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2006 J. Phys. A: Math. Gen. 39 8231

(http://iopscience.iop.org/0305-4470/39/26/001)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **39** (2006) 8231–8255 doi:10.1088/0305-4470/39/26/001

Perturbation theory for path integrals of stiff polymers

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Received 27 January 2006, in final form 21 May 2006
Published 14 June 2006
Online at stacks.iop.org/JPhysA/39/8231

Abstract
The wormlike chain model of stiff polymers is a nonlinear σ-model in one spacetime dimension in which the ends are fluctuating freely. This causes important differences with respect to the presently available theory which exists only for periodic and Dirichlet boundary conditions. We modify this theory appropriately and show how to perform a systematic large-stiffness expansion for all physically interesting quantities in powers of L/ξ, where L is the length and ξ the persistence length of the polymer. This requires special procedures for regularizing highly divergent Feynman integrals which we have developed in previous work. We show that by adding to the unperturbed action a correction term $\mathcal{A}^{\rm corr}$, we can calculate all Feynman diagrams with Green functions satisfying Neumann boundary conditions. Our expansions yield, order by order, a properly normalized end-to-end distribution function in arbitrary dimensions d, its even and odd moments and the two-point correlation function.

PACS number: 05.45.−a

1. Introduction

Recently, the study of biopolymers has become a subject of increasing interest in the research of biological materials. Forming networks, constituent filaments play an important role in the structure and function of living cells and other biological entities [1, 2]. Recent advances in visualizing and manipulating single cytoskeletal filaments [3, 4] and DNA [5, 6] have inspired the study of conformational characteristics of biopolymers in single-molecule experiments [7, 8].

Biopolymers may be *flexible*, such as DNA, *semiflexible* or *stiff*, such as actin, or *rigid*, such as microtubuli. For a polymer with stiffness κ, the *persistence length* of tangent–tangent fluctuations is $\xi = 2\kappa/(d-1)k_BT$. Typical values of ξ in biopolymers range from several nanometres to a few millimetres. Some examples are DNA, $\xi \approx 50\,\mathrm{nm}$ [5]; spectrin, $\xi \approx 10\,\mathrm{nm}$ [4]; actin, $\xi \approx 17\,\mu\mathrm{m}$; and microtubules, $\xi \approx 5\,\mathrm{mm}$ [3].

The length L of a polymer is conveniently measured in units of ξ, which defines a dimensionless parameter characterizing the inverse stiffness, or the *reduced length* $l = L/\xi$, which we shall also call *flexibility*. For high flexibility l, a polymer behaves approximately like an ideal random chain with freely joint links [9]. For small flexibility l, it behaves like a rigid rod. Under the influence of longitudinal compressing forces these filaments exhibit the classical Euler buckling [10].

Most constituent filamentary biopolymers are *semiflexible* with intermediate values of l. If l is of the order of unity, the stiffness is important but not overwhelming. Effects of stiffness have been observed even for large flexibilities up to $l \approx 1000$, for instance in long strands of DNA. Stretching these at large forces has shown significant deviations from a random chain model [6]. It is therefore important to develop a reliable theory to calculate the influence of stiffness upon polymers for the entire range of flexibilities [1, 2].

If a polymer has a sizable stiffness, self-avoidance effects can be neglected due to the energetic suppression of configurations where the filaments fold back onto themselves. An appropriate model for a theoretical description of semiflexible polymers is the *wormlike chain model* proposed by Kratky and Porod in 1949 [11]. This model is formulated most directly in terms of path integrals. The calculation of the statistical properties has mostly been based so far on the equivalent diffusion equation [12]. For a recent review, see Yamakawa's textbook [13], the review article by Chirikjian and Wang [14] and chapter 15 of the textbook of one of the authors [15].

The wormlike chain model is the minimal model of a polymer with arbitrary stiffness. A central feature of this model is the local inextensibility of filaments which is mathematically accounted for by constraining the length of all tangent vectors to unity. Being a sequence of d-component unit vectors, a polymer is equivalent to a particle moving on the surface of a unit sphere in d dimensions, which is described by a quantum-mechanical $O(d)$-symmetric nonlinear σ-model in one spacetime dimension.

Another equivalence exists to the continuum limit of the classical Heisenberg chain of unit magnets. In fact, the partition function of the lattice model was calculated 35 years ago by Stanley [16] in $d = 3$ dimensions. In the magnetic context, however, the quantities of interest in polymer physics were never considered.

Because of the nonlinearity of the wormlike chain model, only a few of the statistical properties of the stiff polymer can be calculated analytically, the most prominent being the mean square $\langle \mathbf{R}^2 \rangle$ of the end-to-end distance $\mathbf{R}$, and a number of higher moments $\langle \mathbf{R}^{2n} \rangle$, for $n \leqslant 14$. The lowest even moments have been calculated a long time ago analytically [17] and numerically [18] by solving recursively the diffusion equation on the unit sphere in three dimensions. The calculations have recently been extended for $d = 3$ up to $n = 13$ in [19] and for arbitrary d up to $n = 14$ in [20]. By this technique it is impossible, however, to derive the end-to-end distribution function for all persistence lengths. To derive this central quantity of the wormlike chain, one has to resort to perturbation schemes. So far, only approximate but highly accurate expressions for the end-to-end distribution of two- and three-dimensional stiff polymers were obtained for all persistence lengths in [19–21].

The end-to-end distribution function $P(\mathbf{R}; L)$ is a principal physical quantity characterizing the statistical properties of a single polymer of length L. For models like the wormlike chain which has only short-range interactions between monomers, it gives also the probability density of finding *any two monomers* at spatial distance $\mathbf{R} = \mathbf{x}(s) - \mathbf{x}(s')$, not just the endpoints, if we identify L with the distance $|s - s'|$ between monomers measured along the chain.

In the random-chain limit of large l, the distribution $P(\mathbf{R}; L)$ is known exactly [13, 15] and can be approximated by a simple Gaussian. For moderately large l, the corrections to the Gaussian distribution were calculated up to the order l^{-2} in three dimensions by Daniels [22], and for arbitrary d by one of the authors [15].

For polymers close to the rod limit, all moments and the distribution function $P(\mathbf{R}; L)$ were calculated as expansions in powers of l for $d = 3$ in [17, 23, 24]. In the same limit, the distribution function has recently been found as an infinite series of parabolic cylinder functions for $d = 2$, and of Hermite polynomials for $d = 3$ in [25]. The generalization to d dimensions is given in chapter 15 of the textbook [15].

These distributions were derived from the path integral of a simple harmonic oscillator [25]. For large stiffness, they are in good quantitative agreement with Monte Carlo data. They disagree, however, with the exact expansions of [23], except for a few lowest orders. Since the failure has a perturbative character, it cannot be compensated by a proper normalization. The reason is that the harmonic path integral approximates correctly the wormlike chain model only at lowest flexibility. It certainly needs *higher-order* corrections.

If we want to calculate such corrections in the path integral formalism, the choice of physically appropriate boundary conditions is essential. The open-end boundary conditions of the wormlike chain model are quite tedious for the perturbative calculation of path integrals. For a harmonic oscillator, they can be replaced by the simpler Neumann boundary conditions, as proposed in [25]. However, to describe the properties of a wormlike chain, the harmonic fluctuations must be suppressed at the endpoints. This can be done by incorporating an important correction factor into the path integral with Neumann boundary conditions.

Calculation schemes based on periodic boundary conditions were considered in [26, 27]. Path integrals for modified wormlike chain models with softened inextensibility conditions have been suggested in [28–31]. These models, however, can describe the behaviour of the stiff polymer only roughly. Some conformational properties were calculated in [32, 33]. Additional insights into the properties of the end-to-end distribution function of polymers with intermediate stiffness have also been provided recently by [34, 35].

Despite a number of recent developments, the theoretical understanding of the statistical properties of a semiflexible chain in isolation remains much less developed than for the flexible chain, and experimental data are often interpreted within the theoretical framework established for random chains or rigid rods, respectively. It is therefore important to find a unified analytic approximation procedure which will yield a reliable end-to-end distribution over the entire range of stiffnesses. In particular, the crossover region between the random chain properties at low stiffness and the rigid-rod limit should be described properly.

In this paper, we develop a systematic path integral approach to find the properties of the wormlike chain model near the rod limit. We shall set up a perturbation theory for a large-stiffness expansion in powers of the flexibility l and show how to calculate all expansion coefficients analytically. All moments, the radial end-to-end distribution function, and the two-point correlation function will be obtained in arbitrary dimensions d. By this unified approach we reproduce correctly the results of [23], and show how to go systematically beyond the approximate large-stiffness result of [25] for a polymer in $d = 3$ dimensions.

2. Wormlike chain model

In the wormlike chain model, the polymer is described by a smooth curve $\mathbf{x}(s)$ in d-dimensional flat space, with the components $x^i(s), i = 1, \ldots, d$. The parameter $s \in (0, L)$ is the arc length along the curve defined by $\mathrm{d}s = \sqrt{(\mathrm{d}\mathbf{x})^2}$. In this parametrization, the derivatives

$\mathrm{d}\mathbf{x}(s)/\mathrm{d}s \equiv \mathbf{u}(s)$ are tangent vectors of unit length:

$$|\mathbf{u}(s)| = 1. \tag{1}$$

This important property accounts for the local inextensibility of a polymer. All vectors $\mathbf{u}(s)$ lie on a surface of a unit sphere in d dimensions which has an area $S_d = 2\pi^{d/2}/\Gamma(d/2)$ and a constant scalar curvature $R = (d-1)(d-2)$.

The local curvature of the polymer is $k(s) = |\dot{\mathbf{u}}(s)|$, where $\dot{\mathbf{u}}(s) = \mathrm{d}\mathbf{u}(s)/\mathrm{d}s$. The bending energy of the wormlike chain model is quadratic in $k(s)$:

$$E_{\mathrm{c}}[\mathbf{u}] = \frac{k_B T}{2\varepsilon} \int_0^L \mathrm{d}s\, \dot{\mathbf{u}}^2(s), \tag{2}$$

where we have introduced the *inverse stiffness* $\varepsilon = k_B T/\kappa$ in units of $k_B T$. The flexibility l is simply related to ε by $l = \varepsilon L(d-1)/2$.

The statistical properties of the model are completely determined by the partition function

$$Z = S_d^{-1} \int \mathrm{d}^d u_b\, \delta(\mathbf{u}_b^2 - 1) \int \mathrm{d}^d u_a\, \delta(\mathbf{u}_a^2 - 1) z(\mathbf{u}_b, \mathbf{u}_a), \tag{3}$$

where $z(\mathbf{u}_b, \mathbf{u}_a)$ is a *partition function density* defined by the path integral

$$z(\mathbf{u}_b, \mathbf{u}_a) = \mathrm{e}^{\varepsilon L R/8} \int_{\mathbf{u}(0)=\mathbf{u}_a}^{\mathbf{u}(L)=\mathbf{u}_b} \mathcal{D}^d u(s) \delta[\mathbf{u}^2(s) - 1] \exp\left(-\frac{1}{2\varepsilon} \int_0^L \mathrm{d}s\, \dot{\mathbf{u}}^2(s)\right). \tag{4}$$

This coincides with the path integral for the imaginary-time evolution amplitude $\langle \mathbf{u}_b L | \mathbf{u}_a 0 \rangle$ of a particle on the surface of the unit sphere in d dimensions which possesses an obvious $O(d)$-symmetry. The length parameter s plays the role of the imaginary time or *pseudo-time*, and the bending energy (2) in the exponent of (4) is proportional to the *Euclidean action* $\mathcal{A}$ of a particle: $E_{\mathrm{c}}[\mathbf{u}] = k_B T \mathcal{A}[\mathbf{u}]$. We shall often use this analogy in the following.

