Critical Phenomena of Single and Double Polymer Strands in a Solution

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Abstract

A universality class describing the statistics of the merging of two single polymer strands to a double polymer strand and the reverse process is examined. The polymers can have an intrinsic direction, and the simpler case, where only single strands aligned parallel bind to a double strand is considered in detail. The critical dimension of the universality class is six, there is a stable fixed point and critical exponents are calculated with renormalization group and loop expansion. The corresponding field theory describes polymer configurations in terms of fields and not in terms of coordinate paths and is second quantized in this sense.

Introduction

It is known since a long time that the configurations of a long polymer chain in a solution exhibit scaling behavior, equivalent to the $n \to 0$ limit of the $O(n)$-symmetric Heisenberg magnet universality class. Such systems can be described with a (“first quantized”) path integral over the monomer coordinates, or with the $O(n)$ symmetric $(\varphi^2)^2$ field theory.\cite{1} \cite{2} \cite{3} \cite{4} The difficult part of the problem is “self avoidance”, the fact that a polymer chain cannot intersect itself.

It also is known since a long time that the formation of a DNA double strand from DNA single strands has aspects of first order phase transitions and second order phase transitions. For instance, it is found to sometimes proceed in steps and sometimes continuously when the temperature is lowered. The real problem of course is complicated by the quasi irregular nucleotide sequences, but a simple argument shows that the problem is nontrivial. An estimate for the configuration entropy of a single polymer strand of length $L$ in $d$ dimensions (ignoring self avoidance) is $k_B \ln (2d-1)^L = k_B L \ln (2d-1)$. A single strand bound to a double strand has half the length and half the configuration entropy. This can be compensated by the binding energy which also is proportional to $L$.

Theoretical models mostly have considered polymer strands with a uniform binding energy, and many methods have been used, see for example ref.\cite{5} A recent review is\cite{6}. In this work we derive a field theory from a microscopic model, which then allows to examine the statistical mechanics of the binding and unbinding of double strands with the renormalization group.

The model

We consider directed polymer chains (i.e., chains with an intrinsic direction) and different binding energies for double strands consisting of single strands aligned parallel and for double strands consisting of single strands aligned antiparallel. This could be realized with DNA chains. Assume there are nucleotide pairs $(Xx)$ and $(Yy)$. Then a strand $...XYxyXYxy...$ binds to itself with offset 2, but

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binds less strongly to the inverted strand ...yxYXyxYX.... The model of course also contains the case of equal binding energies. Similarly the intrinsic direction also contains the case of undirected polymers, the direction then only is a technical device.

The model, as appropriate for critical phenomena, consists of a path integral with action

\[ S = \int d^d x \left\{ \mathcal{L}_0 + \mathcal{L}_1 + \hat{\mathcal{L}}_0 + \hat{\mathcal{L}}_1 \right\}, \]

\[ \mathcal{L}_0 = -\int ds \tilde{\varphi}(s) \left( r_0 - \nabla^2 + \partial_s \right) \varphi(s) - \int ds ds' \tilde{\psi}(s, s') \left( \tau_0 - \nabla^2 + w (\partial_s + \partial_{s'}) \right) \psi(s, s'), \]

\[ \mathcal{L}_1 = \frac{g}{\sqrt{K_d}} \int ds ds' \left\{ \tilde{\psi}(s, s') \varphi(s) \varphi(s') + \tilde{\varphi}(s) \tilde{\varphi}(s') \psi(s, s') \right\}, \]

\[ \hat{\mathcal{L}}_0 = -\int ds ds' \tilde{\chi}(s, s') \left( \tau_0 - \nabla^2 + \tilde{\omega} (\partial_s - \partial_{s'}) \right) \chi(s, s'), \]

\[ \hat{\mathcal{L}}_1 = \frac{\hat{g}}{\sqrt{K_d}} \int ds ds' \left\{ \tilde{\varphi}(s) \varphi(s') (\chi(s, s') + \tilde{\chi}(s, s)) \right\}. \]  

For notational simplicity here all space arguments of fields are suppressed, \( \tilde{\varphi}(s) \) should be read as \( \tilde{\varphi}(x, s) \) etc. The constant \( K_d \) is defined in appendix B. A derivation of the field theory with the help of operators on a lattice can be found in appendix A. However, all terms have a clear meaning.

