t, L) = 0$$ (21)
The expression of $\Psi[J]$ in terms of $R_b$ and $R_q$ is

$$
\Psi[J] = e^{-S_b} \int_{b,c} DR_q D\lambda e^{-\int_0^{t_f} dt \int_0^L ds \left[ eR_b^2 - i\lambda(R_q^2 + 2R_q R_b') + R_q (J - 2eR_b) \right]}
$$

In Eq. (22) we have introduced the notation:

$$
S_b = \int_0^{t_f} dt \int_0^L ds \left[ eR_b^2 + R_b \cdot J \right]
$$

Let us note that it is not necessary that the background field $R_b$ satisfies the classical equations of motion related to the action $\frac{S_0}{4k_BT\tau} + S_1$ appearing in Eq. (13). This would be a severe restriction. We recall in fact that the compatibility with the constraint (18) requires that the solutions of the classical equations of motion $R_{cl}(s)$ are static chain conformations independent of time [10]. The main disadvantage of static background conformations is that with this choice the initial and final conformations of the chain in the boundary conditions (15) must be the same, i.e. $R_f(s) = R_0(s) = R_{cl}(s)$. On the other hand, we have seen here that more general background fields can be considered. Their only effect is the addition to the external current $J$ of the term $2eR_b$, see Eq. (22). Of course, for static solutions $\ddot{R}_b = 0$ and this term vanishes identically.

Let’s now investigate how it is possible to include in our approach the stiffness of the chain. To this purpose, it is convenient to require that $R_b$ is a static background conformation of the chain. Under this hypothesis, Eq. (14) becomes $R(t, s) = R_b(s) + R_q(t, s)$. Taking the derivative with respect to $s$ of both members of this equation, one obtains $R'(t, s) = R'_b(s) + R'_q(t, s)$. At this point, only the fluctuations are responsible for the time variation of the vector field $R'(t, s)$ which is tangent to the chain trajectory for each value of the arc-length $0 \leq s \leq L$. In fact, the contribution of the background vanishes identically: $\dot{R}_b'(s) = 0$. Therefore, we may use the module of $R'_q(t, s)$ as a measure of how fluctuations are effective in bending the chain. Accordingly, we modify the generating functional $\Psi[J]$ in Eq. (22) adding a bending energy term as follows:

$$
\Psi[\alpha J] = e^{-S_b} \int_{b,c} DR_q D\lambda e^{-\int_0^{t_f} dt \int_0^L ds \left[ eR_b^2 + R_b \cdot J + \alpha R_q^2 - i\lambda(R_q^2 + 2R_q R_b') + R_q (J - 2eR_b) \right]}
$$

The term added to the action of the fields $R_q$ and $\lambda$ is:

$$
S_\alpha = \frac{\alpha}{2k_B T\tau} \int_0^{t_f} dt \int_0^L ds R_q^2
$$

It is easy to realize that the parameter $\alpha$ has the dimension of an energy per unit of length. Thus, $H_\alpha(t) = \alpha \int_0^L ds R_q^2$ represents the bending energy measured in energy units of $k_B T$. 

\[ \text{RAW TEXT END} \]
which thermal fluctuations deliver in the unit of time $\tau$ to the system. To have stiff chains, the fluctuations of the tangent vectors must be small, i.e.

$$R_q'^2 \ll 1$$

(26)

This situation is verified in the following cases:

1. $2k_B T \tau$ is small

2. $\alpha$ is big

The first condition implies that either the temperature is so low that fluctuations become negligible or that the chain is fluctuating in a very viscous environment. In both situations one expects that conformational changes due to thermal fluctuations are small, so that the chain may be considered as rigid. The interpretation of the second condition is straightforward. Finally, we notice that it is not possible to substitute naively $R_q'$ with $R'$ in Eq. (25) because in this way the bending energy term would be trivial due to the rigid constraints which require that $R'^2 = 1$.

IV. COMPUTATION OF THE DYNAMICAL FORM FACTOR AND RELATED QUANTITIES

This Section is devoted to the computation of the average values of two physically interesting observables. The average $\langle O \rangle$ of an observable $O$ will be evaluated using the distribution:

$$\int \mathcal{D}\rho(R_q, \lambda) = \int \mathcal{D}R_q \int \mathcal{D}\lambda e^{-\int_0^L dt \int_0^L ds [\dot{R}_q^2 - i\lambda (R_q'^2 + 2R_q'R_b) - S_\alpha(R_q')]}$$

(27)

The boundary conditions satisfied by the fields $R_q$ and $\lambda$ are those specified in the previous Section. Let us note that with this choice of boundary conditions $\mathcal{D}\rho(R_q, \lambda)$ is exactly the measure appearing in the path integral of the generating functional of Eq. (22) as it should be. In writing Eq. (27) we have required that the background field $R_b$ satisfies the classical equations of motion, so that $\ddot{R}_b = 0$. Without this condition, it is very difficult to perform analytical calculations, even in the stiff chain approximation of Eq. (26). We have also neglected the stiffness term $S_\alpha$ of Eq. (25) and the irrelevant normalization factor $e^{-S_b}$. 

