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The asphericity of star polymers: a renormalization group study

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Abstract. The asphericity of a flexible monodisperse f-star polymer in $d = 3$ is calculated in the framework of the standard two-parameter model in the asymptotic limit of infinite molecular weight. In contrast to previous analytical investigations we employ an asphericity measure which takes into account that size and shape of the polymer coils are strongly correlated. We consider ideal non-interacting (NEV) star polymers as well as molecules with excluded-volume (EV) interaction by means of renormalized perturbation theory. We show that in both cases the mean asphericity parameter takes a *universal numerical value* when the molecular weight tends to infinity. The same holds for the corresponding asymptotic distribution functions, which are proved to be universal functions too. These universal properties depend only on the topology, i.e. the number of arms f. For NEV stars we obtain a decrease of the asphericity with increasing number of arms. The numerical values are in excellent agreement with results of previous computer simulations. From the extrapolation of the ε-expansion results for EV stars we conclude that the influence of the EV on the shape asymptotics qualitatively depends on the number of arms. For $f = 1$ and $f = 2$, i.e. a linear chain, we reproduce a previous finding that the EV enlarges the asphericity of the chains by about 5%. For $f > 3$, however, we observe a decrease of the asphericity due to the EV which is intuitively appealing because of the strong steric repulsion for large values of f. These results are also in good agreement with previous computer experiments.

1. Introduction

Investigations on the properties of star polymers in dilute solution have made considerable progress during the last few years. Besides refined experimental techniques, computer simulations [1–4] and field-theoretic renormalization group calculations [5–8] have become especially useful. Star polymers are the simplest representatives of the wide class of branched polymers, but on the other hand they are important as building blocks of polymer networks.

In dilute solution flexible polymers form crumpled coils with a global shape which differs significantly from spherical symmetry on short time scales. This was first recognized by Kuhn [9] for linear polymers in 1934 and has been the focus of many analytical and numerical investigations since then. High flexibility and strong thermal fluctuations make it difficult to measure such shape properties directly. It is nevertheless believed that the equilibrium shape of the polymer coils plays an important role in certain models explaining viscous flow and other hydrodynamic properties of polymeric fluids [10–12].

To begin, consider a fixed configuration of a star polymer consisting of f linear chains connected at one central vertex. Each single chain contains $(N - 1)$ repeating units, say

Kuhnian segments. The end points of these segments are denoted by d-dimensional vectors $\boldsymbol{R}_i^{(a)}$ with Cartesian components

$$\boldsymbol{R}_i^{(a)} = \left(X_{i,1}^{(a)}, X_{i,2}^{(a)} \ldots, X_{i,d}^{(a)}\right) \qquad i = 2, \ldots, N; a = 1, \ldots, f\,. \tag{1.1}$$

Additionally the second end of the first segments which form the vertex of the star polymer are denoted by $\boldsymbol{R}_1^{(a)}$. The global shape of such a configuration can be characterized conveniently by the d eigenvalues q_α of the radius of gyration tensor $\boldsymbol{Q}$ [13–15] which can be generalized for star polymers by

$$Q_{\alpha\beta} = \frac{1}{2(fN)^2} \sum_{a,b=1}^{f} \sum_{i,j=1}^{N} \left[X_{i,\alpha}^{(a)} - X_{j,\alpha}^{(b)}\right]\left[X_{i,\beta}^{(a)} - X_{j,\beta}^{(b)}\right]. \tag{1.2}$$

The present calculations are confined to a very simple invariant of $\boldsymbol{Q}$ quantifying the deviation of a fixed configuration from spherical symmetry. This so-called asphericity [16]

$$A_d = \frac{1}{d(d-1)} \sum_{\alpha=1}^{d} \frac{(q_\alpha - \bar{q})^2}{\bar{q}^2} \tag{1.3}$$

vanishes for configurations with spherical symmetry (all eigenvalues q_α equal) and takes its maximum value 1 for completely elongated shapes (all eigenvalues zero except one). $\bar{q}$ denotes the arithmetic average of the d eigenvalues and is closely related to the well known radius of gyration $\bar{q} = R_{\mathrm{G}}^2/d$. For analytical calculations it is advantageous to rewrite (1.3) in the form [17]

$$A_d = \frac{d}{d-1} \frac{\operatorname{tr}(\hat{\boldsymbol{Q}}^2)}{(\operatorname{tr} \boldsymbol{Q})^2} \tag{1.4}$$

with the traceless tensor

$$\hat{\boldsymbol{Q}} = \boldsymbol{Q} - \frac{\operatorname{tr} \boldsymbol{Q}}{d} \mathbf{1}_d\,. \tag{1.5}$$

In dilute solution thermal fluctuations prevent A_d from taking a sharp value. Even in the limit of infinite molecular weight the asphericity is broadly distributed around a mean value which can, for example, be directly measured in computer experiments.

