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On a path integral description of the dynamics of an inextensible chain and its connection to constrained stochastic dynamics

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Abstract

The dynamics of a freely jointed chain in the continuous limit is described by a field theory which closely resembles the nonlinear sigma model. The generating functional $\Psi[J]$ of this field theory contains nonholonomic constraints, which are imposed by inserting in the path integral expressing $\Psi[J]$ a suitable product of delta functions. The same procedure is commonly applied in statistical mechanics in order to enforce topological conditions on a system of linked polymers. The disadvantage of this method is that the contact with the stochastic process governing the diffusion of the chain is apparently lost. The main goal of this work is to re-establish this contact. For this purpose, it is shown here that the generating functional $\Psi[J]$ coincides with the generating functional of the correlation functions of the solutions of a constrained Langevin equation. In the discrete case, this Langevin equation describes as expected the Brownian motion of beads connected together by links of fixed length.

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1. Introduction

The subject of this work is a chain obtained by performing the continuous limit of a system of $M - 1$ links of fixed length a and M beads of constant mass m. In this limit the number M of beads approaches infinity, the length of the links and the mass of the beads go to zero, while the total length L of the chain remains finite. The dynamics of a chain with rigid constraints of this kind has been studied in a remarkable series of papers [1–3] using an approach based on the Langevin equation. Later on, mainly the statistical mechanics of such chains has been investigated, see e.g. [4–6]. Dynamical models are however interesting by themselves and have also some applications, for instance in modeling the response of a chain to mechanical stresses in micromanipulations [7].

In [8], the dynamics of the constrained chain has been considered using path integral methods. The resulting model is a generalization of the nonlinear sigma model [9], which will be called here the generalized nonlinear sigma model or simply GNLσM. The most striking difference from the standard nonlinear sigma model is that in the GNLσM the constraint is nonholonomic. The relation of the GNLσM with the Rouse model [10, 11] has been discussed in [8]. It has also been shown that it gives the correct equilibrium limit in agreement with [1]. Applications of the GNLσM have been developed in [13, 14], computing for instance the dynamic form factor of the chain in the semiclassical approximation and the probability distribution $Z(\mathbf{r}_{12})$ which measures the probability that in a given interval of time the average distance between two points of the chain is $\mathbf{r}_{12}$.

One point that still needs to be clarified is if the GNLσM can be related to some stochastic process. In fact, the GNLσM has not been derived starting from a Langevin equation and applying for instance the Martin–Siggia–Rose formalism [12] in order to pass to the path integral formulation. The problem is that this approach becomes cumbersome if one has to deal with constraints. For this reason, in [8] the constraints have been added to the path integral describing the fluctuations of the beads with the help of an insertion of Dirac delta functions. This is a widely exploited procedure in the statistical mechanics of polymers in order to impose topological conditions [15–18].

To establish a relation between the GNLσM and a stochastic process is the main goal of the present work. For this purpose, after a brief introduction to the GNLσM, we define in section 3 a two-dimensional vector field φ_ν which satisfies a free Langevin equation and additional nonholonomic constraints. These are exactly the same constraints which appear also in the GLNσM. Our treatment is limited to two dimensions for simplicity. The generating functional $\tilde{\Psi}[J]$ of the correlation functions of the fields φ_ν can be constructed using the prescription of [19]. The discretized version of $\tilde{\Psi}[J]$ describes the Brownian motion of a set of M-beads with diffusion constant D which are connected together by links of fixed length. The difference between $\tilde{\Psi}[J]$ and the generating functional $\Psi[J]$ of the correlation functions of the GNLσM consists in a functional determinant. We show that this determinant is trivial by eliminating the constraints using a special set of variables, called here pseudo-polar coordinates. As a result we prove the equivalence of $\tilde{\Psi}[J]$ and $\Psi[J]$ and thus the connection of the GNLσM with a stochastic process of diffusing particles.

2. A path integral approach to the dynamics of a chain

Let us consider a single free particle in a d-dimensional space. At the time $t = 0$ the particle finds itself at the initial point $\mathbf{R}_0$ and starts to perform a random walk. As is well known, the probability $\psi(t_f; \mathbf{R}_f, \mathbf{R}_0)$ that, after the time t_f, the particle arrives at a given point $\mathbf{R}_f$, satisfies the differential equation: $\frac{\partial\psi}{\partial t_f} = D\frac{\partial^2\psi}{\partial\mathbf{R}^2}$, where D is the diffusion constant. The boundary condition at $t_f = 0$ is chosen in such a way that $\psi(0; \mathbf{R}_f, \mathbf{R}_0) = \delta(\mathbf{R}_f - \mathbf{R}_0)$. The probability function ψ can be expressed in the path integral form

$$\psi(t_f; \mathbf{R}_f, \mathbf{R}_0) = A\int_{\mathbf{R}(0)=\mathbf{R}_0}^{\mathbf{R}(t_f)=\mathbf{R}_f} \mathcal{D}\mathbf{R}(t) \exp\left[-\int_0^{t_f} \frac{\dot{\mathbf{R}}^2(t)}{4D}\,\mathrm{d}t\right], \tag{1}$$

with A being a normalization factor. We note that the diffusion constant D appearing in equation (1) satisfies the relation $D = \frac{k_B T\tau}{m}$, where k_B is the Boltzmann constant and τ is the relaxation time that characterizes the rate of decay of the drift velocity of the particle.