The delta-functional in the integrand of (4) accounts for the local inextensibility (1). At the endpoints $s = 0, L$, this constraint is also accounted for by the two ordinary δ-functions in equation (3). The restricted ordinary integrals over the initial and final $\mathbf{u}$-values lead to the *partition function with open ends* (3). The path integral (4) for the density is calculated with fixed ends, i.e., with Dirichlet boundary conditions (DBC). The extra covariant prefactor $\mathrm{e}^{\varepsilon L R/8}$ is necessary to reproduce the correct diffusion equation on the unit sphere [15, 38] whose Hamiltonian is a Laplace–Beltrami operator.

The principal physical quantity of a semiflexible polymer is the distribution function

$$P(\mathbf{R}; L) = \left\langle \delta^{(d)}\left(\mathbf{R} - \int_0^L \mathrm{d}s\, \mathbf{u}(s)\right)\right\rangle, \tag{5}$$

with $\mathbf{R} = \mathbf{x}(L) - \mathbf{x}(0)$ being the end-to-end vector. It possesses the moments

$$\langle (\mathbf{R}^2)^{n/2} \rangle = \left\langle \left[\int_0^L \int_0^L \mathrm{d}s\, \mathrm{d}s'\, \mathbf{u}(s) \cdot \mathbf{u}(s')\right]^{n/2} \right\rangle, \tag{6}$$

which have been calculated exactly for even n up to high n by solving the diffusion equation on a sphere. From this solution we also know the rotationally invariant two-point correlation function

$$G(s, s') = \langle \mathbf{u}(s) \cdot \mathbf{u}(s') \rangle \tag{7}$$

as being simply

$$G(s, s') = \exp(-|s - s'|/\xi) \tag{8}$$

displaying clearly the exponential decay of tangent–tangent correlations over the persistence length ξ. We shall show that all expectation values (5)–(7) are calculable from the path integral representation (3) of the partition function by inserting the quantities inside the Dirac brackets into the integrand of equation (4).

The inextensibility condition (1) makes the path integral non-Gaussian. For an analytic treatment, we may follow two methods. One may either solve the inextensibility condition (1) explicitly. Then the $O(d)$-symmetry is realized nonlinearly. In geometric language, $O(d)$ is the *isometry* of the metric on a surface of the sphere. This method will be used in this paper to develop the large-stiffness perturbation expansion of path integrals, in which all physical quantities are expressed as power series in l. A second method may be based on enforcing the inextensibility condition (1) with the help of a Lagrange multiplier. This leads to calculations of the physical quantities as power series in $1/d$ to be presented in a forthcoming paper [40]. Both options lead to systematic approximation schemes.

3. Large-stiffness expansion

The large-stiffness expansion of the path integral in powers of $\varepsilon \propto l$ is a special case of weak-coupling perturbation expansions, which have recently been developed by us for quantum-mechanical path integrals of nonlinear σ-models with various boundary conditions [15, 36–39].

3.1. Calculation with Dirichlet boundary conditions

To make contact with the methods developed in the previous papers, we eliminate the δ-functional in (4) by setting $\mathbf{u}(s) = (q^0(s), q^\mu(s),)$ with $\mu = 1, \ldots, d-1$, and integrating over $q^0(s)$, which yields $q^0(s) = \sigma(s) \equiv \sqrt{1-q^2(s)}$. The partition function density becomes

$$z(q_b, q_a) = \int_{\mathrm{DBC}} \mathcal{D}^{d-1}q(s)\sqrt{g(q(s))}\exp\left\{-\frac{1}{2\varepsilon}\int_0^L \mathrm{d}s\, g_{\mu\nu}(q)\dot{q}^\mu(s)\dot{q}^\nu(s) + \varepsilon L\frac{R}{8}\right\}, \tag{9}$$

with the metric $g_{\mu\nu}(q) = \delta_{\mu\nu} + (1-q^2)^{-1}q_\mu q_\nu$ and the determinant $g(q) = (1-q^2)^{-1}$.

The square root in the invariant measure can be rewritten formally as

$$\prod_s \sqrt{g(q(s))} = \exp\left\{\frac{1}{2}\sum_s \log g(q(s))\right\} = \exp\left\{\frac{1}{2}\int_0^L \mathrm{d}s\, \delta(s,s)\log g(q(s))\right\}, \tag{10}$$

where the quantity $\int_0^L \mathrm{d}s\, \delta(s,s) = L\delta(0)$ counts the infinite number of eigenvalues of the operator $-\delta_{\mu\nu}(d/\mathrm{d}s)^2$ in the space of functions $q^\mu(s)$. Including the exponent of (10) into the action we are left with the partition function density

$$z(q_b, q_a) = \int_{\mathrm{DBC}} \mathcal{D}^{d-1}q(s)\exp\{-\mathcal{A}[q]\}, \tag{11}$$

with the Euclidean action

$$\mathcal{A}[q] = \frac{1}{2\varepsilon}\int_0^L \mathrm{d}s[g_{\mu\nu}(q)\dot{q}^\mu(s)\dot{q}^\nu(s) - \varepsilon\delta(s,s)\log g(q(s))] - \varepsilon L\frac{R}{8}. \tag{12}$$

Repeated indices are summed as usual, i.e., $q_\mu q^\mu = q^2$. In a perturbation expansion of the path integral (9), the inverse stiffness $\varepsilon \propto l$ plays the role of a *coupling constant*. The large-stiffness or small-flexibility expansion is a weak-coupling expansion. The subscript DBC in equation (9) emphasizes the Dirichlet boundary conditions $q^\mu(L) = q_b^\mu$, $q^\mu(0) = q_a^\mu$.

To derive the perturbation expansion of [15, 36–39], it is convenient to rescale the coordinates $q^\mu(s) \to \sqrt{\varepsilon}q^\mu(s)$. This removes ε from the quadratic part of the action. The path integral for $\varepsilon = 0$ is therefore Gaussian and determines the basic free correlation function or *propagator*

$$\langle q^{\mu}(s)q^{\nu}(s')\rangle_0 = \delta^{\mu\nu}\Delta(s, s'), \tag{13}$$

where $\Delta(s, s')$ is the Green function of the operator $-d_s^2$ in the space of functions $q(s)$ with appropriate boundary conditions.

An expansion of the action in powers of ε organizes the infinitely many interaction terms. They give rise to fluctuation corrections which are calculated by performing all possible Wick contractions. These consist of multiple integrals over the pseudo-time s containing products of propagators (13) and their s-derivatives. These integrals are mathematically undefined, since derivatives of the propagator (13) contain *generalized functions* or *distributions*, such as Heaviside functions $\Theta(s - s')$ and Dirac δ-functions $\delta(s - s')$. The problem of defining these integrals has, fortunately, been solved in our previous work [36–38]. We have shown that all these highly singular integrals are defined *uniquely* on the basis of the simple physical requirement that the path integrals should be independent of the coordinates used to parametrize the unit sphere. The new integration rules are valid for path integrals with all boundary conditions. Moreover, they are in complete agreement with much more cumbersome calculations in $D = 1 - \epsilon$ dimensions, in which the limit $\epsilon \to 0$ is taken at the end (*dimensional regularization*). For one-dimensional σ-models with Dirichlet and periodic boundary conditions, our rules have led to a perfect cancellation of all UV-divergent diagrams involving powers of $\delta(0)$ in each perturbative order [37–39]. This permitted us to calculate finite fluctuation corrections to any desired order in perturbation theory.

The method developed in [15, 36–39] can be used now to derive the partition function with open ends (3). In coordinates $q^{\mu}(s)$, this quantity takes the form

$$Z = S_d^{-1}\int \mathrm{d}^{d-1}q_b\,\sqrt{g(q_b)}\int \mathrm{d}^{d-1}q_a\,\sqrt{g(q_a)}z(q_b, q_a). \tag{14}$$

This way of writing Z suggests that we must compute the path integral (9) with Dirichlet boundary conditions, and subsequently perform two ordinary integrals over initial and final q^{μ}-values. The advantage of this procedure would be that all necessary tools are available from our previous work in [15, 38]. We would expand the action (12) in powers of the coordinates $q^{\mu}(s)$ around the straight-line solution connecting the endpoints, and evaluate higher-order fluctuation corrections with the help of the basic propagator (13) with Dirichlet boundary conditions

$$\Delta_{\mathrm{D}}(s, s') = -|s - s'|/2 + (s + s')/2 - ss'/L. \tag{15}$$

The resulting expansion of $z(q_b, q_a)$ involves the geometric invariants formed from the curvature tensor on q-space. For the unit sphere in d dimensions, only powers of the curvature scalar $R = (d - 1)(d - 2)$ remain, and the expansion has the form

$$z(q_b, q_a) = \langle q_b L|q_a 0\rangle = \frac{\mathrm{e}^{-\mathcal{A}^{\mathrm{cl}}[\Delta q;\varepsilon]}}{\sqrt{2\pi L}^{d}}\sum_{k=0}^{\infty} L^k a_k(\Delta q; \varepsilon), \tag{16}$$

where the classical action in the exponent depends on $\Delta q^{\mu} \equiv (q_b - q_a)^{\mu}$ as

$$\mathcal{A}^{\mathrm{cl}}[\Delta q; \varepsilon] \equiv \frac{(\Delta q)^2}{2L} + \varepsilon\frac{[(\Delta q)^2]^2}{6L} + \cdots, \tag{17}$$

and the lowest coefficients $a_k(\Delta q; \varepsilon)$ have the small-ε expansions

$$a_0(\Delta q; \varepsilon) \equiv 1 + \varepsilon\frac{(d - 2)}{12}(\Delta q)^2 + \varepsilon^2\frac{(d - 2)(5d - 6)}{1440}[(\Delta q)^2]^2 + \cdots,$$

$$a_1(\Delta q;\varepsilon) \equiv \varepsilon\frac{(d-1)(d-2)}{12} + \varepsilon^2\frac{(d-2)(5d^2-17d+18)}{720}(\Delta q)^2 + \cdots,$$
$$a_2(\Delta q;\varepsilon) \equiv \varepsilon^2\frac{(d-1)(d-2)(5d^2-17d+18)}{1440} + \cdots. \tag{18}$$

From this we can immediately find the partition function (14) with open ends. Inserting (16) into (14) yields

$$Z = 1, \tag{19}$$

to all orders in ε.

3.2. Calculation with Neumann boundary conditions

For a calculation of the important polymer properties (5)–(7) this procedure, although well defined, would be too tedious. To save efforts, we prefer to do the calculations from a path integral in which the ordinary integrals over endpoints in equation (3) are included in the path integral by suitable boundary conditions. For a simple harmonic oscillator, these were shown in [15] to be the *Neumann boundary conditions* (NBC), as anticipated by [25]. These conditions may, however, not be used directly for calculating the fluctuation corrections since they are physically incorrect. The Neumann boundary conditions admit only fluctuations in which the endpoints have zero derivatives $\dot{q}^\mu(0) = \dot{q}^\mu(L) = 0$, thus neglecting all paths with nonzero derivatives. We shall see that this omission can be compensated by adding to the action an important correction term, so that Neumann boundary conditions may be used after deriving the correct perturbation expansions.

We shall evaluate the quantities (5)–(7) from path integrals with Neumann boundary conditions by replacing the combined measure of equations (3) and (9) as follows:

$$\int \mathrm{d}^{d-1}q_b\,\sqrt{g(q_b)}\int \mathrm{d}^{d-1}q_a\,\sqrt{g(q_a)}\int_{\mathrm{DBC}}\mathcal{D}^{d-1}q(s) \to \int_{\mathrm{NBC}}\mathcal{D}^{d-1}q(s)J[q_b,q_a], \tag{20}$$

where the Jacobian factor $J[q_b, q_a]$ corrects for the missing endpoint fluctuations when restricting the paths to zero derivatives at the ends. This factor may be attributed to an extra action at the endpoints,

$$\mathcal{A}^{\mathrm{cor}}[q_b,q_a] = -\log J[q_b,q_a] = -[q^2(0)+q^2(L)]/4, \tag{21}$$

to be added to (12).

