Universal size properties of “star-ring” polymer structure in disordered environment

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We consider the complex polymer system, consisting of ring polymer connected to the $f_1$-branched star-like structure, in good solvent in presence of structural inhomogeneities. We assume, that structural defects are correlated at large distances $x$ according to a power law $x^{-\alpha}$. Applying the direct polymer renormalization approach, we evaluate the universal size characteristics such as the ratio of the radii of gyration of star-ring and star topologies, and compare the effective sizes of single arms in complex structures and isolated polymers of the same total molecular weight. The non-trivial impact of disorder on these quantities is analyzed.

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I. INTRODUCTION

In statistical description of conformational properties of long flexible polymers in a good solvent, one finds a set of characteristics, which are universal, i.e. independent on the details of microscopic chemical structure of macromolecules \cite{1, 2}. As typical example of such properties, we may consider the ratio of the size measures (gyration radii) of linear and closed ring polymers of the same length $L$: $g_{\text{ring}}^{\text{chain}} = \frac{\langle R_g^2 \rangle_{\text{ring}}}{\langle R_g^2 \rangle_{\text{chain}}}$, which is universal $L$-independent quantity and in the idealized case of Gaussian polymer equals $1/2$ \cite{3}. Similarly, one can compare the size measure of a branched star-like polymer structure, consisting of $f_1$ connected arms each of length $L$ connected at one end, and the linear chain of the same length $f_1L$. In the work by Zimm and Stockmayer \cite{3}, an estimate for the size ratio $g_{\text{star}}^{\text{chain}}(f_1)$ in Gaussian case was found analytically:

$$g_{\text{star}}^{\text{chain}} = \frac{3f_1 - 2}{f_1^2}.$$

Inserting $f_1 = 1$ or $f_1 = 2$ in this relation, one restores the trivial result $g_{\text{chain}}^{\text{chain}} = 1$. For any $f_1 \geq 3$, ratio \cite{11} is smaller than 1, reflecting the fact that the size of a branched polymer is always smaller than the size of a linear polymer chain of the same molecular weight.

Let us recall, that the gyration radii of all three above mentioned polymer topologies scale with length $L$ in Gaussian case according to $\langle R_g^2 \rangle \sim L^{2\nu_{\text{Gauss}}}$ with $\nu_{\text{Gauss}} = 1/2$. Introducing the concept of excluded volume, which refers to the idea that any segment (monomer) of macromolecule is not capable of occupying the space that is already occupied by another segment, leads in a good solvent regime to dimensional dependence of scaling exponent: $\langle R_g^2 \rangle \sim L^{2\nu(d)}$ with $\nu(d) = 3/(d+2)$ \cite{4}. Presence of excluded volume effect leads also to $d$-dependence of the size ratios $g_{\text{chain}}$ \cite{5-7} and $g_{\text{star}}^{\text{chain}}$ \cite{8-10}.

Both ring-like and star-like polymers play an important role both in technologies and biophysics. In particular, one can find the circular polymers inside the living cells of bacteria \cite{17} and higher eukaryotes \cite{18}, where DNA occurs in a closed ring shape. Many synthetic polymers form circular structures during polymerization and polycondensation \cite{19, 21}. One can encounters the star-like polymers in studying the complex systems such as gel, rubber, micellar and other polymeric and surfactant systems \cite{22, 24}. In the present paper, we will pay attention to the size properties of the “hybrid” complex polymer structure, consisting of $f_1$ branched linear chains connected with one closed ring (Fig. 1). Such a structure in particular cases $f_1$ and $f_1 = 2$ has a close relation with experimentally synthesized tadpole-shape polystyrene (Ref. \cite{25}). Such structures are very intriguing model polymers from the point of view of viscoelastic properties, since an entanglement of linear parts and closed loops of different macromolecules could lead to formation of strong intermolecular entanglement network. Also, the shape properties of such tadpole structure have been analyzed numerically in \cite{26}. Note that the related more general model of “rosette-like” polymers have been considered in the Gaussian approximation in Ref. \cite{27}. On the other hand, it is related to the process of loop formation in star polymers \cite{28}. It is well known that

![Figure 1: Schematic presentation of complex polymer structure, consisting of $f_1$ linear branches and one closed loop.](image-url)

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the loop formation in macromolecules plays an important role in a number of biochemical processes, such as stabilization of globular proteins \[52\], transcriptional regularization of genes \[33\ \[35\] , DNA compactification in the nucleus \[36\ \[38\] etc. Moreover, such a system can be considered as a part of a general polymer network of a more complicated structure \[32\].

In many physical processes, one faces the problem of presence of structural obstacles (impurities) in the system. One can encounter such situation when considering polymers in gels, colloidal solutions \[40\] , intra- and extracellular environments \[41\ \[43\] etc. Numerous analytical and numerical studies \[44\ \[47\] indicate the considerable impact of structural disorder on the effective polymer size and conformational properties of macromolecules. The density fluctuations of disorder often create the complex fractal structures \[48\] . Such situations are perfectly considered as a part of a general polymer network of a more complicated structure \[32\].

The present paper is dedicated to the universal size of disorder \[49\] . The defects are correlated on large distances \[49\] . The defects are correlated on large distances. Such a model refers to the correlated quenched defects, originally proposed in Ref. \[50\]. The defects are correlated on large distances \[49\] . The defects are correlated on large distances. The defects are correlated on large distances \[49\] . The defects are correlated on large distances. Such situations are perfectly considered as a part of a general polymer network of a more complicated structure \[32\].

