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# The statistical mechanics of a concatenated polymer chain

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**Abstract**

The elastic and configurational properties of mesoscopic structures, which have been formed by linking a finite number of polymer loops to each other, are considered. For simplicity it is assumed that the linking numbers between pairs of loops provides a sufficient description of the topological structure. To conserve the topology the statistical mechanical calculation of the partition sum is restricted to the configuration space labelled by the specified linking numbers.

An expansion of the partition sum is proposed where the linking numbers, corresponding to a particular structure, select a sub-set of terms from the expansion. The case of a linear concatenated chain of loops is studied and it is shown that the first non-zero contribution from this expansion is already able to describe the chain as a re-scaled Gaussian chain capable of supporting stress. This confirms that the approximation maintains the structural integrity of the chain. The effective step length and step length distribution function are also identified together with the elastic properties.

The relationship of linking numbers to the Abelian Chern–Simons gauge field theory is used to illustrate essential parts of the calculation. The relevant term in the partition sum is represented in terms of Feynman diagrams describing the two-particle scattering amplitude for vector gauge bosons. It is shown that the expected re-scaled Gaussian chain result comes from the dominance in the s-channel of a massive scalar boson representing the structure of an individual loop in the chain.

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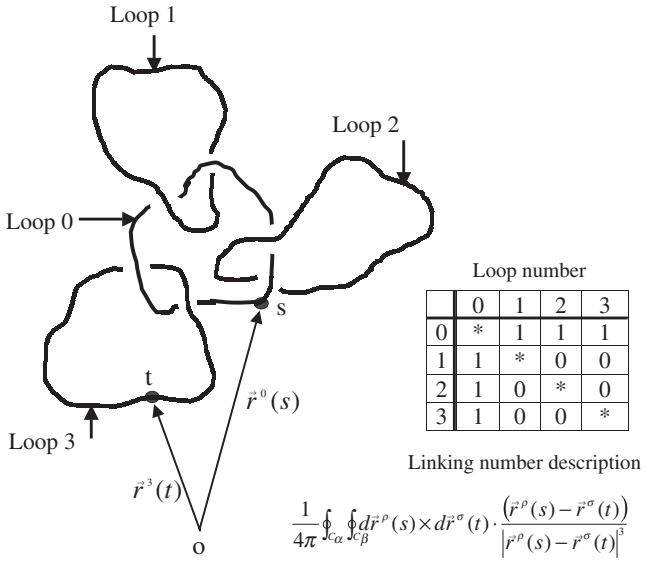
## 1. Introduction: concatenated structures

In this paper the statistical mechanics of mesoscopic structures, formed by linking polymer loops to each other, is developed. For simplicity the only structures considered are those for which the linking numbers between pairs of loops provides a sufficient description of the topology. An example is given in figure 1 together with the description in terms of




| | 0 | 1 | 2 | 3 |
|---|---|---|---|---|
| 0 | * | 1 | 1 | 1 |
| 1 | 1 | * | 0 | 0 |
| 2 | 1 | 0 | * | 0 |
| 3 | 1 | 0 | 0 | * |

**Figure 1.** A concatenated meso-structure and its description in terms of linking numbers. The structure is preserved in a statistical mechanical calculation by confining the partition sum to the configuration space labelled by these linking numbers.

a set of linking numbers. The continuously connected nature of the polymer molecules forming the loops ensures the topological integrity of the meso-structure and confers on it additional configurational and elastic properties. The essential statistical mechanical problem is to calculate the partition sum, restricted to a configuration space labelled by the set of linking numbers describing the structure.

In principle the Boltzmann factor, with a suitable potential function, should be sufficient to stop two polymer chains from passing through each other and thereby changing the topological state. In practice, for polymer chains this is very difficult to implement in an analytic manner because of the continuous nature of the molecule along its arc length. In this paper the Boltzmann factor is not used but instead the partition sum over the phase space is restricted from the outset to those configurations which conserve the given topology (linking numbers). This approach was initiated by Edwards [1, 2] and forms the basis of much of the subsequent work. Previous work, using winding numbers, has considered the linking of two loops [1–4] or the configuration of a polymer chain trapped by obstacles [5–9]. In melt situations the effect of a winding number restriction on the configuration of a single chain was made in [10–12]. The effect of winding number constraints in networks has been considered in [13–16]. The object of this paper is to study the elastic and configurational properties of structures formed by imposing specified linking numbers on a finite collection of polymer loops.

Whilst the problem can be readily formulated, computational problems arise which prevent the direct calculation of the partition sum. In this paper a systematic expansion of the partition sum is proposed where the linking numbers, describing a given structure, are shown to pick out a sub-set (infinite) of terms from the expansion. The calculation can then be completed term by term. However, it is far from clear that picking out a finite number of terms from an expansion will preserve the topological integrity of the problem. To investigate this, the particular case of a concatenated chain of loops will be studied. The reason for this choice is that the major part of the result is known in advance and can be used to guide the calculation.

If the topological of the concatenated chain is preserved by the adopted procedure then it will be expected to behave like a re-scaled Gaussian chain. In particular it should show elastic properties if the two end loops of the concatenated chain are held a fixed distance apart. This example enables the most relevant terms in the expansion to be identified and the procedure can be applied to more complex structures.

The topological content of a general entanglement of loops is an aspect of Knot theory [17]. The linking number is a simple example of a topological invariant but collectively they do not form a complete topological description. Recent progress has led to new and more discriminating invariants [18], which draw heavily on the ideas and formalism of gauge field theories [19–21]. In these so-called topological field theories theory the action, a Chern–Simons 3-form associated with a non-Abelian group, is invariant under general co-ordinate transformations. Linking numbers represent the Abelian version of an otherwise non-Abelian Chern–Simons gauge field theory. The connection between linking numbers and a gauge field theory was already noted by Edwards [1, 2] in 1967. The configuration of a single polymer loop linked into a melt of loops was mapped onto a $n \to 0$ component scalar electrodynamics field theory [10, 22]. The use of Abelian Chern–Simons theory for polymer problems was implemented by Ferrari and Lazzizzera [23]. The interplay between the statistical mechanics of condensed matter and field theories is now well established [24, 25] and frequently one is used to illustrate the other. This paper uses the connection with Abelian gauge fields to represent the topological content of a concatenated chain by a class of Feymann diagrams. It is shown that there is a very close correspondence between the diagrams and the topological structure of the chain.

In the next section the general problem of conserving a linking number description of the topology of a melt of polymer loops is formulated. In section 3, the concatenated chain is considered and the connection with gauge fields and a class of Feynman diagrams explained in section 4. In section 5 the elasticity of the concatenated chain is derived.