For a system of M noninteracting particles, the probability that the mth particle starting from the point $\mathbf{R}_{0,m}$ arrives at the point $\mathbf{R}_{f,m}$ is given by the probability function

$$\psi_M = \prod_{m=1}^{M}\left[A\int_{\mathbf{R}_m(0)=\mathbf{R}_{0,m}}^{\mathbf{R}_m(t_f)=\mathbf{R}_{f,m}}\mathcal{D}\mathbf{R}_m(t)\right]\exp\left[-\frac{1}{2k_BT\tau}\frac{m}{2}\sum_{m=1}^{M}\int_0^{t_f}\dot{\mathbf{R}}_m^2(t)\,\mathrm{d}t\right]. \tag{2}$$

In this form, the connection of the above probability function with the partition function of M free particles in quantum mechanics becomes evident. The quantity $\mathcal{A}_M = \frac{m}{2}\sum_{m=1}^{M}\int_0^{t_f}\dot{\mathbf{R}}_m(t)\,\mathrm{d}t$ represents the action of the system, while

$$\kappa = 2k_BT\tau \tag{3}$$

plays the role of the Planck's constant. Indeed, one may show that the uncertainties in the position and momentum of a Brownian particle in a solution due to the frequent collisions with the surrounding molecules satisfy an analogue of the Heisenberg uncertainty relations: $\Delta p\Delta r \sim \kappa$ [20].

In this work, we would like to consider a more sophisticated system than free particles, namely a chain of length L composed of M beads of mass m joined together by segments of fixed length a. In polymer literature a chain of this kind is also referred to as a freely jointed chain (FJC). Clearly, the quantities L, M and a are related by the identity $L = Ma$. Thus, if $\tilde{M}$ is the total mass of the chain, then the mass of a single bead is $m = \frac{\tilde{M}}{L}a$. In the following, we are going to construct the probability function Ψ_{FJC} which measures the probability that the chain fluctuates in some solution from a given initial configuration $\mathbf{R}_{0,1},\ldots,\mathbf{R}_{0,M}$ at $t=0$ to a final configuration $\mathbf{R}_{f,1},\ldots,\mathbf{R}_{f,M}$ at $t=t_f$. While the chain fluctuates, each bead performs a Brownian motion. The only difference with respect to a free particle is that its radius vector $\mathbf{R}_m(t)$ fulfils also the additional conditions

$$\frac{|\mathbf{R}_m(t)-\mathbf{R}_{m-1}(t)|^2}{a^2} = 1 \qquad m = 2,\ldots,M. \tag{4}$$

These conditions are needed by the requirement that the length of the joining segments is equal to a. It seems thus natural to express Ψ_{FJC} starting from the probability function ψ_M of M free particles and implementing into it the constraints (4) with the help of a product of delta functions:

$$\Psi_{\mathrm{FJC}} = \prod_{m=1}^{M}\left[A'\int_{\mathbf{R}_m(0)=\mathbf{R}_{0,m}}^{\mathbf{R}_m(t_f)=\mathbf{R}_{f,m}}\mathcal{D}\mathbf{R}_m(t)\right]\mathrm{e}^{-a\sum_{m=1}^{M}\int_0^{t_f}c\dot{\mathbf{R}}_m^2(t)\,\mathrm{d}t}\prod_{m=2}^{M}\delta\left(\frac{|\mathbf{R}_m(t)-\mathbf{R}_{m-1}(t)|^2}{a^2}-1\right). \tag{5}$$

The constant c appearing in equation (5) is given by

$$c = \frac{\tilde{M}}{4k_BT\tau L}. \tag{6}$$

There is some arbitrariness in the discrete chain, in the sense that there is no reason for which the massless segments of length a could not be replaced by small massive bars or by small massive cylinders. This would need the introduction of their inertial moments. This arbitrariness can be removed by considering the continuous limit for which a goes to zero, while the number M of segments goes to infinity in such a way that the length L of the chain is preserved. To perform the continuous limit, we define the discrete arc-length $s_m = am$, with $m = 1,\ldots,M$. Moreover, we introduce the new notation for the radius vectors of the beads: $\mathbf{R}(t,s_m) \equiv \mathbf{R}_m(t)$. In a similar way, the final and initial configurations of the chain will be denoted $\mathbf{R}_f(s_m)$ and $\mathbf{R}_0(s_m)$, respectively. To obtain the continuous limit one has to replace everywhere the discrete arc-length s_m with the continuous variable s, i.e. $s_m \to s$. The other recipes for passing from equation (5) to the probability function of the continuous chain are $\frac{\mathbf{R}(t,s_m)-\mathbf{R}(t,s_{m-1})}{a} \rightarrow \mathbf{R}'(t,s)$ with $\mathbf{R}' = \frac{\partial \mathbf{R}}{\partial s}$ and $\sum_{m=1}^{M} a \rightarrow \int_0^L \mathrm{d}s$. The result is

$$\Psi = \int_{\mathbf{R}(0,s)=\mathbf{R}_0(s)}^{\mathbf{R}(t_f,s)=\mathbf{R}_f(s)} \mathcal{D}\mathbf{R}(t,s)\, \mathrm{e}^{-c\int_0^{t_f}\mathrm{d}t\int_0^L \mathrm{d}s \dot{\mathbf{R}}^2(t,s)}\delta(\mathbf{R}'^2(t,s)-1). \tag{7}$$

Let us note that the constraint

$$\mathbf{R}'^2 - 1 = 0 \tag{8}$$

is automatically satisfied if $\mathbf{R}(t,s)$ is differentiable, because the trajectory of the chain at each instant t has been parametrized with the help of the arc-length s. As a consequence, condition (8) restricts the sum over all possible configurations $\mathbf{R}(t,s)$ in the path integral (7) to those which are differentiable with respect to s. From the physical point of view, we have already seen that the meaning of the constraint (8) is the inextensibility of the chain.