Here, \(Z_0\) is partition function of Gaussian chain given by

\[
Z_0 = \frac{f_1+1}{Z_0} \prod_{i=1}^{f_1+1} \int ds_i \exp \left( \frac{\int_{0}^{L} ds \left( \frac{d\vec{r}_i(s)}{ds} \right)^2}{2} \right).
\]

\[
Z_{f_1} = \frac{f_1+1}{Z_0} \prod_{i=1}^{f_1+1} \int ds_i \exp \left( \frac{\int_{0}^{L} ds \left( \frac{d\vec{r}_i(s)}{ds} \right)^2}{2} \right).
\]

\[
H = \sum_{i=1}^{f_1+1} \int_{0}^{L} ds \left( \frac{d\vec{r}_i(s)}{ds} \right)^2
\]

\[
+ \frac{u}{2} \sum_{i,j=1}^{f_1+1} \int_{0}^{L} ds' \int_{0}^{L} ds'' \delta(\vec{r}_i(s') - \vec{r}_j(s''))
\]

\[
+ \sum_{i,j=1}^{f_1+1} \int_{0}^{L} ds V(\vec{r}_i(s)).
\]

Here, the first term describes the connectivity of trajectories, the second one corresponds to the excluded volume interactions governed by a coupling constant \(u\) and the last term describes potential that arises due to presence of obstacles in the system. We consider the case when impurities are correlated on the large distances according to power law \[49\] :

\[
V(\vec{r}_i(s')) V(\vec{r}_j(s'')) = v|\vec{r}_i(s') - \vec{r}_j(s'')|^{-a},
\]

where \(\langle \ldots \rangle\) denotes averaging over different realizations of disorder and \(v\) is a corresponding coupling constant.

Performing dimensional analysis of the terms in \[4\] , one finds the dimensions of the couplings in terms of dimension of contour length \(L\) : \(\langle u \rangle = [L]^{(4-d)/2}, \langle v \rangle = [L]^{(4-a)/2}\). The “upper critical” values of the space dimension \(d_c = 4\) and the correlation parameter \(a_c = 4\), at which the couplings are dimensionless, play an important role in the renormalization scheme, as outlined below.

\[
\delta\text{-function describes the closed loop structure and } H \text{ is the system Hamiltonian:}
\]

\[
H = \sum_{i=1}^{f_1+1} \int_{0}^{L} ds \left( \frac{d\vec{r}_i(s)}{ds} \right)^2
\]

\[
+ \frac{u}{2} \sum_{i,j=1}^{f_1+1} \int_{0}^{L} ds' \int_{0}^{L} ds'' \delta(\vec{r}_i(s') - \vec{r}_j(s''))
\]

\[
+ \sum_{i,j=1}^{f_1+1} \int_{0}^{L} ds V(\vec{r}_i(s)). \quad (4)
\]

Performing dimensional analysis of the terms in \[4\] , one finds the dimensions of the couplings in terms of dimension of contour length \(L\) : \(\langle u \rangle = [L]^{(4-d)/2}, \langle v \rangle = [L]^{(4-a)/2}\). The “upper critical” values of the space dimension \(d_c = 4\) and the correlation parameter \(a_c = 4\), at which the couplings are dimensionless, play an important role in the renormalization scheme, as outlined below.
III. THE METHOD

The observables calculated on the basis of continuous chain model, contain divergences in the limit of infinitely long chain, that correspond to the case of infinite number of monomers. In order to receive the universal values of parameters under consideration, those divergences need to be eliminated. The direct polymer renormalization method developed by des Cloizeaux allows to remove those divergences by adsorbing them into a set of so-called renormalization factors, directly connected to the observable physical quantities. The finite values of observables are obtained while evaluated at stable fixed points (FPs) of renormalization group. The method is described in more details in our previous works, e.g. [53].

It is important to note that FPs do not depend on the topology of the polymer under consideration, and thus can be obtain in the simplest case of single linear chain. The renormalized coupling constants $\lambda_R = \{u_R, v_R\}$ are defined by:

$$\lambda_R(\{\lambda\}) = -[Z(\lambda)](L)^{-2}Z(\lambda)(L, L) \times [2\pi \chi_0(L, \{\lambda_0\})]^{2-d_\lambda},$$

where $Z_L(\{\lambda_0\})$ is a partition function of a single chain, $Z(t(\lambda))(L, L)$ - partition function of two interacting chains, $\chi_0(L, \{\lambda_0\})$ is a so-called renormalization swelling factor, and $d_\lambda$ are dimensions of corresponding coupling constants, introduced after Eq. (6): $d_u = (4-d)/2, d_v = (4-a)/2.$

In the limit of infinite linear size of macromolecules, the renormalized theory remains finite, such that:

$$\lim_{L \to \infty} \lambda_R(\{\lambda\}) = \lambda^*_R.$$  

For negative values of $d_\lambda < 0,$ macromolecules are expected to behave like Gaussian chains in spite of the interactions between monomers, thus each $\lambda^*_R = 0$ for corresponding $d_\lambda < 0.$ The concept of expansion in small deviations from the upper critical dimensions ($\epsilon = d_u - d, \delta = a_c - a$) of the coupling constants thus naturally arises. Stable fixed points govern the asymptotical scaling properties of macromolecules in solutions and make it possible, e.g., to obtain the reliable values of universal size ratios.