Our correction term (21) should no be confused with a similar-looking but completely unrelated term $\lambda\{[\mathbf{u}^2(0)-1]+[\mathbf{u}^2(L)-1]\}$ in harmonic models of stiff polymers [29–31], where it serves to enforce *approximately* the inextensibility (1) at the endpoints, which in our approach is satisfied *exactly* for the entire polymer.

Thus we shall calculate the polymer properties (5)–(7) by performing the averages inside with respect to the path integral representation for Z with Neumann boundary conditions

$$Z = S_d^{-1}\int_{\mathrm{NBC}}\mathcal{D}^{d-1}q(s)\exp\{-\mathcal{A}[q]-\mathcal{A}^{\mathrm{cor}}[q_b,q_a]\}. \tag{22}$$

The perturbation expansion of this expression is not straightforward since with Neumann boundary conditions the fluctuations of the free part of the action contain $d-1$ zero modes. These are due to the $d-1$ constant solutions $q^\mu(s) = c^\mu$ of the 'equation of motion' $-(\mathrm{d}/\mathrm{d}s)^2q^\mu(s) = 0$. Their symmetry origin lies in the $d-1$ isometries of a sphere in d dimensions. They prevent us from inverting the operator $-(\mathrm{d}/\mathrm{d}s)^2$ to obtain a perturbative propagator (13). The zero modes must first be extracted from the path integral.

The proper way of doing this has recently been exhibited for one-dimensional path integrals of a nonlinear σ-model with periodic paths in [39]. The method can easily be modified to apply to Neumann boundary conditions. To avoid overcounting of the constant paths in the elimination process, we have to fix a coordinate system $q^\mu(s)$, for example, by placing the centre of mass of a polymer at the origin. Let us assume that the end-to-end distance vector $\mathbf{R} = \int_0^L \mathrm{d}s\, \mathbf{u}(s)$ points towards the dth direction. In coordinates $q^\mu(s)$, this yields the zero average

$$L^{-1}\int_0^L \mathrm{d}s\, q^\mu(s) = 0, \qquad \mu = 1, \ldots, d-1. \tag{23}$$

We therefore introduce the measure of fluctuations without the dangerous $d-1$ zero modes as

$$\mathcal{D}'^{d-1}q(s) = \mathcal{D}^{d-1}q(s)\delta^{(d-1)}\left[\int_0^L \mathrm{d}s\, q^\mu(s)\right] \tag{24}$$

to be used instead of the measure in equation (20).

This can be done most directly for the distribution function (5). Introducing the *reduced end-to-end distance* $r \equiv |\mathbf{R}|/L$, we represent this quantity via the path integral

$$P(r; L) = S_d^{-1}\int_{\mathrm{NBC}} \mathcal{D}'^{d-1}q(s)\delta\left(r - L^{-1}\int_0^L \mathrm{d}s\,\sqrt{1-q^2(s)}\right)\exp\{-\mathcal{A}[q] - \mathcal{A}^{\mathrm{cor}}[q_b, q_a]\}. \tag{25}$$

In turn, the partition function (22) can be obtained from the distribution (25) as

$$Z = S_d\int_0^\infty \mathrm{d}r\, r^{d-1}P(r; L), \tag{26}$$

where the prefactor S_d reflects the rotation invariance of $P(r; L)$. Since the zero modes are already excluded from the path integration in equation (25), we integrate simply over r in equation (26) with help of the δ-function in equation (25) to define the path integral (22). This produces a further contribution to the action (12),

$$\mathcal{A}^{\mathrm{FP}}[q] = -(d-1)\log\left(L^{-1}\int_0^L \mathrm{d}s\,\sqrt{1-q^2(s)}\right), \tag{27}$$

to be referred to as *Faddeev–Popov action*. For periodic paths this action was found in our paper [39]. It is a logarithmic Jacobian which compensates the distorting effect of condition (23) on the measure of path integration. This procedure of extracting the zero modes guarantees therefore the independence of path integrals of the choice of the coordinate system (23) used in the perturbative calculation.

Thus we rewrite the partition function (22) as a path integral

$$Z = \int_{\mathrm{NBC}} \mathcal{D}'^{d-1}q(s)\exp\left\{-\mathcal{A}[q] - \mathcal{A}_{\mathrm{e}}^{\mathrm{cor}}[q_b, q_a] - \mathcal{A}^{\mathrm{FP}}[q]\right\}, \tag{28}$$

where the paths not only satisfy the Neumann boundary conditions, but have also no zero modes. Note that the prefactor S_d in (22), the volume of the isometries, is now absent.

The expectation values in equations (5)–(7) can now be defined with respect to this partition function as follows:

$$\langle\cdots\rangle \equiv \int_{\mathrm{NBC}} \mathcal{D}'^{d-1}q(s)(\cdots)\exp\{-\mathcal{A}[q] - \mathcal{A}^{\mathrm{cor}}[q_b, q_a] - \mathcal{A}^{\mathrm{FP}}[q]\}. \tag{29}$$

Note that there is no need to normalize the path integral (29) by $Z = Z_0$, since the partition function (28) is equal to unity as in equation (19). This will be verified order by order in perturbation expansion of the path integral (28).

With the definition (29), the radial distribution function is given by the path integral

$$
\begin{aligned}
P^{\text{rad}}(r;L) &= \left\langle \delta\left(r - L^{-1}\int_0^L \mathrm{d}s\,\sqrt{1-q^2(s)}\right)\right\rangle \\
&= \int_{\text{NBC}} \mathcal{D}'^{d-1}q(s)\delta\left(r - L^{-1}\int_0^L \mathrm{d}s\,\sqrt{1-q^2(s)}\right) \\
&\quad\times \exp\{-\mathcal{A}[q] - \mathcal{A}^{\text{cor}}[q_b,q_a] - \mathcal{A}^{\text{FP}}[q]\} \\
&= S_d r^{d-1} P(r;L),
\end{aligned} \tag{30}
$$

where the Faddeev–Popov action (27) is illuminated by the δ-function, whereas the moments (6) of the reduced distance r are found from

$$
\begin{aligned}
\langle(\mathbf{R}^2/L^2)^{n/2}\rangle = \langle r^n\rangle &= \left\langle \left(L^{-1}\int_0^L \mathrm{d}s\,\sqrt{1-q^2(s)}\right)^n\right\rangle \\
&= \int_{\text{NBC}} \mathcal{D}'^{d-1}q(s)\left(L^{-1}\int_0^L \mathrm{d}s\,\sqrt{1-q^2(s)}\right)^n \\
&\quad\times \exp\{-\mathcal{A}[q] - \mathcal{A}^{\text{cor}}[q_b,q_a] - \mathcal{A}^{\text{FP}}[q]\} \\
&= \int_{\text{NBC}} \mathcal{D}'^{d-1}q(s)\exp\big\{-\mathcal{A}[q] - \mathcal{A}^{\text{cor}}_{\text{e}}[q_b,q_a] - \mathcal{A}^{\text{FP}}_n[q]\big\} \equiv Z_n.
\end{aligned} \tag{31}
$$

This looks similar to equation (28) except for the last action term which now is

$$
\mathcal{A}^{\text{FP}}_n[q] = -(n+d-1)\log\left(L^{-1}\int_0^L \mathrm{d}s\,\sqrt{1-q^2(s)}\right), \tag{32}
$$

rather than (27). The path integral (31) abbreviated by Z_n comprises for $n = 0$ the unit partition function (28): $Z_0 = Z = 1$.

With the zero modes subtracted, the Green function with Neumann boundary conditions representing the lines in the Feynman diagrams acquires the form

$$
\Delta'_{\text{N}}(s,s') = L/3 - |s-s'|/2 - (s+s')/2 + (s^2+s'^2)/2L, \tag{33}
$$

$$
\int_0^L \mathrm{d}s\,\Delta'_{\text{N}}(s,s') = 0. \tag{34}
$$

In the following we shall simply write $\Delta(s,s')$ for $\Delta'_{\text{N}}(s,s')$, for brevity.

4. Partition function and all moments up to four loops

We present now the explicit perturbative calculation of the partition function (28) and all moments (31) to order $\varepsilon^2 \propto l^2$. This requires evaluating Feynman diagrams up to four loops. As mentioned before, the fluctuation corrections involve integrals over products of distributions, which will be calculated unambiguously using the rules derived in [37, 38].

For perturbation calculation, we rescale the coordinates $q^\mu(s) \to \sqrt{\varepsilon}q^\mu(s)$ and rewrite the path integral (31) as

$$
Z_n = \int_{\text{NBC}} \mathcal{D}'^{d-1}q(s)\exp\big\{-\mathcal{A}^{\text{tot}}_{,n}[q;\varepsilon]\big\}, \tag{35}
$$

where the total action $\mathcal{A}^{\text{tot}}_{,n}[q;\varepsilon] \equiv \mathcal{A}[q;\varepsilon] + \mathcal{A}^{\text{cor}}[q_b,q_a;\varepsilon] + \mathcal{A}^{\text{FP}}_{,n}[q;\varepsilon]$ reads explicitly,

$$
\begin{aligned}
\mathcal{A}^{\text{tot}}_{,n}[q;\varepsilon] &= \int_0^L \mathrm{d}s\left[\frac{1}{2}\left(\dot{q}^2 + \varepsilon\frac{(q\dot{q})^2}{1-\varepsilon q^2}\right) + \frac{1}{2}\delta(0)\log(1-\varepsilon q^2)\right] \\
&\quad - \sigma_n\log\left[\frac{1}{L}\int_0^L \mathrm{d}s\,\sqrt{1-\varepsilon q^2}\right] - \frac{1}{4}\varepsilon[q^2(0)+q^2(L)] - \varepsilon L\frac{R}{8}.
\end{aligned} \tag{36}
$$

The constant σ_n is an abbreviation for $\sigma_n \equiv n + (d-1)$. For $n = 0$ the path integral (35) must yield the normalized partition function $Z = Z_0 = 1$.