This mean value $\langle A_d \rangle$ has been calculated for the first time analytically for non-interacting linear polymers [18]. The simple method which allows the averaging of ratios such as (1.4) with fluctuating numerator and denominator (within a Gaussian model) was later used to calculate this shape parameter also for linear polymers with EV interaction by means of renormalized perturbation theory [19]. The results of these calculations corroborated the findings of Monte Carlo simulations [20, 21] stating the asphericity to be enlarged by the EV asymptotically by about 5–10%. Previous analytical investigations underestimated this effect as they used a simplified mean asphericity measure [17]

$$\hat{A}_d = \frac{d}{d-1} \frac{\langle \operatorname{tr}(\hat{\boldsymbol{Q}}^2) \rangle}{\langle (\operatorname{tr} \boldsymbol{Q})^2 \rangle}\,. \tag{1.6}$$

The reason for this difference is the neglecting of important correlations between size and shape of the polymer coils in (1.6). As pointed out by Cannon *et al* [21] this definition overestimates the influence of larger polymer configurations on the mean shape properties and suppresses the influence of compact ones. This artificially leads to larger absolute values for the mean asphericity, whereas the influence of the EV on the asymmetry is underestimated by nearly one order of magnitude [19, 21]. After all, the large difference between the two mean asphericity measures $\langle A_d \rangle$ and $\hat{A}_d$ (about 30% for NEV linear chains in $d = 3$) illustrates the strong fluctuations in the shape of diluted polymers.

In this paper we apply the methods of [18] and [19] to star polymers and calculate for the first time analytically the mean asphericity $\langle A_d \rangle$ for NEV and EV stars. We show that in both cases the mean asphericity takes a universal numerical value when the chain lengths tend to infinity. These universal numbers only depend on the space dimension d and the functionality f, i.e. the number of arms. The same holds for all higher moments of the asphericity. By that means the distribution function of A_d is proved to be a universal function, too.

In section 2 we calculate exact expressions for the mean asphericity of non-interacting star polymers which are compared with the results of Monte Carlo simulations [20]. Here we also take the opportunity to explain the method of ratio-averaging [18] leading to a somewhat unusual propagator which we later need to set up the perturbation series. The next section deals with the asphericity of EV stars and starts with some remarks on universality, the method of renormalized perturbation theory and the ε-expansion. In the second subsection we present explicit results of the first order ε-expansion for $\langle A_{d=4-\varepsilon} \rangle$ and the extrapolation to the physical dimension $d = 3$. Comparing these results with data from Monte Carlo simulations [20] and the numbers from the non-interacting case, we discuss the influence of the EV on the asphericity of star polymers. The last section summarizes our results and contains some concluding remarks.

2. Ideal star polymers

To describe the asymptotic shape properties of non-interacting ideal star polymers we choose one of the simplest representatives from the universality class of RW-like polymer models without any true many-body interaction. As usual, the Kuhnian segments are modelled as simple harmonic springs tied together at their end points. The Hamiltonian of this model is given by

$$\mathcal{H}_0\{\boldsymbol{R}_i^{(a)}\} = \sum_{\alpha=1}^{d} h_0\{X_{i,\alpha}^{(a)}\} \tag{2.1}$$

where h_0 denotes one single Cartesian contribution

$$h_0\{X_i^{(a)}\} = \frac{1}{4\ell^2} \sum_{i=2}^{N} \sum_{a=1}^{f} \left(X_i^{(a)} - X_{i-1}^{(a)} \right)^2 . \tag{2.2}$$

To guarantee star topology for this model of f independent Gaussian chains all thermodynamic averages which are denoted by $\langle \cdot \rangle_0$ are calculated under the restriction

$$\prod_{a=1}^{f} \delta^d(\boldsymbol{R}_1^{(a)}) . \tag{2.3}$$

Besides, equation (2.3) eliminates divergent contributions from the massless translational mode, since we are only interested in translational invariant properties.