The field \( \tilde{\varphi}(x, s) \) creates a start of a single strand at position \( x \) with initial length variable \( s \), the field \( \varphi(x, s) \) terminates a single strand with length variable \( s \) at position \( x \). The \( \varphi \) propagator \( \mathcal{L}_0 \) with \( r_0 = 0 \) describes diffusion of the \( \varphi \)-field in \( s \)-direction (this is not a diffusion that takes place step by step in \( s \), it simply is part of the partition sum).

The nonlinear terms in \( \mathcal{L}_1 \) can be identified as the transition of two aligned single strands \( \varphi \) to an (aligned) double strand \( \tilde{\psi}(x, s, s') \) and the reverse process. The terms in \( \hat{\mathcal{L}}_1 \) can be identified as the transition of two oppositely aligned single strands \( \varphi, \tilde{\varphi} \) to an (oppositely aligned) double strand \( \tilde{\chi}(x, s, s') \) and the reverse process. The double strands \( \psi \) and \( \chi \) take over the length variables of the single strands. Along a double strand of course one has \( s - s' = const \) or \( s + s' = const \), but field theory and perturbation theory are simpler when both length variables are kept. One might introduce fields like \( \psi_a(x, s) \), where \( a \) is the length offset of the single strands. But then the interaction terms would be more complicated.

The interactions \( \mathcal{L}_1 \) and \( \hat{\mathcal{L}}_1 \) are local in space but non-local and even translationally invariant in the length variables. This means that the interaction of two strands at the same point in space is the same, for any length index. Technically this implies that in Fourier space (with “frequencies” \( \omega \) and \( \omega' \) dual to \( s \) and \( s' \)) no frequency is transferred between single strands, even when the strands combine to a double strand and separate again - the perturbation theory does not contain any frequency integrals.

The redundancy (or gauge invariance) of length variables in the double strand fields \( \psi, \tilde{\psi}, \chi, \tilde{\chi} \) reflects itself in their propagators. In wavevector space the harmonic equations of motion (functional derivative of \( \mathcal{L}_0 \) and \( \hat{\mathcal{L}}_0 \) with respect to \( \tilde{\psi} \) or \( \tilde{\chi} \) read (the quantities \( w \) and \( \tilde{\omega} \) are constants)

\[ (\tau_0 + \mathbf{k}^2 + w (\partial_s + \partial_{s'}) ) \psi_k(s, s') = 0, \]

\[ (\tilde{\tau}_0 + \mathbf{k}^2 + \tilde{\omega} (\partial_s - \partial_{s'}) ) \chi_k(s, s') = 0. \]

The generic solutions of these homogeneous equations are

\[ \psi_k(s, s') = \exp \left( -\frac{1}{2w} (\tau_0 + \mathbf{k}^2) (s + s') \right) \gamma_k(s - s'), \]

\[ \chi_k(s, s') = \exp \left( -\frac{1}{2\tilde{\omega}} (\tilde{\tau}_0 + \mathbf{k}^2) (s - s') \right) \tilde{\gamma}_k(s + s'), \]
where $\gamma_k(s-s')$ and $\hat{\gamma}_k(s+s')$ are arbitrary functions. But in the perturbation expansion there actually only occur the “causal” response functions

\[
G_k (s_2, s'_2; s_1, s'_1) = \theta(s_2 - s_1) \exp\left(-\frac{1}{w} (\tau_0 + k^2) (s_2 - s_1)\right) \delta((s_2 - s_1) - (s'_2 - s'_1)), \tag{2}
\]

\[
\hat{G}_k (s_2, s'_2; s_1, s'_1) = \theta(s_2 - s_1) \exp\left(-\frac{1}{\hat{w}} (\hat{\tau}_0 + k^2) (s_2 - s_1)\right) \delta((s_2 - s_1) + (s'_2 - s'_1)),
\]

where $(s_1, s'_1)$ are the initial and $(s_2, s'_2)$ the final length variables. The delta functions enforce the length variable constraints. In frequency space the propagators simply are

\[
G_k (\omega, \omega') = 1/\left(\tau_0 + k^2 - w (i\omega + i\omega')\right),
\]

\[
\hat{G}_k (\omega, \omega') = 1/\left(\hat{\tau}_0 + k^2 - \hat{w} (i\omega - i\omega')\right).
\]

And in fact, the perturbation theory can also be done in the traditional way by combining segments of trajectories of different types of polymers and integrating over coordinates, carefully taking account of the segment length constraints (an example is eq. (3) below). The phenomenology of the model and the meaning of the relevant parameters $r_0$, $\tau_0$ and $\hat{\tau}_0$ are examined after the renormalization group calculation in the next section.