At $\varepsilon = 0$, the total action (36) contains only the kinetic term

$$\mathcal{A}^0[q] = \frac{1}{2}\int_0^L \mathrm{d}s\, \dot{q}^2(s). \tag{37}$$

With this free action, the path integral (35) becomes Gaussian which will be defined as

$$Z^0 \equiv \int_{\mathrm{NBC}} \mathcal{D}'^{d-1}q(s)\,\mathrm{e}^{-\mathcal{A}^0[q]} = \int_{\mathrm{NBC}} \mathcal{D}'^{d-1}q(s)\,\mathrm{e}^{-(1/2)\int_0^L \mathrm{d}s\,\dot{q}^2(s)} = 1. \tag{38}$$

To find the corrections, we split

$$\mathcal{A}^{\mathrm{tot}}_{,n}[q;\varepsilon] = \mathcal{A}^0[q] + \mathcal{A}^{\mathrm{int}}_{,n}[q;\varepsilon], \tag{39}$$

where the interaction action $\mathcal{A}^{\mathrm{int}}_{,n}[q;\varepsilon]$ has to be expanded in powers of small ε. Its large-stiffness expansion starts out as

$$\mathcal{A}^{\mathrm{int}}_{,n}[q;\varepsilon] = \varepsilon\mathcal{A}^{\mathrm{int}\,1}_{,n}[q] + \varepsilon^2\mathcal{A}^{\mathrm{int}\,2}_{,n}[q] + \cdots. \tag{40}$$

The first expansion term is

$$\mathcal{A}^{\mathrm{int}\,1}_{,n}[q] = \frac{1}{2}\int_0^L \mathrm{d}s\{[q(s)\dot{q}(s)]^2 - \rho_n(s)q^2(s)\} - L\frac{R}{8}, \tag{41}$$

where $\rho_n(s) \equiv \delta_n + [\delta(s) + \delta(s-L)]/2$ with $\delta_n = \delta(0) - \sigma_n/L$. The second expansion term is given by

$$\begin{aligned}\mathcal{A}^{\mathrm{int}\,2}_{,n}[q] = \frac{1}{2}\int_0^L \mathrm{d}s\left\{[q(s)\dot{q}(s)]^2 - \frac{1}{2}\left[\delta(0) - \frac{\sigma_n}{2L}\right]q^2(s)\right\}q^2(s)\\ + \frac{\sigma_n}{8L^2}\int_0^L \mathrm{d}s\int_0^L \mathrm{d}s'\,q^2(s)q^2(s').\end{aligned} \tag{42}$$

The perturbation expansion of the path integral (35) in powers of ε is an expansion in terms of expectation values to be calculated with respect to the Gaussian integral (38). For an arbitrary functional $F[q]$ of $q(s)$, these will be denoted by

$$\langle F[q]\rangle_0 \equiv \int_{\mathrm{NBC}} \mathcal{D}'^{d-1}q(s)F[q]\,\mathrm{e}^{-(1/2)\int_0^L \mathrm{d}s\,\dot{q}^2(s)}. \tag{43}$$

With this notation, the perturbative expansion of (35) reads

$$\begin{aligned}Z_n &= 1 - \left\langle\mathcal{A}^{\mathrm{int}}_{,n}[q;\varepsilon]\right\rangle_0 + \tfrac{1}{2}\left\langle\mathcal{A}^{\mathrm{int}}_{,n}[q;\varepsilon]^2\right\rangle_0 - \cdots\\ &= 1 - \varepsilon\left\langle\mathcal{A}^{\mathrm{int}\,1}_{,n}[q]\right\rangle_0 + \varepsilon^2\left(-\left\langle\mathcal{A}^{\mathrm{int}\,2}_{,n}[q]\right\rangle_0 + \tfrac{1}{2}\left\langle\mathcal{A}^{\mathrm{int}\,1}_{,n}[q]^2\right\rangle_0\right) - \cdots.\end{aligned} \tag{44}$$

The expectation values $\langle\cdots\rangle_0$ are evaluated by performing all possible Wick contractions with the basic propagator (13) and the Green function (33) of the unperturbed action (37). The relevant loop integrals I_i and H_i are calculated with our regularization rules when necessary and are listed in appendices A and B.

We now state the results for various terms appearing in equation (44):

$$\left\langle\mathcal{A}^{\mathrm{int}\,1}_{,n}[q]\right\rangle_0 = \frac{(d-1)}{2}\left[\frac{\sigma_n}{L}I_1 + \mathrm{d}I_2 - \frac{1}{2}\Delta(0,0) - \frac{1}{2}\Delta(L,L)\right] - L\frac{R}{8} = L\frac{(d-1)n}{12}, \tag{45}$$

$$\begin{aligned}\left\langle\mathcal{A}^{\mathrm{int}\,2}_{,n}[q]\right\rangle_0 &= \frac{(d^2-1)}{4}\left[\left(\delta(0) + \frac{\sigma_n}{2L}\right)I_3 + 2(d+2)I_4\right] + \frac{(d-1)\sigma_n}{8L^2}\left[(d-1)I_1^2 + 2I_5\right]\\ &= L^3\frac{(d^2-1)}{120}\delta(0) + L^2\frac{(d-1)}{1440}[(25d^2+36d+23) + n(11d+5)],\end{aligned} \tag{46}$$

$$\frac{1}{2}\left\langle \mathcal{A}^{\text{int}\,1}_{,\text{n}}[q]^2\right\rangle_0 = \frac{L^2}{2}\left\{\frac{(d-1)L}{12}\left[\left(\delta(0)+\frac{d}{2L}\right)-\left(\delta_n+\frac{2}{L}\right)\right]-\frac{R}{8}\right\}^2$$
$$+\frac{(d-1)}{4}\left[H_1^n-2\left(H_2^n+H_3^n-H_5\right)+H_6-4d\left(H_4^n-H_7-H_{10}\right)\right.$$
$$\left.+H_{11}+2d^2(H_8+H_9)\right]+\frac{(d-1)}{4}[\mathrm{d}H_{12}+2(d+2)H_{13}+\mathrm{d}H_{14}]$$
$$=\frac{L^2}{2}\left[\frac{(d-1)n}{12}\right]^2+L^3\frac{(d-1)}{120}\delta(0)$$
$$+L^2\frac{(d-1)}{1440}[(25d^2-22d+25)+4(n+4d-2)]$$
$$+L^3\frac{(d-1)d}{120}\delta(0)+L^2\frac{(d-1)}{720}(29d-1). \tag{47}$$

Inserting these results into equation (44), we obtain the partition function and all moments up to order $\varepsilon^2 \propto l^2$:

$$Z_n = 1-\varepsilon L\frac{(d-1)n}{12}+\varepsilon^2L^2\left[\frac{(d-1)^2n^2}{288}+\frac{(d-1)(4n+5d-13)n}{1440}\right]-\mathcal{O}(\varepsilon^3)$$
$$=1-\frac{n}{6}l+\left[\frac{n^2}{72}+\frac{(4n+5d-13)n}{360(d-1)}\right]l^2-\mathcal{O}(l^3). \tag{48}$$

For $n=0$, this yields the properly normalized partition function $Z=Z_0=1$. For $n=2,4$, we obtain the known even moments in d dimensions

$$\langle r^2\rangle = 1-\frac{l}{3}+\frac{1}{12}l^2+\cdots, \tag{49}$$

$$\langle r^4\rangle = 1-\frac{2l}{3}+\frac{25d-17}{90(d-1)}l^2+\cdots. \tag{50}$$

In addition, we find all odd moments up to order l^2, the lowest being

$$\langle r\rangle = 1-\frac{l}{6}+\frac{5d-7}{180(d-1)}l^2+\cdots, \tag{51}$$

$$\langle r^3\rangle = 1-\frac{l}{2}+\frac{25d-4}{30(d-1)}l^2+\cdots. \tag{52}$$

Restricted to $d=3$ dimensions, all moments (48) are in full agreement with the exact expansions of [23] obtained by solving the diffusion equation on a unit sphere.

5. Correlation function up to four loops

As an important test of this perturbation theory, we calculate the correlation function (7) up to four loops and verify its agreement with the exact expression (8).

Starting point is the path integral representation (29) with Neumann boundary conditions for the two-point correlation function

$$G(s,s') = \langle \mathbf{u}(s)\cdot\mathbf{u}(s')\rangle = \int_{\text{NBC}}\mathcal{D}'^{d-1}q(s)U[q,q';\varepsilon]\exp\left\{-\mathcal{A}^{\text{tot}}_{,0}[q;\varepsilon]\right\}, \tag{53}$$

with the action of equation (36) for $n=0$. The functional in the integrand $U[q,q'] \equiv U(q(s),q(s'))$ is the scalar product $\mathbf{u}(s)\cdot\mathbf{u}(s')$ expressed in terms of independent coordinates q^μ as

$$U(q(s),q(s')) \equiv \mathbf{u}(s)\cdot\mathbf{u}(s') = \sqrt{1-q^2(s)}\sqrt{1-q^2(s')}+q(s)q(s'). \tag{54}$$

After rescaling $q^\mu \to \sqrt{\varepsilon} q^\mu$ and expanding in powers of ε, this becomes

$$U[q, q'; \varepsilon] = 1 + \varepsilon U_1[q, q'] + \varepsilon^2 U_2[q, q'] + \cdots, \tag{55}$$

with

$$U_1[q, q'] \equiv U_1(q(s), q(s')) = q(s)q(s') - \tfrac{1}{2}q^2(s) - \tfrac{1}{2}q^2(s'), \tag{56}$$

$$U_2[q, q'] \equiv U_2(q(s), q(s')) = \tfrac{1}{4}q^2(s)q^2(s') - \tfrac{1}{8}[q^2(s)]^2 - \tfrac{1}{8}[q^2(s')]^2. \tag{57}$$

We shall attribute the integrand $U[q, q'; \varepsilon]$ to an interaction $\mathcal{A}^{\rm U}[q; \varepsilon]$ defined by

$$U[q, q'; \varepsilon] \equiv \exp(-\mathcal{A}^{\rm U}[q; \varepsilon]), \tag{58}$$

which has to be added to the interaction action in equation (36) with $n = 0$. The small ε-expansion, similar to equation (40), reads

$$\mathcal{A}^{\rm U}[q; \varepsilon] = -\varepsilon U_1[q, q'] + \varepsilon^2 \left[-U_2[q, q'] + \tfrac{1}{2}U_1^2[q, q']\right] - \cdots. \tag{59}$$

Thus, the perturbation expansion of the path integral (53) takes the form

$$G(s, s') = 1 - \left\langle \left(\mathcal{A}^{\rm int}_{,0}[q; \varepsilon] + \mathcal{A}^{\rm U}[q; \varepsilon]\right)\right\rangle_0 + \tfrac{1}{2}\left\langle \left(\mathcal{A}^{\rm int}_{\rm e,0}[q; \varepsilon] + \mathcal{A}^{\rm U}_{\rm e}[q; \varepsilon]\right)^2\right\rangle_0 - \cdots. \tag{60}$$

Collecting the expansions terms of equations (40) and (59) in equation (60) and taking into account the unit normalization of the partition function $Z = Z_0 = 1$ reduces this to

$$G(s, s') = 1 + \varepsilon \langle U_1[q, q']\rangle_0 + \varepsilon^2 \left[\langle U_2[q, q']\rangle_0 - \langle U_1[q, q']\mathcal{A}^{\rm int\,1}_{,0}[q]\rangle_0\right] + \cdots, \tag{61}$$

where the expectation values can be calculated, as before, using the propagator (13) with the Green function (33). For the calculation of the rotationally invariant quantity $G(s, s') = G(s - s')$, however, the Green function $\Delta(s, s') + C$ must be just as good a Green function satisfying Neumann boundary conditions as $\Delta(s, s')$.

We illustrate this explicitly by setting $C = L(a - 1)/3$ with an arbitrary constant a, and calculating the expectation values in equation (61) using the modified Green function. Details are given in appendix C (see equation (C.1)), where we list various expressions and integrals appearing in the Wick contractions of expansion (61). Using these results, we find the manifestly a-independent terms up to second order in ε:

$$\langle U_1[q, q']\rangle_0 = (d - 1)\Delta_{\rm F}(s - s') = -\frac{(d - 1)}{2}|s - s'|, \tag{62}$$

$$\begin{aligned} &\langle U_2[q, q']\rangle_0 - \left\langle U_1[q, q']\mathcal{A}^{\rm int\,1}_{,0}[q]\right\rangle_0 \\ &\quad = (d - 1)\left[\frac{1}{2}D_1 - \frac{1}{8}(d + 1)D_2^2 - K_1 - {\rm d}K_2 - \frac{(d - 1)}{L}K_3 + \frac{1}{2}K_4 + \frac{1}{2}K_5\right] \\ &\quad = \frac{1}{8}(d - 1)^2(s - s')^2. \end{aligned} \tag{63}$$

This leads to the two-point correlation function

$$\begin{aligned} G(s, s') &= 1 - \varepsilon\frac{(d - 1)}{2}|s - s'| + \varepsilon^2\frac{(d - 1)^2}{8}(s - s')^2 - \mathcal{O}(\varepsilon^3) \\ &= 1 - \frac{|s - s'|}{\xi} + \frac{(s - s')^2}{2\xi^2} - \cdots \end{aligned} \tag{64}$$

in agreement with the small-flexibility expansion of the exact expression (8) up to the second order in $1/\xi$.