## 2. The partition sum and linking number conservation

The Gauss linking number $G(C_\rho, C_\sigma)$ between two closed space curves $C_\rho$ and $C_\sigma$ is a positive or negative integer and a topological invariant given by

$$G(C_\rho, C_\sigma) = \frac{1}{4\pi} \oint_{C_\alpha} \oint_{C_\beta} \mathrm{d}\vec{r}^{\rho}(s) \times \mathrm{d}\vec{r}^{\sigma}(t) \cdot \frac{(\vec{r}^{\rho}(s) - \vec{r}^{\sigma}(t))}{|\vec{r}^{\rho}(s) - \vec{r}^{\sigma}(t)|^3}. \tag{2.1}$$

The notation is shown in figure 1, $\vec{r}^{\rho}(s)$ is a position on the $C_\rho$ curve at a point described by the arc length $s$. It measures the number of times one curve wraps around the other. Its use in the statistical mechanics of polymer systems has been considered in previous papers [1–16]. When the system is first fabricated it is assumed that the particular topology formed can be adequately described by a set of linking numbers $\{m_{\rho\sigma}\}$ between all the loops in the system. The example in figure 1 is a particular case where the linking numbers are either 1 or 0. These linking numbers are to be rigorously conserved by restricting the configurational phase space used in the partition sum to this initial set. Since the $\{m_{\rho\sigma}\}$ are integer variables, a product of Kronecker delta functions is used and the partition sum $Z(\{m_{\rho\sigma}\})$ is written as

$$Z\left(\{m_{\rho\sigma}\}\right) = \left\langle \prod_{\rho\sigma} \left[\delta\left(G(C_\rho, C_\sigma) - m_{\rho\sigma}\right) + \delta\left(G(C_\rho, C_\sigma) + m_{\rho\sigma}\right)\right] \right\rangle. \tag{2.2}$$

The brackets $\langle \cdots \rangle$ represent an unrestricted average over all the configurations of all the loops in the system.

The statistical mechanical calculation to be described in this paper proceeds from the following parametrization of the delta function:

$$\delta\left(G_{\rho\sigma} \pm m_{\rho\sigma}\right) = \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}g_{\rho\sigma}\, \exp[\mathrm{i}g_{\rho\sigma}(G(C_\rho, C_\sigma) \pm m_{\rho\sigma})] \tag{2.3}$$

to give

$$Z(\{m_{\rho\sigma}\}) = \prod_{\rho'\sigma'}\left\{\frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}g_{\rho'\sigma'}\cos\left(g_{\rho'\sigma'}m_{\rho'\sigma'}\right)\right\}\left\langle \exp\left[\mathrm{i}\sum_{\rho\sigma} g_{\rho\sigma}G(C_\rho, C_\sigma)\right]\right\rangle. \tag{2.4}$$

The central statistical mechanical problem consists of evaluating the term

$$Z(\{g_{\rho\sigma}\}) = \left\langle \exp\left[\mathrm{i}\sum_{\rho\sigma} g_{\rho\sigma}G(C_\rho, C_\sigma)\right]\right\rangle. \tag{2.5}$$

There have been two main approaches to this problem: one is to further transform the problem either to a gauge field theory [7, 10], while the other [15, 16] attempts to identify suitable collective polymer variables. Both approaches attempt to preserve the integrity of the exponential function in (2.5), however, the subsequent results do not readily lend themselves to the final integrations over the $\{g_{\rho\sigma}\}$ variables conjugate to the linking numbers $\{m_{\rho\sigma}\}$. This last operation encapsulates the essential aspects of the physics of these systems. A system with all the linking numbers set equal to zero should not support an imposed large-scale deformation, whereas the presence of structures formed by non-zero linking numbers will, when they reach the scale of the deformation. This physical difference should be reflected and identified in the calculation.

The approach adopted in this paper starts with the expansion of the exponential in the statistical term

$$\left\langle \exp\left[\mathrm{i}\sum_{\rho\sigma} g_{\rho\sigma}G_{\rho\sigma}\right]\right\rangle = 1 + \mathrm{i}\sum_{\rho\sigma} g_{\rho\sigma}\langle G_{\rho\sigma}\rangle - \frac{1}{2!}\sum_{\rho\sigma;\rho'\sigma'} g_{\rho\sigma}g_{\rho'\sigma'}\langle G_{\rho\sigma}G_{\rho'\sigma'}\rangle - \cdots. \tag{2.6}$$

The averaging is taken over unrestricted loop configurations. The actual structure to be imposed on the loops is contained in the product of the cosine terms, involving the winding numbers:

$$\left\{\prod_{\rho'\sigma'}\cos\left(g_{\rho'\sigma'}m_{\rho'\sigma'}\right)\right\}. \tag{2.7}$$

When this is applied to the expansion (2.6) and integrated over the $\{g_{\rho\sigma}\}$, the presence of non-zero linking numbers in the set $\{m_{\rho\sigma}\}$ has a very immediate effect. To see this consider the simplest situation when all the winding numbers are zero. This describes an amorphous melt of unlinked loops, no mesoscopic structures can be present. In this case the product of cosine factors (2.7) is just unity and all terms in the expansion (2.6), as well as each loop term in the summations contribute to the integrals over the $\{g_{\rho\sigma}\}$ factors. There are no special terms present and the series must be re-summed in its entirety. This was considered in a previous paper [15] and achieved with the use of appropriately defined collective variables.

The situation is radically altered by the presence of non-zero winding numbers between loops, indicating the presence of linked meso-structures. Now specific terms in the expansion (2.6) are identified which reflect the concatenated structures and which will be shown to provide the major contribution to the partition sum. For example, if a loop 1 is linked to loop 2, then $m_{12} \neq 0$ and the product (2.7) becomes $\cos(g_{12}m_{12})$. Then, in sharp contrast to the un-linked amorphous melt where all terms contributed, no term contributes in the expansion (2.6) unless it contains the factor$g_{12}$, since

$$\int_0^{2\pi} \mathrm{d}g_{12}\cos(g_{12}m_{12}) = 0 \qquad \text{if} \quad m_{12} \neq 0.$$

Furthermore since

$$\int_0^{2\pi} \mathrm{d}g_{12} \cos(g_{12}m_{12})\, g_{12} = 0$$

the first non-zero contribution for each pair of linked loops occurs when a $g_{12}^2$ term is present, since

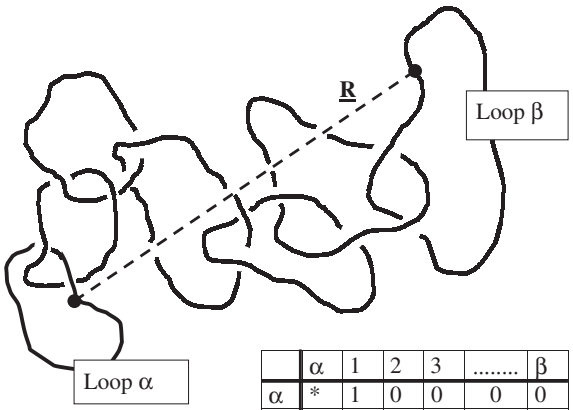
$$\frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}g_{12} \cos(g_{12}m_{12})\, g_{12}^2 = \frac{2}{m_{12}^2}.$$

The winding numbers $\{m_{\rho\sigma}\}$ are chosen to represent physical structures. For example, the star-shaped meso-structure shown in figure 1, described by the non-zero linking number sequence $m_{10}, m_{20}, m_{30}$, will pick out terms in the expansion (2.6) which at least contain the sequence $g_{10}^2 g_{20}^2 g_{30}^2$. In the expansion these only begin to occur at the sixth order. The more complex the structure being modelled, the higher one must go in the expansion (2.6) before any contribution to the partition sum is made.