IV. RESULTS AND DISCUSSIONS

A. Partition function

We start our calculations by considering the partition function of the star-ring polymer structure. We exploit the Fourier-transform of the $\delta$-function with wave vectors $\vec{q}$ for the one corresponding to a loop structure and with wave vector $p_u^*$ for those describing excluded volume interaction:

$$\delta(\vec{r}_{f_1+1}(L) - \vec{r}_{f_1+1}(0)) = \frac{1}{(2\pi)^d} \times$$

$$\times \int \frac{d\vec{q}}{(2\pi)^d} e^{-(i\vec{q}(\vec{r}_{f_1+1}(L) - \vec{r}_{f_1+1}(0))},$$

$$\delta(\vec{r}_{s'}(s) - \vec{r}_{j}(s'')) = \frac{1}{(2\pi)^d} \times$$

$$\times \int d^d p_u e^{-(i\vec{p}_u(\vec{r}_{s'}(s) - \vec{r}_{j}(s''))}.$$  

The Fourier transform of 15 can be presented as:

$$\frac{u}{2(2\pi)^d} \int d\vec{p}_u |p_u|^{d-a} e^{-(i\vec{p}_u(\vec{r}_{s'}(s) - \vec{r}_{j}(s''))},$$

where $i$ is an imaginary unit. As a result, $Z^{f_1,1}$ can be presented as:

$$Z^{f_1,1} = \frac{1}{Z_0} \int d\vec{r} \left( \frac{1}{(2\pi)^d} e^{-\frac{f_{1,+1}}{i} \int_0^L ds \left( d\vec{p}_u^* \right)^2} \right.$$

$$\times \int \frac{d\vec{q}}{(2\pi)^d} e^{-(i\vec{q}(\vec{r}_{f_1+1}(L) - \vec{r}_{f_1+1}(0)))}$$

$$\times \left( 1 - \frac{u}{2(2\pi)^d} \sum_{i,j=1}^{f_{1,+1}} \int_0^L ds' \int_0^L ds'' \int d\vec{p}_u \right.$$

$$\times \exp \left(-i\vec{p}_u^*(\vec{r}_{s'}(s) - \vec{r}_{j}(s'')) \right)$$

$$+ \frac{v}{2(2\pi)^d} \sum_{i,j=1}^{f_{1,+1}} \int_0^L ds' \int_0^L ds'' \int d\vec{p}_v |p_v|^{d-a}$$

$$\times \exp \left(-i\vec{p}_v^*(\vec{r}_{s'}(s) - \vec{r}_{j}(s'')) \right) \bigg) \bigg)$$

Here, $\int d\vec{r} = \prod_{i=1}^{f_{1,+1}} \int d\vec{r}_i.$ Performing the corresponding integrations and taking into account that $Z_0 = (2\pi L)^{-\frac{d}{2}}$ we receive:

$$Z^{f_1,1} = (2\pi L)^{-\frac{d}{2}} \left( 1 - z_u f_1 (f_1 - 3) + 4 (f_1 + 1) \right)$$

$$+ z_v f_1 (f_1 - 3) + 4 (f_1 + 1) - (z_u - z_v)$$

$$\times \left( 2(f_1 - 1) - \frac{f_1 (f_1 - 1)}{\delta} \ln(2) + \frac{f_1 (f_1 - 3)}{2} \right.$$

$$+ f_1 \left( \frac{2\sqrt{5}}{5} \ln \left( \frac{2}{\sqrt{5} + 3} \right) \right) \bigg) \bigg)$$

with $z_u$ and $z_v$ being dimensionless coupling constants:

$$z_u = \frac{u L^{2-d/2}}{(2\pi)^d},$$

$$z_v = \frac{v L^{2-d/2}}{(2\pi)^d}.$$  

B. Gyration radius of a star-ring structure and corresponding size ratios

Gyration radius of a polymer structure under consideration in terms of continuous model can be presented
Figure 2: Diagrammatic presentation of contributions into \( \langle \xi(\vec{k}) \rangle \) in Gaussian approximation. The solid line on a diagram is a schematic presentation of a polymer path of length \( L \), and arrows denote so-called restriction points \( s_1 \) and \( s_2 \).

\[
\langle R_g^2 \rangle = \frac{1}{2L^2(f_1 + 1)^2} \times \sum_{i,j=1}^{f_1+1} \int_0^L \int_0^L ds_1 ds_2 ((\vec{r}_i(s_2) - \vec{r}_j(s_1))^2). \tag{15}
\]

Here and below, \( \langle \ldots \rangle \) denotes averaging with an effective Hamiltonian \( (6) \) according to:

\[
\langle \ldots \rangle = \frac{f_1+1 \prod_{i=1}^{f_1+1} \int dr_i(s) \delta(\vec{r}_{f_1+1}(L) - \vec{r}_{f_1+1}(0)) e^{-H_{eff}}}{Z_{f_1+1}}.
\]

We make use of identity:

\[
\langle (\vec{r}_i(s_2) - \vec{r}_j(s_1))^2 \rangle = -2 \frac{d}{d|\vec{k}|^2} \xi(\vec{k})|_{k=0},
\]

\[
\xi(\vec{k}) \equiv \langle e^{-i\vec{k}(\vec{r}_i(s_2) - \vec{r}_j(s_1))} \rangle, \tag{16}
\]

and evaluate \( \xi(\vec{k}) \) in path integration approach. In calculations of the contributions into \( \xi(\vec{k}) \), it is convenient to use the diagrammatic presentation, as given in Figs. 2-3.

In the simplified case of Gaussian polymer we have only four diagrams (see Fig. 2). The example of diagram calculations is given in the Appendix A. It is also important to note that different diagrams are included in final expressions with different pre-factors arising from combinatorics, so that diagram \( D_{01} \) is taken with pre-factor \( f_1 \), diagram \( D_{02} \) with \( 1 \), \( D_{03} \) with \( f_1(f_1 - 1)/2 \) and \( D_{04} \) with \( f_1 \). As a result, the gyration radius of star-ring structure in Gaussian approximation reads:

\[
\langle R_g^2 \rangle_{\text{Gauss}} = \frac{Ld(6f_1^2 + 6f_1 + 1)}{12(f_1 + 1)^2}. \tag{17}
\]

In the first order of perturbation theory in couplings \( z_u, z_v \), the gyration radius can be in general presented as:

\[
\langle R_g^2 \rangle = \langle R_g^2 \rangle_{\text{Gauss}} + z_u \langle R_g^2 u \rangle - z_v \langle R_g^2 v \rangle,
\]

where \( z_u, z_v \) are dimensionless coupling constants given by \( (14) \) and \( \langle R_g^2 u \rangle, \langle R_g^2 v \rangle \) are contributions of a set of diagrams presented on Fig. 3 with interactions governed by corresponding coupling constants. Again, all the diagrams should be taken into account with corresponding combinatorial pre-factors. Both the pre-factors and \( \epsilon, \delta \)-expansions for each of the diagram are given in Table I in the Appendix B.

