Topological Constraints at the Theta Point: Closed Loops at Two Loops

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We map the problem of self-avoiding random walks in a Θ solvent with a chemical potential for writhe to the three-dimensional symmetric $U(N)$-Chern-Simons theory as $N \to 0$. We find a new scaling regime of topologically constrained polymers, with critical exponents that depend on the chemical potential for writhe, which gives way to a fluctuation-induced first-order transition.

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The statistics and properties of random walks are central to our understanding of a large class of phenomena in mathematics, biology, physics and even economics. The broad applicability of random walks in modelling physical situations is, in part, due to the Gaussian statistics of its correlations, rendering it attractive from an analytical viewpoint. In polymer physics, self-avoiding random walks model polymers in a good solvent that are much longer than their persistence length. This identification establishes a theoretical basis for the computation of scaling exponents of critical phenomena.

Without a topological constraint, the individual monomers suffer two interactions: a chemical interaction which depends on the solvent and a hard-core interaction which is entropic. In the case of good solvents, these interactions of chain connectivity and excluded volume are described by de Gennes’ mapping [8] of the $O(N)$-symmetric $\phi^4$-theory in the $N \to 0$ limit. The Wilson-Fisher fixed point controls the scaling in $d = 4 - \epsilon$ dimensions where $\nu \approx 0.588$ in $d = 3$ [1]. In poor solvents, the polymers collapse into compact globules and $R_G \sim L^{\nu}$.

At the $\Theta$ point, the exponent $\nu$ is the correlation length exponent at the tricritical point $\mu = u = 0$ of the following free energy density for the $N$-component, complex scalar $\vec{\phi}$ [8, 9]:

$$ f = |\partial_\mu \vec{\phi}|^2 + \mu |\vec{\phi}|^2 + u \left( |\vec{\phi}|^2 \right)^2 + w \left( |\vec{\phi}|^2 \right)^3, \quad (1) $$

in the $N \to 0$ limit. In three dimensions, renormalization group analysis shows that although there are logarithmic corrections to mean-field behavior, the scaling exponents agree simply with predictions from dimensional analysis [15, 16]. To incorporate the topological constraints found in closed polymers, we introduce an Abelian Chern-Simons gauge field with the free energy density [1]:

$$ f = \frac{1}{2} \epsilon^{\mu\nu\rho} A_\mu \partial_\nu A_\rho, \quad (2) $$

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Since we are interested in the critical behavior of our theory near the \( \Theta \) point, we perform our analysis at the tricritical point where \( \mu \) and \( u \) vanish. The energy is the sum \( F = F_{\text{CS}} + F_b + F_{\text{gf}} \) where

\[
F_{\text{CS}} = \frac{1}{2} \int d^3x \epsilon_{\mu\nu\rho} A_\mu \partial_\nu A_\rho \\
F_b = \int d^3x (\partial_\mu \phi_i - iy_0 A_\mu \phi_i)^2 + V(\phi_i) \\
F_{\text{gf}} = \frac{1}{2\Delta} \int d^3x (\partial_\mu A_\mu)^2 \\
V(\phi_i) = \mu_0 |\phi|^2 + w_0 \left(|\phi|^2\right)^3
\]

We impose the Landau gauge \((\Delta \to 0)\) in \( F_{\text{gf}} \) for all our subsequent calculations. Because the graphs first diverge at two-loops, standard dimensional regularization is adequate and leads to \( \frac{1}{2} \) poles in \( d = 3 - \epsilon \) dimensions. To evaluate each two-loop diagram, we perform the first momentum integral in \( d = 3 \) and then use dimensional regularization on the remaining single integral. This scheme works because the first integral can only give power law divergences since any integrand with odd powers of momenta vanishes, leaving only even powers of the momenta compared to the three-dimensional measure. Moreover, by power-counting, the remaining integral must diverge logarithmically and cannot cancel the power-law divergence from the first integral. Thus the logarithms only arise in the second of the two integrations. A more sophisticated treatment suggests that this scheme is consistent to all orders \([17]\).

As is usual, we first perform the necessary tensor algebra in physical dimensions before analytically continuing the dimensions of the resulting scalar integrand. The correlation functions satisfy the Slavnov-Taylor identities \([18]\) and the Ward identities \([17]\); gauge invariance is therefore preserved.