To complete the definition of the path integral in equation (7) we specify the boundary conditions of the vector field $\mathbf{R}(t,s)$ with respect to the variable s. The physics of the problem suggests for those boundary conditions the following two alternatives:

(a) Periodic boundary conditions $\mathbf{R}(t,s+L) = \mathbf{R}(t,s)$.
(b) Fixed end conditions: $\mathbf{R}(t,0) = \mathbf{r}_1$ and $\mathbf{R}(t,L) = \mathbf{r}_2$, where $\mathbf{r}_1$ and $\mathbf{r}_2$ are fixed points satisfying the requirement $|\mathbf{r}_2 - \mathbf{r}_1| \leqslant L$.

Case (a) corresponds to a closed chain, while case (b) describes an open chain with the two ends fixed at the points $\mathbf{r}_1$ and $\mathbf{r}_2$.

The connection of the path integral in equation (7) to field theory becomes evident after passing to dimensionless coordinates $\sigma_1 = \frac{t}{t_f}$ and $\sigma_2 = \frac{s}{L}$. In these coordinates Ψ is given by

$$\Psi = \int_{\mathbf{R}(0,\sigma_2)=\mathbf{R}_0(\sigma_2)}^{\mathbf{R}(t_f,\sigma_2)=\mathbf{R}_f(\sigma_2)} \mathcal{D}\mathbf{R}(\sigma_1,\sigma_2)\, \mathrm{e}^{-\int_0^1 \mathrm{d}\sigma_1 \mathrm{d}\sigma_2 \frac{\tilde{M}}{2\kappa t_f}[(\frac{\partial \mathbf{R}}{\partial \sigma_1})^2 + (\frac{\partial \mathbf{R}}{\partial \sigma_2})^2]}\delta\left(\frac{1}{L^2}\left|\left(\frac{\partial \mathbf{R}}{\partial \sigma_2}\right)^2\right| - 1\right). \tag{9}$$

Let us note that the constraint $\frac{1}{L^2}\left|\left(\frac{\partial \mathbf{R}}{\partial \sigma_2}\right)^2\right| - 1 = 0$ fixes the second term in the exponent appearing in the right-hand side of the above equation in such a way that $\int_0^1 \mathrm{d}\sigma_1\, \mathrm{d}\sigma_2 \frac{\tilde{M}}{2\kappa t_f}\left(\frac{\partial \mathbf{R}}{\partial \sigma_2}\right)^2 = \frac{\tilde{M}L^2}{2\kappa t_f}$, i.e. this term is an irrelevant constant. The right-hand side of equation (9) closely resembles that of a nonlinear sigma model. For this reason, the field theory described in equation (7) has been called the generalized nonlinear sigma model. The most relevant difference of the GNLσM from the nonlinear sigma model lays in the fact the in the latter the constraints are imposed on the modulus of the vector field $\mathbf{R}(t,s)$, while in equation (7) what is constrained is the modulus of $\frac{\partial \mathbf{R}}{\partial \sigma_2}$.

3. The generalized nonlinear sigma model and its relation to the Langevin equation

The starting point of this section is the generating functional $\Psi[J]$ associated with the probability function (7):

$$\Psi[J] = \int \mathcal{D}\mathbf{R}(t,s)\, \mathrm{e}^{-c\int_0^{t_f}\mathrm{d}t\int_0^L \mathrm{d}s \dot{\mathbf{R}}^2(t,s)}\delta(|\mathbf{R}'(t,s)|^2 - 1)\, \mathrm{e}^{-\int_0^{t_f}\mathrm{d}t\int_0^L \mathrm{d}s \mathbf{J}(t,s)\cdot\mathbf{R}(t,s)}. \tag{10}$$

The boundary conditions of the field $\mathbf{R}(t,s)$ are here implicitly understood. The way in which equation (10) has been obtained is different from the usual approach to the dynamics of a chain, which is based on a Langevin equation. In this section we are going to show that the GNLσM can be related to a Langevin equation too. For simplicity, we restrict ourselves to the two-dimensional case.

Since the GNLσM ignores all interactions, it is natural to suppose that it should be related to a free Langevin equation

$$\dot{\varphi}_{\nu} = \boldsymbol{\nu}, \tag{11}$$

where φ_{ν} is a two-dimensional vector field and $\boldsymbol{\nu}$ is a white noise source, whose components $\nu^{(i)}$, $i = 1, 2$ satisfy the basic correlation functions

$$\langle \nu^{(i)}(t,s)\rangle = 0 \tag{12}$$

$$\langle \nu^{(i)}(t,s)\nu^{(j)}(t',s')\rangle = \frac{\delta^{ij}}{c}\delta(t-t')\delta(s-s') \qquad i,j = 1,2. \tag{13}$$