To average ratios like (1.4) with fluctuating numerator and denominator with a statistical weight induced by (2.1) and (2.2) it was shown to be useful to exponentiate the denominator by the identity [18]

$$(\operatorname{tr} Q)^{-m} = \frac{1}{(m-1)!} \int_0^\infty \mathrm{d}y\, y^{m-1}\, \mathrm{e}^{-y \operatorname{tr} Q}\,. \tag{2.4}$$

With $m = 2$ the average of (1.4) can be rewritten as [18]

$$\langle A_d \rangle_0 = \frac{d}{d-1} \int_0^\infty \mathrm{d}y\, y \big\langle \operatorname{tr}(\hat{Q}^2) \big\rangle_{0,y} \big\langle \mathrm{e}^{-y \operatorname{tr} Q} \big\rangle_0 \tag{2.5}$$

where $\langle \cdot \rangle_{0,y}$ is calculated with a modified Hamiltonian

$$\mathcal{H}_{0,y}\{R_i^{(a)}\} = \mathcal{H}_0\{R_i^{(a)}\} + y \operatorname{tr} Q\,. \tag{2.6}$$

Note that (2.6) is also of the form (2.1) with

$$h_{0,y}\{X_i^{(a)}\} = h_0\{X_i^{(a)}\} + \frac{y}{2(fN)^2} \sum_{i,j=1}^{N} \sum_{a,b=1}^{f} \left(X_i^{(a)} - X_j^{(b)}\right)^2. \tag{2.7}$$

Since $h_{0,y}$ is quadratic in X, too (which is the crucial point of this trick), we can use a simple orthogonal transformation (see appendix A)

$$X_i^{(a)} \longrightarrow \xi_\nu^{(t)} \tag{2.8}$$

to cast the Hamiltonian in diagonal form

$$h_{0,y}\{\xi_\nu^{(t)}\} = \sum_{\nu=0}^{N-1} \sum_{t=0}^{f-1} (1 - \delta_{\nu 0}\delta_{t0})\ \varepsilon_\nu(y)\, |\xi_\nu^{(t)}|^2 \tag{2.9}$$

with mode energies given by

$$\varepsilon_\nu(y) = \ell^{-2} \sin^2\left(\frac{\pi\nu}{2N}\right) + \frac{y}{fN}\,. \tag{2.10}$$

It is important to notice that $\varepsilon_\nu(y)$ does not depend on the mode index t which reflects the permutation symmetry of the polymer arms. As $\xi_0^{(0)}$ describes translations of the whole polymer star, this mode gives no contribution in (2.9).

According to (2.9) the second average in (2.5) can now be expressed in terms of the Rouse eigenmodes $\varphi_\nu(i)$ of a single chain and the energies $\varepsilon_\nu(y)$. The result of this calculation, which we explain in appendix B, reads

$$\big\langle \mathrm{e}^{-y \operatorname{tr} Q} \big\rangle_0 = \left(\frac{y}{f}\right)^{(d/2)(1-f)} \prod_{\nu=1}^{N-1} \left[\frac{\varepsilon_\nu(0)}{\varepsilon_\nu(y)}\right]^{df/2} \left[\sqrt{\sum_{\nu=0}^{N-1} \frac{(\varphi_\nu(1))^2}{\varepsilon_\nu(y)}}\right]^{d(1-f)}. \tag{2.11}$$

As we are only interested in asymptotic properties, the continuum limit

$$N \to \infty \qquad \ell \to 0 \qquad \text{with} \quad N\ell^2 \equiv L \quad \text{fixed} \tag{2.12}$$

simplifies our results considerably. Introducing

$$\beta = 2\sqrt{\frac{yL}{f}} \tag{2.13}$$

as a new integration variable, equation (2.11) takes the final form

$$\left\langle \mathrm{e}^{-y\,\mathrm{tr}\,Q} \right\rangle_0 = (\cosh\beta)^{(d/2)(1-f)} \left[\frac{\beta}{\sinh\beta}\right]^{d/2} . \tag{2.14}$$

For $f = 1$ equation (2.14) obviously reduces to the result for linear chains [18]. The same holds for $f = 2$ after proper rescaling of the integration variable β.