We first introduce the renormalized free energy as follows:

\[
F = \int d^3x \left\{ Z_\phi |\partial_\mu \phi_i|^2 + \tilde{\mu} Z_{\phi}|\bar{\phi}|^2 - i\tilde{g} Z_{\phi}^0 [(A_\mu \phi_i)^\ast(\partial_\mu \phi_i) + (\partial_\mu \phi_i)^\ast A_\mu \phi_i] + Z''_{\phi} \tilde{g}^2 |A_\mu \phi|^2 \\
+ \frac{1}{2} Z_A \epsilon^{\mu\nu\rho} A_\mu \partial_\nu A_\rho + \frac{1}{2\Delta} (\partial_\mu A_\mu)^2 + Z_w \tilde{w} \left(|\bar{\phi}|^2\right)^3 \right\}
\]

where \( \tilde{g} = gM^{(3-d)/2} \), \( \tilde{\mu} = \mu M^2 \), \( \tilde{w} = w M^{6-2d} \), and \( M \) is the momentum scale at which we are renormalizing. Denoting \( \Gamma_R^{(N_\phi, N_A)} \) as the renormalized proper vertex of \( N_\phi \) scalar fields and \( N_A \) gauge fields, the Callan-Symanzik equation is:

\[
\left[ M \frac{\partial}{\partial M} + \beta_\mu \frac{\partial}{\partial \mu} + \beta_w \frac{\partial}{\partial w} + \beta_g \frac{\partial}{\partial g} - \frac{1}{2} N_\phi \eta_\phi - \frac{1}{2} N_A \eta_A \right] \Gamma_R^{(N_\phi, N_A)} = 0,
\]

where \( M \) is the renormalization scale. The engineering dimension of any correlation function \( \Gamma \) depends on its field content so that \( d(\Gamma) = 3 - \frac{4}{3} N_\phi - N_A \). We have

\[
\eta_\phi = M \frac{\partial}{\partial M} \ln Z_\phi \\
\eta_A = M \frac{\partial}{\partial M} \ln Z_A \\
\mu_0 = \mu M^2 Z_\phi \]

\[
g_0 = g M^{(3-d)/2} \frac{Z_{\phi}^0}{Z_{\phi} \sqrt{Z_A}} \\
w_0 = w M^{6-2d} \frac{Z_w}{Z_{\phi}^3}
\]

Perturbatively, the underlying symmetry of our action provides a tight constraint on the divergences in our calculations. The odd parity of the Chern-Simons field prevents any correction to the scalar field at the one-loop level: by rescaling \( A_\mu \to g^{-1} A_\mu \), we see that under parity \( g^2 \to -g^2 \), and so correlations of \( \phi \) which are parity invariant can only depend on \( g^2 \) and thus the first corrections are at two loops. Accordingly, we do not find any one-loop contributions to \( Z_{\phi} \) or \( Z_A \). Further, the Coleman-Hill theorem shows that the \( \beta \)-function of the Chern-Simons gauge
coupling receives no contribution beyond one-loop [19, 20, 21, 22] in perturbation. More simplification results from the vanishing of diagrams at any order with closed scalar loops: they necessarily introduce a combinatoric factor of \( N \) and do not provide corrections to the gauge field as \( N \to 0 \) and so a Maxwell term, \( F_{\mu\nu}^2 \), though allowed by symmetry, is not generated. The details of the combinatoric argument go as follows: consider a graph with only external gauge-field legs. Since an external gauge-field leg must necessarily connect to two internal \( \phi \) legs (and possibly one internal gauge-field leg) and since the \( U(N) \) index of \( \phi \) is not carried by any of the other external legs, there must be a sum over that index. Since that sum is proportional to \( N \), this graph vanishes as \( N \to 0 \). More complex internal topologies only add factors of \( N \) to the graph and do not change this result, thus \( Z_A = 1 \). For the same reason there exists only a handful of potential two-loop contributions to the renormalization functions \( Z_X \).

All the non-vanishing two-loop Feynman diagrams are shown in Figures 1 and 2. Figs. 1a and 1b are contributions to \( Z_\phi \), while Fig. 1c through 1f are corrections to the cubic gauge vertex. Fig. 1g is the same as Fig. 1a but evaluated at zero external momentum, contributing to \( Z_\mu \). The evaluation of these graphs is straightforward, since their singularity structures involve only simple poles by power counting. Our results for each graph agree with those in [17].

Employing the results in the table, we have

\[
Z_\phi = 1 - \frac{5g^4}{24\pi^2\epsilon} \\
Z_g' = 1 - \frac{5g^4}{24\pi^2\epsilon} \\
Z_\mu = 1 - \frac{g^4}{8\pi^2\epsilon} \\
Z_w = 1 + \frac{7g^8}{4w\pi^2\epsilon} + \frac{27g^4}{8\pi^2\epsilon} + \frac{33w}{4\pi^2\epsilon} \\
Z_A = 1
\]
FIG. 2: Two-loop contributions to $\Gamma^{(6,0)}$. Figures (c), (d) and (e) are representative of the topology; we have accounted for other contractions of $\phi$ with $\phi^*$. 