First of all, we consider the quantity:

\[ \Psi(\xi_1) = \left\langle e^{- \int_{0}^{t_f} dt \int_{0}^{L} ds R_q(t,s) \cdot \xi_1(t,s)} \right\rangle \] (28)

where

\[ \xi_1(t, s) = i k [\delta(t - t_2) \delta(s - l_2) - \delta(t - t_1) \delta(s - l_1)] \] (29)

In the above equation \( k \) is a constant vector and we have assumed that \( 0 \leq t_1 \leq t_2 \leq t_f \). Let us note that the observable (28) is related to the dynamical form factor, see Ref. [12] for an introduction to that quantity. As a matter of fact, substituting the current (29) in Eq. (28) and integrating over \( l_1 \) and \( l_2 \) we obtain:

\[ \frac{1}{L^2} \int_{0}^{L} dl_1 \int_{0}^{L} dl_2 \left[ e^{- \int_{0}^{t_f} dt \int_{0}^{L} ds R_q \cdot \xi_1} \Psi(\xi_1) \right] = \frac{1}{L^2} \int_{0}^{L} dl_1 \int_{0}^{L} dl_2 \left\langle e^{ik(R(t_1, l_1) - R(t_2, l_2))} \right\rangle \] (30)

where we have added the normalization factor \( \frac{1}{L^2} \). The quantity in the right hand side of the above equation is nothing but the dynamical form factor of the chain.

We are now going to compute the expression of \( \Psi(\xi_1) \). Looking at the integration measure of Eq. (27), it is easy to realize that \( \Psi(\xi_1) \) coincides with the generating functional \( \Psi[J] \) in the special case in which \( J \) is the external current \( \xi_1 \) of Eq. (29). As we will see, the presence of Dirac delta functions in \( \xi_1 \) produces ultraviolet divergences in the expectation value \( \Psi(\xi_1) \) which should be properly regulated. For simplicity, we will consider here stiff chains. As explained above, see Eq. (26), this means that the changes due to the fluctuations of the vectors tangent to the chain’s trajectory are relatively small, so that it is possible to neglect in the probability distribution (27) the quadratic term in \( R'_q \):

\[ R_q'^2 + 2R_q' \cdot R_b' \sim 2R_q' \cdot R_b' \] (31)

Taking into account Eq. (31), the expression of \( \Psi(\xi_1) \) may be approximated as follows:

\[ \Psi(\xi_1) \sim \int \mathcal{D}R_q \int \mathcal{D}\lambda e^{- \int_{0}^{t_f} dt \int_{0}^{L} ds [2R_q'^2 + j R_q]} \] (32)

where

\[ j = \xi_1 - i \frac{\partial}{\partial s} (\lambda R_b') \] (33)

After a straightforward gaussian integration over \( R_q \) in Eq. (32), we obtain

\[ \Psi(\xi_1) = \int \mathcal{D}\lambda e^{S(\lambda)} \] (34)
with

\[ S(\lambda) = \frac{1}{4} \int_0^{t_f} dt dt' \int_0^L ds \mathbf{j}(t, s) G(t, t') \mathbf{j}(t', s) \]  

(35)

In the above formula \( G(t, t') \) denotes the Green function satisfying the equation

\[ 2c \frac{\partial^2 G(t, t')}{\partial t^2} = -\delta(t, t') \]  

(36)

The boundary conditions of \( G(t, t') \) at both initial and final instants \( t = 0 \) and \( t_f = 0 \) are the same Dirichlet boundary conditions of the fields \( R_q \) given in Eq. (19). The Green function \( G(t, t') \) may be written in closed form as follows [29]:

\[ G(t, t') = -\frac{1}{2c} \left[ \frac{t(t - t_f)}{t_f} \theta(t - t') + \frac{t(t' - t_f)}{t_f} \theta(t' - t) \right] \]  

(37)

Here \( \theta(t) \) is the theta function of Heaviside. Later on it will be necessary to evaluate \( G(t, t') \) on the line \( t = t' \). In this case the right hand side of Eq. (37) becomes proportional to \( \theta(0) \), which is not a well defined quantity. This is rather a problem of the chosen representation than an intrinsic flaw of the solution of Eq. (37). For this reason, it will be useful to derive a series representation for \( G(t, t') \), which is regular when \( t = t' \). To this purpose, we use the definition of a Green function in terms of its eigenvalues and eigenfunctions:

\[ G(t, t') = -\sum_n f_n(t) f_n(t') \lambda_n \]  

(38)

where the eigenfunctions \( f_n(t) \)'s satisfy the equation

\[ 2c \frac{\partial^2 f_n(t)}{\partial t^2} = \lambda_n f_n(t) \]  

(39)

It is easy to show that

\[ f_n(t) = \sqrt{\frac{2}{t_f}} \sin \left( \frac{n\pi (t_f - t)}{t_f} \right) \]  

(40)

and that

\[ \lambda_n = -\frac{2n^2 \pi^2 c}{t_f^2} \]  

(41)

where \( n > 0 \) in both Eqs. (40) and (41). Inserting Eqs. (40) and (41) back in (38) we obtain:

\[ G(t, t') = \sum_{n>0} \frac{t_f}{cn^2 \pi^2} \sin \left( \frac{n\pi (t_f - t)}{t_f} \right) \sin \left( \frac{n\pi (t_f - t')}{t_f} \right) \]  

(42)