The remaining first average in (2.5) involves the calculation of four-point functions with the somewhat unusual Gaussian weight associated with $\mathcal{H}_{0,y}$. Using the continuum version of (1.2)

$$Q_{\alpha\beta} = \frac{1}{2(fL)^2} \sum_{a,b=1}^{f} \int_0^L \mathrm{d}t_1\, \mathrm{d}t_1' \left[X_\alpha^{(a)}(t_1) - X_\alpha^{(b)}(t_1')\right]\left[X_\beta^{(a)}(t_1) - X_\beta^{(b)}(t_1')\right] \tag{2.15}$$

Wick's theorem and simple combinatorics lead to

$$\left\langle \mathrm{tr}\left(\hat{Q}^2\right)\right\rangle_{0,y} = \frac{(d-1)(d+2)}{4(fL)^4} \sum_{a,a',b,b'=1}^{f} \int_0^L \mathrm{d}t_1\, \mathrm{d}t_1'\, \mathrm{d}t_2\, \mathrm{d}t_2' \left\langle C_d^{(a,a')}(t_1, t_1')\, C_d^{(b,b')}(t_2, t_2')\right\rangle_{0,y}^2 \tag{2.16}$$

where

$$C_\alpha^{(a,a')}(t, t') = X_\alpha^{(a)}(t) - X_\alpha^{(a')}(t') . \tag{2.17}$$

Here we used the diagonality of the two-point function in the Cartesian indices

$$\begin{aligned} &\left\langle \left[X_\alpha^{(a)}(t) - X_\alpha^{(a)}(0)\right]\left[X_\beta^{(b)}(t') - X_\beta^{(b)}(0)\right]\right\rangle_{0,y} \\ &\qquad = \delta_{\alpha\beta} \left\langle \left[X_d^{(a)}(t) - X_d^{(a)}(0)\right]\left[X_d^{(b)}(t') - X_d^{(b)}(0)\right]\right\rangle_{0,y} \\ &\qquad = \delta_{\alpha\beta}\, G(a, b; t, t') . \end{aligned} \tag{2.18}$$

In appendix B we show that the propagator for our model is given by

$$\begin{aligned} G(a, b; t, t') = \frac{1}{f}\frac{2L}{\beta\sinh\beta} \Big\{ & \tfrac{1}{2}\cosh\left[\beta\left(1 - |t - t'|/L\right)\right] + \tfrac{1}{2}\cosh\left[\beta\left(1 - (t + t')/L\right)\right] \\ & - \cosh\left[\beta\left(1 - t/L\right)\right] - \cosh\left[\beta\left(1 - t'/L\right)\right] + \cosh\beta \Big\} \\ & - \left(\delta_{ab} - \frac{1}{f}\right) \frac{L}{\beta\cosh\beta} \Big\{ \sinh\left[\beta\left(1 - (t + t')/L\right)\right] \\ & - \sinh\left[\beta\left(1 - |t - t'|/L\right)\right] \Big\} . \end{aligned} \tag{2.19}$$

Note that the two-point function only depends on whether the two segments at t and t' belong to the same or to different arms of the star polymer. The case of a linear chain is also included in (2.19) for $f = 1$ or $f = 2$ (after proper transformation of the segments indices and rescaling of L and β).

Substituting (2.18), (2.19) in (2.16), the summations over the arm indices are easily carried out. The remaining integrations yield the quite simple result

$$\langle \mathrm{tr}(\hat{Q}^2)\rangle_{0,y} = \frac{(d+2)(d-1)L^2}{f^2\beta^4\,[\cosh(4\beta)-1]}\{2+4f\beta^2-2(f-2)\beta\sinh(2\beta) \\ -4(f-2)\beta^2\cosh(2\beta)+f\beta\sinh(4\beta)-2\cosh(4\beta)\}\,. \tag{2.20}$$

Together with (2.14) this leads to our final formula for the mean asphericity of a NEV f-star polymer in d dimensions

$$\langle A_d(f)\rangle_0 = \frac{d(d+2)}{8}\int_0^\infty \mathrm{d}\beta \frac{(\cosh\beta)^{(d/2)(1-f)}}{\beta\,[\cosh(4\beta)-1]}\left[\frac{\beta}{\sinh\beta}\right]^{d/2}\{2+4f\beta^2-2(f-2)\beta\sinh(2\beta) \\ -4(f-2)\beta^2\cosh(2\beta)+f\beta\sinh(4\beta)-2\cosh(4\beta)\}\,. \tag{2.21}$$

As expected, this asymptotic mean value only depends on f and d, whereas the chain length L drops out in the integral (2.5). For $f = 1$ and $f = 2$ equation (2.21) reduces to the result for NEV linear chains [18].

In table 1 we listed our estimates for the mean asphericity in $d = 3$ for arm numbers up to $f = 6$ which we calculated via numerical integration of (2.21). The next column shows the data from Monte Carlo simulations by Bishop *et al* [20]. We also included the results of a previous analytical investigation by Wei and Eichinger [22] who calculated the asphericity approximant (1.6) for NEV f-stars.

Table 1. Estimates for the mean asphericity in $d = 3$ for arm numbers up to $f = 6$.