6. Alternative calculation of all moments

It is interesting to recapitulate the result (48) by calculating all moments (6) once more in the way used in the previous section. To this end, we start from the path integral with Neumann boundary conditions

$$\langle r^n\rangle = \int_{\mathrm{NBC}} \mathcal{D}'^{d-1}q(s)R^n[q;\varepsilon]\exp\{-\mathcal{A}^{\mathrm{tot}}_{,0}[q;\varepsilon]\}, \tag{65}$$

where the action $\mathcal{A}^{\mathrm{tot}}_{,0}[q;\varepsilon]$ is the same as in equation (53), while the functional $R^2[q]$ corresponds to the square of the reduced distance r^2 represented now in terms of the $d-1$ coordinates $q^\mu(s)$ with the help of equation (54) as

$$R^2[q] = L^{-2}\int_0^L \mathrm{d}s\int_0^L \mathrm{d}s'\,U(q(s),q(s')). \tag{66}$$

Note that in terms of the reduced distance r, the moments (65) make sense *initially* for all n.

Using equations (55)–(57) yields the small ε-expansion

$$R^2[q;\varepsilon] = 1 + \varepsilon R_1^2[q] + \varepsilon^2 R_2^2[q] + \cdots, \tag{67}$$

with

$$R_1^2[q] = L^{-2}\int_0^L \mathrm{d}s\int_0^L \mathrm{d}s'\,U_1(q(s),q(s')) = -L^{-1}\int_0^L \mathrm{d}s\,q^2(s), \tag{68}$$

$$\begin{aligned} R_2^2[q] &= L^{-2}\int_0^L \mathrm{d}s\int_0^L \mathrm{d}s'\,U_2(q(s),q(s')) \\ &= -(4L)^{-1}\int_0^L \mathrm{d}s[q^2(s)]^2 + (2L)^{-2}\int_0^L \mathrm{d}s\int_0^L \mathrm{d}s'\,q^2(s)q^2(s'), \end{aligned} \tag{69}$$

where we have used condition (23).

The interaction associated with $R^n[q;\varepsilon]$ is

$$\mathcal{A}^{\mathrm{R}}[q;\varepsilon] = -\frac{n}{2}\log R^2[q;\varepsilon] = -\varepsilon\frac{n}{2}R_1^2[q] + \varepsilon^2\frac{n}{2}\left\{-R_2^2[q] + \frac{1}{2}\left(R_1^2[q]\right)^2\right\} - \cdots. \tag{70}$$

Adding (70) to the action $\mathcal{A}^{\mathrm{tot}}_{,0}[q;\varepsilon]$ leads to the perturbation expansion of the path integral (65) up to second order in ε:

$$\begin{aligned} \langle r^n\rangle &= 1 - \left\langle\left(\mathcal{A}^{\mathrm{int}}_{\mathrm{e},0}[q;\varepsilon] + \mathcal{A}^{\mathrm{R}}_{\mathrm{e}}[q;\varepsilon]\right)\right\rangle_0 + \frac{1}{2}\left\langle\left(\mathcal{A}^{\mathrm{int}}_{,0}[q;\varepsilon] + \mathcal{A}^{\mathrm{R}}[q;\varepsilon]\right)^2\right\rangle_0 \\ &= 1 + \varepsilon\frac{n}{2}\left\langle R_1^2[q]\right\rangle_0 + \varepsilon^2\frac{n}{2}\left[\left\langle R_2^2[q]\right\rangle_0 - \left\langle R_1^2[q]\mathcal{A}^{\mathrm{int}\,1}_{\mathrm{e},0}[q]\right\rangle_0 + \frac{1}{4}(n-2)\left\langle\left(R_1^2[q]\right)^2\right\rangle_0\right]. \end{aligned} \tag{71}$$

Most of the expectation values appeared here are related through equations (68) and (69) to those obtained before in equations (62) and (63). For these, we find

$$\begin{aligned} \left\langle R_1^2[q]\right\rangle_0 &= \frac{1}{L^2}\int_0^L \mathrm{d}s\int_0^L \mathrm{d}s'\langle U_1(q(s),q(s'))\rangle_0 \\ &= -\frac{(d-1)}{2L^2}\int_0^L \mathrm{d}s\int_0^L \mathrm{d}s'|s-s'| = -L\frac{(d-1)}{6}, \end{aligned} \tag{72}$$

$$\begin{aligned} &\left\langle R_2^2[q]\right\rangle_0 - \left\langle R_1^2[q]\mathcal{A}^{\mathrm{int}\,1}_{\mathrm{e},0}[q]\right\rangle_0 \\ &\quad = \frac{1}{L^2}\int_0^L \mathrm{d}s\int_0^L \mathrm{d}s'\left[\langle U_2(q(s),q(s'))\rangle_0 - \left\langle U_1(q(s),q(s'))\mathcal{A}^{\mathrm{int}\,1}_{\mathrm{e},0}[q]\right\rangle_0\right] \\ &\quad = \frac{(d-1)^2}{8L^2}\int_0^L \mathrm{d}s\int_0^L \mathrm{d}s'(s-s')^2 = L^2\frac{(d-1)^2}{48}. \end{aligned} \tag{73}$$

The last expectation value in equation (71) is calculated as

$$\left\langle \left(R_1^2[q]\right)^2\right\rangle_0 = \frac{1}{L^2}\int_0^L \mathrm{d}s \int_0^L \mathrm{d}s' \langle q^2(s) q^2(s')\rangle_0$$
$$= \frac{(d-1)}{L^2}\left[(d-1)I_1^2 + 2I_5\right] = L^2\frac{(d-1)(5d-1)}{180}. \tag{74}$$

Inserting the results (72)–(74) into equation (71), we obtain the same perturbation expansion for all moments up to order l^2 as in equation (48), but in the slightly different form

$$\langle r^n\rangle = 1 - \varepsilon L\frac{(d-1)n}{12} + \varepsilon^2 L^2\left[\frac{(d-1)^2 n}{96} + \frac{(d-1)(5d-1)n(n-2)}{1440}\right] - \mathcal{O}(\varepsilon^3)$$
$$= 1 - \frac{n}{6}l + \left[\frac{n}{24} + \frac{(5d-1)n(n-2)}{360(d-1)}\right]l^2 - \mathcal{O}(l^3). \tag{75}$$

7. Radial distribution up to four loops

We now turn to the calculation of the most important quantity characterizing a polymer, the distribution function (25). Going over to the Fourier transform of the δ-function, which enforces the reduced end-to-end distance $r = L^{-1}\int_0^L \mathrm{d}s\,\sqrt{1-q^2(s)}$ in equation (25), yields the Fourier decomposition

$$P(r;L) = S_d^{-1}\int \frac{\mathrm{d}k}{2\pi}\,\mathrm{e}^{-\mathrm{i}k(r-1)}P(k;L), \tag{76}$$

where $P(k;L)$ has to be calculated from the path integral with Neumann boundary conditions

$$P(k;L) = \int_{\mathrm{NBC}} \mathcal{D}'^{d-1}q(s)\exp\left\{-\mathcal{A}^{\mathrm{tot}}_{,k}[q;\varepsilon]\right\}. \tag{77}$$

The resulting total action

$$\mathcal{A}^{\mathrm{tot}}_{,k}[q] \equiv \mathcal{A}[q] + \mathcal{A}^{\mathrm{cor}}[q_b,q_a] - (\mathrm{i}k/L)\int_0^L \mathrm{d}s\left(\sqrt{1-q^2(s)} - 1\right), \tag{78}$$

after rescaling the coordinates $q^\mu(s) \to \sqrt{\varepsilon}q^\mu(s)$, reads explicitly

$$\mathcal{A}^{\mathrm{tot}}_{,k}[q;\varepsilon] = \int_0^L \mathrm{d}s\left\{\frac{1}{2}\left[\dot{q}^2 + \varepsilon\frac{(q\dot{q})^2}{1-\varepsilon q^2}\right] + \frac{1}{2}\delta(0)\log(1-\varepsilon q^2) - \frac{\mathrm{i}k}{L}\left(\sqrt{1-\varepsilon q^2} - 1\right)\right\}$$
$$- \frac{1}{4}\varepsilon[q^2(0) + q^2(L)] - \varepsilon L\frac{R}{8} \equiv \mathcal{A}^0[q] + \mathcal{A}^{\mathrm{int}}_{,k}[q;\varepsilon]. \tag{79}$$

As before in equation (40), we expand the interaction in powers of a small coupling constant ε. The first term coincides with equation (41), except that $\rho_n(s)$ is now replaced by $\rho_k(s) = \delta_k + [\delta(s) + \delta(s-L)]/2$ with $\delta_k = \delta(0) - \mathrm{i}k/L$:

$$\mathcal{A}^{\mathrm{int}\,1}_{,k}[q] = \int_0^L \mathrm{d}s\,\frac{1}{2}[(q(s)\dot{q}(s))^2 - \rho_k(s)q^2(s)] - L\frac{R}{8}. \tag{80}$$

The second expansion term $\mathcal{A}^{\mathrm{int}\,2}_{,k}[q]$ is simpler than that in equation (42) by not containing the last non-local contribution

$$\mathcal{A}^{\mathrm{int}\,2}_{,k}[q] = \int_0^L \mathrm{d}s\,\frac{1}{2}\left\{[q(s)\dot{q}(s)]^2 - \frac{1}{2}\left(\delta(0) - \frac{\mathrm{i}k}{2L}\right)q^2(s)\right\}q^2(s). \tag{81}$$

Apart from that, the perturbation expansion of the path integral (77) has the same general form as in equation (44) and, therefore, reads

$$P(k;L) = 1 - \left\langle \mathcal{A}^{\mathrm{int}}_{,k}[q;\varepsilon]\right\rangle_0 + \tfrac{1}{2}\left\langle \mathcal{A}^{\mathrm{int}}_{\mathrm{e},k}[q;\varepsilon]^2\right\rangle_0 - \cdots$$
$$= 1 - \varepsilon\left\langle \mathcal{A}^{\mathrm{int}\,1}_{,\mathrm{k}}[q]\right\rangle_0 + \varepsilon^2\left(-\left\langle \mathcal{A}^{\mathrm{int}\,2}_{\mathrm{e},k}[q]\right\rangle_0 + \tfrac{1}{2}\left\langle \mathcal{A}^{\mathrm{int}\,1}_{,k}[q]^2\right\rangle_0\right) - \cdots. \tag{82}$$