Remembering the definition of the current \( \mathbf{j} \) of Eq. (33), it is easy to realize that the action \( S(\lambda) \) of Eq. (35) is gaussian in the Lagrange multiplier \( \lambda \):

\[ S(\lambda) = \frac{1}{2} \int_0^{t_f} dt dt' \int_0^L ds G(t, t') \left[ \mathbf{\xi}_1(t, s) : \mathbf{\xi}_1(t', s) + i\lambda(t, s) \mathbf{R}'_b(s) : \frac{\partial}{\partial s} \mathbf{\xi}_1(t', s) \right. \]  

\[ + i\lambda(t', s) \mathbf{R}'_b(s) : \frac{\partial}{\partial s} \mathbf{\xi}_1(t, s) + \left. \lambda(t, s) \mathbf{R}'_b(s) : \frac{\partial^2}{\partial s^2} (\lambda(t', s) \mathbf{R}'_b(s)) \right] \]  

(43)
At this point we require that the background conformation $R_b(s)$ describes a ring-shaped chain placed in a two-dimensional subspace. For instance, we may choose

$$R_b(s) = \int_{s_0}^{s} \, du \, (\cos \varphi(u), \sin(\varphi(u)), 0, \ldots, 0) + R_{b,0}$$  \hspace{1cm} (44)$$

$s_0$ is the arc-length of the point $R_{b,0}$ belonging to the background conformation. Clearly, the above expression of the background field $R_b(s)$ satisfies the constraint (18) and the periodicity conditions (16) provided the function $\varphi(u)$ is periodic modulo $2\pi$: $\varphi(u + L) = \varphi(u) + 2k\pi$, $k = 0, \pm 1, \pm 2, \ldots$. Using the ansatz (44) it is easy to show that in the action $S(\lambda)$ of Eq. (43) the last term in the right hand side may be rewritten as follows:

$$\frac{1}{2} \int_{t}^{t_f} dt \, dt' \int_0^L ds G(t, t') \lambda(t, s) R'_b(s) \cdot \frac{\partial^2}{\partial s^2}(\lambda(t', s) R'_b(s)) =$$

$$\frac{1}{2} \int_{t}^{t_f} dt \, dt' \int_0^L ds G(t, t') \left[ \lambda(t, s) \left( \lambda''(t', s) - \lambda(t', s) \varphi'^2(s) \right) \right]$$  \hspace{1cm} (45)$$

In deriving Eq. (45) it has been exploited the fact that $R'_b$ is an orthonormal vector satisfying the relations $R'_b^2 = 1$ and $R'_b \cdot R''_b = 0$. Thanks to Eq. (45), the path integral over $\lambda$ (34) becomes:

$$\Psi(\xi_1) = \int \mathcal{D}\lambda e^{\frac{i}{2} \int_{t}^{t_f} dt \, dt' \int_0^L ds G(t, t') \xi_1(t, s) \xi_1(t', s) + i \lambda(t, s) \xi_{1,T}(t, s) + i \lambda(t', s) \xi_{1,T}(t', s)} \times e^{-\frac{i}{2} \int_{t}^{t_f} dt \, dt' \int_0^L ds G(t, t') \left[ \lambda(t, s) \lambda'(t', s) + \varphi'^2(s) \lambda(t, s) \lambda(t', s) \right]}$$

$$\times e^{I_1 + I_2}$$  \hspace{1cm} (46)$$

where we have set

$$\xi_{1,T}(t, s) = R'_b(s) \cdot \xi'_1(t, s)$$  \hspace{1cm} (47)$$

After a straightforward integration over $\lambda$, we obtain:

$$\Psi(\xi_1) = e^{I_1 + I_2}$$  \hspace{1cm} (48)$$

with

$$I_1 \equiv \frac{1}{2} \int_{t}^{t_f} dt \, dt' \int_0^L ds G(t, t') \xi_1(t, s) \xi_1(t', s)$$  \hspace{1cm} (49)$$

and

$$I_2 \equiv -\frac{1}{2} \int_{t}^{t_f} dt \, dt' \int_0^L ds ds' G(t, t') K(s, s') \xi_{1,T}(t, s) \xi_{1,T}(t', s')$$  \hspace{1cm} (50)$$

In Eq. (50) $K(s, s')$ denotes the Green function satisfying the equation

$$\left[ \frac{\partial^2}{\partial s^2} - (\varphi'(s))^2 \right] K(s, s') = -\delta(s - s')$$  \hspace{1cm} (51)$$
At this point, we may proceed our calculation of $\Psi(\xi_1)$ considering general background conformations of the form (44). However, one should keep in mind that, if the function $\varphi$ is too complicated, the solution of Eq. (51) is not known explicitly. For this reason, we will concentrate here on the particular case in which $\varphi(s) = \frac{2\pi s}{L}$, so that the background conformation $R_b(s)$ has the shape of a circle of length $L$:

$$R_b(s) = \frac{L}{2\pi} \left( \cos \frac{2\pi s}{L}, \sin \frac{2\pi s}{L}, 0, \ldots, 0 \right)$$  \hspace{1cm} (52)