	$\langle A_3(f)\rangle_0$		$\hat{A}_{3,0}(f)$
f	Exact	MC	
1	0.3943...	0.397 ± 0.001	0.5263...
2	0.3943...	0.397 ± 0.001	0.5263...
3	0.3044...	0.304 ± 0.001	0.3609...
4	0.2427...	0.242 ± 0.001	0.2732...
5	0.2006...	0.199 ± 0.001	0.2195...
6	0.1706...	0.171 ± 0.001	0.1834...

The agreement of our analytical result for $\langle A_d(f)\rangle_0$ with the extrapolated asphericities from the MC experiment is very good. Both data show a smooth decay of the mean asphericity with increasing values of f. Even when there is no repulsive interaction between the segments, star polymers with high functionality are more spherical than those with a smaller number of arms. Figure 1 illustrates this trend and shows $\langle A_3(f)\rangle_0$ as a continuous function of f. Additionally, we plotted the values from the MC simulation.

The comparison of the numerical values for $\langle A_3(f)\rangle_0$ and $\hat{A}_{3,0}(f)$ again shows that the mean asphericity is overestimated by (1.6) due to the enhanced influence of larger polymer configurations. As this difference shrinks from 33% for linear chains to less than

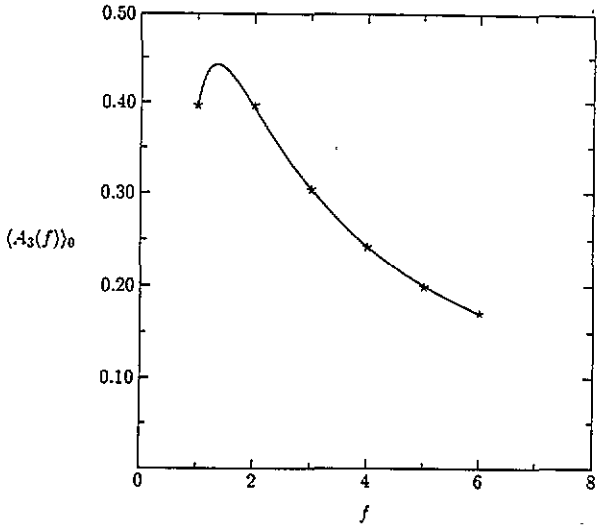

Figure 1. Asymptotic mean asphericity for NEV stars (— exact solution, ⋆ Monte Carlo simulation [20]).

8% for $f = 6$ we conclude that shape fluctuations are suppressed when the number of arms increases. Indeed, asymptotic expansions of [22]

$$\hat{A}_{3,0}(f) = \frac{10(15f - 14)}{15(3f - 2)^2 + 4(15f - 14)} \tag{2.22}$$

and (2.21) for large values of f show the same leading behaviour of the mean asphericity, which vanishes like $\frac{10}{9} f^{-1}$.

3. Star polymers with EV interaction

In the limit of infinite molecular weight the global properties of polymers in a good solvent are dominated by a short-range repulsive force preventing the segments occupying the same position in space. In this section we are going to investigate the influence of this EV interaction on the shape asymptotics of star polymers. For that purpose we set up a perturbation expansion for the mean asphericity $\langle A_d \rangle$ up to first order in the EV potential, which we conveniently choose as

$$\mathcal{V}\{\boldsymbol{R}\} = \tfrac{1}{6} u \sum_{a,b=1}^{f} \int_0^L \mathrm{d}t\, \mathrm{d}t'\, \delta^d \left(\boldsymbol{R}^{(a)}(t) - \boldsymbol{R}^{(b)}(t') \right) . \tag{3.1}$$

The simple continuous form of $\mathcal{V}$ is justified by universality in the asymptotic limit. The perturbation theory for the mean asphericity

$$\langle A_d \rangle = \frac{d}{d-1} \int_0^\infty \mathrm{d}y\, y \left\langle \mathrm{tr}\,(\hat{Q}^2) \right\rangle_y \left\langle \mathrm{e}^{-y\,\mathrm{tr}\,Q} \right\rangle \tag{3.2}$$

is well defined if all segment indices in the perturbation expansion of (3.2) are at least separated by some microscopic cutoff [23]. For technical reasons we will use a dimensional regularization scheme [23] to calculate an estimate for $\langle A_d \rangle$ which orders asymptotically in powers of $\varepsilon = 4 - d$ [19].

Note that the second mean value in (3.2) now involves the usual Hamiltonian $\mathcal{H} = \mathcal{H}_0 + \mathcal{V}$, whereas the first one is calculated with a weight according to $\mathcal{H}_y = \mathcal{H}_{0,y} + \mathcal{V}$ (see (2.6)).