### Renormalization group calculation for model A

In this work we restrict ourselves to the case where only single strands oriented in the same direction form a double strand (model A. Model B is when only oppositely aligned strands bind, like a sequence ...XYZzyx...). This means $\bar{q} = 0$ and $\chi$ and $\bar{\chi}$ can be ignored.

The first step is to examine the scaling behavior of the microscopic field theory \(^{(1)}\). Because of the symmetries $\varphi \leftrightarrow \bar{\varphi}$, $\psi \leftrightarrow \bar{\psi}$ and $s \leftrightarrow s'$ one concludes that the model is of order 4 - there are four different scaling exponents, say, for $k$, $\omega$, $\varphi$ and $\psi$. The (naive) scaling exponents are denoted as $[k] = 1$, $[\omega]$, $[\varphi]$ and $[\psi]$. The scaling of the wavevector (or length) is purely geometric and the exponent 1 is exact by definition. Dimensional analysis (the action must be dimensionless) then requires that a wave vector dimension also is assigned to the coupling constant $g$. The result of the linear algebra is $[s^{-1}] = [\omega] = 2$, $[\varphi] = [\bar{\varphi}] = 3 - \epsilon/2$, $[\psi] = [\bar{\psi}] = 4 - \epsilon/2$ and $[g] = \epsilon/2$ as well as $[w] = 0$.

As usual $\epsilon = d - d_c$, the critical dimension $d_c$ is 6. With these scaling exponents it can already be checked that the excluded volume effect (between all sorts of polymers) is strongly irrelevant in the renormalization group sense in the vicinity of $d_c = 6$. One final remark is in order here. $\mathcal{L}_0$ and $\mathcal{L}_1$ together provide 5 linear equations (ignoring the relevant $r_0$ and $\tau_0$ terms). Four of them already suffice to determine $[\varphi]$, $[\psi]$, $[\omega]$ and $[g]$. This is the reason for introducing the “coupling constant” $w$. The physical scaling exponents are written as $[f] + \eta_f$, for instance $[\varphi] + \eta_{\varphi}$.

The model A perturbation theory generates no one loop contributions to the 3-point vertex $g\psi\bar{\varphi}\bar{\varphi}$ and likewise to $g\bar{\psi}\varphi\varphi$. There only remain the self energy renormalizations, see fig.(1). The contributions to the action \(^{(1)}\) are

\[
\Gamma^{(1)}_{\varphi\bar{\varphi}} |_{k=\mu} = -g_0^2 \left\{ 2k^2 I_1 (\epsilon) - (4w + 2) i\omega I_2 (\epsilon) \right\},
\]

\[
\Gamma^{(1)}_{\psi\bar{\psi}} |_{k=\mu} = -g_0^2 \left\{ 2k^2 I_1 (\epsilon) - 2i (\omega_1 + \omega_2) I_2 (\epsilon) \right\}.
\]
The dimensionless bare coupling constant is \( g_0 = g \mu^{-\epsilon/2} \), where \( \mu \) is an arbitrary small wave vector. The integrals \( I_1 \) and \( I_2 \) are defined in appendix A. The mapping to the renormalized field theory then amounts to the rescalings \( \varphi = Z \varphi_R \), \( \tilde{\psi} = Z \tilde{\psi}_R \), \( \psi = Z \psi_s \), \( s = Z_s s_R \) (only considering the critical point \( r_R = \tau_R = 0 \)). The formalism is standard and need not be described in detail here.\[7\] One result are the flow equations

\[
\mu \partial_\mu g_R = -\frac{\epsilon}{2} g_R \left\{ 1 - 6 g_R^2 I_1 \right\},
\]

\[
\mu \partial_\mu w_R = \frac{\epsilon}{w_R} g_R^2 \left( 2 w_R^2 + w_R - 1 \right) I_2
\]

for the renormalized dimensionless coupling constants \( g_R \) and \( w_R \). For \( \mu \to 0 \) one finds the infrared stable fixed point \( g_R^2 = \frac{\epsilon}{2} \) and \( w_R = \frac{1}{2} \). The flow equation for \( w \) is remarkable, it is nonlinear and has a second (unphysical) stable fixed point \( w_R = -1 \). The value \( \frac{1}{2} \) means that a double strand has a larger size than a single strand for a given end-to-end length.