The final expression for the gyration radius of star-ring structure reads:

\[
\langle R_g^2 \rangle = \frac{Ld(6f_1^2 + 6f_1 + 1)}{12(f_1 + 1)^2}.
\]
structure is thus given by:

\[
\overline{R_g^2} = \frac{dL(6f_1^2 + 4f_1 + 1)}{12(f_1 + 1)^2} \left( 1 + \frac{2z_u - 2z_v}{\epsilon} \right) - \frac{(z_u - z_v)}{\delta} \left( \frac{13}{12} \right)
\]

\[
\left( f_1 \left( f_1 + 1 \right) - 4 \ln(2) \left( \frac{1}{3f_1 + 1} \right) \right).
\]

(18)

Let us recall the gyration radius of a star-like polymer of the same molecular weight \((f_1 + 1)\) arm polymer\(53\):  

\[
\overline{R_{g,\text{star}}^2} = \frac{dL(3f_1 + 1)}{12(f_1 + 1)^2} \left( 1 + \frac{2z_u - 2z_v}{\epsilon} \right) - \frac{(z_u - z_v)}{\delta} \left( \frac{13}{12} \right)
\]

\[
\left( f_1 \left( f_1 + 1 \right) - 4 \ln(2) \left( \frac{1}{3f_1 + 1} \right) \right).
\]

(19)

and the expression for the gyration radius of a single chain of the same molecular weight (chain with total length \((f_1 + 1)L\)) \(53\):

\[
\overline{R_{g,\text{chain}}^2} = \frac{dL(f_1 + 1)}{6} \left( 1 + \frac{2z_u - 2z_v}{\epsilon} \right) - \frac{(z_u - z_v)}{\delta} \left( \frac{13}{12} \ln(f_1 + 1) \right).
\]

(20)

With expressions \(18\) - \(20\) we can obtain the corresponding universal size ratios \(g_{\text{star}} = \frac{\overline{R_{g,\text{star}}^2}}{\overline{R_{g,\text{star}}^2}}\) and \(g_{\text{chain}} = \frac{\overline{R_{g,\text{chain}}^2}}{\overline{R_{g,\text{chain}}^2}}\) which will allow us to estimate the relative effective size of polymers of the same molecular weight but different topology. These ratios are given by the following expressions:

\[
g_{\text{star}} = \frac{6f_1^2 + 4f_1 + 1}{6f_1^2 + 8f_1 + 2} \times 
\]

\[
\left( 1 - \frac{(z_u - z_v)}{\epsilon} \right) \left( 1 + \frac{4f_1(8f_1 + 3)(3f_1 - 2) \ln(2)}{3f_1 + 1} \right) \left( \frac{1}{1 + 2 \left( 3f_1 + 1 \right)} \right)
\]

\[
- \frac{4 f_1 \sqrt{5} (30f_1^2 + 132f_1 - 1) \arctan(\sqrt{5}/5)}{25} \left( \frac{1}{3f_1 + 1} \right) \left( 6f_1^2 + 4f_1 + 1 \right) \left( \frac{1}{1 + 2 \left( 3f_1 + 1 \right)} \right)
\]

\[
\left( 1 - \frac{(z_u - z_v)}{\delta} \right) \left( \frac{13}{12} \ln(f_1 + 1) \right).
\]

(21)

\[
g_{\text{chain}} = \frac{6f_1^2 + 4f_1 + 1}{2(f_1 + 1)^3} \times 
\]

\[
\left( 1 - \frac{(z_u - z_v)}{\epsilon} \right) \left( \frac{1}{30} \right) \left( 6f_1^2 + 4f_1 + 1 \right) \left( 3f_1 + 1 \right) \left( 30f_1^2 + 132f_1 - 1 \right) \left( \frac{1}{1 + 2 \left( 3f_1 + 1 \right)} \right)
\]

\[
- \frac{8 \ln(2) f_1(3f_1 - 2) \ln(2)}{6f_1^2 + 4f_1 + 1} \left( \frac{1}{1 + 2 \left( 3f_1 + 1 \right)} \right)
\]

\[
\left( 1 - \frac{(z_u - z_v)}{\delta} \right) \left( \frac{13}{12} \ln(f_1 + 1) \right).
\]

(22)
We make use of results for fixed point values found previously for the linear polymer chains in long-range correlated disorder \[50\]. There are three distinct fixed points governed by the properties of macromolecule in various regions of parameters \(d\) and \(a\):

\[
\text{Gaussian} : z^*_u = 0, z^*_v = 0, \quad (23)
\]

\[
\text{Pure} : z^*_u = \frac{\epsilon}{8}, z^*_v = 0, \quad (24)
\]

\[
LR : z^*_u = \frac{\delta^2}{4(\epsilon - \delta)} z^*_v = \frac{\delta(\epsilon - 2\delta)}{4(\delta - \epsilon)}. \quad (25)
\]