In this paper only the first term to contribute will be considered. In the above example of a star-shaped meso-structure this will be the term

$$g_{10}^2 g_{20}^2 g_{30}^2 \langle G_{10}^2 G_{20}^2 G_{30}^2 \rangle.$$

The question remains whether picking out this minimal term will maintain anything of the integrity of the original meso-structure. In the next section this is investigated using a linear concatenated chain of loops, shown in figure 2. The loops at either end will be held a fixed distance apart and the approximation of picking out the minimal term in the expansion (2.6) will be used. We will show that this approximation preserves the integrity of the chain by demonstrating its elastic properties. In fact, at a scale larger than an individual loop size, we are able to recover the usual partition sum of a Gaussian chain.




| | α | 1 | 2 | 3 | ..... | β |
|---|---|---|---|---|---|---|
| α | * | 1 | 0 | 0 | 0 | 0 |
| 1 | 1 | * | 1 | 0 | 0 | 0 |
| 2 | 0 | 1 | * | 1 | 0 | 0 |
| 3 | 0 | 0 | 1 | * | …… | 0 |
| : | : | : | : | : | * | : |
| β | 0 | 0 | 0 | 0 | …… | * |

Linking number description of the linear concatenated chain.

**Figure 2.** A linear concatenated chain. The structural integrity is tested by holding the end loops $C_\alpha$ and $C_\beta$ a fixed distance $\boldsymbol{R}$ apart.

## 3. A concatenated chain

A concatenated chain of $n$ links, connecting a loop $C_\alpha$ to another loop $C_\beta$, will be described by a sequence of non-zero linking numbers $m_{\alpha 1}m_{12}m_{23}\cdots m_{n\beta}$ with the linking numbers associated with all the other permutations of loop labels being set equal to zero, figure 2. In view of the previous discussion the first contribution to the partition sum from the expansion (2.6) will occur for the term

$$g^2_{\alpha 1}g^2_{12}g^2_{23}\cdots g^2_{n\beta}\langle G^2_{\alpha 1}G^2_{12}G^2_{23}\cdots G^2_{n\beta}\rangle. \tag{3.1}$$

If the essential features of the topology are conserved then the system will be able to support a stress. To investigate this a point $\vec{r}^{\,\alpha}(s^\alpha_0)$ on the loop $C_\alpha$ and a point $\vec{r}^{\,\beta}(s^\beta_0)$ on the loop $C_\beta$ are held a distance $\vec{R}$ apart. The free energy and in particular the restoring force can then be calculated from the partition sum. The constraint is expressed by inserting the factor $\delta(\vec{R}-\vec{r}^{\,\alpha}(s^\alpha_0)+\vec{r}^{\,\beta}(s^\beta_0))$ into the configurational average for the partition sum given by (2.4).

Higher terms in the expansion will also contribute provided that they have the basic grouping $(g^2_{\alpha 1}g^2_{12}g^2_{23}\cdots g^2_{n\beta})$. For example, the information that $C^\alpha$ is *not* linked to $C^2(m_{\alpha 2}=0)$ would be entered through the terms containing the sequence $(g^2_{\alpha 1}g^2_{12}g^2_{23}\cdots g^2_{n\beta})g^2_{\alpha 2}$ as a minimum group of factors. The effect of these terms will be examined in a future paper. In this paper the partition sum $Z(\boldsymbol{R})$ for a concatenated chain with the end loops $C_\alpha$ and $C_{\alpha'}$ are held a distance $\boldsymbol{R}$ apart is taken to be given by the first non-zero contribution to the partition sum:

$$\begin{aligned} Z(R) \approx \prod_{\rho'\sigma'}\left\{\frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}g_{\rho'\sigma'}\cos\left(g_{\rho'\sigma'}m_{\rho'\sigma'}\right)\right\}\Big\langle g^2_{\alpha 1}g^2_{12}\cdots g^2_{n\beta}\langle G^2_{\alpha 1}G^2_{12}\cdots G^2_{n\beta}\rangle \\ \times\delta\big(\vec{R}-\vec{r}^{\,\alpha}(s^\alpha_0)+\vec{r}^{\,\beta}(s^\beta_0)\big)\Big\rangle \\ = \text{constant}\,\big\langle G^2_{\alpha 1}G^2_{12}\cdots G^2_{n\beta}\delta\big(\vec{R}-\vec{r}^{\,\alpha}(s^\alpha_0)+\vec{r}^{\,\beta}(s^\beta_0)\big)\big\rangle. \end{aligned} \tag{3.2}$$

The term *constant* contains the integrals over the $g$ variables and combinatorial factors. $G_{\rho\sigma}\equiv G(C_\rho,C_\sigma)$ represents the Gauss winding number (2.1).

The calculation of the statistical average

$$\big\langle G^2_{\alpha 1}G^2_{12}\cdots G^2_{n\beta}\delta\big(\vec{R}-\vec{r}^{\,\alpha}(s^\alpha_0)+\vec{r}^{\,\beta}(s^\beta_0)\big)\big\rangle \tag{3.3}$$

is performed using the Gaussian model for the individual polymer loops. It is in principle (but not in practice) straightforward and the details are presented in appendix A. There it is shown that, by averaging over the end loops $C_\alpha$ and $C_\beta$, the partition sum can be written in the form

$$Z(R)=\int\mathrm{d}\vec{Q}\,Z(\vec{Q})\exp\left(-\mathrm{i}\vec{Q}\cdot\vec{R}\right) \tag{3.4}$$

where

$$Z(\vec{Q})=\int\mathrm{d}\vec{p}\,\mathrm{d}\vec{p}\,'\,S_\alpha(\vec{Q})T_n\big\lfloor\vec{p},(\vec{Q}-\vec{p});\vec{p}\,',(\vec{Q}-\vec{p}\,')\big\rfloor S_\beta(\vec{Q}). \tag{3.5}$$

$S_{\alpha/\beta}(\vec{Q})$ is the structure factor of the end loops and given by

$$S(Q)=\frac{1}{L}\int_0^L\mathrm{d}s\,\mathrm{d}s_0\left\langle\exp[-\mathrm{i}\vec{Q}\cdot(\vec{r}(s)-\vec{r}(s_0))]\right\rangle. \tag{3.6}$$

The term $T_n(\vec{p},\vec{k};\vec{p}\,',\vec{k}\,')$ describes the topological connectivity of the intermediate $n$ loops in the chain. As a reflection of the concatenated nature of the chain, the structure of the general term can be obtained by iteration. The result from appendix A is

$$T_n(p,k;\vec{p}\,',\vec{k}\,')=\int\frac{\mathrm{d}^3p_1}{(2\pi)^3}\frac{\mathrm{d}^3k_1}{(2\pi)^3}T_1(p,k;\vec{p}_1,\vec{k}_1)T_{n-1}(p_1,k_1;\vec{p}\,',\vec{k}\,'). \tag{3.7}$$

$T_1(\vec{p},\vec{k};\,\vec{p}',\vec{k}')$ is the result for a chain of one intermediate loop $C_\alpha - C_1 - C_\beta$. In the appendix it is shown that $T_1(p,k;\,\vec{p}',\vec{k}')$ can be written as

$$T_1(p,k;\,\vec{p}',\vec{k}') = D_{aa'}(p)D_{ab'}(k)\Gamma^{a'b'c'd'}(p,k;\,p',k')D_{cc'}(p')D_{cd'}(k'). \quad (3.8)$$