The anomalous contributions to the scaling dimensions at the stable fixed point to order \( O(\epsilon) \) are

\[
\eta_\varphi = \epsilon, \quad \eta_\psi = \frac{11}{6} \epsilon, \quad \eta_\omega = \frac{5}{3} \epsilon.
\]

The scaling exponent for \( \omega \) thus is \( z = [\omega] + \eta_\omega \). As a first result one can conclude from the scaling equivalences \( \omega \sim k^z \) and \( s \sim x^z \) (where \( x \) is a length) that \( x \sim s^{1/z} = s^{1/(2 + 5\epsilon/3)} \). Normal diffusive behavior would be \( x \sim \sqrt{s} \). A single strand thus has a much smaller extension. This is plausible - binding to a double strand as in fig.(1) counteracts diffusion.

**Phenomenology of model A**

In this section we attempt to understand the physics at and near the stable fixed point. The simplest and most important scenario is a single one-strand polymer. The relevant parameter \( r_0 \) (or its renormalized counterpart) always is zero. A nonzero value would be equivalent to a Boltzmann factor for \( \varphi \) segments in the partition sum. However, the polymer is of fixed length and there is no reservoir of \( \varphi \) molecules. This is analogous to first quantized models, where contributions to \( \varphi \) segments, and \( \varphi \) acts as a reservoir for \( \psi \). The parameter \( \tau \) in principle can be changed by changing the temperature or the composition of the solution.

As long as \( \tau \) is nonnegative, one would expect that the amount of double strands \( \psi \) is small. In this sense \( \psi \) plays the role of an order parameter. This does not mean that the \( \psi \) field has no effect for \( \tau \geq 0 \). There could be many short \( \psi \) segments with a small statistical weight in the partition sum. This can be compared with the excluded volume effect, where there also is no binding energy. The critical exponents depend on the interaction nevertheless. The region \( \tau > 0 \) in the parameter space of the system then would be a region of a transition from excluded volume behavior to model A behavior with exponents \( 1, 4 \). For \( \tau < 0 \) the binding energy becomes positive and there will be many \( \psi \) segments.

To estimate the amount of double strands with the field theory \( 1 \), one should introduce an external field \( h_{\psi \varphi}(x, s) \) which couples to \( \int ds' \psi(x, s, s') \varphi(x, s) \). This "sink" in principle is a normal \( \varphi \) sink, but it describes the case where a single strand terminates within a double strand, converting it to a single strand. The one-loop contribution to this sink looks like graph A in fig.1 without the propagator on the r.h.s.

If \( u \) denotes the length of the \( \psi \) and \( v \) the length of the \( \varphi \) propagator, then the total single strand length in in the loop of graph A of fig.1 is \( s = 2u + v \). In \( (k, s) \) - space the propagators are (eq.2)
Figure 2: Some diagrams for model B. Double lines without arrow consist of oppositely aligned single strands. There also is a hairpin diagram H of order $g$, which can be inserted into single strand polymers.

$$\theta(s) e^{-k^2 s} \text{ and } \theta(s) e^{-(\tau + k^2) s/\omega} \text{ and one gets}$$

$$K(\tau, s) = g \int_0^s d\nu e^{-\tau s^a/\omega} \int \frac{d^d k}{(2\pi)^d} e^{-k^2(v + \frac{s - \nu}{\omega})} \left[1 + \frac{1}{2} \left(1 - e^{-\frac{k^2 s}{\omega}} \right) \right] = \frac{g}{(2\pi)^{\frac{d}{2}}} s^{1 - \frac{d}{2}} f(\tau s),$$

where factors $\frac{1}{2}$ originate from the constraint $\delta(2u - v - s)$. Performing the momentum integral without cutoff $\Lambda$ is allowed when $\Lambda \sqrt{s} \gg 1$. The scaling function $f(y)$ only depends on $y = \tau s$, the negative total binding energy of a double polymer of length $s$.