Evaluating (21) and (22) in these three cases, we obtain:

\[
g_{\text{star-ring}}^\text{Gaussian}[\text{Gaussian}] = \frac{6f^2_1 + 4f_1 + 1}{6f^2_1 + 8f_1 + 2} \quad (26)
\]

\[
g_{\text{star-ring}}^\text{Pure} = \frac{6f^2_1 + 4f_1 + 1}{6f^2_1 + 8f_1 + 2} \left(1 - \frac{\epsilon}{8}(\ldots)\right) \quad (27)
\]

\[
g_{\text{star-ring}}^\text{LR} = \frac{6f^2_1 + 4f_1 + 1}{6f^2_1 + 8f_1 + 2} \left(1 - \frac{\delta}{4}(\ldots)\right), \quad (28)
\]

\[
g_{\text{chain}}^\text{Gaussian}[\text{Gaussian}] = \frac{6f^2_1 + 4f_1 + 1}{2f_1(1+\delta)} \quad (29)
\]

\[
g_{\text{chain}}^\text{Pure} = \frac{6f^2_1 + 4f_1 + 1}{2f_1(1+\delta)} \left(1 - \frac{\epsilon}{8}(\ldots)\right) \quad (30)
\]

\[
g_{\text{chain}}^\text{LR} = \frac{6f^2_1 + 4f_1 + 1}{2f_1(1+\delta)} \left(1 - \frac{\delta}{4}(\ldots)\right), \quad (31)
\]

where \((\ldots)\) denotes a factor that depends only on \(f_1\) and is different for different ratios.

Comparing (26) and (29), one easily notices, that at any \(f_1\) both \(g_{\text{star-ring}}^\text{Gaussian}\) and \(g_{\text{chain}}^\text{Gaussian}\) are smaller than 1. Thus, in Gaussian approximation the effective size of branched polymer structure with one loop is more compact than both of that of star polymer or linear chain of the same molecular weight. The value of \(g_{\text{star-ring}}^\text{Gaussian}\) is growing with increasing of \(f_1\) and gradually reaches the value of 1, which can be explained by diminishing of the role played by presence of single loop with growing number of linear arms. On the other hand, \(g_{\text{chain}}^\text{Gaussian}\) is decreasing with \(f_1\): the polymer of complex branched structure becomes more and more compact comparing with linear chain. To find the quantitative values for the size ratios (27), (28), (30), we estimate them at fixed values of space dimension \(d = 3\) and various values of correlation parameter \(a\). Results are presented on Figs. [4] [5]. Note, that our results in pure solvent at \(d = 3\) can be compared with experimental values for single-tail \((f_1 = 1)\) and twin-tail \((f_1 = 2)\) tadpole-shape polystyrene molecules (Ref. 29): \(g_{\text{star-ring}}^\text{Pure} = 0.86 \) and 0.80 correspondingly. Note however, that our analytical results are obtained in one-loop approximation and are rather of qualitative character. To obtain the reliable estimates for the values, one need to proceed to higher order calculations and apply the special resummation techniques to the obtained perturbation theory expansions (see, e.g. 30). Presence of excluded volume interactions as well as presence of structural disorder in the system makes the effect of compactification of the effective size of complex branched structure less pronounced: the corresponding size ratios become closer to 1. It is interesting to mention, that when correlations of disorder become strong enough, the corresponding size ratios gradually overcome the value of 1. Thus, the complex star-ring structure becomes more extended in space, than structures without closed loops.

C. Gyration radius of a single linear arm in a complex structure

Another parameter of our interest is the gyration radius of a single linear arm within the complex polymer structure, which can be presented as:

\[
\left\langle R^2_{g,\text{arm}}\right\rangle = \frac{1}{2L^2} \times \int_0^L ds \int_0^L ds' (\langle r_1^2(s_2) - r_2^2(s_1)\rangle). \quad (32)
\]

In this case, we need to take into account only those diagrams on Figs. 2 and 3 which are shown in purple color, with corresponding pre-factors: \((f_1 - 1)\) for \(D_s, D_{2s}, D_{2t}, D_{1s}, D_{1t}, D_{3s}, D_{3t}, D_{5s}, D_{5t}, D_{12s}, D_{12t}, D_{15s}, D_{15t}, D_{30s}, D_{30t}, D_{31}, D_{32}, D_{34}, D_{35}, D_{36}\) should be accounted for without pre-factors. As a result we receive the following expression:

\[
\left\langle R^2_{g,\text{arm}}\right\rangle = \frac{dL}{6} \left(1 + \frac{(2z_u - 2z_v)}{\epsilon} - (z_u - z_v)\right)
\]

\[
\times \left(\frac{463}{120} - \frac{35}{8} f_1 + 6(f_1 - 1)\ln(2)\right)
\]

\[
- \frac{2}{5} f_1 \sqrt{5} \ln\left(\frac{2}{\sqrt{5} + 3}\right)
\]

\[
+ \sqrt{5} \arctan\left(\sqrt{5/5}\right)\right)\right). \quad (33)
\]

Let us recall the expression for the gyration radius of a single chain of length \(L\) [33]:

\[
\left\langle R^2_{g,\text{chain}}\right\rangle = \frac{dL}{6} \left(1 + \frac{(2z_u - 2z_v)}{\epsilon} - (z_u - z_v)\right)
\]

\[
- \frac{(z_u - z_v)}{12}. \quad (34)
\]

Thus, we can consider a size ratio \(g_{\text{arm}} = \left\langle R^2_{g,\text{arm}}\right\rangle / \left\langle R^2_{g,\text{chain}}\right\rangle\) which reads:

\[
\left\langle R^2_{g,\text{arm}}\right\rangle = \left\langle R^2_{g,\text{arm}}\right\rangle = 1 - (z_u - z_v)
\]

\[
\times \left(\frac{111}{40} - \frac{35}{8} f_1 + 6(f_1 - 1)\ln(2)\right)
\]

\[
- \frac{2}{5} f_1 \sqrt{5} \ln\left(\frac{2}{\sqrt{5} + 3}\right) + \sqrt{5} \arctan\left(\sqrt{5/5}\right)\right)\right). \quad (35)
\]
Figure 6: Size ratio $g_{\text{arm}}$ as function of parameter $f_1$, estimated at different fixed points values. Squares: Eq. (36); stars: Eq. (37) estimated at $d = 3$ ($\epsilon = 1$); triangles, diamonds and circles correspond to results given by Eq. (38) at different values of correlation parameter $a = 3$ ($\delta = 1$), $a = 2$ ($\delta = 2$), $a = 1$ ($\delta = 3$) correspondingly.