In this expression $a, b, c, \ldots$ are Cartesian co-ordinates and

$$D_{ab}(p) = \varepsilon_{abc}p^c/p^2. \quad (3.9)$$

$\Gamma(p,k;\,p',k')$ is calculated from the four-point single-chain correlation function:

$$\Gamma(p,k;\,p',k') = \oint\!\!\oint\!\!\oint\!\!\oint \langle \mathrm{d}\vec{r}_1\,\mathrm{d}\vec{r}_2\,\mathrm{d}\vec{r}_3\,\mathrm{d}\vec{r}_4 \exp \mathrm{i}\big(-\vec{p}\cdot\vec{r}_1 - \vec{k}\cdot\vec{r}_2 - \vec{p}'\cdot r_{31} - \vec{k}'\cdot\vec{r}_4\big)\rangle. \quad (3.10)$$

While the calculations described in appendices A and B have been entirely in terms of polymer variables, the results (3.7)–(3.9) can be interpreted in terms of two-body scattering amplitudes for vector gauge bosons. This draws attention to the close connection that exists between topology and Gauge field theories [5–7] and leads directly to a simplification of the term $\Gamma(p,k;\,p',k')$. This aspect is considered in the next section where it is also shown how certain classes of Feynman diagrams describing the interaction of a gauge field with a massive scalar field precisely mirror the topological content of the concatenated chain. The section can be omitted, the main result is that $Z(\vec{Q})$ from (3.5) can be written as

$$\begin{aligned} Z(\vec{Q}) &= \int \mathrm{d}\vec{p}\,\mathrm{d}\vec{p}' S_\alpha(\vec{Q})T_n\big[\vec{p},(\vec{Q}-\vec{p});\,\vec{p}',(\vec{Q}-\vec{p}')\big]S_\beta(\vec{Q}) \\ &\cong [S(Q)]^{n+2} \end{aligned}$$

and this reflects the dominance of a certain class of Feynman diagrams.

## 4. Concatenated chains, gauge fields and Feynman diagrams

The term $D_{ab}(p) = \varepsilon_{abc}p^c/p^2$ can be regarded as the propagator for a vector gauge field $\vec{A}(q)$. The following is a mathematical identity first used by Edwards in 1967 [1]:

$$\begin{aligned} D_{ab}(p) &= \langle A_a(p)A_b(-p)\rangle \\ &= \frac{\int D\vec{A}_q A_a(p)A_b(-p)\exp\big(-\int \mathrm{d}^3q\;\vec{A}_q\cdot\mathrm{curl}\vec{A}_{-q}\big)\delta(\vec{q}\cdot\vec{A}_q)}{\int D\vec{A}_q \exp\big(-\int \mathrm{d}^3q\;\vec{A}_q\cdot\mathrm{curl}\vec{A}_{-q}\big)\delta(\vec{q}\cdot\vec{A}_q)} \\ &= \frac{\varepsilon_{abc}p^c}{p^2}. \end{aligned} \quad (4.1)$$

The term $\int \mathrm{d}^3q\;\vec{A}_q\cdot\mathrm{curl}\vec{A}_{-q}$ is now recognized as the Abelian version of a Chern–Simons Lagrangian [20,21].

The term $T_1(p,k;\,\vec{p}',\vec{k}')$, given by (3.8), then represents the scattering amplitude of two gauge bosons with the four-point correlation function $\Gamma^{a'b'c'd'}(p,k;\,p',k')$ acting as a vertex function. It can be diagrammatically represented as shown in figure 3.

For a concatenated chain of $n$ intermediate links, $T_n(p,k;\,\vec{p}',\vec{k}')$ is given by the iteration (3.7). This leads to the ladder diagram, shown in figure 4.

The vertex function $\Gamma(p,k;\,p',k')$ is the only input required to calculate $T_n(p,k;\,\vec{p}',\vec{k}')$. $\Gamma(p,k;\,p',k')$ reflects the structure of a single loop in the chain and is calculated from the four-point correlation function (3.10). The calculation is considered in detail in appendix B, where it is shown that for long loops it can be approximated as the sum of three terms:

$$\Gamma^{abcd}(\vec{p},\vec{k},\vec{p}',\vec{k}') = \frac{bL}{9}\delta_{ab}\delta_{cd}S(\vec{p}+\vec{k}) + \delta_{ac}\delta_{bd}S(\vec{p}+\vec{p}') + \delta_{ad}\delta_{bc}S(\vec{p}+\vec{k}') \quad (4.2)$$

where $S(\vec{q})$ is once again the structure factor, given by (3.6), of the intermediate chain.

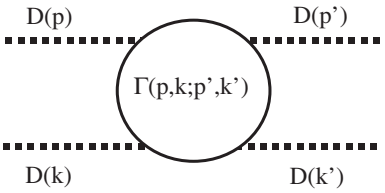



**Figure 3.** The diagrammatic representation of $T_1(p, k; \vec{p}', \vec{k}')$. The dotted lines represent massless vector bosons and $\Gamma(p, k; p', k')$ is a vertex function calculated from the four-point single chain correlation function (3.10).

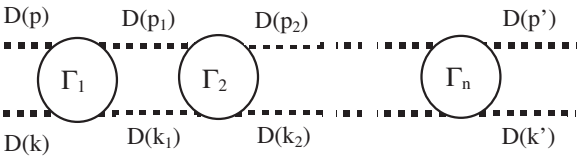



**Figure 4.** Diagrammatic representation of $T_n(p, k; \vec{p}', \vec{k}')$ for a concatenated chain of $n$ intermediate links. Integration over the wavenumber variables $\vec{p}_1, \vec{k}_1$, etc is implied in the diagram.

The three combinations of wavevectors in the structure factors of this result (4.2) define the $s$, $t$ and $u$ channels through the Mandelstam variables:

$$\begin{aligned} s &= (p+k)^2 \\ t &= (p+p')^2 \\ u &= (p+k')^2. \end{aligned} \tag{4.3}$$

These were originally defined for the relativistic 4 vector momentum variables occurring in the quantum field theory description of particle scattering theory.

The contribution of these three terms to the scattering amplitude $T_1(\vec{p}, \vec{k}; \vec{p}', \vec{k}')$ is diagrammatically shown in figure 5.

For a Gaussian chain of length $L$ and average step length $b$, the structure factor can be approximated by [26]

$$S(q) = 12\left[\frac{1}{\frac{12}{Nb^2} + q^2}\right]. \tag{4.4}$$

The term in the square bracket can be interpreted as the propagator for a scalar boson of 'mass' $12/Lb$. The scattering amplitude $T_1(\vec{p}, \vec{k}; \vec{p}', \vec{k}')$ then describes the exchange of a scalar boson between Chern–Simons gauge bosons in the $s$, $t$ and $u$ channels respectively.

In appendix C it is shown that the s-channel contribution is the dominant one, when the integration over the wavenumbers carried by the gauge boson is completed. Using this term, the fourier transform $Z(\vec{Q})$ of the partition sum $Z(\vec{R})$ expressed by (3.5) and (3.7) can be represented by the 'necklace' diagram shown in figure 6.