This leads to a consistent picture. For $y$ large (high temperature, negative binding energy) $f(y) \approx 2^{-d/2}/y$ and $K(\tau, s) \sim s^{-d/2}/\tau$. Therefore the amount of double strands first grows like $1/\tau$ when the temperature is lowered. This growth slows down near $\tau = 1/s$ because $f(0) = \text{const.}$ Below the critical temperature (positive binding energy) $f(y)$ grows exponentially.

The creation of double strands below the critical temperature takes place in a temperature interval $\tau \sim 1/s$ and looks like a first order phase transition when the chain length $s$ is large. However, the process is still described by universal critical exponents and a universal scaling function. Of course, the scaling function and the critical exponents calculated here only are correct near $d = 6$, but the general picture should be the same in lower dimensions.

Two somewhat technical remarks are in order. To get a complete response function one should calculate $\int_S^{\Lambda - 2} ds K(\tau, s)$, the combination of $K(\tau, s)$ with a $\varphi$ propagator with length $S - s$ and with $k = 0$ (which has value one) on the l.h.s. of diagram A. This does not change the general picture. The factor $s^{1 - d/2}$ can be understood as the ratio of the volume of the polymer ($\sim s$) to the volume of a box containing the polymer ($\sim \sqrt{s^d}$).

**Some remarks concerning model B**

In model B oppositely oriented single strands bound to a double strand do not have an intrinsic direction. In the perturbation theory there automatically appears a diagram with a $\langle \tilde{\chi} \chi \rangle$ and a diagram with a $\langle \chi \tilde{\chi} \rangle$ propagator. Both diagrams contribute the same value.

Model B also allows hairpin configurations. A single polymer strand can form a loop and then bind to itself to a hairpin configuration, thus generating a single $\chi$ field. Hairpin configurations are a well known phenomenon in real DNA physics.

All this is nothing new in principle, diagram H simply is another single strand self energy. But the greater number of fields and coupling constants require more effort. As can be seen from fig. [2] the perturbation theory now also generates one loop contributions to the coupling constants.

**Conclusions and open problems**

The field theory [1] defines at least three universality classes with upper critical dimension $d_c = 6$. The high critical dimension makes it difficult to get accurate values for $d = 3$. But the qualitative
behavior in \( d = 3 \) could be similar nevertheless. At least this is the case for comparable models with also \( d_c = 6 \), for instance static and dynamic percolation.

To get realistic results for \( d = 3 \) the excluded volume effect also must be considered. This effect is simple in principle. The Flory argument gives exact critical exponents in dimensions 1, 2 and 4, the critical exponent for \( d = 3 \) is close to the exact value. A realistic scenario is that the excluded volume effect also must be considered. This effect also is a technical device.

The phenomenology of model A still is not completely clear. The flow of parameter \( w \) to the value \( \frac{1}{2} \) in the crossover region is a nonlinear effect, but might still have a simple explanation. One also should try to calculate more measurable quantities. For instance, the length of the double strands is determined by the scaling dimension of the relevant parameter \( \tau \) (the temperature). A two loop diagram contributing to the critical exponent is shown in fig. (1).

Also open are the model B case and the case of (normal) undirected polymers, where the internal direction only is a technical device.

**Appendix A: Derivation of the field theory**

The principal idea is to consider directed polymers on the edges of a finite rectangular lattice. The goal is to count the number of polymer configurations. To simplify the steps we first consider a simplified model.

**A simple model without length variables**

We first assume a Boltzmann factor \( p \) for a polymer link. When \( k \) enumerates the chain configurations and \( l_k \) is the number of links then the partition sum is \( Z = \sum_k p^{l_k} \).