Let’s now evaluate the integrals appearing in the two exponents in the right hand side of Eq. (48). The explicit calculation of $I_1$ and $I_2$ will be performed in Appendix A. Only the final results are provided here:

$$I_1 = 0$$  \hspace{1cm} (53)

and

$$I_2 = \sum_{\alpha=1}^{2} \left[ \frac{\sigma}{L} g(t_f, t_\alpha, c) \sum_{i,j=1}^{2} \frac{k_i k_j}{2} x'_{b,i}(l_\alpha) x'_{b,j}(l_\alpha) + \frac{\sigma L}{4\pi^2} g(t_f, t_\alpha, c) \sum_{i,j=1}^{2} \frac{k_i k_j}{2} x''_{b,i}(l_\alpha) x''_{b,j}(l_\alpha) \right]$$

$$- \sum_{i,j=1}^{2} \left( \frac{1}{2} k_i k_j \left[ G(t_1, t_2) \frac{\partial^2 K(l_1, l_2)}{\partial l_1 \partial l_2} x'_{b,i}(l_1) x'_{b,j}(l_2) + \frac{\partial K(l_1, l_2)}{\partial l_1} x''_{b,i}(l_1) x'_{b,j}(l_2) \right] + \left[ G(t_1, t_2) \frac{\partial^2 K(l_1, l_2)}{\partial l_1 \partial l_2} x''_{b,i}(l_1) x''_{b,j}(l_2) + \frac{\partial K(l_1, l_2)}{\partial l_1} x'_{b,i}(l_1) x''_{b,j}(l_2) \right] \right)$$  \hspace{1cm} (54)

In the above equation we have put

$$g(t_f, t_\alpha, c) = \sum_{n>0}^{n} \frac{t_f}{cn^2 \pi^2} \sin^2 \frac{n\pi(t_f - t_\alpha)}{t_f} \equiv G(t_\alpha, t_\alpha)$$  \hspace{1cm} (55)

with $\alpha = 1, 2$ and $\sigma$ being a constant defined in Eq. (A19).

The function $K(s, s')$ appearing in Eq. (54) is the Green function of Eq. (51). If the background conformation is given by Eq. (52), $K(s, s')$ satisfies the relation:

$$\left[ \frac{\partial^2}{\partial s^2} - \frac{4\pi^2}{L^2} \right] K(s, s') = -\delta(s, s')$$  \hspace{1cm} (56)

An explicit expression of the solution of Eq. (56) in the form of a Fourier series is given in the Appendix, Eqs. (A13) and (A14). Finally, in Eq. (54) the components of the background conformation field $R'_b$ have been denoted with the symbols $x'_{b,i}(s)$, $i = 1, 2$. The particular choice of $R_b(s)$ made in Eq. (52) implies

$$x'_{b,1}(s) = \cos \varphi(s) \quad x'_{b,2}(s) = \sin \varphi(s)$$  \hspace{1cm} (57)
with \( \varphi(s) = \frac{2\pi s}{L} \). Let us note that the delta functions present in the external current \( \xi_1(t, s) \) of Eq. (29) are responsible for the self-interactions of the two points on the chain corresponding to the values of the arc-length \( s = l_1 \) and \( s = l_2 \). These self-interactions introduce infinities in both integrals \( I_1 \) and \( I_2 \). Such infinities have been regulated in order to obtain the final result of Eqs. (53) and (54) with the help of a \( \zeta \)-function regularization \[19\]. At the end it is possible to write:

\[
\Psi(\xi_1) = e^{I_2}
\]

(58)

where \( I_2 \) is given in Eq. (54).

In a way which is analogous to that used to calculate the quantity (28) one may compute also the following observable:

\[
\Psi(\xi_2) = \left\langle e^{-\int_0^{t_f} dt \int_0^L ds \xi_2(t,s) \cdot R_q(t,s)} \right\rangle
\]

(59)

where

\[
\xi_2(t, s) = \frac{ik}{t_2 - t_1} \theta(t - t_1) \theta(t_2 - t) \left[ \delta(s - l_1) - \delta(s - l_2) \right]
\]

(60)

\( \Psi(\xi_2) \) provides a measure of the average distance between two points of the chain over the time \( t_2 - t_1 \). However, \( \Psi(\xi_2) \) may also be used in order to estimate the distance between two points at any given instant \( t_1 \). As a matter of fact, substituting the expression of the current (60) in Eq. (59) and taking the limit \( t_2 \longrightarrow t_1 \), it turns out that:

\[
e^{-\int_0^{t_f} dt \int_0^L ds \xi_2(t,s) \cdot R_q(t,s)} \Psi(\xi_2) \bigg|_{t_1=t_2} = \left\langle e^{ik(R(t_1,t_2) - R(t_1,l_1))} \right\rangle
\]

(61)

where \( x_i(t, s) \) denotes the \( i \)-th component of the vector \( R(t, s) \). Expanding the exponent in the right hand side of the above equation up to the second order we obtain

\[
\Psi(\xi_2)|_{t_1=t_2} \sim \left\langle 1 + ik \cdot (R(t_1, l_2) - R(t_1, l_1)) - \sum_{i,j=1}^d k_i k_j (x_i(t_1, l_2) - x_i(t_1, l_1)) \right. \\
\left. \times (x_j(t_1, l_2) - x_j(t_1, l_1)) + \ldots \right\rangle
\]

(62)

It is easy to show that, for instance:

\[
-\frac{\partial^2}{\partial k^2} \Psi(\xi_2) \bigg|_{k=0} = \left\langle |R(t_1, l_2) - R(t_1, l_1)|^2 \right\rangle
\]