Substituting the fixed point values \((23)-(25)\) into \((35)\), we obtain:

\[ g_{\text{arm}}[\text{Gaussian}] = 1, \]
\[ g_{\text{arm}}[\text{Pure}] = 1 - \frac{\epsilon}{8}(\ldots), \]
\[ g_{\text{arm}}[\text{LR}] = 1 - \frac{\delta}{4}(\ldots), \]

where \((\ldots)\) denotes a factor that depends only on $f_1$ and is different for different ratios. We estimate the numerical value of \((37)\) at fixed $d = 3$ ($\epsilon = 1$) and \((38)\) at various values of correlation parameter $a$. Results are presented on Fig. 6. We note that the ratio is always larger than 1 and grows with increasing $f_1$. Thus, the effective size of an arm in a complex polymer structure is more extended in space than the size of free single polymer chain. The presence of structural disorder makes this effect more pronounced.

**D. Gyration radius of a single loop in a complex structure**

In the same way as in the previous subsection, we can calculate the gyration radius of a single loop in a complex star-ring structure. We take into account only diagrams that marked with pink color on the figures 2 and 3. As a result, we obtain the following expression:

\[
\langle R^2_{g\text{loop}} \rangle = \frac{dL}{12} \left( 1 + \left( \frac{2z_u}{\epsilon} - \frac{2z_v}{\delta} \right) - 
\left( z_u - z_v \right) \frac{f_1}{5} - \frac{36\sqrt{5}f_1}{25} \arctan \left( \frac{\sqrt{5}}{\delta} \right) \right) - \frac{2f_1\sqrt{5}}{5} \ln \left( \frac{2}{\sqrt{5} + 3} \right). \tag{39}
\]

It is interesting to compare this result with that of gyration radius of isolated ring polymer [54]:

\[
\langle R^2_{g\text{ring}} \rangle = \frac{dL}{12} \left( 1 + \left( \frac{2z_u}{\epsilon} - \frac{2z_v}{\delta} \right) \right), \tag{40}
\]

so that the corresponding size ratio $g_{\text{loop}} = \frac{\langle R^2_{g\text{loop}} \rangle}{\langle R^2_{g\text{ring}} \rangle}$ reads:

\[
g_{\text{loop}} = 1 - (z_u - z_v) \left( \frac{f_1}{5} - \frac{36\sqrt{5}f_1}{25} \arctan \left( \frac{\sqrt{5}}{\delta} \right) - \frac{2f_1\sqrt{5}}{5} \ln \left( \frac{2}{\sqrt{5} + 3} \right) \right). \tag{41}
\]

Evaluating (41) at different fixed points \((23)-(25)\), we obtain:

\[
g_{\text{loop}}[\text{Gaussian}] = 1, \tag{42}
\]
\[
g_{\text{loop}}[\text{Pure}] = 1 - \frac{\epsilon}{8}(\ldots), \tag{43}
\]
\[
g_{\text{loop}}[\text{LR}] = 1 - \frac{\delta}{4}(\ldots), \tag{44}
\]

where \((\ldots)\) denotes a factor that depends only on $f_1$. To find the quantitative estimates for the size ratio \((43)\) we evaluate it at fixed values of space dimension $d = 3$ and various values of parameter $f_1$. Results are presented on Fig. 7. We note, that presence of excluded volume interactions causes the extension of effective size of a loop.
as a part of the complex polymer structure as comparing with isolated polymer ring. This effect becomes more pronounced in presence of correlated disorder in system. Evaluating the size ratio \( \frac{a}{d} \) at various fixed values of parameter \( \delta \), we note an increase of this value with growing correlations of disorder.

V. CONCLUSIONS

In the present paper, we analyzed the universal conformational properties of complex branched polymer structure, consisting of \( f_1 \) linear chains connected with one closed ring. Such a polymer system could be of interest in processes of loop formation in branched star polymers \( \text{(45)} \). On the other hand, such a system can be considered as a part of a general polymer network of a more complicated structure \( \text{(46)} \).

Since in most of real physical processes one encounters the problem of presence of structural obstacles (impurities) in the system, which often have complex fractal structures \( \text{(48)} \), we turn our attention to analysis of star-ring polymer behavior in solution in presence of defects correlated on large distances according to a power law with a pair correlation function \( h(x) \sim x^{-a} \) with \( a < d \).

Applying the direct polymer renormalization approach, we evaluate the expression for the universal ratios of the radii of gyration of star-ring structure and star polymer \( \text{(49)} \) and linear chain \( \text{(50)} \) of the same total molecular length. In Gaussian approximation, the effective size of branched polymer structure with one loop is more compact than both of that of star polymer or linear chain of the same molecular weight. However, presence of excluded volume interactions as well as presence of structural disorder makes the effect of compactification of the effective size of complex branched structure less pronounced. Moreover, as can be seen on Figs. \( \text{(51)} \) \( \text{(52)} \) when correlations of disorder become strong enough, the corresponding size ratios gradually overcome the value of 1 and the star-ring structure becomes more extended in space, than structures without closed loops. Also, we analyzed the size ratio \( \text{(53)} \) of the radii of gyration of single arm in complex structure and free linear polymer chain of the same length. We found, that the effective size of an arm is more extended in space that of free chain, and this extension grows in presence of long-range-correlated disorder. Finally, we evaluate the size ratio \( \text{(54)} \) of the radii of gyration of a loop in complex structure and free ring polymer of the same length. Again, we found that presence of correlated disorder in system causes the extension of effective size of a loop within the complex polymer structure as comparing with isolated polymer ring, and this effect is more pronounced with growing correlations of disorder.