One may also expect that, together with equation (11), the field φ_{ν} must also satisfy the constraint

$$\varphi_{\nu}'^{2} = 1. \tag{14}$$

The generating functional $\tilde{\Psi}[J]$ of the correlation functions of the field φ_{ν} is then given by [19]:

$$\tilde{\Psi}[J] = \int_{\varphi_{\nu}'^{2}=1} \mathcal{D}\boldsymbol{\nu}\, \mathrm{e}^{-c\int_0^{t_f}\mathrm{d}t\int_0^L \mathrm{d}s\boldsymbol{\nu}^2}\, \mathrm{e}^{\int_0^{t_f}\mathrm{d}t\int_0^L \mathrm{d}s\mathbf{J}\cdot\varphi_{\nu}}. \tag{15}$$

The meaning of the statistical sum in the right-hand side of the above equation becomes clear if we rewrite it as follows:

$$\tilde{\Psi}[J] = \int \mathcal{D}\boldsymbol{\nu} \int_{\mathbf{R}'^2=1} \mathcal{D}\mathbf{R}\, \mathrm{e}^{-c\int_0^{t_f}\mathrm{d}t\int_0^L \mathrm{d}s\boldsymbol{\nu}^2}\delta(\mathbf{R}-\varphi_{\nu})\, \mathrm{e}^{\int_0^{t_f}\mathrm{d}t\int_0^L \mathrm{d}s\mathbf{J}\cdot\mathbf{R}}. \tag{16}$$

The path integration over $\boldsymbol{\nu}$ is now unconstrained, while that over the new field $\mathbf{R}$ is limited to the configurations which, in the case of periodic boundary conditions, are of the form

$$\mathbf{R}(t,s) = \int_0^s \mathrm{d}u(\cos\phi(t,u), \sin\phi(t,u)), \tag{17}$$

where $\phi(t, u+L) = \phi(t,u)$. If we have fixed end boundary conditions, then equation (17) is replaced by

$$\mathbf{R}(t,s) = \int_0^s \mathrm{d}u(\cos\phi(t,u), \sin\phi(t,u)) + \mathbf{r}_1 \tag{18}$$

with the additional constraints $\mathbf{r}_2 = \int_0^L \mathrm{d}u(\cos\phi(t,u), \sin\phi(t,u)) + \mathbf{r}_1$. In both cases the only left degree of freedom is the angle $\phi(t,s)$. Let us note that the definition and computation of path integrals in polar field coordinates have been discussed in [18, 21] and, more recently, an interesting conjecture about the passage to polar field variables has been presented in [22]. These results cannot be applied however to the present case, in which the passage to polar fields is also accompanied by an integration over the s variable.

The probability function $\tilde{\Psi}[J]$ of equation (16) should be compared with the generating functional $\Psi[J]$ of equation (10). The latter may be written as follows:

$$\Psi[J] = \int \mathcal{D}\boldsymbol{\nu} \int \mathcal{D}\mathbf{R}\, \mathrm{e}^{-c\int_0^{t_f}\mathrm{d}t\int_0^L \mathrm{d}s\boldsymbol{\nu}^2}\delta(\mathbf{R}'^2-1)\delta(\dot{\mathbf{R}}-\boldsymbol{\nu})\, \mathrm{e}^{-\int_0^{t_f}\mathrm{d}t\int_0^L \mathrm{d}s\mathbf{J}\cdot\mathbf{R}}. \tag{19}$$

The connection with the Langevin equation (11) is made by noting that, for any solution φ_{ν} of that equation, it is possible to write the formula

$$\delta(\dot{\mathbf{R}}-\boldsymbol{\nu}) = \det{}^{-1}\partial_t\delta(\mathbf{R}-\varphi_{\nu}). \tag{20}$$

Applying equation (20) to equation (19) we obtain, up to an irrelevant constant

$$\Psi[J] = \int \mathcal{D}\mathbf{R}\mathcal{D}\boldsymbol{\nu}\, \mathrm{e}^{-c\int_0^{t_f}\mathrm{d}t\int_0^L \mathrm{d}s\boldsymbol{\nu}^2}\delta(\mathbf{R}-\varphi_{\nu})\delta(\mathbf{R}'^2-1)\, \mathrm{e}^{-\int_0^{t_f}\mathrm{d}t\int_0^L \mathrm{d}s\mathbf{J}\cdot\mathbf{R}}. \tag{21}$$

As already announced, this expression of the generating functional $\Psi[J]$ differs from $\tilde{\Psi}[J]$ only by the fact that the condition $\mathbf{R}'^2 = 1$ is imposed with the help of the delta function $\delta(\mathbf{R}'^2 - 1)$. In the following sections the degrees of freedom which are frozen by the condition $\mathbf{R}'^2 = 1$ will be projected out from the path integral (21) and it will be shown that what remains is exactly the generating functional $\tilde{\Psi}[J]$ related to the constrained stochastic process of equations (11) and (14).