(63)

confirming the close relation of the observable \( \Psi(\xi_2) \) with the average distance of two points of the chain.
The computation of $\Psi(\xi_2)$ can be performed in a way that is analogous to the calculation of $\Psi(\xi_1)$. We report here only the result

$$\langle \Psi(\xi_2) \rangle = \exp \left[ \sum_{i,j=1}^{2} k_i k_j B_{ij} \right]$$

(64)

where

$$B_{ij} = \frac{A}{2} x'_{b,i}(l_1)x'_{b,j}(l_1) \frac{\sigma}{L} + \frac{A}{2} x'_{b,i}(l_2)x'_{b,j}(l_2) \frac{\sigma}{L} + \frac{A}{2} \frac{\partial^2 K(l_1,l_2)}{\partial l_1 \partial l_2} x'_{b,i}(l_1)x'_{b,j}(l_2)$$

$$+ \frac{A}{2} \frac{\partial^2 K(l_2,l_1)}{\partial l_2 \partial l_1} x'_{b,i}(l_1)x'_{b,j}(l_2) + A \frac{\partial K(l_1,l_2)}{\partial l_1} x'_{b,i}(l_1)x''_{b,j}(l_2)$$

$$+ A \frac{\partial K(l_2,l_1)}{\partial l_2} x'_{b,i}(l_2)x''_{b,j}(l_2) - \frac{\sigma AL}{8\pi^2} \left( x''_{b,i}(l_1)x''_{b,j}(l_1) + x''_{b,i}(l_2)x''_{b,j}(l_2) \right) + \frac{A}{2} \left( K(l_1,l_2)x''_{b,i}(l_1)x''_{b,j}(l_2) + K(l_2,l_1)x''_{b,i}(l_2)x''_{b,j}(l_1) \right)$$

(65)

and

$$A = \int_{t_1}^{t_2} dt \int_{t_2}^{t_2} dt' G(t,t')$$

(66)

V. A MODEL OF THE DYNAMICS OF TWO TOPOLOGICALLY ENTANGLED CHAINS

In this Section we discuss the physically relevant case in which $d = 3$. The single chain model will be extended to two chains including topological interactions, which in three space dimensions become relevant, in particular when the chains are near the $\Theta$–condition. Let us consider 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 radius vectors $R_1(t,s_1)$ and $R_2(t,s_2)$, 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 $\chi$:

$$\chi(t,C_1,C_2) = \frac{1}{4\pi} \oint_{C_1} dR_1 \cdot \oint_{C_2} dR_2 \times \frac{(R_1 - R_2)}{|R_1 - R_2|^2}$$

(67)

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 repulsive interactions between the two chains which could prevent their crossing, we just require that, during the time $t_f$, the average value of the Gauss linking number is an arbitrary constant.
\( m, \) i.e.:  
\[
m = \frac{1}{t_f} \int_0^{t_f} \chi(t, C_1, C_2) dt
\]  
(68)

Our starting point is the probability function of two free chains:
\[
\Psi(C_1, C_2) = \int \prod_{i=1}^{2} [\mathcal{D}R_i \mathcal{D}\lambda_i] e^{-(S^{(1)} + S^{(2)})}
\]  
(69)

where, in agreement with Eq. (3), the actions \( S^{(1)} \) and \( S^{(2)} \) are given by:
\[
S^{(i)} = \int_0^{t_f} dt \int_0^L ds_i [cR^2_i - i\lambda_i(R_i^2 - 1)] \quad i = 1, 2
\]  
(70)

In order to add the topological interactions, we introduce in the above functional a Dirac \( \delta \)-function which imposes the constraint (68). In this way we obtain the new probability function:
\[
\Psi_m(C_1, C_2) = \int \prod_{i=1}^{2} [\mathcal{D}R_i \mathcal{D}\lambda_i] \delta \left( m - \int_0^{t_f} dt \int_{C_1} dR_1 \cdot \int_{C_2} dR_2 \times \frac{(R_1 - R_2)}{|R_1 - R_2|^3} \right) \times e^{-(S^{(1)} + S^{(2)})}
\]  
(71)

Exploiting the Fourier representation of the Dirac \( \delta \)-function, the probability function \( \Psi_m(C_1, C_2) \) takes the form
\[
\Psi_m(C_1, C_2) = \int_{-\infty}^{+\infty} d\Lambda \Psi_\Lambda(C_1, C_2) e^{-im\Lambda}
\]  
(72)

where
\[
\Psi_\Lambda(C_1, C_2) = \int \prod_{i=1}^{2} [\mathcal{D}R_i \mathcal{D}\lambda_i] e^{-(S^{(1)} + S^{(2)})} e^{i\Lambda \int_0^{t_f} \frac{dt}{4\pi t_f} \oint_{C_1} dR_1 \cdot \oint_{C_2} dR_2 \times \frac{(R_1 - R_2)}{|R_1 - R_2|^3}}
\]  
(73)

At this point, after introduction the three dimensional spatial indices \( \mu, \nu, \rho = 1, 2, 3 \), we state the identity:
\[
\Lambda \int_0^{t_f} \frac{dt}{4\pi t_f} \oint_{C_1} dR_1 \cdot \oint_{C_2} dR_2 \times \frac{(R_1 - R_2)}{|R_1 - R_2|^3} = \int_{-\infty}^{+\infty} d\eta \int d^3 x \int_{-\infty}^{+\infty} d\eta' \int d^3 y J^\mu_1(\eta, x) G^{\mu\nu}(\eta, \eta'; x, y) J^\nu_2(\eta', y)
\]  
(74)

In the above equation we have defined the following currents:
\[
J^\mu_i(\eta, x) = \gamma_i \int_0^{t_f} \frac{dt}{t_f} \delta(\eta - t) \int_0^{L_i} ds_i \frac{\partial R_i(t, s_i)}{\partial s_i} \delta^{(3)}(x - R_i(t, s_i))
\]  
(75)
with $\gamma_1 = \frac{1}{2t_f}$ and $\gamma_2 = \Lambda$.