Appendix A

Here, we present an example of diagram calculations. As an example we choose a diagram \( D_1 45 \) from Fig. \( \text{9} \) which is presented in more details on Fig. \( \text{8} \). According to the general rules of diagram calculations \( \text{(2)} \), each segment between any two points and is oriented and bears a wave vector given by a sum of incoming and outgoing wave vectors injected at interaction points and end points. Here, points \( s \) and \( z \) are interaction points associated with wave vector \( \vec{p} \), \( s_1 \), \( s_2 \) are so-called restriction points with wave vector \( \vec{k} \), the wave vector \( \vec{q} \) corresponds to the loop and has restriction points at 0 and \( L \) of the corresponding trajectory. Each segment of a diagram bears a factor \( \frac{2}{L} (s_a - s_b) \) where \( q_{ab} \) is given by a sum of incoming and outgoing vectors injected at points \( s_a, s_b \). The expression has to be integrated over all wave vectors and over all independent restriction points and end points:

\[
D_1 45 = \frac{(2\pi)^{-2d}}{L} \int_0^L ds_1 ds_2 \times \int \frac{d\tilde{q}}{2\pi} e^{-\frac{q^2}{2} (L - s)} s - \frac{s^2}{2} s_1 = \frac{s_2}{2} (s_2 + s_1). \tag{45}
\]

Integrating over wave vectors \( \vec{q} \) and \( \vec{p} \) and taking a derivative over \( \vec{k} \) according to \( \text{(10)} \) we receive:

\[
D_1 45 = \frac{(2\pi)^{-d} L^{-d/2}}{L} \int_0^L ds_1 ds_2 (s_2 + s_1) \times \int \frac{ds}{2\pi} \int_0^L dz \left( s + z - \frac{s^2}{L} \right)^{-d/2}. \tag{46}
\]

Performing the integration over \( s_1 \) and \( s_2 \) and passing to dimensionless variables \( s = s/L, \frac{z}{L} \) we come to the expression:

\[
D_1 45 = \frac{(2\pi)^{-d} L^{-d/2} L^{5-d}}{1 - d/2} \int_0^1 ds \frac{d\tilde{z}}{\tilde{z}^2} (\tilde{s} + \tilde{z} - \tilde{s}^2)^{-d/2}. \tag{47}
\]

Integration over \( \tilde{z} \) will give:

\[
D_1 45 = \frac{(2\pi)^{-d} L^{-d/2} L^{5-d}}{1 - d/2} \times \tag{48}
\]

Figure 8: (Color online) Example of diagrammatic contribution into the gyration radius of star-ring polymer.
\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|}
\hline
Name & Pre-factor & $\epsilon(\delta)$-expansion \\
\hline
$D_{i1}$ & $f_1 f_2$ & $\frac{3\sqrt{2}}{100} \arctan \left( \frac{\sqrt{2}}{5} \right) + \frac{1}{5}$ \\
$D_{i2}$ & $f_1 f_2$ & $\frac{3\sqrt{2}}{100} \arctan \left( \frac{\sqrt{2}}{5} \right) + \frac{1}{5}$ \\
$D_{i3}$ & $f_1 f_2$ & $\frac{4}{15} - \frac{16\sqrt{2}}{15} \arctan \left( \frac{\sqrt{2}}{3} \right) - \frac{5}{6}$ \\
$D_{i4}$ & $f_1 f_2$ & $\frac{4}{15} - \frac{16\sqrt{2}}{15} \arctan \left( \frac{\sqrt{2}}{3} \right) + \frac{5}{6}$ \\
$D_{i5}$ & $f_1 f_2$ & $\frac{1}{3}$ \\
$D_{i6}$ & $f_1 f_2$ & $-\frac{1}{3} + \frac{d}{2}$ \\
$D_{i7}$ & $f_1 f_2$ & $-\frac{1}{3} - \frac{2}{3}$ \\
$D_{i8}$ & $f_1 f_2$ & $-\frac{1}{3} + \frac{1}{3}$ \\
$D_{i9}$ & $f_1 f_2 (f_1 - 1)/(f_1 - 2)$ & $-\frac{1}{3} - \frac{20}{21} \ln(2) + \frac{4}{3}$ \\
$D_{i10}$ & $f_1 f_2$ & $-\frac{1}{3} - \frac{2}{3}$ \\
$D_{i11}$ & $f_1 f_2 (f_1 - 1)$ & $-\frac{1}{3} - \frac{1}{3}$ \\
$D_{i12}$ & $f_1 f_2$ & $\frac{1}{3}$ \\
$D_{i13}$ & $f_1 f_2 (f_1 - 1)$ & $\frac{4}{27} - \frac{28\sqrt{2}}{45} \arctan \left( \frac{\sqrt{2}}{3} \right) + \frac{7}{10}$ \\
$D_{i14}$ & $f_1 f_2 (f_1 - 1)$ & $\frac{4}{27} - \frac{28\sqrt{2}}{45} \arctan \left( \frac{\sqrt{2}}{3} \right) + \frac{7}{10}$ \\
$D_{i15}$ & $f_1 f_2 (f_1 - 1)$ & $\frac{1}{3} + \frac{5}{3} - \frac{12}{7} \ln(2)$ \\
$D_{i16}$ & $f_1 f_2 (f_1 - 1)$ & $\frac{1}{3} + \frac{5}{3} - \frac{12}{7} \ln(2)$ \\
$D_{i17}$ & $f_1 f_2$ & $\frac{1}{3}$ \\
$D_{i18}$ & $f_2$ & $\frac{1}{3} - \frac{1}{n}$ \\
$D_{i19}$ & $f_1 f_3$ & $\frac{1}{3} - \frac{1}{n}$ \\
$D_{i20}$ & $f_2$ & $\frac{1}{3} - \frac{1}{n}$ \\
$D_{i21}$ & $f_1 f_2 (f_1 - 1)$ & $\frac{1}{3} - \frac{1}{n} \ln(2) + \frac{1}{3}$ \\
$D_{i22}$ & $f_2$ & $\frac{1}{3} - \frac{1}{n}$ \\
$D_{i23}$ & $f_2$ & $\frac{1}{3} - \frac{1}{n}$ \\
$D_{i24}$ & $f_2$ & $\frac{1}{3} - \frac{1}{n}$ \\
$D_{i25}$ & $f_1 f_2 (f_1 - 1)$ & $\frac{2}{3} - \frac{28\sqrt{2}}{15} \arctan \left( \frac{\sqrt{2}}{3} \right) + \frac{1}{3}$ \\
$D_{i26}$ & $f_1 (f_1 - 1)$ & $\frac{2}{3} - \frac{28\sqrt{2}}{15} \arctan \left( \frac{\sqrt{2}}{3} \right) + \frac{1}{3}$ \\
$D_{i27}$ & $f_1 (f_1 - 1)$ & $\frac{2}{3} - \frac{28\sqrt{2}}{15} \arctan \left( \frac{\sqrt{2}}{3} \right) + \frac{1}{3}$ \\
$D_{i28}$ & $f_1 (f_1 - 1)$ & $\frac{2}{3} - \frac{28\sqrt{2}}{15} \arctan \left( \frac{\sqrt{2}}{3} \right) + \frac{1}{3}$ \\
$D_{i29}$ & $f_1 f_2$ & $\frac{2}{3} - \frac{1}{3}$ \\
$D_{i30}$ & $f_1$ & $\frac{2}{3} - \frac{1}{3}$ \\
\hline
\end{tabular}
\caption{$\epsilon$-expansion of expressions, corresponding to diagrams on Fig. 8}
\end{table}