4. The discrete generating functional in pseudo-polar coordinates

As a first step to show the equivalence of the generating functionals $\Psi[J]$ and $\tilde{\Psi}[J]$, we replace the continuous variables s and t with discrete variables s_m and t_n, with $0 \leqslant m \leqslant M$ and $0 \leqslant n \leqslant N$. The spacings in the discrete s and t-lines are respectively given by

$$s_m - s_{m-1} = a \qquad m = 2, \ldots, M \tag{22}$$

$$t_n - t_{n-1} = b \qquad n = 2, \ldots, N, \tag{23}$$

where a and b are supposed to be very small. The continuous limit is recovered in the limit $M, N \longrightarrow +\infty, a, b \longrightarrow 0$ and $Ma = L, Nb = t_f$. To simplify formulae, it will be used in the following the shorthand notation:

$$\mathbf{R}(t_n, s_m) \equiv \mathbf{R}_{nm} \qquad \boldsymbol{\nu}(t_n, s_m) \equiv \boldsymbol{\nu}_{nm} \qquad \varphi_{\nu}(t_n, s_m) \equiv \varphi_{\nu,nm}. \tag{24}$$

In this way the discrete version of the constraint $\mathbf{R}'^2(t, s) = 1$ is replaced by the set of conditions

$$\frac{(\mathbf{R}_{nm} - \mathbf{R}_{n(m-1)})}{a^2} = 1 \qquad \begin{array}{l} n = 1, \ldots, N \\ m = 2, \ldots, M. \end{array} \tag{25}$$

With the above settings the generating functional $\Psi[J]$ of equation (21) may be rewritten as follows[1]:

$$\begin{aligned}\Psi[J] = \lim_{N\to\infty} \lim_{M\to\infty} \int_{-\infty}^{+\infty} \left[\prod_{n,m} \mathrm{d}\boldsymbol{\nu}_{nm}\, \mathrm{d}\mathbf{R}_{nm}\right] \exp\left\{-abc\sum_{n,m} \boldsymbol{\nu}_{nm}^2\right\} \\ \times \prod_{n,m} \delta(\mathbf{R}_{nm} - \varphi_{\nu,nm}) \exp\left\{ab\sum_{n,m} \mathbf{J}_{nm}\cdot\mathbf{R}_{nm}\right\} \\ \times \prod_{n}\prod_{m=2}^{M} \frac{2}{a}\delta\left(\frac{|\mathbf{R}_{nm} - \mathbf{R}_{n(m-1)}|^2}{a^2} - 1\right).\end{aligned} \tag{26}$$

Let us also note in the last line of equation (26) the normalization factor $\prod_n \prod_{m=2}^{M} \frac{2}{a}$ in the definition of the delta function imposing the constraints. The reason of this normalization will be clear later.

To eliminate the constraints (25), we pass to a new set of coordinates, which in the following will be called pseudo-polar:

$$\mathbf{R}_{nm} = \sum_{m'=1}^{m} l_{nm'} (\cos\phi_{nm'}, \sin\phi_{nm'}). \tag{27}$$

The ranges of variation of the variables l_{mn} and ϕ_{nm} are respectively given by

$$0 \leqslant l_{mn} < +\infty \qquad 0 \leqslant \phi_{nm} \leqslant 2\pi. \tag{28}$$

[1] Unless otherwise specified, from now on it will be understood that the indices n and m in sums and products will take all possible values in their respective ranges, i.e. $1 \leqslant n \leqslant N$ and $1 \leqslant m \leqslant M$.

The coordinate l_{nm} for $n = 1, \ldots, N$ and $m = 2, \ldots, M$, describes the length of the mth segment at the instant t_n. The coordinate l_{n1} is very special, because it gives the position with respect to the origin of the reference system of the first bead in the chain at the time t_n. Finally, the angles ϕ_{nm} tell us how the $M - 1$ segments are reciprocally oriented. After the transformation (27), the vector $\mathbf{R}_{nm}$ depends on the variables l_{nm} and ϕ_{nm}, i.e.

$$\mathbf{R}_{nm} = \mathbf{R}_{nm}(\{l_{nm}\}, l_{n1}; \{\phi_{nm}\}), \tag{29}$$

where $\{l_{nm}\}$ is the set of all l_{nm}'s for which $m \neq 2$ and $\{\phi_{nm}\}$ is the set of all ϕ_{nm}'s. Analogously, we denote with $\{\mathbf{R}_{nm}\}$ the set of all $\mathbf{R}_{nm}$'s for $m = 1, \ldots, M$ and $n = 1, \ldots, N$. We are now able to explain the reason of the normalization factor $\prod_n \prod_{m=2}^{M} \frac{2}{a}$ in equation (26). In the pseudo-polar variables the constraints (25) become: $\frac{l_{nm}^2}{a^2} = 1$. The factor $\frac{2}{a}$ is necessary in order to normalize the delta functions imposing these constraints. As a matter of fact, it is possible to check that $\frac{2}{a} \int_0^{+\infty} \mathrm{d}l_{nm} \delta\left(\frac{l_{nm}^2}{a^2} - 1\right) = 1$.

In order to perform the transformations (27) in the expression of the generating functional $\Psi[J]$ of equation (26), we need to compute the associated Jacobian determinant. In the rest of this section we will prove for a general functional $f(\{\mathbf{R}_{nm}\})$ the following formula:

$$\int \prod_{n,m} \mathrm{d}\mathbf{R}_{nm} f(\{\mathbf{R}_{nm}\}) = \int_0^{+\infty} \prod_{n,m} \mathrm{d}l_{nm} \int_0^{2\pi} \prod_{n,m} \mathrm{d}\phi_{nm} f(\{R_{nm}(\{l_{nm}\}, l_{n1}; \{\phi_{nm}\})\}) J_{NM}, \tag{30}$$

where the Jacobian J_{NM} of the transformation (27) is given by

$$J_{NM}(\{l_{nm}\}, l_{n1}; \{\phi_{nm}\}) = \prod_n l_{nM} l_{n(M-1)} \cdots l_{n1}. \tag{31}$$