$G_{\mu\nu}(\eta, \eta'; x, y)$ is the propagator of the field theory

$$S_{CS} = \frac{1}{t_f} \int_{-\infty}^{+\infty} d\eta \int d^3x A^{(1)}(\eta, x) \cdot (\nabla_x \times A^{(2)}(\eta, x))$$

(76)

$\nabla_x$ being the gradient with respect to the spatial variable $x$. Moreover, the $A^{(i)}(\eta, x)$'s, $i = 1, 2$, are two vector fields defined in the Euclidean four dimensional space $(\eta, x)$ and having three spatial components $A^{(i)}_\mu$. Explicitly, $G_{\mu\nu}(\eta, \eta'; x, y)$ is given by

$$G_{\mu\nu}(\eta, \eta'; x, y) = \frac{t_f}{2\pi} \varepsilon_{\mu\nu\rho} \frac{(x - y)^\rho}{|x - y|^3} \delta(\eta - \eta')$$

(77)

Apparently, $S_{CS}$ is similar to the multi-component Chern-Simons field theory used to impose the topological constraints in the case of a static chain [30]. It differs however from it by the addition of the fourth dimension spanned by the coordinate $\eta$, with $-\infty < \eta < +\infty$. This new coordinate is necessary to deal with the time variable $t$ appearing in the dynamical case. Using the identity (74), it is possible to formulate the probability function $\Psi_\Lambda(C_1, C_2)$ of Eq. (73) as a Chern-Simons field theory

$$\Psi_\Lambda(C_1, C_2) = \int \prod_{i=1}^2 [DR_i D\lambda_i D\mathbf{A}^{(i)}] e^{-iS_{CS} + S^{(1)} + S^{(2)}} e^{-i\sum_{i=1}^2 \int_{-\infty}^{+\infty} d\eta \int d^3x J^\mu_i(\eta, x) A^{(i)}_\mu(\eta, x)}$$

(78)

where the actions $S_{CS}, S^{(1)}, S^{(2)}$ have been defined respectively defined respectively in Eqs. (76) and (70), while the currents $J^\mu_i(\eta, x)$ are given in Eq. (75).

**VI. CONCLUSIONS**

The main goal of this paper was to make the GNL$\sigma$M of Ref. [10] more suitable to describe realistic systems and to compute the average of concrete physical quantities. In the introductory Section II, the continuous limit of a freely jointed chain consisting of $N - 1$ segments of fixed length $a$ and $N$ beads of mass $m$ attached at the joints has been discussed in $d$ dimensions. The final model describing the dynamics of the continuous chain is a generalized nonlinear sigma model. The difference from the two dimensional case discussed in Ref. [10] is that the underlying symmetry group is $O(d)$ and not $O(2)$. This slight difference is enough to complicate the calculation of the generating functional $\Psi[J]$ of Eq. (13) even in the approximation of Eq. (26). To obtain analytical results, one is forced to assume that the background conformations $\mathbf{R}_b$ are lying on a plane as it has been done in Eq. (14).
In Section III we have introduced in our approach the notion of chain stiffness. The bending energy term \( S_\alpha \) of Eq. \( \text{(25)} \) has been added to the action of the GNL\( \sigma \)M in Eq. \( \text{(24)} \). Let us note that, due to the constraint \( R'_q^2 + 2R'_b \cdot R'_q = 0 \), \( S_\alpha \) may be treated as a linear term, in which the fluctuation \( R'_q \) is coupled to an external current proportional to \( R''_b \).

The expectation values of two important observables have been derived in Section IV. The first observable \( \Psi(\xi_1) \) is the dynamical form factor. The second observable \( \Psi(\xi_2) \) may be related both to the average distance between two arbitrary points of the chain at a given time \( t_1 \) or to the average of that distance over a finite time interval. We have seen that the calculation of these observables is complicated by ultraviolet divergences, which have been cured using the zeta function regularization. The closed form of \( \Psi(\xi_1) \) and \( \Psi(\xi_2) \) in the approximation \( \text{(26)} \) has been presented in Eqs. \( \text{(54)}-\text{(58)} \) and \( \text{(64)}-\text{(66)} \) respectively.

Finally, we have proposed in Section V a way to describe the topological relations between two ring-shaped chains via the Gauss linking number. This result generalizes to dynamics the treatment of topological constraints presented in the case of statistical mechanics in \[30\].