The expectation values can be expressed in terms of the same integrals listed in appendices A and B as follows:

$$\left\langle \mathcal{A}^{\text{int}\,1}_{,k}[q]\right\rangle_0 = \frac{(d-1)}{2}\left[\frac{\mathrm{i}k}{L}I_1 + \mathrm{d}I_2 - \frac{1}{2}\Delta(0,0) - \frac{1}{2}\Delta(L,L)\right] - L\frac{R}{8}$$
$$= -L\frac{(d-1)\,[(d-1)-\mathrm{i}k]}{12}, \tag{83}$$

$$\left\langle \mathcal{A}^{\text{int}\,2}_{,k}[q]\right\rangle_0 = \frac{(d^2-1)}{4}\left[\left(\delta(0)+\frac{\mathrm{i}k}{2L}\right)I_3 + 2(d+2)I_4\right]$$
$$= L^3\frac{(d^2-1)}{120}\delta(0) + L^2\frac{(d^2-1)\,[7(d+2)+3\mathrm{i}k]}{720}, \tag{84}$$

$$\frac{1}{2}\left\langle \mathcal{A}^{\text{int}\,1}_{,k}[q]^2\right\rangle_0 = \frac{L^2}{2}\left\{\frac{(d-1)L}{12}\left[\left(\delta(0)+\frac{d}{2L}\right) - \left(\delta_k + \frac{2}{L}\right)\right] - \frac{R}{8}\right\}^2$$
$$+ \frac{(d-1)}{4}\big[H_1^k - 2\big(H_2^k + H_3^k - H_5\big) + H_6 - 4d\big(H_4^k - H_7 - H_{10}\big)$$
$$+ H_{11} + 2d^2(H_8+H_9)\big] + \frac{(d-1)}{4}[\mathrm{d}H_{12} + 2(d+2)H_{13} + \mathrm{d}H_{14}]$$
$$= L^2\frac{(d-1)^2[(d-1)-\mathrm{i}k]^2}{2\cdot 12^2} + L^3\frac{(d-1)}{120}\delta(0) + L^2\frac{(d-1)}{1440}[(13d^2-6d+21)$$
$$+ 4\mathrm{i}k(2d+\mathrm{i}k)] + L^3\frac{(d-1)d}{120}\delta(0) + L^2\frac{(d-1)}{720}(29d-1). \tag{85}$$

In this way, we find the large-stiffness expansion of the path integral (77) up to order ε^2:

$$P(k;L) = 1 + \varepsilon L\frac{(d-1)}{12}[(d-1)-\mathrm{i}k] + \varepsilon^2 L^2\frac{(d-1)}{1440}[(\mathrm{i}k)^2(5d-1)$$
$$- 2\mathrm{i}k(5d^2-11d+8) + (d-1)(5d^2-11d+14)] + \mathcal{O}(\varepsilon^3). \tag{86}$$

The Fourier transform (76) of expansion (86) yields the end-to-end distribution function

$$P(r;l) = S_d^{-1}\left\{\delta(r-1) + \frac{l}{6}[\delta'(r-1) + (d-1)\delta(r-1)] + \frac{l^2}{360(d-1)}[(5d-1)\delta''(r-1)\right.$$
$$\left. + 2(5d^2-11d+8)\delta'(r-1) + (d-1)(5d^2-11d+14)\delta(r-1)] + \mathcal{O}(l^3)\right\}. \tag{87}$$

This representation is convenient to calculate the moments

$$\langle r^n\rangle = S_d\int \mathrm{d}r\, r^{n+(d-1)}P(r;l). \tag{88}$$

Indeed, inserting the distribution function (87) into equation (88) yields directly the moments (48) found before by the independent calculation.

To make the contact with the results of [23] derived in $d=3$ dimensions, we rewrite the distribution function (87) in the form

$$P(r;l) = \frac{1}{4\pi}[p_0(l)\delta(r-1) + p_1(l)\delta'(r-1) + p_2(l)\delta''(r-1) + p_3(l)\delta'''(r-1) + \cdots], \tag{89}$$

where the coefficients $p_i(l)$ are expanded for $d = 3$ up to order l^3

$$p_0(l) = 1 + \frac{1}{3}l + \frac{13}{180}l^2 + \frac{38}{2^3 \cdot 315}l^3 + \cdots = 1 + \frac{2}{3}t + \frac{13}{45}t^2 + \frac{38}{315}t^3 + \cdots, \tag{90}$$

$$p_1(l) = \frac{1}{6}l + \frac{1}{18}l^2 + \frac{34}{2^3 \cdot 315}l^3 + \cdots = \frac{1}{3}t + \frac{2}{9}t^2 + \frac{34}{315}t^3 + \cdots, \tag{91}$$

$$p_2(l) = \frac{7}{360}l^2 + \frac{1}{2^3 \cdot 21}l^3 + \cdots = \frac{7}{90}t^2 + \frac{1}{21}t^3 + \cdots \tag{92}$$

$$p_3(l) = \frac{31}{2^3 \cdot 1890}l^3 + \cdots = \frac{31}{1890}t^3 + \cdots. \tag{93}$$

Inserting $l = 2t$ in the last lines of equations (90)–(93) shows the agreement with the end-to-end distribution function $G(r; t)$ of [23] reduced to the form (89) after re-expansion in appendix D.

Let us make now the contact with the distribution functions of [25]. To this end, expansion (86) can be reassembled as

$$P(k; L) = P_0(k; L)\left\{1 + \frac{(d-1)}{6}l + \left[\frac{(d-3)}{180(d-1)}\,\mathrm{i}k + \frac{(5d^2 - 11d + 14)}{360}\right]l^2 + \mathcal{O}(l^3)\right\}, \tag{94}$$

where we have factored out the series containing the expansion terms with the same powers of ε, k and L,

$$P_0(k; L) = 1 - \frac{(d-1)}{2^2 \cdot 3}(\mathrm{i}k\varepsilon L) + \frac{(d-1)(5d-1)}{2^5 \cdot 3^2 \cdot 5}(\mathrm{i}k\varepsilon L)^2 - \cdots. \tag{95}$$

By setting $\hat{\omega}^2 \equiv \mathrm{i}k\varepsilon L$, we identify this with the beginning of the expansion of a functional determinant,

$$P_0(\hat{\omega}) = \left(\frac{\hat{\omega}}{\sinh\hat{\omega}}\right)^{(d-1)/2} = 1 - \frac{d-1}{12}\hat{\omega}^2 + \frac{(d-1)(5d-1)}{1440}\hat{\omega}^4 + \cdots, \tag{96}$$

valid for $\hat{\omega}$ small. One can replace, however, expansion (95) by the exact expression (96) for $P_0(\hat{\omega})$ and integrate over $\hat{\omega}$ in the Fourier transform (76). This would ignore the smallness of $\hat{\omega}$. In such a way, the distribution function with the only determinant (96) was calculated for $d = 2, 3$ in [25] from the $\hat{\omega}$-integral

$$P_0(r; l) \propto \frac{1}{l}\int_{-\mathrm{i}\infty}^{\mathrm{i}\infty} \frac{\mathrm{d}\hat{\omega}}{2\pi\mathrm{i}}\,\mathrm{e}^{-\hat{\omega}^2(d-1)(r-1)/2l}\,\hat{\omega}P_0(\hat{\omega}), \tag{97}$$

which was found to give, after a proper normalization, good radial end-to-end distribution functions for large stiffness. It represents the leading contribution to the distribution function (76), since $P_0(\hat{\omega})$ enters equation (94) as a prefactor with no dependence on the flexibility l. To find corrections, the rest of expansion (94) in powers of small l must be known for all $\hat{\omega}$. This can be done by reorganizing the perturbation theory as follows.

The determinant (96) can directly be obtained from the path integral of a simple harmonic oscillator with Neumann boundary conditions [15]:

$$Z^0_\omega \equiv \int_{\mathrm{NBC}} \mathcal{D}'^{d-1}q(s)\,\mathrm{e}^{-\mathcal{A}^0_{,\omega}[q]} = P_0(\hat{\omega}), \tag{98}$$

where $\mathcal{A}^0_{,\omega}[q]$ is the harmonic action

$$\mathcal{A}^0_{,\omega}[q] = \frac{1}{2}\int_0^L \mathrm{d}s[\dot{q}^2(s) + \omega^2 q^2(s)]. \tag{99}$$

With the redefinition $\omega^2 \equiv \mathrm{i}k\varepsilon/L$, it represents a 'free' part of the total action (79), whose expansion in powers of small ε becomes

$$\mathcal{A}^{\mathrm{tot}}_{,k}[q;\varepsilon] = \mathcal{A}^{0}_{,\omega}[q] + \varepsilon\mathcal{A}^{\mathrm{int}\,1}_{\mathrm{e},\omega}[q] + \cdots, \tag{100}$$

while the first expansion term reads

$$\mathcal{A}^{\mathrm{int}\,1}_{,\omega}[q] = \int_0^L \mathrm{d}s\left[\frac{1}{2}(q\dot{q})^2 - \frac{1}{2}\delta(0)q^2 + \frac{1}{8}\omega^2(q^2)^2\right] - \frac{1}{4}[q^2(0)+q^2(L)] - L\frac{R}{8}. \tag{101}$$

Note that the interaction (101) contains the harmonic terms even at lowest order in ε.

The result (98) represents the leading term in the large-stiffness expansion for the path integral (77). By expanding the path integral (77) with respect to the harmonic integral (98), we find the higher-order fluctuation corrections. This yields

$$P(\hat{\omega};L) = Z^0_{\omega}\left(1 - \varepsilon\left\langle\mathcal{A}^{\mathrm{int}\,1}_{,\omega}[q]\right\rangle_0 + \cdots\right), \tag{102}$$

where the expectation values are evaluated using the basic propagator (13), which contains now a harmonic Green function of the unperturbed action (99). With the zero-mode subtracted, this Green function explicitly reads

$$\Delta_{\omega}(s,s') = \frac{2}{L}\sum_{n=1}^{\infty}\frac{\cos(n\pi s/L)\cos(n\pi s'/L)}{\omega^2+n^2\pi^2/L^2}$$
$$= \frac{\cosh\omega(L-|s-s'|)+\cosh\omega(L-(s+s'))}{2\omega\sinh\omega L} - \frac{1}{L\omega^2}. \tag{103}$$

As a result, we obtain the next-to-leading contribution

$$\left\langle\mathcal{A}^{\mathrm{int}\,1}_{,\omega}[q]\right\rangle_0 = -L\frac{(d-1)^2}{8} - L\frac{(d-1)}{4}\left(\frac{\coth\hat{\omega}}{\hat{\omega}} - \frac{1}{\hat{\omega}^2}\right)$$
$$+L\frac{(d^2-1)}{32}\left(\coth^2\hat{\omega} + \frac{\coth\hat{\omega}}{2\hat{\omega}} - \frac{3}{2\sinh^2\hat{\omega}}\right). \tag{104}$$

Substituting now the leading (98) and the next-to-leading (104) terms into expansion (102) yields

$$P(\hat{\omega};l) = P_0(\hat{\omega})R(\hat{\omega};l), \tag{105}$$

where the factor $R(\hat{\omega};l)$ for all $\hat{\omega}$ has the small-l expansion

$$R(\hat{\omega};l) = 1 + l\frac{(3d-5)}{16} - l\frac{(d+1)}{32}\left(\frac{\coth\hat{\omega}}{\hat{\omega}} - \frac{1}{\sinh^2\hat{\omega}}\right) + l\frac{1}{2}\left(\frac{\coth\hat{\omega}}{\hat{\omega}} - \frac{1}{\hat{\omega}^2}\right) + \mathcal{O}(l^2). \tag{106}$$

Expanding (105) in powers of $\hat{\omega}$ for $\hat{\omega}$ small yields, of course, expansion (94) to the order of l. Nevertheless the analytic form (105) is convenient for the use in the Fourier representation (76) in terms of $\hat{\omega}$:

$$P(r;l) = \frac{(d-1)}{l}S_d^{-1}\int_{-\mathrm{i}\infty}^{\mathrm{i}\infty}\frac{\mathrm{d}\hat{\omega}}{2\pi\mathrm{i}}\,\mathrm{e}^{-\hat{\omega}^2(d-1)(r-1)/2l}\,\hat{\omega}P(\hat{\omega};l). \tag{107}$$