Let us show that J_{NM} is really that given in equation (31). In order to proceed, it is convenient to introduce the components $x_{nm}^{(1)}$ and $x_{nm}^{(2)}$ of the vectors $\mathbf{R}_{nm}$, i.e. $\mathbf{R}_{nm} = \left(x_{nm}^{(1)}, x_{nm}^{(2)}\right)$. Thus, equation (27) becomes

$$x_{nm}^{(1)} = \sum_{m'=1}^{m} l_{nm'} \cos\phi_{nm'} \qquad x_{nm}^{(2)} = \sum_{m'=1}^{m} l_{nm'} \sin\phi_{nm'} \tag{32}$$

and J_{NM} may be written as follows:

$$J_{NM}(\{l_{nm}\}, l_{n1}; \{\phi_{nm}\}) = \det \begin{vmatrix} \dfrac{\partial x_{nm}^{(1)}}{\partial l_{n'm'}} & \dfrac{\partial x_{nm}^{(2)}}{\partial l_{n'm'}} \\ \dfrac{\partial x_{nm}^{(1)}}{\partial \phi_{n'm'}} & \dfrac{\partial x_{nm}^{(2)}}{\partial \phi_{n'm'}} \end{vmatrix}. \tag{33}$$

Strictly speaking, J_{NM} is the determinant of a block matrix $A_{nm;n'm'}$ with composite indices nm and $n'm'$. $A_{nm;n'm'}$ is composed by four $NM \times NM$ matrices, since $n, n' = 1, \ldots, N$ and $m, m' = 1, \ldots, M$. Due to the fact that $\frac{\partial x_{nm}^{(i)}}{\partial l_{n'm'}} = \frac{\partial x_{nm}^{(i)}}{\partial \phi_{n'm'}} = 0$ for $i = 1, 2$ if $n \neq n'$, $A_{nm;n'm'}$ is a block diagonal matrix. As a consequence, it is possible to write its determinant as follows:

$$J_{NM} = \prod_n J_{nM}, \tag{34}$$

where

$$J_{nM} = \det \begin{vmatrix} \dfrac{\partial x_{nm}^{(1)}}{\partial l_{nm'}} & \dfrac{\partial x_{nm}^{(2)}}{\partial l_{nm'}} \\ \dfrac{\partial x_{nm}^{(1)}}{\partial \phi_{nm'}} & \dfrac{\partial x_{nm}^{(2)}}{\partial \phi_{nm'}} \end{vmatrix}. \tag{35}$$

Using equations (32), it is found after a few calculations that J_{nM} is the determinant of the block matrix

$$J_{nM} = \det \begin{vmatrix} A(n) & B(n) \\ C(n) & D(n) \end{vmatrix}, \tag{36}$$

where $A(n)$, $B(n)$, $C(n)$, $D(n)$ are lower triangular $M \times M$ matrices with elements

$$A_{mm'}(n) = \theta_{mm'} \cos\phi_{nm'} \qquad B_{mm'}(n) = \theta_{mm'} \sin\phi_{nm'} \tag{37}$$

$$C_{mm'}(n) = -l_{nm'}\theta_{mm'} \sin\phi_{nm'} \qquad D_{mm'}(n) = l_{nm'}\theta_{mm'} \cos\phi_{nm'}. \tag{38}$$

Here the matrix $\theta_{mm'}$ denotes the discrete equivalent of the Heaviside theta-function

$$\theta_{mm'} = 1 \qquad \text{if} \quad m' \leqslant m \tag{39}$$

$$\theta_{mm'} = 0 \qquad \text{if} \quad m' > m. \tag{40}$$

If the matrices $A(n)$, $B(n)$, $C(n)$, $D(n)$ would commute, one could use a known theorem of linear algebra and write $J_{nM} = \det(A(n)D(n) - B(n)C(n))$. In our case these matrices do not commute, but it is still possible to compute the determinant J_{nM} by induction on M.

If $M = 1$, it is easy to show that

$$J_{n1} = l_{n1}. \tag{41}$$

Next, we prove that

$$J_{nM} = l_{nM} J_{n(M-1)}. \tag{42}$$

For this purpose, it will be convenient to introduce new indices $\alpha, \beta = 1, \ldots, M-1$. At this point, we note that the Mth column of the $2M \times 2M$ block matrix whose determinant we wish to compute in equation (35) has only two elements which are not zero. Thus, we expand J_{nM} with respect to the Mth column. Taking into account the necessary permutations and the fact that the two nonvanishing elements are $A_{MM}(n) = \cos\phi_{nM}$ and $C_{MM}(n) = -l_{nm} \sin\phi_{nM}$ we obtain

$$J_{nM} = \cos\phi_{nM} \det \begin{vmatrix} \theta_{\alpha\beta}\cos\phi_{n\beta} & \theta_{\alpha\beta}\sin\phi_{n\beta} & 0 \\ -l_{n\beta}\theta_{\alpha\beta}\sin\phi_{n\beta} & l_{n\beta}\theta_{\alpha\beta}\cos\phi_{n\beta} & 0 \\ -l_{n\beta}\theta_{M\beta}\sin\phi_{n\beta} & l_{n\beta}\theta_{M\beta}\cos\phi_{n\beta} & l_{nM}\cos\phi_{nM} \end{vmatrix}$$
$$+ (-1)^M l_{nM} \sin\phi_{nM} \det \begin{vmatrix} \theta_{\alpha\beta}\cos\phi_{n\beta} & \theta_{\alpha\beta}\sin\phi_{n\beta} & 0 \\ \theta_{M\beta}\cos\phi_{n\beta} & \theta_{M\beta}\sin\phi_{n\beta} & \sin\phi_{nM} \\ -l_{n\beta}\theta_{\alpha\beta}\sin\phi_{n\beta} & l_{n\beta}\theta_{\alpha\beta}\cos\phi_{n\beta} & 0 \end{vmatrix}. \tag{43}$$