The integration over the wavenumbers carried by the gauge boson 'bubbles' lead to a product of constants, dependent on a small-distance cut-off. In the partition sum $Z(R)$ multiplicative constants are irrelevant as they only contribute a constant term to the free energy. The essential contribution of figure 4 to $Z(R)$ can be written as

$$Z(R) \approx \int \mathrm{d}^3 Q\, [S(Q)]^{n+2} \exp(\mathrm{i}\vec{Q} \cdot \vec{R}). \tag{4.5}$$

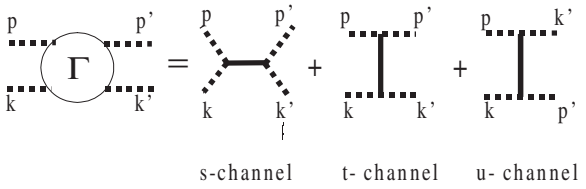



**Figure 5.** The structure of the scattering amplitude $T_1(\vec{p},\vec{k};\vec{p}',\vec{k}')$ according to the approximation (4.2). The solid lines represent the structure factor of a single chain and the broken lines are the gauge bosons.

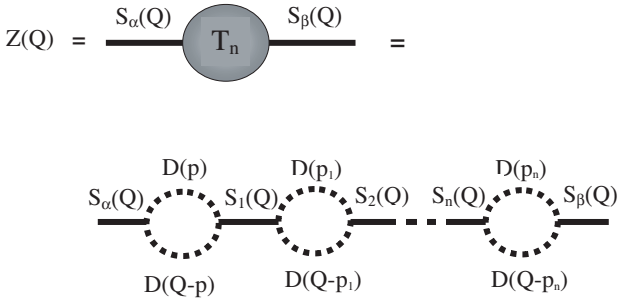



**Figure 6.** The diagrammatic structure of the fourier transform of the partition function. The solid 'boson' lines represent the physical structure of the polymer loops. The broken 'gauge bosons' lines mediate the topological connectivity of the chain. The 'necklace' structure mirrors the linearity of the concatenated chain. Integration over the intermediate wavenumber variables is implied. This is the dominant diagram that gives rise to rubber elasticity.

In the next section the result (4.5) will be interpreted in terms of an equivalent freely jointed chain of variable bond lengths $\{\vec{l}_j\}$. The form of the bond length distribution function $p(\vec{l}_j)$ will be found and the expected rubber elasticity verified.

## 5. The equivalent freely jointed chain and rubber elasticity

The partition function $Z_0(R)$ for a chain of $n+2$ bonds of variable bond lengths $\{\vec{l}_j\}$ with the ends held a distance $R$ apart is given by

$$Z_0(R) = \left\langle \delta\left[\sum_{j=1}^{n+2}\vec{l}_j - \vec{R}\right]\right\rangle = \frac{1}{(2\pi)^3}\int \mathrm{d}^3Q\,\exp\left(-\mathrm{i}\vec{Q}\cdot\vec{R}\right)\left\langle \exp\left(\mathrm{i}\vec{Q}\cdot\sum_{j=1}^{n+2}\vec{l}_j\right)\right\rangle. \tag{5.1}$$

For a freely jointed chain with a bond length distribution function $p(\vec{l}_j)$

$$\left\langle \exp\left(\mathrm{i}\vec{Q}\cdot\sum_{j=1}^{n+2}\vec{l}_j\right)\right\rangle = \left[\int \mathrm{d}^3l\; p(l)\exp\left(\mathrm{i}\vec{Q}\cdot\vec{l}\right)\right]^{n+2} = [p(Q)]^{n+2} \tag{5.2}$$

and

$$Z_0(R) = \frac{1}{(2\pi)^3}\int \mathrm{d}^3Q\,[p(Q)]^{n+2}\exp\left(-\mathrm{i}\vec{Q}\cdot\vec{R}\right). \tag{5.3}$$

Comparing (4.5) with (5.3) the distribution function $p(l)$ for the equivalent chain can be identified (apart from a normalization factor) with the single chain structure factor

$$p(Q) \approx S(Q) \tag{5.4}$$

$S(Q)$ has the well known Yukawa form and consequently

$$p(l) \approx \frac{1}{l} \exp\left(-l\sqrt{\frac{12}{Nb^2}}\right). \tag{5.5}$$

The usual simple models for a polymer chain either consider freely jointed bonds of a fixed length or bonds with a Gaussian distribution. The distribution function (5.5) does not lead to any significant differences from the simple models. The Gaussian result for a chain of $n$ links is obtained by using the approximation

$$\begin{aligned}[S(Q)]^{n+2} &\approx \left[\frac{1}{1+\frac{Q^2Nb^2}{12}}\right]^{n+2} \\ &\approx \exp\left(-\frac{Q^2(n+2)Nb^2}{12}\right). \end{aligned} \tag{5.6}$$

Then the partition sum is given by

$$\begin{aligned} Z(R) &\approx \sum_Q \exp\left(-\frac{Q^2(n+2)Nb^2}{12}\right)\exp(\mathrm{i}\vec{Q}\cdot\vec{R}) \\ &\approx \left(\frac{12\pi}{(n+2)Nb^2}\right)^{3/2} \exp\left(-\frac{3R^2}{(n+2)Nb^2}\right). \end{aligned} \tag{5.7}$$

This is the classic Gaussian result for a chain of $n+2$ statistical segments. The rubber elasticity of the chain follows directly (5.7).

## 6. Conclusions

Topological connectivity in a melt of polymer loops has been formulated in terms of the Gauss winding number between pairs of loops. The resulting statistical mechanical average cannot be done exactly and approximation procedures are required. In a previous paper only zero winding numbers between all loops were considered and suitable collective variables were identified. The inclusion of non-zero winding numbers radically alters the methodology of the calculation and reflects the changed physical nature of the system. In this paper a straightforward expansion of the statistical factor has been considered and used to investigate the elasticity of a concatenated chain. It was shown that the first non-zero term in the expansion is able to reproduce the results of Gaussian rubber elasticity theory. This term only contains the minimal information of which loops are linked to each other, that is the non-zero linking numbers. Higher terms, which were not discussed in the paper, carry the information of which loops are not linked to each other, that is have zero linking numbers. The paper also demonstrated how this minimal term represents the concatenated chain very directly in terms of gauge particles scattering off scalar particles. The gauge particles carry the topological information and the scalar particles the structure of the individual elements of the chain. The 'necklace' structure of the corresponding Feymann diagram mirrors precisely the topological structure of the chain.

## Appendix A

In this appendix the result:

$$\begin{aligned} Z(\vec{Q}) &= \left\langle G^2_{\alpha 1} G^2_{12} \cdots G^2_{n\beta} \exp\left(\vec{Q}\cdot(\vec{r}^{\,\alpha}(s^\alpha_0) + \vec{r}^{\,\beta}(s^\beta_0))\right)\right\rangle \\ &= \int \mathrm{d}\vec{p}\,\mathrm{d}\vec{p}\,' \, S_\alpha(\vec{Q}) T_n\big[\vec{p}, (\vec{Q}-\vec{p}); \vec{p}\,', (\vec{Q}-\vec{p}\,')\big] S_\beta(\vec{Q}) \end{aligned} \tag{A.1}$$

is derived.