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**APPENDIX A: PROOF OF Eqs. \( \text{(53)} \) AND \( \text{(54)} \)**

First we evaluate the integral \( I_1 \) of Eq. \( \text{(49)} \), which we rewrite here for convenience:

\[
I_1 = \frac{1}{2} \int_0^{t_f} dt dt' \int_0^L ds G(t, t') \xi_1(t, s) \xi_1(t', s)
\]  
(A1)

where \( \xi_1(t, s) \) is given in Eq. \( \text{(29)} \). The only potentially non-zero contributions come from the self-interactions of the two points located at arc-lengths \( s = l_1 \) and \( s' = l_2 \):

\[
I_1 = -\frac{k^2}{2} \sum_{\alpha=1}^2 \int_0^{t_f} dt dt' \int_0^L ds ds' G(t, t') \delta(t - t_\alpha) \delta(t' - t_\alpha) \delta(s - s') \delta(s - l_\alpha) \delta(s' - l_\alpha)
\]  
(A2)
There are in principle other two contributions which are proportional to $\delta(l_1 - l_2)$ and thus vanish identically, since $l_1 \neq l_2$. The time integrations in Eq. (A2) do not pose particular problems. Using the prescription (42) to evaluate the Green function $G(t, t')$ at coinciding points, we obtain

$$I_1 = -\frac{k^2}{2} \sum_{\alpha=1}^{2} g(t_f, t_\alpha, c) \int_0^L dsds' \delta(s - s')\delta(s - l_\alpha)\delta(s' - l_\alpha) \quad (A3)$$

Here $g(t_f, t_\alpha, c)$ is the series given in Eq. (55). Unfortunately, the integrals over the arc-length $s$ and $s'$ are divergent and require regularization. To this purpose, we first expand the periodic $\delta$-function $\delta(s)$ in Fourier series:

$$\delta(s) = \sum_{\kappa=-\infty}^{+\infty} \frac{e^{2\pi i \kappa s}}{L} \quad (A4)$$

After some calculations, it is possible to show in this way that:

$$\int_0^L dsds' \delta(s - s')\delta(s - l_\alpha)\delta(s' - l_\alpha) = \frac{1}{L} \sum_{\kappa=-\infty}^{+\infty} 1 \quad (A5)$$

Of course, $\sum_{\kappa=-\infty}^{+\infty} 1$ is divergent if left without treatment. To remove the singularities, we will use the zeta function regularization. This kind of regularization is based on the Riemann $\zeta$-function:

$$\zeta(s) = \sum_{\kappa=0}^{+\infty} \frac{1}{\kappa^s} \quad (A6)$$

and on the fact that, in the sense of the analytic continuation, one may write the following formal identity:

$$\zeta(0) = \sum_{\kappa=0}^{+\infty} 1 \quad (A7)$$

On the other side, Eq. (A7) implies that:

$$\sum_{\kappa=-\infty}^{+\infty} 1 = 2\zeta(0) - 1 \quad (A8)$$

Applying Eqs. (A7) and (A8) to Eq. (A5) and substituting the result in the expression of $I_1$ given in (A3), it is easy to realize that the integral $I_1$ becomes:

$$I_1 = -\frac{k^2}{2} \sum_{\alpha=1}^{2} g(t_f, t_\alpha, c) \frac{1}{L}(2\zeta(0) - 1) \quad (A9)$$

After an analytic continuation of the function $\zeta(s)$ to the point $s = 0$, one finds that $\zeta(0) = \frac{1}{2}$. Substituting this value of $\zeta(0)$ in Eq. (A9), we obtain

$$I_1 = 0 \quad (A10)$$
This completes the proof of Eq. (53). As expected, the self-interactions of the points at \( s = l_1 \) and \( s = l_2 \) with themselves do not give any contribution to \( \Psi(\xi_1) \).

The situation is more complicated in the case of the second integral \( I_2 \) of Eq. (50):

\[
I_2 = -\frac{1}{2} \int_0^{t_L} dt dt' \int_0^{L} ds ds' G(t, t') K(s, s') \xi_{1,T}(t, s) \xi_{1,T}(t', s')
\]  

(A11)

Using the definition (17) of the current \( \xi_{1,T} \) one obtains:

\[
I_2 = \sum_{i,j=1}^{2} \sum_{\alpha=1}^{2} \frac{k_i k_j}{2} g(t_f, t, c) \int_0^{L} ds ds' \left[ K(s, s') x''_{b,i}(s) x''_{b,j}(s') + \frac{\partial^2 K(s, s')}{\partial s \partial s'} x'_{b,i}(s) x'_{b,j}(s') \right]
\]

\[
+ \frac{\partial K(s, s')}{\partial s} x'_{b,i}(s) x'_{b,j}(s') + \frac{\partial K(s, s')}{\partial s'} x'_{b,i}(s) x'_{b,j}(s') \right] \delta(s - l_\alpha) \delta(s' - l_\alpha)
\]

(A12)

To write Eq. (A12), we have made some integrations by parts in the variables \( s \) and \( s' \). These are allowed because of the choice of the boundary condition and of the fact that the current \( \xi_1 \) vanishes at the boundary: \( \xi_1(t, 0) = \xi_1(t, L) = 0 \). It is not difficult to show that, for symmetry reasons, \( \frac{\partial K(s, s')}{\partial s} \bigg|_{s= l_\alpha, s' = l_\alpha} = 0 \). As a matter of fact, using the Fourier representation of \( K(s, s') \):

\[
K(s, s') = \sum_{\kappa = -\infty}^{+\infty} e^{2\pi i \kappa (s-s')} \tilde{K}(\kappa)
\]  

(A13)

where

\[
\tilde{K}(\kappa) = \frac{L}{4\pi^2 \kappa^2 + 1}
\]  

(A14)

we obtain:

\[
\frac{\partial K(s, s')}{\partial s} \bigg|_{s= l_\alpha, s' = l_\alpha} = \frac{i}{2\pi} \sum_{\kappa = -\infty}^{+\infty} \frac{\kappa}{\kappa^2 + 1} = 0
\]  

(A15)

Analogously, one may show that \( \frac{\partial K(s, s')}{\partial s} \bigg|_{s= l_\alpha, s' = l_\alpha} = 0 \).