\[
\times \left( \int_0^1 ds \left( \bar{s} + 1 - \bar{s}^2 \right)^{1-d/2} - \int_0^1 ds \left( \bar{s} - \bar{s}^2 \right)^{1-d/2} \right).
\]

Making the change of variables in first integral $\bar{s} = t + 1/2$ and performing both integrations we came to the final expression:

\[
D_{45} = \frac{(2\pi)^{-d} L^{d/2} L^{5-d/2}}{1-d/2} \times \left( \left( \frac{5}{4} \right)^{1-d/2} \right.
\]

\[
\times \left. _2 F_1 \left( 1/2, 1/2; d - 1; 3/2; 1/5 \right) - B(2 - d/2, 2 - d/2) \right),
\]

where $B$ is a Euler’s Beta function and $_2 F_1$ is a hypergeometric function.

**Appendix B**

Here, we present the results of $\epsilon$-expansions for the expressions corresponding to diagrams on Fig. 8 (tables I II). Note that in order to receive the $\delta$-expansions, one needs just to replace $\epsilon$ with $\delta$. However, it is important to note that this type of symmetry exists only in one loop approximation.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|}
\hline
Name & $f_1$ \\
\hline
$D_{31}$ & $f_1$ \\
$D_{32}$ & $f_1$ \\
$D_{33}$ & $f_1 (f_1 - 1)/(f_1 - 2)$ \\
$D_{34}$ & $f_1$ \\
$D_{35}$ & $f_2$ \\
$D_{36}$ & $f_2$ \\
$D_{37}$ & $f_1 (f_1 - 1)$ \\
$D_{38}$ & $f_1 (f_1 - 1)/(f_1 - 2)$ \\
$D_{39}$ & $f_1 (f_1 - 1)/(f_1 - 2)$ \\
$D_{40}$ & $f_1 (f_1 - 1)/2$ \\
$D_{41}$ & $f_1 (f_1 - 1)$ \\
$D_{42}$ & $f_1 (f_1 - 1)$ \\
$D_{43}$ & $f_1 (f_1 - 1)$ \\
$D_{44}$ & $f_1 (f_1 - 1)$ \\
$D_{45}$ & $f_1 (f_1 - 1)/(f_1 - 2)$ \\
$D_{46}$ & $f_1 (f_1 - 1)$ \\
$D_{47}$ & $f_1 (f_1 - 1)$ \\
$D_{48}$ & $f_1 (f_1 - 1)$ \\
$D_{49}$ & $f_1 (f_1 - 1)$ \\
$D_{50}$ & $f_1 (f_1 - 1)$ \\
$D_{51}$ & $f_1 f_2$ \\
$D_{52}$ & $f_1 f_2$ \\
$D_{53}$ & $f_1 f_2$ \\
$D_{54}$ & $f_1 f_2 (f_1 - 1)/(f_1 - 2)$ \\
$D_{55}$ & $f_1 f_2$ \\
$D_{56}$ & $f_1 f_2$ \\
$D_{57}$ & $f_1 f_2$ \\
$D_{58}$ & $f_1 (f_1 - 1)/(f_1 - 2)$ \\
\hline
\end{tabular}
\caption{$\epsilon$-expansion of expressions, corresponding to diagrams on Fig. 8}
\end{table}