It is expedient to begin the statistical averaging in (A.1) with the two end loops $C_\alpha$ and $C_\beta$. These support the constraint that the end-to-end distance of the concatenated chain is a fixed distance $R$. The calculation is achieved by expressing the Gauss linking number formula (2.1) in terms of wavevector variables as

$$G(C_\rho, C_\sigma) = \int \frac{\mathrm{d}^3 q}{(2\pi)^3} \frac{\vec{u}_\rho(q) \times \vec{u}_\sigma(-q) \cdot \mathrm{i}\vec{q}}{q^2} \tag{A.2}$$

where $\vec{u}_\rho(q)$ are the Fourier components of the tangent vector density to the single loop $C_\rho$

$$\vec{u}_\rho(q) = \oint_{C_\rho} \mathrm{d}\vec{r} \exp(\mathrm{i}\vec{q} \cdot \vec{r}^\sigma) = \oint_{C_\rho} \mathrm{d}s\, \dot{\vec{r}}(s) \exp(\mathrm{i}\vec{q} \cdot \vec{r}^\sigma(s)). \tag{A.3}$$

The term $\langle G_{\alpha 1}^2 \rangle_\alpha$ is given by

$$\left\langle G_{\alpha 1}^2 \right\rangle_\alpha = -\int \frac{\mathrm{d}^3 p}{(2\pi)^3} \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \frac{(\vec{u}_1(p) \times \vec{p}) \cdot \langle \vec{u}_\alpha(-p)\vec{u}_\alpha(-k)\rangle_\alpha \cdot \left(\vec{u}_1(k) \times \vec{k}\right)}{p^2 k^2}. \tag{A.4}$$

The Cartesian components of the bond vector correlation function $\langle \vec{u}_\alpha(-p)\vec{u}_\alpha(-k)\rangle_\alpha$ are given as (all loops in the chain will be considered identical and in general chain labels will be omitted when there is no confusion):

$$\begin{aligned}
\langle u_a(-p)u_b(-k)\rangle_\alpha &= \int_0^L \mathrm{d}s \int_0^L \mathrm{d}t \left\langle \dot{r}_a(s)\dot{r}_b(t) \exp\left[ -\mathrm{i}\left(\vec{p} \cdot \vec{r}(s) + \vec{k} \cdot \vec{r}(t)\right)\right]\right\rangle \\
&= \exp\left[-\mathrm{i}\vec{r}^\alpha(s_0) \cdot \left(\vec{p} + \vec{k}\right)\right] \int_0^L \mathrm{d}s \int_0^L \mathrm{d}t \\
&\quad \times \left\langle \dot{r}_a(s)\dot{r}_b(t) \exp\left[ -\mathrm{i}\vec{p} \cdot \int_{s_0}^s \mathrm{d}t\, \dot{\vec{r}}(t) - \mathrm{i}\vec{k} \cdot \int_{s_0}^t \mathrm{d}t\, \dot{\vec{r}}(t)\right]\right\rangle.
\end{aligned} \tag{A.5}$$

$\vec{r}^\alpha(s_0)$ is the position vector to an arbitrary point on the loop $C_\alpha$. The tangent vectors $\{\dot{r}_i(t)\}$ are treated as Gaussian random variables

$$\left\langle \dot{r}_i(t)\dot{r}_j(t')\right\rangle = \frac{b}{3}\delta_{ij}\delta(t - t'). \tag{A.6}$$

For sufficiently long chains, two approximations will be constantly used in this paper:

(i) the tangent vectors correlations will be factorized from the position vector correlations:

$$\begin{aligned}
&\int_0^L \mathrm{d}s \int_0^L \mathrm{d}t \left\langle \dot{r}_a(s)\dot{r}_b(t) \exp\left[ -\mathrm{i}\vec{p} \cdot \int_{s_0}^s \mathrm{d}t\, \dot{\vec{r}}(t) - \mathrm{i}\vec{k} \cdot \int_{s_0}^t \mathrm{d}t\, \dot{\vec{r}}(t)\right]\right\rangle \\
&\qquad \cong \int_0^L \mathrm{d}s \int_0^L \mathrm{d}t\, \langle \dot{r}_a(s)\dot{r}_b(s)\rangle \left\langle \exp\left[ -\mathrm{i}\vec{p} \cdot \int_{s_0}^s \mathrm{d}t\, \dot{\vec{r}}(t) - \mathrm{i}\vec{k} \cdot \int_{s_0}^t \mathrm{d}t\, \dot{\vec{r}}(t)\right]\right\rangle
\end{aligned} \tag{A.7}$$

(ii) the loop constraint will be neglected when averaging over the configuration of the chains.

With these approximations

$$\begin{aligned}
\langle u_{a\alpha}(-p)u_{b\alpha}(-k)\rangle_\alpha &= \frac{b}{3}\delta_{ij} \exp\left[-\mathrm{i}\vec{r}^\alpha(s_0) \cdot \left(\vec{p} + \vec{k}\right)\right] \int_0^L \mathrm{d}s \left\langle \exp\left[ -\mathrm{i}\left(\vec{p} + \vec{k}\right) \cdot \int_{s_0}^s \mathrm{d}t\, \dot{\vec{r}}(t)\right]\right\rangle \\
&= \frac{b}{3}\delta_{ij} \exp\left[-\mathrm{i}\vec{r}^\alpha(s_0) \cdot \left(\vec{p} + \vec{k}\right)\right] \rho(p + k; s_0)
\end{aligned} \tag{A.8}$$

where

$$\rho(p + k; s_0) = \int_0^L \mathrm{d}s \left\langle \exp\left[ -\mathrm{i}\left(\vec{p} + \vec{k}\right) \cdot \int_{s_0}^s \mathrm{d}t\, \dot{\vec{r}}(t)\right]\right\rangle$$

is the fourier transform of the density of chain segments round the point $\vec{r}_\alpha(s_0)$. This is related to the structure factor $S(Q)$ of the molecule by

$$\begin{aligned} S(Q) &= \frac{1}{L}\int_0^L \mathrm{d}s\,\mathrm{d}s_0 \left\langle \exp[-\mathrm{i}\vec{Q}\cdot(\vec{r}(s)-\vec{r}(s_0))]\right\rangle \\ &= \frac{1}{L}\int_0^L \mathrm{d}s\,\mathrm{d}s_0 \left\langle \exp[-\mathrm{i}\vec{Q}\cdot\int_{s_0}^{s}\mathrm{d}t\dot{\vec{r}}(t)]\right\rangle \\ &= \frac{1}{L}\int_0^L \mathrm{d}s_0\,\rho(p+k;s_0). \end{aligned} \tag{A.9}$$

Hence

$$\begin{aligned} \left\langle G^2_{\alpha 1}\right\rangle_\alpha = -\frac{b}{3}\int\frac{\mathrm{d}^3p}{(2\pi)^3}\int\frac{\mathrm{d}^3k}{(2\pi)^3}\frac{(\vec{u}_1(p)\times\vec{p})\cdot(\vec{u}_1(k)\times\vec{k})}{p^2k^2} \\ \times\exp\left[-\mathrm{i}\vec{r}^{\alpha}(s_0)\cdot(\vec{p}+\vec{k})\right]\rho(p+k;s_0^\alpha). \end{aligned} \tag{A.10}$$