3.1. Renormalization and universality

It is well known that a naive perturbation expansion in u fails in the limit of diverging chain lengths when the space dimension d is less than four. The reason is that the expansion parameter itself, which is not u but uL^{4-d}, diverges in the asymptotic limit. As usual we shall adopt the renormalization group (RG) transformation to circumvent this problem. By that means the universal properties of star polymers in the limit $L \to \infty$ are linked together with those of molecules where each arm effectively consists of only one segment. After this mapping simple perturbation theory in some renormalized coupling constant works [23].

In the following we will make use of the close relation of polymer chain statistics to a (Landau–Ginzburg-type) field theory in the limit $n \to 0$ [24] and employ a well developed field-theoretic renormalization scheme [25, 26]. In appendix C we show how mean values, which typically appear in the calculation of any shape parameter, are related to special composite operators in field theory. From the well known renormalization of these operators we conclude that all UV-divergencies (simple pole terms in ε in dimensional regularization) of the perturbation expansion of (3.2) can be absorbed in a reparametrization of the chain length L and the coupling constant u which read

$$L = \mu^{-2}(Z_t)^{-1}\, L^{\mathrm{R}} \tag{3.3}$$

$$u = 16\pi^2\mu^{\varepsilon} Z_u\, u^{\mathrm{R}}\,. \tag{3.4}$$

By that means the two mean values in (3.2) can now be expressed by two dimensionless functions F_1 and F_2

$$\left\langle \mathrm{tr}(\hat{Q}^2)\right\rangle_y = \mu^{-4}\; F_1\left(L^{\mathrm{R}}, u^{\mathrm{R}}, \mu^{-2}y\right) \tag{3.5}$$

$$\left\langle \mathrm{e}^{-y\,\mathrm{tr}\,Q}\right\rangle = F_2\left(L^{\mathrm{R}}, u^{\mathrm{R}}, \mu^{-2}y\right) \tag{3.6}$$

which are finite for $\varepsilon \to 0$ if their renormalized arguments are kept fixed. Here μ denotes some arbitrary inverse length scale. All ε-poles are now contained in some Z-factors of the reparametrization which are known from n-component ϕ^4 field theory in the limit $n \to 0$

$$Z_t = 1 + \tfrac{2}{3}\frac{u^{\mathrm{R}}}{\varepsilon} + \mathrm{O}\left(\left(u^{\mathrm{R}}\right)^2\right) \tag{3.7}$$

$$Z_u = 1 + \tfrac{8}{3}\frac{u^{\mathrm{R}}}{\varepsilon} + \mathrm{O}\left(\left(u^{\mathrm{R}}\right)^2\right). \tag{3.8}$$

The reparametrization $(L, u) \to (\mu, L^{\mathrm{R}}, u^{\mathrm{R}})$ is not unique since the inverse length scale μ is arbitrary. A simultaneous variation of $(\mu, L^{\mathrm{R}}, u^{\mathrm{R}})$ with (L, u) kept fixed then implies 'renormalization group' equations for renormalized quantities [23, 25–27]. For $F_{1,2}$ in (3.5), (3.6) these read

$$\left\{\mu\frac{\partial}{\partial\mu} + \beta(u^{\mathrm{R}})\frac{\partial}{\partial u^{\mathrm{R}}} + \vartheta(u^{\mathrm{R}})\, L^{\mathrm{R}}\frac{\partial}{\partial L^{\mathrm{R}}} + E_i\right\} F_i\left(L^{\mathrm{R}}, u^{\mathrm{R}}, \mu^{-2}y\right) = 0 \tag{3.9}$$

with $E_1 = -4$, $E_2 = 0$ and the Wilson functions given by $\beta(u^{\mathrm{R}}) = \mu\partial_\mu u^{\mathrm{R}}\big|_{L,u}$ and $\vartheta(u^{\mathrm{R}}) = \mu\partial_\mu \ln L^{\mathrm{R}}\big|_{L,u}$. As usual equation (3.9) can be solved by the method of characteristics. Defining a variable inverse length scale

$$\bar{\mu}(\lambda) = \mathrm{e}^{-\lambda}\mu \tag{3.10}$$

with a flow parameter λ, equation (3.9) can easily be solved if we also introduce flowing renormalized variables $\bar{u}^{\mathrm{R}}(\lambda)$ and $\bar{L}^{\mathrm{R}}(\lambda)$ which obey