An important observation for performing the $\hat{\omega}$-integral (107) is now that the integrand (105) can be expressed in terms of $P_0(\hat{\omega})$, and the derivatives $P_0'(\hat{\omega})$ and $P_0''(\hat{\omega})$ with respect to $\hat{\omega}$. To show this, we set

$$P_0(\hat{\omega}) = \left(\frac{\hat{\omega}}{\sinh\hat{\omega}}\right)^{(d-1)/2} = \mathrm{e}^{-f(\hat{\omega})}, \tag{108}$$

with

$$f(\hat{\omega}) = \frac{(d-1)}{2}\,(\log\sinh\hat{\omega} - \log\hat{\omega})\,. \tag{109}$$

In terms of $f(\hat{\omega})$, the factor (106) becomes

$$R(\hat{\omega}; l) = 1 + \frac{(3d-5)l}{16} - \frac{(d-15)l}{16(d-1)}\frac{f'(\hat{\omega})}{\hat{\omega}} - \frac{(d+1)l}{16(d-1)}f''(\hat{\omega}). \tag{110}$$

Substituting equations (108) and (110) into equation (105), we use the identities

$$\begin{aligned} &-f'(\hat{\omega})\,\mathrm{e}^{-f(\hat{\omega})} = P_0'(\hat{\omega}),\\ &-f''(\hat{\omega})\,\mathrm{e}^{-f(\hat{\omega})} = \frac{2}{(d+1)}P_0''(\hat{\omega}) - \frac{2(d-1)}{(d+1)\hat{\omega}}P_0'(\hat{\omega}) - \frac{(d-1)^2}{2(d+1)}P_0(\hat{\omega}). \end{aligned} \tag{111}$$

This brings, finally, expansion (105) in the form

$$P(\hat{\omega}; l) = \left[1 + \frac{(5d-9)l}{32}\right]P_0(\hat{\omega}) - \frac{(d+13)l}{16(d-1)\hat{\omega}}P_0'(\hat{\omega}) + \frac{l}{8(d-1)}P_0''(\hat{\omega}). \tag{112}$$

With the representation (112), the integration of equation (107) is straightforward. We substitute the binomial series

$$P_0(\hat{\omega}) = \left(\frac{\hat{\omega}}{\sinh\hat{\omega}}\right)^{(d-1)/2} = (2\hat{\omega})^{(d-1)/2}\sum_{k=0}^{\infty}(-1)^k\binom{-(d-1)/2}{k}\,\mathrm{e}^{-(2k+(d-1)/2)\hat{\omega}} \tag{113}$$

and express the resulting integrals in terms of a parabolic cylinder functions. In the physical case of three dimensions, where $\hat{\omega}^2 = \mathrm{i}kl$, the answer reads

$$\begin{aligned} P(r; l) = \frac{1}{4\pi\sqrt{\pi}l}\sum_{n=1}^{\infty}\frac{1}{[(1-r)/l]^{3/2}}\exp\left[-\frac{(n-1/2)^2}{(1-r)/l}\right]\\ \times\left\{\left[1 + \frac{(n^2-n+1)l}{4}\right]H_2\left[\frac{n-1/2}{\sqrt{(1-r)/l}}\right] + \frac{3(n-1/2)^2 l}{\sqrt{2}} - (1-r)\right\}, \end{aligned} \tag{114}$$

where the second Hermite polynomial is $H_2(x) = 4x^2 - 2$. The first term in the brackets represents the leading contribution found before in [25], the others are the new next-to-leading corrections. The proper normalization is ensured automatically in each perturbative order l in the small-flexibility expansion. Since the next-to-leading terms are suppressed as $l \sim 1/\kappa$, there is no drastic change in the behaviour of the radial distribution with respect to the leading contribution.

8. Conclusion

In conclusion, we have developed a systematic perturbation theory capable of yielding the polymer properties near the rod limit from a path integral formulation. This has yielded the large-stiffness expansions for the experimentally relevant end-do-end distribution, all the even and odd moments, and the correlation function in d dimensions as power series in the flexibility l up to the order l^2. All these results have been obtained without the use of the diffusion equation on a unit sphere. In subsequent work we shall use variational perturbation theory [15, 41] to extend the results from small to large flexibility, i.e., to find results connecting the above results smoothly with the random-chain limit.

Appendix A. Basic integrals

The following well-defined integrals appear throughout the calculation of the Feynman diagrams:

$$\Delta(0,0) = \Delta(L,L) = \frac{L}{3}, \tag{A.1}$$

$$I_1 = \int_0^L \mathrm{d}s\, \Delta(s,s) = \frac{L^2}{6}, \tag{A.2}$$

$$I_2 = \int_0^L \mathrm{d}s\, {}^{\cdot}\Delta^2(s,s) = \frac{L}{12}, \tag{A.3}$$

$$I_3 = \int_0^L \mathrm{d}s\, \Delta^2(s,s) = \frac{L^3}{30}, \tag{A.4}$$

$$I_4 = \int_0^L \mathrm{d}s\, \Delta(s,s)\, {}^{\cdot}\Delta^2(s,s) = \frac{7L^2}{360}, \tag{A.5}$$

$$I_5 = \int_0^L \mathrm{d}s \int_0^L \mathrm{d}s'\, \Delta^2(s,s') = \frac{L^4}{90}, \tag{A.6}$$

$$\Delta(0,L) = \Delta(L,0) = -\frac{L}{6}, \tag{A.7}$$

$$I_6 = \int_0^L \mathrm{d}s[\Delta^2(s,0) + \Delta^2(s,L)] = \frac{2L^3}{45}, \tag{A.8}$$

$$I_7 = \int_0^L \mathrm{d}s \int_0^L \mathrm{d}s'\, \Delta(s,s)\, {}^{\cdot}\Delta^2(s,s') = \frac{L^3}{45}, \tag{A.9}$$

$$I_8 = \int_0^L \mathrm{d}s \int_0^L \mathrm{d}s'\, {}^{\cdot}\Delta(s,s)\Delta(s,s')\, {}^{\cdot}\Delta(s,s') = \frac{L^3}{180}, \tag{A.10}$$

$$I_9 = \int_0^L \mathrm{d}s\, \Delta(s,s)[{}^{\cdot}\Delta^2(s,0) + {}^{\cdot}\Delta^2(s,L)] = \frac{11L^2}{90}, \tag{A.11}$$

$$I_{10} = \int_0^L \mathrm{d}s\, {}^{\cdot}\Delta(s,s)[\Delta(s,0)\, {}^{\cdot}\Delta(s,0) + \Delta(s,L)\, {}^{\cdot}\Delta(s,L)] = \frac{17L^2}{360}, \tag{A.12}$$

$${}^{\cdot}\Delta(0,0) = -{}^{\cdot}\Delta(L,L) = -\frac{1}{2}, \tag{A.13}$$

$$I_{11} = \int_0^L \mathrm{d}s \int_0^L \mathrm{d}s'\, \Delta(s,s)\Delta^{\cdot}(s,s')\, {}^{\cdot}\Delta(s',s') = \frac{L^3}{360}, \tag{A.14}$$

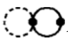
$$I_{12} = \int_0^L \mathrm{d}s \int_0^L \mathrm{d}s'\, \Delta(s,s')\, {}^{\cdot}\Delta^2(s,s') = \frac{L^3}{90}. \tag{A.15}$$

Appendix B. Loop integrals

We list here the Feynman integrals evaluated with dimensional regularization rules whenever necessary. In the calculation, they occur either from the expectations (45)–(47), or from the expectations (83)–(85). Accordingly, we encounter the integrals depending either on $\rho_n(s) = \delta_n + [\delta(s) + \delta(s-L)]/2$ with $\delta_n = \delta(0) - \sigma_n/L$, or on $\rho_k(s) = \delta_k + [\delta(s) + \delta(s-L)]/2$ with $\delta_k = \delta(0) - \mathrm{i}k/L$:

$$H_1^{n(k)} = \int_0^L \mathrm{d}s \int_0^L \mathrm{d}s'\, \rho_{n(k)}(s)\rho_{n(k)}(s')\Delta^2(s,s') \\ = \delta^2_{n(k)} I_5 + \delta_{n(k)} I_6 + \frac{1}{2}[\Delta^2(0,0) + \Delta^2(0,L)], \tag{B.1}$$

$$H_2^{n(k)} = \int_0^L \mathrm{d}s \int_0^L \mathrm{d}s'\, \rho_{n(k)}(s')\Delta(s,s)\dot{\Delta}^2(s,s') = \delta_{n(k)} I_7 + \frac{I_9}{2}, \tag{B.2}$$



$$H_3^{n(k)} = \int_0^L \mathrm{d}s \int_0^L \mathrm{d}s'\, \rho_{n(k)}(s')\dot{\Delta}(s,s)\Delta^2(s,s') = \left[\delta_{n(k)} I_5 + \frac{I_6}{2}\right]\delta(0), \tag{B.3}$$

$$H_4^{n(k)} = \int_0^L \mathrm{d}s \int_0^L \mathrm{d}s'\, \rho_{n(k)}(s')\dot{\Delta}(s,s)\dot{\Delta}(s,s')\Delta(s,s') = \delta_{n(k)} I_8 + \frac{I_{10}}{2}. \tag{B.4}$$

When calculating Z_n, we need to insert here $\delta_n = \delta(0) - \sigma_n/L$, thus obtaining

$$H_1^n = \frac{L^4}{90}\delta^2(0) + \frac{L^3}{45}(3-d-n)\delta(0) + \frac{L^2}{360}[(45 - 24d + 4d^2) - 4n(6-2d-n)], \tag{B.5}$$

$$H_2^n = \frac{L^3}{45}\delta(0) + \frac{L^2}{180}(15 - 4d - 4n), \tag{B.6}$$

$$H_3^n = \frac{L^4}{90}\delta^2(0) + \frac{L^3}{90}(3-d-n)\delta(0), \tag{B.7}$$

$$H_4^n = \frac{L^3}{180}\delta(0) + \frac{L^2}{720}(21 - 4d - 4n), \tag{B.8}$$

where the values for $n = 0$ correspond to the partition function $Z = Z_0$. The substitution $\delta_k = \delta(0) - \mathrm{i}k/L$, required for the calculation of $P(k; L)$, yields

$$H_1^k = \frac{L^4}{90}\delta^2(0) + \frac{L^3}{45}\,[2 + (-\mathrm{i}k)]\,\delta(0) + \frac{L^2}{90}(-\mathrm{i}k)\,[4 + (-\mathrm{i}k)] + \frac{5L^2}{72}, \tag{B.9}$$

$$H_2^k = \frac{L^3}{45}\delta(0) + \frac{L^2}{180}[11 + 4(-\mathrm{i}k)], \tag{B.10}$$

$$H_3^k = \frac{L^4}{90}\delta^2(0) + \frac{L^3}{90}\,[2 + (-\mathrm{i}k)]\,\delta(0), \tag{B.11}$$

$$H_4^k = \frac{L^3}{180}\delta(0) + \frac{L^2}{720}[17 + 4(-\mathrm{i}k)]. \tag{B.12}$$