The configurations can be generated with the help of a simple operator algebra (similar techniques have been used for percolation problems). For each lattice site \( i \) there are operators \( \bar{a}_i \) and \( a_i \). The operator \( \bar{a}_i \) creates the start of a polymer link at site \( i \), the operator \( a_i \) terminates a link at site \( i \). All these operators commute and are nilpotent, \( a_i^2 = a_i \bar{a}_i = 0 \). Nilpotency guarantees that links cannot converge or diverge - there are no branches and no overlaps. The last property of the operator algebra is an expectation value \( \langle \bar{a}_i a_j \rangle_0 = \delta_{i,j} \). The expectation value connects a link end to a link start. A formal expression for the partition sum then is

\[
Z(p) = \left( \prod_{i,j} (1 + \bar{a}_i U_{i,j} a_j) \right)_0,
\]

where \( U_{i,j} = p \) for next neighbors and 0 otherwise. The product, when multiplied out, generates a huge sum. Each combination of next neighbor links occurs exactly once, but because of the operator algebra only valid configurations contribute. Pairing \( \bar{a}_i \) with \( a_i \) operators generates chains of \( U_{i,j} \) operators, and each link produces a factor \( p \). The partition sum describes the statistical mechanics of polymer loops. Loops of length two like \( U_{1,2} U_{2,1} \) \( \langle \bar{a}_1 a_1 \rangle_0 \langle \bar{a}_2 a_2 \rangle_0 = p^2 \) also are allowed.

For a given \( i, j \) pair \( 1 + \bar{a}_i U_{i,j} a_j = e^{\bar{a}_i U_{i,j} a_j} \), and in matrix notation it follows \( Z = \langle e^{\bar{a}_i U_{i,j} a_j} \rangle_0 \). A field theory can now be derived with the help of a Hubbard-Stratonovich transformation

\[
Z(p) = \left( \int D\bar{\varphi} D\varphi e^{-\bar{\varphi} U^{-1} \varphi + \bar{\varphi} a + a \varphi} \right)_0 = \left( \int D\bar{\varphi} D\varphi e^{-\bar{\varphi} U^{-1} \varphi} \left( \prod_i (1 + \bar{\varphi}_i a_i) \prod_j (1 + \bar{\varphi}_j a_j) \right) \right)_0.
\]

The integrals over \( \bar{\varphi}_i \) run along the imaginary and the integrals over \( \varphi_i \) along the real axis. The expectation value can now be evaluated

\[
\langle ... \rangle_0 = \prod_i (1 + \bar{\varphi}_i \varphi_i) = e^{\sum_i \ln(1 + \bar{\varphi}_i \varphi_i)} = e^{\sum_i \left\{ \bar{\varphi}_i \varphi_i + \frac{1}{2} (\bar{\varphi}_i \varphi_i)^2 + \frac{3}{3!} (\bar{\varphi}_i \varphi_i)^3 + \frac{1}{4!} (\bar{\varphi}_i \varphi_i)^4 + ... \right\} }.
\]
The first term in the exponent contributes to the propagator, the second term is the excluded volume interaction. The third and fourth term are strongly irrelevant in the renormalization group sense but are kept to render the $\bar{\varphi}$-integrals finite. To use this model in a meaningful way one could simply omit all closed loops in the perturbation theory and add external sources. Perturbation theory and renormalization group then reproduce the critical exponents of the $n \to 0$ limit of the $O(n)$ system.

**The actual model**

Closed polymer loops disappear automatically when the operators also have a length index $\mu \in \mathbb{Z}$ which is incremented by 1 in every link. Furthermore, we anyway need the partition sum of a polymer of fixed length. This is achieved with the help of commuting operators $\bar{a}^{\mu}_{i}$ and $a_{i}^{\mu}$ with a site index $i$ and a length index $\mu$ and the properties $\bar{a}^{\mu}_{i}a^{\nu}_{i} = a^{\mu}_{i}\bar{a}^{\nu}_{i} = 0$ and $\langle \bar{a}^{\mu}_{i}a^{\nu}_{j} \rangle_{0} = \delta_{i,j}\delta_{\mu,\nu}$. The meaning of the operators is the same except that they now start or terminate a link with given length index. At a given site two operators are nilpotent for any length indexes. A formal expression for the partition sum now is

$$Z = \left\langle \prod_{i,j,\mu,\nu} \left( 1 + \bar{a}^{\mu}_{i}U_{i,j}^{\mu,\nu}a^{\nu}_{j} \right) \right\rangle_{0} = \left\langle e^{\bar{a}Ua} \right\rangle_{0}.$$