from which we find that at two-loop order in $d = 3 - \epsilon$

$$\beta_g = -\frac{\epsilon g^2}{2\pi^2}$$  \hspace{1cm} (19) \\
$$\eta_\phi = \frac{5g^4}{12\pi^2}$$  \hspace{1cm} (20) \\
$$\beta_\mu = \mu \left(-2 + \frac{g^4}{6\pi^2}\right)$$  \hspace{1cm} (21) \\
$$\beta_w = -w \left(2\epsilon - \frac{7g^8}{2w\pi^2} - \frac{8g^4}{\pi^2} - \frac{33w}{2\pi^2}\right) = \frac{33}{2\pi^2}(w - w_+)(w - w_-)$$  \hspace{1cm} (22) \\

where

$$w_\pm(g) = \frac{1}{33} \left[ 2\pi^2\epsilon - 8g^4 \pm \sqrt{4\pi^4\epsilon^2 - 32\pi^2g^4\epsilon - 167g^8} \right]$$  \hspace{1cm} (23) \\

For nonvanishing $g$, as $\epsilon \to 0$ both roots are complex and there is no physical $w$ fixed point. However, for $g^4 \leq 0.851\epsilon$, the radicand in (23) is real and $w_+$ is a stable fixed point for $\epsilon > 0$. Note, however, that for $\epsilon > 0$ the gauge coupling runs away to large values and thus the only stable fixed point in $d = 3 - \epsilon$ is at $(g, w) = (0, 4\pi^2\epsilon/33)$. Focussing on $d = 3$, we see that $g$ is exactly marginal and $w_\pm = -g^4(0.242 \mp 0.392i)$. Writing $M = M_0 e^{-\ell},$ we have

$$w(\ell) = \Re w_+ + 3w_+ \cot \left( \cot^{-1} \left[ \frac{w_0 - \Re w_+}{3w_+} \right] + \kappa \ell \right)$$  \hspace{1cm} (24) \\

where $\kappa = \frac{33}{2\pi^2} 3w_+ = 0.655$. Note that this solution is unstable and as $\ell$ grows runs away to negative values of $w$, reminiscent of the behavior in a superconductor [23] and signaling a first-order transition. However, until any new fixed point controls the scaling, the critical exponents $\nu$ and $\eta$ are determined entirely by the exactly marginal coupling $g$:  

$$\eta = \frac{5g^4}{24\pi^2}$$  \hspace{1cm} (25) \\
$$\nu = \frac{1}{2 - g^4/6\pi^2} \approx \frac{1}{2} + \frac{g^4}{24\pi^2}$$  \hspace{1cm} (26) \\

We thus see that a chemical potential for writhe can alter the radius of gyration exponent $\nu$ and therefore writhe alters the universality class of a self-avoiding walk before driving it to collapse. The gauge field is not perturbatively renormalized and thereby preserves its topological character. As in [1] the scaling behavior of the average writhe $\langle Wr \rangle$ and the average squared writhe $\langle Wr^2 \rangle$ are given in terms of the specific heat exponent $\alpha = 2 - d\nu = \frac{1}{2} - \frac{g^4}{6\pi^2}$:

$$\langle Wr \rangle \sim -\frac{d}{dg^2} \ln (L^{\alpha-2}) = \frac{g^2}{4\pi^2} \ln L$$  \hspace{1cm} (27) \\
$$\langle Wr^2 \rangle \sim \frac{d^2}{dg^2} \ln (L^{\alpha-2}) = -\frac{1}{4\pi^2} \ln L$$  \hspace{1cm} (28) \\

we see that if the chemical potential vanishes then $\langle Wr \rangle = 0$ as expected. These logarithmic corrections are in addition to the writhe that is stored is polymer segments comparable to the persistence length (e.g. plectonemes)
which scales as $L$, a result which does not violate the rigorous bound $\ln(\langle |\mathcal{W}_r| \rangle) \geq \frac{1}{2} \ln L$ \cite{24, 25}. Our expressions of scaling exponents $\eta$ and $\nu$ depend continuously on $g^2$ and are thus similar to those in the two-dimensional XY model. There, topological defects are responsible for this uncommon behavior; here the topological link constraint is responsible.

In conclusion, we have mapped the study of the statistics of self-avoiding random walks in a $\Theta$ solvent to a Chern-Simons field theory and have found a new scaling regime for topologically constrained polymers by calculating the scaling exponents $\eta$ and $\nu$ to two-loop order at the $\Theta$ point. We conjecture that even in a good solvent the scaling behavior will be altered, though as prior work indicates \cite{1} it is difficult to establish results in a controlled approximation. Since taking $N \to 0$ amounts to canceling a functional determinant, progress in this problem might be made by introducing fermionic partners to the complex scalars to have the same effect. It is possible that supersymmetric formulation of this field theory would yield a more complete understanding of the effect of topological constraints.

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