The other loop integrals are

$$H_5 = \int_0^L \mathrm{d}s \int_0^L \mathrm{d}s'\, \Delta(s,s)\dot{\Delta}^2(s,s')\dot{\Delta}(s',s') = \delta(0) I_7 = \frac{L^3}{45}\delta(0), \tag{B.13}$$

$$H_6 = \int_0^L \mathrm{d}s \int_0^L \mathrm{d}s'\, \dot{\Delta}(s,s)\Delta^2(s,s')\dot{\Delta}(s',s') = \delta^2(0) I_5 = \frac{L^4}{90}\delta^2(0), \tag{B.14}$$


$$H_7 = \int_0^L \mathrm{d}s \int_0^L \mathrm{d}s' \, {}^{\cdot}\Delta(s,s)\, {}^{\cdot}\Delta(s,s')\Delta(s,s')\, {}^{\cdot}\Delta^{\cdot}(s',s') = \delta(0) I_8 = \frac{L^3}{180}\delta(0), \tag{B.15}$$


$$H_8 = \int_0^L \mathrm{d}s \int_0^L \mathrm{d}s' \, {}^{\cdot}\Delta(s,s)\, {}^{\cdot}\Delta(s,s')\Delta^{\cdot}(s,s')\, {}^{\cdot}\Delta(s',s') = -\frac{L^2}{720}, \tag{B.16}$$


$$H_9 = \int_0^L \mathrm{d}s \int_0^L \mathrm{d}s' \, {}^{\cdot}\Delta(s,s)\Delta(s,s')\, {}^{\cdot}\Delta^{\cdot}(s,s')\, {}^{\cdot}\Delta(s',s')$$
$$= \frac{I_{10}}{2} - \frac{I_8}{L} - H_8 = \frac{7L^2}{360}, \tag{B.17}$$


$$H_{10} = \int_0^L \mathrm{d}s \int_0^L \mathrm{d}s' \, \Delta(s,s)\, {}^{\cdot}\Delta(s,s')\, {}^{\cdot}\Delta^{\cdot}(s,s')\, {}^{\cdot}\Delta(s',s') = \frac{I_9}{4} - \frac{I_7}{2L} = \frac{7L^2}{360}, \tag{B.18}$$


$$H_{11} = \int_0^L \mathrm{d}s \int_0^L \mathrm{d}s' \, \Delta(s,s)\, {}^{\cdot}\Delta^{\cdot 2}(s,s')\Delta(s',s')$$
$$= \delta(0) I_3 + \left(\frac{I_1}{L}\right)^2 - \frac{2(I_3 - I_{11})}{L} - 2I_4 + 2[\Delta^2(L,L)\Delta^{\cdot}(L,L)$$
$$- \Delta^2(0,0)\Delta^{\cdot}(0,0)] - 2H_{10} = \frac{L^3}{30}\delta(0) + \frac{L^2}{9}, \tag{B.19}$$


$$H_{12} = \int_0^L \mathrm{d}s \int_0^L \mathrm{d}s' \, {}^{\cdot}\Delta^2(s,s')\Delta^{\cdot 2}(s,s') = \frac{L^2}{90}, \tag{B.20}$$


$$H_{13} = \int_0^L \mathrm{d}s \int_0^L \mathrm{d}s' \, \Delta(s,s')\, {}^{\cdot}\Delta(s,s')\Delta^{\cdot}(s,s')\, {}^{\cdot}\Delta^{\cdot}(s',s)$$
$$= \frac{I_4}{2} - \frac{I_{12}}{2L} - \frac{H_{12}}{2} = -\frac{L^2}{720}, \tag{B.21}$$


$$H_{14} = \int_0^L \mathrm{d}s \int_0^L \mathrm{d}s' \, \Delta^2(s,s')\, {}^{\cdot}\Delta^{\cdot 2}(s,s')$$
$$= \delta(0) I_3 - \frac{2(I_3 - I_{12})}{L} - 2I_4 + \frac{I_5}{L^2}, +2[\Delta^2(L,L)\Delta^{\cdot}(L,L)$$
$$- \Delta^2(0,0)\Delta^{\cdot}(0,0)] - 2H_{13} = \frac{L^3}{30}\delta(0) + \frac{11L^2}{72}. \tag{B.22}$$

Calculating the integrals (B.17)–(B.22) required the regularization rules of [37, 38]. To compute these unambiguously, we must first use partial integrations together with Neumann boundary conditions so that we can apply subsequently the equation ${}^{\cdot\cdot}\Delta(s,s') = \Delta^{\cdot\cdot}(s,s') = 1/L - \delta(s,s')$. In this way, most of the integrals can be expressed in terms of the basic integrals in appendix A. For the integrals (B.19) and (B.22), the above procedure had to be applied twice.

Appendix C. Integrals involving Green functions with arbitrary constant

To demonstrate the translational invariance of results showed in the main text we use the modified Green function

$$\Delta(s,s') = \frac{L}{3}a - \frac{|s-s'|}{2} - \frac{(s+s')}{2} + \frac{(s^2+s'^2)}{2L}, \tag{C.1}$$

with an arbitrary constant a. The various relations fulfilled by this Green function are listed below assuming $s \geqslant s'$, for brevity.

The useful relations are

$$\Delta_{\rm F}(s,s') = \Delta_{\rm F}(s-s') = \Delta(s,s') - \frac{1}{2}\Delta(s,s) - \frac{1}{2}\Delta(s',s') = -\frac{1}{2}(s-s'), \tag{C.2}$$

$$\begin{aligned} D_1(s,s') &= \Delta^2(s,s') - \Delta(s,s)\Delta(s',s') \\ &= (s-s')\left[\frac{s(L-s)}{L} + \frac{(s-s')(s+s')^2}{4L^2} - \frac{La}{3}\right], \end{aligned} \tag{C.3}$$

$$D_2(s,s') = \Delta(s,s) - \Delta(s',s') = \frac{(s-s')(s+s'-L)}{L}. \tag{C.4}$$

The useful integrals are

$$\begin{aligned} J_1(s,s') &= \int_0^L \mathrm{d}t\, \Delta(t,t)\,{}^{\cdot}\Delta(t,s)\,{}^{\cdot}\Delta(t,s') = \frac{(s^4+s'^4)}{4L^2} - \frac{(2s^3+s'^3)}{3L} \\ &\qquad + \frac{((a+3)s^2+as'^2)}{6} - \frac{sa}{3}L + \frac{(20a-9)}{180}L^2, \end{aligned} \tag{C.5}$$

$$\begin{aligned} J_2(s,s') &= \int_0^L \mathrm{d}t\, {}^{\cdot}\Delta(t,t)\Delta(t,s)\,{}^{\cdot}\Delta(t,s') \\ &= \frac{(-2s^4+6s^2s'^2+3s'^4)}{24L^2} + \frac{(3s^3-3s^2s'-6ss'^2-s'^3)}{12L} \\ &\quad - \frac{(5s^2-12ss'-4as'^2)}{24} - \frac{s'a}{6}L + \frac{(20a-3)}{720}L^2, \end{aligned} \tag{C.6}$$

$$\begin{aligned} J_3(s,s') &= \int_0^L \mathrm{d}t\, \Delta(t,s)\Delta(t,s') = -\frac{(s^4+6s^2s'^2+s'^4)}{60L} + \frac{(s^2+3s'^2)s}{6} \\ &\qquad - \frac{(s^2+s'^2)}{6}L + \frac{(5a^2-10a+6)}{45}L^3. \end{aligned} \tag{C.7}$$

These are the building blocks for other relations

$$\begin{aligned} \langle U_2(s,s')\rangle &= \frac{(d-1)}{2}\left[D_1(s,s') - \frac{(d+1)}{4}D_2^2(s,s')\right] \\ &= -\frac{(d-1)(s-s')}{4}\left[\frac{2La}{3} + \frac{(d-3)s-(d+1)s'}{2}\right. \\ &\qquad \left. - \frac{(d-1)s^2-(d+1)s'^2}{L} + \frac{d(s-s')(s+s')^2}{2L^2}\right], \end{aligned} \tag{C.8}$$

$$\begin{aligned} K_1(s,s') &= J_1(s,s') - \frac{1}{2}J_1(s,s) - \frac{1}{2}J_1(s',s') \\ &= -(s-s')\left[\frac{La}{6} - \frac{(s+s')}{4} + \frac{(s^2+ss'+s'^2)}{6L}\right], \end{aligned} \tag{C.9}$$

$$\begin{aligned} K_2(s,s') &= J_2(s,s') + J_2(s',s) - J_2(s,s) - J_2(s',s') \\ &= -(s-s')^2\left[\frac{1}{4} - \frac{(5s+7s')}{12L} + \frac{(s+s')^2}{4L^2}\right], \end{aligned} \tag{C.10}$$

$$\begin{aligned} K_3(s,s') &= J_3(s,s') - \frac{1}{2}J_3(s,s) - \frac{1}{2}J_3(s',s') \\ &= -(s-s')^2\left[\frac{(s+2s')}{6} - \frac{(s+s')^2}{8L}\right], \end{aligned} \tag{C.11}$$

$$K_4(s, s') = \Delta(0, s)\Delta(0, s') - \frac{1}{2}\Delta^2(0, s) - \frac{1}{2}\Delta^2(0, s')$$
$$= -\frac{(s - s')^2(s + s' - 2L)^2}{8L^2}, \tag{C.12}$$
$$K_5(s, s') = \Delta(L, s)\Delta(L, s') - \frac{1}{2}\Delta^2(L, s) - \frac{1}{2}\Delta^2(L, s') = -\frac{(s^2 - s'^2)^2}{8L^2}. \tag{C.13}$$

Appendix D. Relation with distribution from diffusion equation

The distribution function derived in [23] for $d = 3$ dimensions has the form

$$G(r; t) = \frac{1}{4\pi}\left[f_0(t)\delta(r-1) + \frac{f_1(t)}{r}\delta'(r-1) + \frac{f_2(t)}{r}\delta''(r-1) + \frac{f_3(t)}{r}\delta'''(r-1) + \cdots\right], \tag{D.1}$$

where the coefficients $f_i(t)$ are the polynomials in powers of t. To order t^3, their expansions read

$$f_0(t) = 1 + \frac{1}{3}t + \frac{1}{15}t^2 + \frac{4}{315}t^3 + \cdots, \tag{D.2}$$
$$f_1(t) = f_0(t) - 1, \tag{D.3}$$
$$f_2(t) = \frac{7}{90}t^2 - \frac{1}{630}t^3 + \cdots, \tag{D.4}$$
$$f_3(t) = \frac{31}{1890}t^3 - \cdots. \tag{D.5}$$

Depending on the reduced distance r, expression (D.1) cannot be directly comparable with the distribution function (89). To remove this, we expand

$$\frac{1}{r} = \frac{1}{(r-1)+1} = 1 - (r-1) + (r-1)^2 - (r-1)^3 + \cdots. \tag{D.6}$$

Substituting expansion (D.6) into equation (D.1), we use the properties of δ-function

$$x\delta'(x) = -\delta(x), \qquad x^n\delta'(x) \equiv 0, \qquad n > 1, \tag{D.7}$$
$$x\delta''(x) = -2\delta'(x), \qquad x^2\delta''(x) = 2\delta(x), \qquad x^n\delta'(x) \equiv 0, \qquad n > 2, \tag{D.8}$$
$$x\delta'''(x) = -3\delta''(x), \qquad x^2\delta'''(x) = 6\delta'(x), \qquad x^3\delta'''(x) = -6\delta(x),$$
$$x^n\delta'(x) \equiv 0, \qquad n > 3. \tag{D.9}$$

This brings the distribution function (D.1) in the form (89) with

$$p_0(t) = 2f_0(t) + 2\frac{f_2(t)}{t} + 6\frac{f_3(t)}{t^2} - 1 + \cdots = 1 + \frac{2}{3}t + \frac{13}{45}t^2 + \frac{38}{315}t^3 + \cdots, \tag{D.10}$$
$$p_1(t) = f_0(t) + 2\frac{f_2(t)}{t} + 6\frac{f_3(t)}{t^2} - 1 + \cdots = \frac{1}{3}t + \frac{2}{9}t^2 + \frac{34}{315}t^3 + \cdots, \tag{D.11}$$
$$p_2(t) = \frac{f_2(t)}{t} + 3\frac{f_3(t)}{t^2} + \cdots = \frac{7}{90}t^2 + \frac{1}{21}t^3 + \cdots, \tag{D.12}$$
$$p_3(t) = \frac{f_3(t)}{t^2} + \cdots = \frac{31}{1890}t^3 + \cdots. \tag{D.13}$$

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