A corresponding expression holds for the other end loop term $\langle G^2_{n\beta}\rangle_\beta$.

$$\begin{aligned} \left\langle G^2_{n\beta}\right\rangle_\beta = -\frac{b}{3}\int\frac{\mathrm{d}^3p'}{(2\pi)^3}\int\frac{\mathrm{d}^3k'}{(2\pi)^3}\frac{(\vec{u}_n(p')\times\vec{p}')\cdot(\vec{u}_n(k')\times\vec{k}')}{p'^2k'^2} \\ \times\exp\left[-\mathrm{i}\vec{r}^{\beta}(s_0)\cdot(\vec{p}'+\vec{k}')\right]\rho(p'+k';s_0^\beta). \end{aligned}$$

The combination of terms $\langle G^2_{\alpha 1}\rangle_\alpha\langle G^2_{n\beta}\rangle_\beta$ has still to be averaged over the position of the two loops in space subject to the constraint that $\vec{r}^{\alpha}(s_0^\alpha)-\vec{r}^{\beta}(s_0^\beta)=\vec{R}$. Furthermore, since the positions $s_0^\alpha, s_0^\beta$ along each loop of the end points of the vector $\boldsymbol{R}$ are also arbitrary they are also averaged. These averages are given by

$$\begin{aligned} &\int_0^L\frac{\mathrm{d}s_0^\alpha}{L}\int_0^L\frac{\mathrm{d}s_0^\beta}{L}\int\frac{\mathrm{d}^3r^\alpha(s_0^\alpha)}{\Omega}\frac{\mathrm{d}^3r^\beta(s_0^\beta)}{\Omega}\left\langle \mathrm{G}^2_{\alpha 1}\right\rangle_\alpha\left\langle \mathrm{G}^2_{n\beta}\right\rangle_\beta\delta(\vec{R}-\vec{r}^{\alpha}(s_0^\alpha)-\vec{r}^{\beta}(s_0^\beta)) \\ &\quad=\frac{1}{\Omega^2}\left(\frac{b}{3}\right)^2\int\frac{\mathrm{d}^3p}{(2\pi)^3}\int\frac{\mathrm{d}^3k}{(2\pi)^3}\int\frac{\mathrm{d}^3p'}{(2\pi)^3}\int\frac{\mathrm{d}^3k'}{(2\pi)^3}\delta(\vec{p}+\vec{k}+\vec{p}'+\vec{k}') \\ &\quad\times S(p+k)S(p'+k')\frac{(\vec{u}_1(p)\times\vec{p})\cdot(\vec{u}_1(k)\times\vec{k})}{p^2k^2}\frac{(\vec{u}_n(p')\times\vec{p}')\cdot(\vec{u}_n(k')\times\vec{k}')}{p'^2k'^2} \\ &\quad\times\exp(-\mathrm{i}(\vec{p}+\vec{k})\cdot\vec{R}). \end{aligned} \tag{A.11}$$

Finally, using (A.11), the partition sum (3.2) for the concatenated chain can be written as

$$\begin{aligned} Z(R) = \frac{1}{\Omega^2}\left(\frac{b}{3}\right)^2\int\frac{\mathrm{d}^3p}{(2\pi)^3}\int\frac{\mathrm{d}^3k}{(2\pi)^3}\int\frac{\mathrm{d}^3p'}{(2\pi)^3}\int\frac{\mathrm{d}^3k'}{(2\pi)^3}\delta(\vec{p}+\vec{k}+\vec{p}'+\vec{k}') \\ \times S^2(p+k)T_n(\vec{p},\vec{k};\vec{p}',\vec{k}')\exp(-\mathrm{i}(\vec{p}+\vec{k})\cdot\vec{R}) \end{aligned} \tag{A.12}$$

where $T_n(\vec{p},\vec{k};\vec{p}',\vec{k}')$ is given by

$$\begin{aligned} T_n(\vec{p},\vec{k};\vec{p}',\vec{k}') = \left\langle\frac{(\vec{u}_1(-p)\times\vec{p})\cdot(\vec{u}_1(-k)\times\vec{k})}{p^2k^2}G^2_{12}G^2_{23}\cdots G^2_{n-1,n}\right. \\ \left.\times\frac{(\vec{u}_n(-p')\times\vec{p}')\cdot(\vec{u}_n(-k')\times\vec{k}')}{p'^2k'^2}\right\rangle_{C_1\cdots C_n}. \end{aligned} \tag{A.13}$$

By repeating the process and averaging over the loop $C_1$, it can readily be shown that $T_n(\vec{p},\vec{k};\vec{p}',\vec{k}')$ is generated by iteration. The result is

$$T_n(p,k;\vec{p}',\vec{k}') = \int\frac{\mathrm{d}^3p_1}{(2\pi)^3}\frac{\mathrm{d}^3k_1}{(2\pi)^3}T_1(p,k;\vec{p}_1,\vec{k}_1)T_{n-1}(p_1,k_1;\vec{p}',\vec{k}') \tag{A.14}$$

where

$$T_1(p,k;\vec{p}',\vec{k}') = \frac{1}{p^2k^2}\frac{1}{p'^2k'^2} \times\left\langle(\vec{u}_1(-p)\times\vec{p})\cdot(\vec{u}_1(-k)\times\vec{k})(\vec{u}_1(-p')\times\vec{p}')\cdot(\vec{u}_1(-k')\times\vec{k}')\right\rangle_{C_1}. \quad \text{(A.15)}$$

Set

$$D_{ab}(p) = \varepsilon_{abc}p^c/p^2$$

and

$$\Gamma^{abcd}(p,k;p',k') = \left\langle u^a(-p)u^b(-k)u^c(-p')u^d(-k')\right\rangle = \oint\oint\oint\oint \left\langle \mathrm{d}\vec{r}_1^{\,a}\,\mathrm{d}\vec{r}_2^{\,b}\,\mathrm{d}\vec{r}_3^{\,c}\,\mathrm{d}\vec{r}_4^{\,d}\exp\left[\mathrm{i}\left(-\vec{p}\cdot\vec{r}_1-\vec{k}\cdot\vec{r}_2-\vec{p}'\cdot r_{31}-\vec{k}'\cdot\vec{r}_4\right)\right]\right\rangle$$

to get the result quoted in the paper. i.e.

$$T_1(p,k;\vec{p}',\vec{k}') = D_{aa'}(p)D_{ab'}(k)\Gamma^{a'b'c'd'}(p,k;p',k')D_{cc'}(p')D_{cd'}(k'). \quad \text{(A.16)}$$

## Appendix B

In this appendix the vertex function

$$\Gamma^{abcd}(p,k;p',k') = \oint\oint\oint\oint \left\langle \mathrm{d}\vec{r}_1^{\,a}\,\mathrm{d}\vec{r}_2^{\,b}\,\mathrm{d}\vec{r}_3^{\,c}\,\mathrm{d}\vec{r}_4^{\,d}\exp\left[\mathrm{i}\left(-\vec{p}\cdot\vec{r}_1-\vec{k}\cdot\vec{r}_2-\vec{p}'\cdot r_{31}-\vec{k}'\cdot\vec{r}_4\right)\right]\right\rangle \quad \text{(B.1)}$$

is calculated for a Gaussian chain.