$$\beta\big(\bar{u}^{\mathrm{R}}(\lambda)\big) = -\frac{\mathrm{d}}{\mathrm{d}\lambda}\bar{u}^{\mathrm{R}}(\lambda) \qquad \bar{u}^{\mathrm{R}}(0) = u^{\mathrm{R}} \tag{3.11}$$

$$\vartheta\big(\bar{u}^{\mathrm{R}}(\lambda)\big) = -\frac{\mathrm{d}}{\mathrm{d}\lambda}\ln \bar{L}^{\mathrm{R}}(\lambda) \qquad \bar{L}^{\mathrm{R}}(0) = L^{\mathrm{R}}. \tag{3.12}$$

Then the solution of (3.9) simply reads

$$F_i\left(L^{\mathrm{R}}, u^{\mathrm{R}}, \mu^{-2}y\right) = F_i\left(\bar{L}^{\mathrm{R}}(\lambda), \bar{u}^{\mathrm{R}}(\lambda), \left(\mathrm{e}^{-\lambda}\mu\right)^{-2}y\right)\mathrm{e}^{-E_i\lambda}. \tag{3.13}$$

The zeros of (3.11) determine the fixed-point value of $\bar{u}^{\mathrm{R}}(\lambda)$. For $\varepsilon > 0$ and not too large positive values of u one gets

$$\overset{*}{u}{}^{\mathrm{R}} = \tfrac{3}{8}\varepsilon + \mathrm{O}\left(\varepsilon^2\right) \tag{3.14}$$

which is an attractive infrared-stable fixed point as $\lambda \to \infty$.

The second flow equation is formally solved by

$$\bar{L}^{\mathrm{R}}(\lambda) = L^{\mathrm{R}}\exp\left\{-\int_0^{\lambda}\mathrm{d}\lambda'\,\vartheta\big(\bar{u}^{\mathrm{R}}(\lambda')\big)\right\}. \tag{3.15}$$

As we are interested in $L^{\mathrm{R}} \to \infty$, equation (3.15) allows us to choose λ so that $\bar{L}^{\mathrm{R}}(\lambda) = 1$, i.e. the long-chain problem is thereby mapped on a simple short-chain problem. This requires $\lambda \to \infty$ since $\overset{*}{\vartheta} = \vartheta(\overset{*}{u}{}^{\mathrm{R}}) > 0$. We can now determine the behaviour of the mean asphericity under the RG flow. For $L^{\mathrm{R}} \to \infty$ equation (3.13) implies

$$F_i\left(L^{\mathrm{R}}, u^{\mathrm{R}}, \mu^{-2}y\right) \overset{\lambda\to\infty}{\simeq} \psi_i\left(\mathrm{e}^{2\lambda}\mu^{-2}y\right)\mathrm{e}^{-E_i\lambda} \tag{3.16}$$

with a non-universal flow factor e^{λ}, which depends on $u^{\mathrm{R}} = \bar{u}^{\mathrm{R}}(0)$, and

$$\psi_i(Y) = F_i\left(1, \overset{*}{u}{}^{\mathrm{R}}, Y\right). \tag{3.17}$$

Respecting (3.2), (3.5) and (3.6), the mean asphericity is now given by

$$a\big(L^{\mathrm{R}}, u^{\mathrm{R}}\big) := \frac{d}{d-1}\int_0^{\infty}\mathrm{d}y\,y\,\mu^{-4}\,F_1\left(L^{\mathrm{R}}, u^{\mathrm{R}}, \mu^{-2}y\right)F_2\left(L^{\mathrm{R}}, u^{\mathrm{R}}, \mu^{-2}y\right). \tag{3.18}$$

As the F_i are finite functions for $\varepsilon \to 0$ the same holds for (3.18) as a function of renormalized parameters. Substituting $Y = \mathrm{e}^{2\lambda}\mu^{-2}y$ equations (3.16) and (3.18) yield the $L^{\mathrm{R}} \to \infty$ limit of the mean asphericity

$$a\big(1, \overset{*}{u}{}^{\mathrm{R}}\big) := \frac{d}{d-1}\int_0^{\infty}\mathrm{d}Y\,Y\,\psi_1(Y)\,\psi_2(Y). \tag{3.19}$$

Note that the non-universal flow factor e^{λ} drops out in (3.19) so that $a\big(1, \overset{*}{u}{}^{\mathrm{R}}\big)$ takes a *universal numerical value* at the EV fixed point depending only on d and f. In the next subsection we show how these numbers can be calculated within a first-order ε-expansion and extrapolate the results to $d = 3$.