The matrix $U_{i,j}^{\mu,\nu} = v_{ij}\delta_{\mu,\nu+1}$ has value 1 for next neighbor sites and incremented length index, otherwise it has value zero. The algebra is exactly the same except that the matrix $U$ now increments the length index. Matrix products comprise $i$ and $\mu$. Since closed loops cannot occur anymore $Z$ actually is trivial, but this changes when external sources are added. The transition to a field theory proceeds as above. The harmonic part of the action becomes $S_{0}^{(\psi)} = -\bar{\varphi}U^{-1}\varphi$, where the matrix product runs over lattice sites and length indexes. Only the evaluation of the expectation value differs, because now operators with different length indexes interact,

$$\left\langle e^{\bar{a}^{\mu}a^{\nu}} \right\rangle_{0} = \left\langle \prod_{i,\mu} \left( 1 + \bar{a}^{\mu}_{i}a^{\nu}_{i} \right) \prod_{j,\nu} \left( 1 + \bar{a}^{\nu}_{j}a^{\mu}_{j} \right) \right\rangle_{0} = \prod_{i} \left( 1 + \sum_{\mu} \bar{a}^{\mu}_{i}a_{i}^{\mu} \right) = \prod_{i} \left( 1 + \sum_{\mu} \bar{a}^{\mu}_{i}a_{i}^{\mu} \right) = \prod_{i} \left( 1 + \sum_{\mu} \bar{a}^{\mu}_{i}a_{i}^{\mu} \right).$$

The first product over $\mu$ becomes a sum over $\mu$ because of $a^{\mu}_{i}a^{\nu}_{i} = 0$ and likewise the product over $\nu$. The excluded volume interaction (the last product) now acts between two polymers strands with arbitrary length index.

Double polymers are completely identical except that their operators $\bar{b}^{\mu}_{i}, b^{\nu}_{j}$ and $\bar{c}^{\mu}_{i}, c^{\nu}_{i}$ carry two length indexes which are incremented or decremented accordingly from link to link with matrices

$$V_{i,j}^{\mu,\nu,\rho,\tau} = v_{ij}\delta_{\mu,\rho+1}\delta_{\nu,\tau+1},$$

$$W_{i,j}^{\mu,\nu,\rho,\tau} = v_{ij}\delta_{\mu,\rho+1}\delta_{\nu,\tau-1}.$$

The expectation value is $\left\langle \bar{b}^{\mu}_{i}b^{\nu}_{j} \right\rangle_{0} = \delta_{i,j}\delta_{\mu,\nu}\delta_{\rho,\tau}$ and likewise for $c$. The matrix $V$ propagates operators $b$ with single strands aligned parallel, the matrix $W$ propagates operators $c$ with single strands aligned oppositely. As for the single strand above the harmonic part of the field theory simply becomes $S_{0}^{(\psi,\chi)} = -\bar{\varphi}V^{-1}\varphi - \bar{\chi}W^{-1}\chi$, where the field $\psi$ corresponds to $b$ and the field $\chi$ corresponds to $c$. The matrix products run over the lattice sites and two length indexes.

The model now is complete except for transforming $S_{0}^{(\psi,\chi)}$ to a continuum (coordinate) representation and except for the interaction between the different types of polymer strands. The propagator of the $\psi$ field in $S_{0}^{(\psi)}$ is the inverse of the matrix $V$ from eq. (7). The inverse of $V$ can be found by solving the equation $\sum_{j,\rho,\tau} V_{i,j}^{\mu,\nu,\rho,\tau} f_{j}^{\rho,\tau} = \sum_{j} v_{i,j} f_{j}^{\mu,\nu-1} = h_{j}^{\mu,\nu}$ or $\sum_{j} v_{i,j} f_{j}^{\mu,\nu} = h_{j}^{\mu+1,\nu+1}$. The next
neighbor matrix \( v_{i,j} \) is diagonal in wave vector space, like \( v(k) = (A + Bk^2 + \ldots)^{-1} \). The solution of the equation then is
\[
f^{\mu,\nu}(k) = (A + Bk^2 + \ldots) \left( 1 + \partial_\mu + \partial_\nu + \frac{1}{2} \partial^2_\mu + \ldots \right) h^{\mu,\nu}(k).
\]

This leads to the \( \psi \) propagator of the field theory when the length indexes \( \mu, \nu \) are identified with the length variables \( s \) and \( s' \). The matrix \( W \) for the \( \chi \) propagator has a minus sign for the second length index.