There is only one term in the expression of \( I_2 \) which is divergent and needs regularization.

This is given by:

\[
I_{2, sing} = \sum_{i,j=1}^{2} \sum_{\alpha=1}^{2} \frac{k_i k_j}{2} g(t_f, t, c) \int_0^{L} ds ds' \frac{\partial^2 K(s, s')}{\partial s \partial s'} x'_{b,i}(s) x'_{b,j}(s') \delta(s - l_\alpha) \delta(s' - l_\alpha)
\]  

(A16)
Exploiting the Fourier representation \[^{[A13]}\] of \(K(s, s')\), it turns out that \(I_{2,\text{sing}}\) may be rewritten as follows:

\[
I_{2,\text{sing}} = -\frac{2}{L} \sum_{i,j=1}^{2} \sum_{\alpha=1}^{2} \frac{k_i k_j}{2} g(t_f, t, c) x'_{b,i}(l_\alpha) x'_{b,j}(l_\alpha) \frac{1}{L} \sum_{\kappa=-\infty}^{+\infty} \frac{\kappa^2}{\kappa^2 + 1} \quad (A17)
\]

Applying also the identity \(\sum_{\kappa=-\infty}^{+\infty} \frac{\kappa^2}{\kappa^2 + 1} = \sum_{\kappa=-\infty}^{+\infty} \left(1 - \frac{1}{\kappa^2 + 1}\right)\) and the fact that \(\sum_{\kappa=-\infty}^{+\infty} 1 = 0\) as we have previously seen, we arrive at the final result in which the singularity of \(I_{2,\text{sing}}\) has been regulated:

\[
I_{2,\text{sing}} = \frac{\sigma}{L} \sum_{i,j=1}^{2} \sum_{\alpha=1}^{2} \frac{k_i k_j}{2} g(t_f, t, c) x'_{b,i}(l_\alpha) x'_{b,j}(l_\alpha) \quad (A18)
\]

In the above equation we have put:

\[
\sigma = \sum_{\kappa=-\infty}^{+\infty} \frac{1}{\kappa^2 + 1} \quad (A19)
\]

Let’s now simplify the following term contained in \(I_2\):

\[
I_{2,0} = \frac{2}{L} \sum_{i,j=1}^{2} \sum_{\alpha=1}^{2} \frac{k_i k_j}{2} g(t_f, t, c) \int_0^L dsds' x''_{b,i}(s) x''_{b,j}(s') \delta(s - l_\alpha) \delta(s' - l_\alpha) \quad (A20)
\]

After the integrations over \(s\) and \(s'\), one obtains from \(I_{2,0}\) an expression which is proportional to the Green function \(K(s, s')\) computed at coinciding points \(s = s' = l_\alpha\). Exploiting the Fourier representation \[^{[A13]}\], it is possible to check that \(K(l_\alpha, l_\alpha)\) is convergent and is equal to:

\[
K(l_\alpha, l_\alpha) = \frac{\sigma L}{4\pi^2} \quad (A21)
\]

where \(\sigma\) is the constant given in Eq. \[^{(A19)}\]. Thus, we may write:

\[
I_{2,0} = \sum_{i,j=1}^{2} \sum_{\alpha=1}^{2} \frac{k_i k_j}{2} g(t_f, t, c) \frac{\sigma L}{4\pi^2} x''_{b,i}(l_\alpha) x''_{b,j}(l_\alpha) \quad (A22)
\]

All the other terms present in \(I_2\) are divergenceless. At the end, remembering the expressions of the contributions \(I_{2,\text{sing}}\) and \(I_{2,0}\) to \(I_2\) given in Eqs. \[^{(A18)}\] and \[^{(A22)}\] respectively, we obtain the final result:

\[
I_2 = I_{2,\text{sing}} + I_{2,0} - \left\{ \sum_{i,j=1}^{2} \frac{k_i k_j}{2} G(t_1, t_2) \left[ \frac{\partial^2 K(l_1, l_2)}{\partial l_1 \partial l_2} x'_{b,i}(l_1) x'_{b,j}(l_2) + \frac{\partial K(l_1, l_2)}{\partial l_1} x'_{b,i}(l_1) x''_{b,j}(l_2) + \frac{\partial K(l_1, l_2)}{\partial l_2} x''_{b,i}(l_1) x'_{b,j}(l_2) + K(l_1, l_2)x''_{b,i}(l_1)x''_{b,j}(l_2) + \begin{pmatrix} t_1 & \leftrightarrow & t_2 \\ l_1 & \leftrightarrow & l_2 \end{pmatrix} \right] \right\} \quad (A23)
\]
The above equation coincides exactly with Eq. (54).

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[31] See also the pearl-necklace model proposed in [2] and the Verdier–Stockmayer model [3].