The calculation of the four-point correlation function generates a variety of terms, even when the same approximations employed for the two-point function are used. The first approximation is to de-couple the tangent vectors $\{\mathrm{d}\vec{r}\,(s)\}$ from the phase factors $\{\exp\mathrm{i}\,(\vec{q}\cdot\vec{r}(s))\}$ so that

$$\Gamma^{abcd}(p,k;p',k') \approx \oint\oint\oint\oint \left\langle \mathrm{d}\vec{r}_1^{\,a}\,\mathrm{d}\vec{r}_2^{\,b}\,\mathrm{d}\vec{r}_3^{\,c}\,\mathrm{d}\vec{r}_4^{\,d}\right\rangle\left\langle\exp\left[\mathrm{i}\left(-\vec{p}\cdot\vec{r}_1-\vec{k}\cdot\vec{r}_2-\vec{p}'\cdot r_3-\vec{k}'\cdot\vec{r}_4\right)\right]\right\rangle. \quad \text{(B.2)}$$

The second approximation is to ignore the loop constraint. Then the four-point correlation function of the tangent vectors generates three separate terms:

$$\langle\dot{r}_a(s_1)\dot{r}_b(s_2)\dot{r}_c(s_3)\dot{r}_d(s_4)\rangle \cong \left(\frac{b}{3}\right)^2 \times\left[\delta_{ab}\delta_{cd}\delta(s_1-s_2)\delta(s_3-s_4)+\delta_{ac}\delta_{bd}\delta(s_1-s_3)\delta(s_2-s_4) +\delta_{ad}\delta_{bc}\delta(s_1-s_4)\delta(s_2-s_3)\right]. \quad \text{(B.3)}$$

Using this result the calculation of $\Gamma^{a'b'c'd'}(p,k;q,l)$can be completed and the result written as

$$\Gamma^{abcd}(p,k,p',k') = \frac{bL}{9}\delta_{ab}\delta_{cd}S(p+k)+\delta_{ac}\delta_{bd}S(p+p')+\delta_{ad}\delta_{bc}S(p+k') \quad \text{(B.4)}$$

where $S(q)$ is the structure factor, given by (3.6) for the intermediate chain $C_1$.

## Appendix C

In this appendix the dominance of the s-channel contribution is established.

It is sufficient to consider the term $T_1(p,k;\vec{p}',\vec{k}')$ since the result for $n$ intermediate loops is generated by iterating this term. Using (3.9) and (4.2) in (3.8) and performing the sums over the Cartesian indices on the vector gauge bosons, each channel contributes to the term $T_1(p,k;\vec{p}',\vec{k}')$ according to

$$T_1(p,k;\vec{p}',\vec{k}') = T_s(p,k;\vec{p}',\vec{k}') + T_t(p,k;\vec{p}',\vec{k}') + T_u(p,k;\vec{p}',\vec{k}') \tag{C.1}$$

where

$$\begin{aligned} T_s(p,k;\vec{p}',\vec{k}') &= \frac{(\vec{p}\cdot\vec{k})}{p^2k^2}\frac{(\vec{p}'\cdot\vec{k}')}{p'^2k'^2}S(p+k) \\ T_t(p,k;\vec{p}',\vec{k}') &= \frac{(\vec{p}\cdot\vec{k})(\vec{p}'\cdot\vec{k}') + (\vec{p}\cdot\vec{p}')(\vec{k}\cdot\vec{k}')}{p^2k^2p'^2k'^2}S(p+p') \\ T_u(p,k;\vec{p}',\vec{k}') &= \frac{(\vec{p}\cdot\vec{k})(\vec{p}'\cdot\vec{k}') + (\vec{p}\cdot\vec{k}')(\vec{k}\cdot\vec{p}')}{p^2k^2p'^2k'^2}S(p+k'). \end{aligned} \tag{C.2}$$

The partition sum is given by

$$\begin{aligned} Z(R) = \frac{1}{\Omega^2}\left(\frac{b}{3}\right)^2 \int \frac{\mathrm{d}^3p}{(2\pi)^3}\int \frac{\mathrm{d}^3k}{(2\pi)^3}\int \frac{\mathrm{d}^3p'}{(2\pi)^3}\int \frac{\mathrm{d}^3k'}{(2\pi)^3}\delta\big(\vec{p}+\vec{k}+\vec{p}'+\vec{k}'\big) \\ \times S^2(p+k)T_1(\vec{p},\vec{k};\vec{p}',\vec{k}')\exp\big[\big(-\mathrm{i}\big(\vec{p}+\vec{k}\big)\cdot\vec{R}\big)\big]. \end{aligned} \tag{C.3}$$

Define the variables

$$\begin{aligned} \vec{Q} &= \frac{\vec{p}+\vec{k}}{2} = -\frac{\vec{p}'+\vec{k}'}{2} \\ \vec{q} &= \frac{\vec{p}-\vec{k}}{2} \qquad \vec{q}' = \frac{\vec{p}'-\vec{k}'}{2}. \end{aligned}$$

Then the contribution to the partition sum from the s-channel term can be written as

$$Z_s(R) \sim \int \mathrm{d}^3Q\, S^3(Q)I_s^2(Q)\exp\big(-\mathrm{i}\vec{Q}\cdot\vec{R}\big) \tag{C.4}$$

where $I_s(Q)$ arises from the gauge boson terms $(\vec{p}\cdot\vec{k})/p^2k^2$ and is given by

$$I_s(Q) = \int \mathrm{d}^3q\,\frac{Q^2-q^2}{(Q^2-q^2)^2-(2\vec{Q}\cdot\vec{q})^2}. \tag{C.5}$$

This integral is divergent and requires a small distance cut-off. However the leading term is independent of $Q$ and consequently only occurs as a factor in the partition sum.

The contribution to the partition sum from the t-channel term can be written down in a similar fashion as

$$Z_t(R) \sim \int \mathrm{d}^3Q\, S^2(Q)I_t(Q)\exp\big(-\mathrm{i}\vec{Q}\cdot\vec{R}\big) \tag{C.6}$$

where, from (C.2), $I_t(Q)$ is given by

$$2\int \mathrm{d}^3q'\int \mathrm{d}^3q\,\frac{Q^2-q^2}{(Q^2-q^2)^2-(2\vec{Q}\cdot\vec{q})^2}\,\frac{Q^2-q'^2}{(Q^2-q'^2)^2-(2\vec{Q}\cdot\vec{q}')^2}S\left(2(\vec{q}+\vec{q}')\right). \tag{C.7}$$

The intermediate chain structure factor,

$$S\left(2(q+q')\right) \sim \frac{1}{\frac{12}{Nb^2}+4(\vec{q}+\vec{q}')^2}$$

is convoluted in the term $I_t(Q)$ and reduces the degree of divergence of the integral to a logarithmic dependent on the cut-off. The same argument also applies to the u-channel contribution. Hence the dominant term comes from the s-channel term.

The topological connectivity is carried by the gauge bosons and the structure of the intermediate links is carried by the massive boson. For this channel the sequence of terms factorize and the result can be written as a generalization of (C.4)

$$Z_s(R) \sim \int \mathrm{d}^3 Q \, S^{n+2}(Q) \exp\left(-\mathrm{i}\vec{Q} \cdot \vec{R}\right). \tag{C.8}$$

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