The determinants of the remaining two $(2M-1) \times (2M-1)$ matrices may be expanded according to the $(2M-1)$ th column, because these columns contain only one nonvanishing element. After simple calculations one finds

$$J_{nM} = l_{nM} \det \begin{vmatrix} \theta_{\alpha\beta}\cos\phi_{n\beta} & \theta_{\alpha\beta}\sin\phi_{n\beta} \\ -l_{n\beta}\theta_{\alpha\beta}\sin\phi_{n\beta} & l_{n\beta}\theta_{\alpha\beta}\cos\phi_{n\beta} \end{vmatrix}, \tag{44}$$

which is exactly equation (42) because

$$J_{n(M-1)} = \det \begin{vmatrix} \theta_{\alpha\beta}\cos\phi_{n\beta} & \theta_{\alpha\beta}\sin\phi_{n\beta} \\ -l_{n\beta}\theta_{\alpha\beta}\sin\phi_{n\beta} & l_{n\beta}\theta_{\alpha\beta}\cos\phi_{n\beta} \end{vmatrix}. \tag{45}$$

Using equations (41) and (42) it is easy to show by induction that $J_{nM} = l_{nM} l_{n(M-1)} \cdots l_{n1}$. With a straightforward application of equation (34) it is now possible to prove equation (31).

5. Recovering the generating functional $\tilde{\Psi}[J]$ of the constrained stochastic process of equations (11)–(14)

Let us now go back to the generating functional $\Psi[J]$ of equation (26). After the change of variables (27), the delta functions imposing the constraints simplify as follows: $\delta\left(\frac{|\mathbf{R}_{nm}-\mathbf{R}_{n(m-1)}|^2}{a^2}-1\right)=\delta\left(\frac{l_{nm}^2}{a^2}-1\right)$. Further simplifications are obtained after applying the two delta function identities $\delta\left(\frac{l_{nm}^2}{a^2}-1\right)=a^2\delta\left(l_{nm}^2-a^2\right)$ and $\delta\left(l_{nm}^2-a^2\right)=\frac{1}{2a}\left[\delta(l_{nm}-a)+\delta(l_{nm}+a)\right]$. Remembering that in our case $l_{nm}\geqslant 0$, it is possible to put: $\delta\left(l_{nm}^2-a^2\right)=\frac{1}{2a}\delta(l_{nm}-a)$. As a consequence, the expression of the generating functional $\Psi[J]$ in pseudo-polar coordinates becomes

$$\Psi[J]=\lim_{N\to\infty}\lim_{M\to\infty}\int_{-\infty}^{+\infty}\prod_{n,m}\mathrm{d}\boldsymbol{\nu}_{nm}\int_0^{+\infty}\prod_{n,m}\mathrm{d}l_{nm}\int_0^{2\pi}\prod_{n,m}\mathrm{d}\phi_{nm}\exp\left\{-abc\sum_{n,m}\boldsymbol{\nu}_{nm}^2\right\}$$
$$\times\prod_{n,m}\delta(\mathbf{R}_{nm}(\{l_{nm}\},l_{n1};\{\phi_{nm}\})-\varphi_{\nu,nm})\exp\left\{ab\sum_{n,m}\mathbf{J}_{nm}\cdot\mathbf{R}_{nm}(\{l_{nm}\},l_{n1};\{\phi_{nm}\})\right\}$$
$$\times\prod_n l_{n1}\left[\prod_n\prod_{m=2}^{M}\delta\left(l_{nm}-a\right)\right]\prod_{m=2}^{M}l_{nM}\cdots l_{n2}.\tag{46}$$

In writing the above equation we have separated from the Jacobian determinant J_{NM} the contribution coming from the $l_{n1}'s$, because these quantities denote the distance with respect to the origin of the first bead at different times t_n's and are thus not fixed by the constraints. The integration in equation (46) over the l_{nm}'s, for $n=1,\ldots,N$ and $m=2,\ldots,M$, produces as a result

$$\Psi[J]=\lim_{N\to\infty}\lim_{M\to\infty}a^{N(M-1)}\int_{-\infty}^{+\infty}\prod_{n,m}\mathrm{d}\boldsymbol{\nu}_{nm}\int_0^{+\infty}\prod_{n}\mathrm{d}l_{n1}l_{n1}\int_0^{2\pi}\prod_{n,m}\mathrm{d}\phi_{nm}\exp\left\{-abc\sum_{n,m}\boldsymbol{\nu}_{nm}^2\right\}$$
$$\times\prod_{n,m}\delta(\mathbf{R}_{nm}(\{a\},l_{n1};\{\phi_{nm}\})-\varphi_{\nu,nm})\exp\left\{ab\sum_{n,m}\mathbf{J}_{nm}\cdot\mathbf{R}_{nm}(\{a\},l_{n1};\{\phi_{nm}\})\right\}.\tag{47}$$