**Interaction between single and double strands**

The interactions \( \mathcal{L}_1 \) and \( \hat{\mathcal{L}}_1 \) of eq.(1) now could be immediately written down, for completeness the derivation is sketched here. It is assumed that at any lattice point \( i \) only “diagonal” operator products \( \hat{a}_i^\mu a_i^\nu \), \( \hat{b}_i^{\mu\nu} b_i^\rho_\tau \) and \( \hat{c}_i^{\mu\nu} c_i^\rho_\tau \) are different from zero. All other products vanish, \( a_i^\mu c_i^{\rho\tau} a_i^\nu c_i^{\rho\tau} = \ldots = 0 \). This naturally leads to the excluded volume interaction between all three types of polymers.

The binding of single strands to double strands is generated by inserting an additional factor
\[
Y = \prod_{(i,j,m)\mu\nu} \left( 1 + g_1 a_i^\mu a_j^\nu b_{m\mu} \right) \prod_{(i,j,m)\mu\nu} \left( 1 + g_2 \hat{a}_i^\mu \hat{a}_j^\nu \hat{b}_{m\mu} \right) \prod_{(i,j,m)\mu\nu} \left( 1 + g_3 a_i^\mu \hat{a}_j^\nu \hat{c}_{m\mu} \right) \prod_{(i,j,m)\mu\nu} \left( 1 + g_4 \hat{a}_i^\mu a_j^\nu \hat{c}_{m\mu} \right)
\]

into the expectation value of the partition sum. The constants \( g_1, g_2 \) are weights for transitions between two single strands \( \varphi \) and a double strand \( \psi \), the constants \( g_3, g_4 \) analogously for a double strand \( \chi \). The products run over all length indexes \( \mu, \nu \) and all triangles of next neighbor lattice points \( (i, j, m) \), with \( m \) not in the middle. All terms in \( Y \) are quasi local. The length indexes are not arbitrary. In the \( g_3 \) term the index \( \mu \) of an incoming single strand becomes the first index of a double strand, in the \( g_4 \) term the first index \( \mu \) of a double strand becomes the index of an outgoing single strand, in accord with the fact that the matrix \( W \) (the \( \chi \) propagator) increments the first length index. When the Hubbard transformations have been performed there remains the expectation value
\[
\left\langle Y \prod (1 + \tilde{\varphi} a) \prod (1 + \tilde{a} \varphi) \prod (1 + \tilde{\psi} b) \prod (1 + \tilde{b} \psi) \prod (1 + \tilde{c} \chi) \prod (1 + \tilde{\chi} c) \right\rangle_0.
\]

Contraction of the operators of \( Y \) among themselves only produces uninteresting constants. Mixed contractions produce local terms which are irrelevant or relevant and present in the model anyway. Contraction of \( Y \) only with the other factors leads to the interactions \( \mathcal{L}_1 \) and \( \hat{\mathcal{L}}_1 \).

**Appendix B: One loop integrals**

Required are the \( k^2, i\omega \) and \( i\omega_1 + i\omega_2 \) parts of the integrals
\[
J_1 = \frac{1}{K_4 (2\pi)^d} \int \frac{d^dp}{(\tau_0 + (p+k)^2 - 2wi\omega)(r_0 + p^2 - i\omega)},
\]
\[
J_2 = \frac{1}{K_4 (2\pi)^d} \int \frac{d^dp}{(r_0 + (p+k)^2 - i\omega_1)(r_0 + p^2 - i\omega_2)}
\]
for \( d = 6 - \epsilon \) and \( |k| = \mu \), calculated with dimensional regularization. The constant \( K_4 \) is \( K_4 = 2^{-d+1}\pi^{-d/2}/\Gamma(d/2) \). The \( i\omega \) contributions come from
\[
I_2 = \frac{1}{K_4 (2\pi)^d} \int \frac{d^dp}{(p+k)^2 (p^2)^2} = \frac{\mu^{-\epsilon}}{\epsilon} + ...
\]
The $k^2$ contributions come from

$$I_1 = -\frac{\partial^2}{\partial k^2} \frac{1}{K_d (2\pi)^d} \int \frac{d^dp}{(p+k)^2 p^2} = \frac{\mu^{-\epsilon}}{3\epsilon} \left( 1 - \frac{\epsilon}{4} + \ldots \right).$$

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