Here the symbol $\{a\}$ denotes the set of all l_{nm}'s for $m\neq 2$ after the imposition of the constraints $l_{nm}=a$. We can now rewrite equation (47) as an integral over a restricted domain D:

$$\Psi[J]=\lim_{N\to\infty}\lim_{M\to\infty}\int_D\prod_{n,m}\mathrm{d}l_{nm}\mathrm{d}\phi_{nm}\int_{-\infty}^{+\infty}\prod_{n,m}\mathrm{d}\boldsymbol{\nu}_{nm}\exp\left\{-abc\sum_{n,m}\boldsymbol{\nu}_{nm}^2\right\}\prod_n l_{nM}\cdots l_{n1}$$
$$\times\prod_{n,m}\delta(\mathbf{R}_{nm}(\{l_{nm}\},l_{n1};\{\phi_{nm}\})-\varphi_{\nu,nm})\exp\left\{ab\sum_{n,m}\mathbf{J}_{nm}\cdot\mathbf{R}_{nm}(\{l_{nm}\},l_{n1};\{\phi_{nm}\})\right\},\tag{48}$$

where D is the domain of all l_{nm}'s and ϕ_{nm}'s with the constraints $l_{nm}=a$ for $m=2,\ldots,M$ and $n=1,\ldots,N$:

$$D=\left\{\{l_{nm}\},\{\phi_{nm}\}\,\middle|\,\begin{array}{lll}l_{nm}=a & m=2,\ldots,M & \text{and}\quad n=1,\ldots,N\\ 0\leqslant l_{n1}\leqslant+\infty & n=1,\ldots,N & \\ 0\leqslant\phi_{nm}\leqslant 2\pi & m=1,\ldots,M & \text{and}\quad n=1,\ldots,N\end{array}\right\}.\tag{49}$$

At this point, using equations (30) and (31) we go back to Cartesian coordinates

$$\Psi[J] = \lim_{N\to\infty}\lim_{M\to\infty}\int_D \prod_{n,m} \mathrm{d}\mathbf{R}_{nm} \int_{-\infty}^{+\infty} \prod_{n,m} \mathrm{d}\boldsymbol{\nu}_{nm} \exp\left\{-abc\sum_{n,m}\boldsymbol{\nu}_{nm}^2\right\}$$
$$\times \prod_{n,m}\delta(\mathbf{R}_{nm} - \varphi_{\nu,nm})\exp\left\{ab\sum_{n,m}\mathbf{J}_{nm}\cdot\mathbf{R}_{nm}\right\}. \qquad (50)$$

The domain D in Cartesian coordinates is given by all $\mathbf{R}_{nm}$'s in the two-dimensional plane subjected to the constraints (25):

$$D = \left\{ \{\mathbf{R}_{nm}\} \,\middle|\, \begin{array}{lll} \mathbf{R}_{nm} \in \mathbb{R}^2 & m = 1, \ldots, M & n = 1, \ldots, N \\ \frac{|\mathbf{R}_{nm} - \mathbf{R}_{n(m-1)}|^2}{a^2} = 1 & m = 2, \ldots, M & n = 1, \ldots, N \end{array} \right\}. \qquad (51)$$

Finally, we rewrite the path integral in equation (50) in its continuous form. The result is

$$\Psi[J] = \int_{\mathbf{R}'^2=1} \mathcal{D}\mathbf{R} \int \mathcal{D}\boldsymbol{\nu}\, \mathrm{e}^{-c\int_0^{t_f}\mathrm{d}t\int_0^L \mathrm{d}s\boldsymbol{\nu}^2}\delta(\mathbf{R}-\varphi_\nu)\,\mathrm{e}^{\int_0^{t_f}\mathrm{d}t\int_0^L \mathrm{d}s\mathbf{J}\cdot\mathbf{R}}. \qquad (52)$$

The right-hand side of the above equation coincides exactly with the right-hand side of equation (16). This proves the equivalence between the generating functional $\Psi[J]$ of the GNLσM and the generating functional $\tilde{\Psi}[J]$ of the stochastic process of equations (11)–(14).

6. Conclusions

In this work it has been shown that the GNLσM is related to a stochastic process which, after discretization of the arc-length variable s, describes the Brownian motion of M beads subjected to the constraints (25). These constraints enforce the conditions that the links connecting the beads are of fixed length. More in details, it has been proved that the generating functional $\Psi[J]$ of the GNLσM coincides with the generating functional $\tilde{\Psi}[J]$ of the solutions of the Langevin equation (11) and of the constraint (14). The fact that the two functionals are equal was not *a priori* obvious, because they differ by the delta function $\delta(\mathbf{R}'^2 - 1)$ which contains quadratic powers of the fields. If $\delta(g(\mathbf{R}))$ is a delta function imposing the condition $g(\mathbf{R}) = 0$, then in general the following identity is valid:

$$\int \mathcal{D}\mathbf{R} f(\mathbf{R})\delta(g(\mathbf{R})) = \int_{g(\mathbf{R})=0} \mathcal{D}\mathbf{R} f(\mathbf{R})\det{}^{-1}\left|\frac{\delta g(\mathbf{R})}{\delta\mathbf{R}}\right|. \qquad (53)$$

If in our case the functional determinant appearing in the right-hand side of equation (53) would be not trivial, then there would be no chance that (16) and (21) coincide. Luckily, it turns out that, after passing to the pseudo-polar coordinates (27), the delta function $\delta(\mathbf{R}'^2 - 1)$ produces just a functional determinant which is a trivial constant.

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