Finally let us draw another important conclusion. In appendix C we demonstrated how the renormalization of products like $\left\langle Q_{\alpha_1\beta_1}\dots Q_{\alpha_s\beta_s}\right\rangle$ can be derived from the renormalization of special composite operators in field theory. The same arguments apply when higher moments of the asphericity $\langle (A_d)^m\rangle$ are calculated. Substituting $\mathrm{d}y\,y\,\langle\mathrm{tr}\,(\hat{Q}^2)\rangle_y$ in (3.2) by $\mathrm{d}y\,y^{2m-1}\big\langle\big[\mathrm{tr}\,(\hat{Q}^2)\big]^m\big\rangle_y$ (see also (2.4)) it immediately follows that the flow factor e^{λ} always drops out in the analogous Y-integral. By that means, all higher moments of A_d are proved to take universal numerical values at the EV fixed point so that the asymptotic distribution function $\mathcal{P}(A) \equiv \big\langle\delta\big(A - A_d\big)\big\rangle$ is a universal function, too.

3.2. ε-expansion and extrapolation to $d = 3$

In this subsection we actually carry through the RG program of the previous section to calculate an estimate for the mean asphericity of EV star polymers. Below $d = 4$ ($\varepsilon > 0$) the fixed-point value $\overset{*}{u}^{\mathrm{R}}$ deviates from zero and $a(1, \overset{*}{u}^{\mathrm{R}})$ takes a different numerical value as its random walk counterpart $a(1, 0)$. For $d > 4$ the EV is an irrelevant interaction ($\overset{*}{u}^{\mathrm{R}} \equiv 0$) so that NEV and EV stars show the same shape asymptotics.

To eliminate trivial d-dependent factors we perform a *systematic* ε-expansion to first order of the ratio $a(1, \overset{*}{u}^{\mathrm{R}})/a(1, 0)$ and try to extrapolate the results towards $d = 3$ [19]. According to (3.2) we need the first order in $\mathcal{V}$ contributions to (3.5) and (3.6), which are given by

$$\langle \mathrm{e}^{-y\,\mathrm{tr}\,Q} \rangle_1 = \langle \mathrm{e}^{-y\,\mathrm{tr}\,Q} \rangle_0 \left[\langle \mathcal{V} \rangle_0 - \langle \mathcal{V} \rangle_{0,y} \right] \tag{3.20}$$

$$\langle \mathrm{tr}(\hat{Q}^2) \rangle_{1,y} = -\langle \mathrm{tr}(\hat{Q}^2)\, \mathcal{V} \rangle_{0,y} + \langle \mathrm{tr}(\hat{Q}^2) \rangle_{0,y} \langle \mathcal{V} \rangle_{0,y} . \tag{3.21}$$

The strategy to calculate these averages is quite analogous to that of section 2. Writing $\mathcal{V}$ in its Fourier representation

$$\mathcal{V}\{\boldsymbol{R}\} = \tfrac{1}{6} u \sum_{a,b=1}^{f} \int_0^L \mathrm{d}t\, \mathrm{d}t' \int_k \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot[\boldsymbol{R}^{(a)}(t) - \boldsymbol{R}^{(b)}(t')]} \tag{3.22}$$

where

$$\int_k \equiv \int \frac{\mathrm{d}^d k}{(2\pi)^d} \tag{3.23}$$

a Taylor expansion in $\boldsymbol{k}$ leads to simple Wick contractions within Gaussian $(0, y)$-statistics. The resulting expressions can be summed up again and the $\boldsymbol{k}$-integration can easily be performed. For (3.20) we find

$$\langle \mathrm{e}^{-y\,\mathrm{tr}\,Q} \rangle_1 = \langle \mathrm{e}^{-y\,\mathrm{tr}\,Q} \rangle_0 \frac{1}{(2\sqrt{\pi})^d} \frac{u}{6} \sum_{a,b=1}^{f} \int_0^L \mathrm{d}t\, \mathrm{d}t' \left\{ \left[S_y^{(a,b)}(t,t') \right]^{-2+\varepsilon/2} - \left[S_0^{(a,b)}(t,t') \right]^{-2+\varepsilon/2} \right\} \tag{3.24}$$

where we have introduced the abbreviation

$$S_y^{(a,b)}(t,t') = \tfrac{1}{2} \langle [C_d^{(a,b)}(t,t')]^2 \rangle_{0,y} = \tfrac{1}{2} G(a,a;t,t) - G(a,b;t,t') + \tfrac{1}{2} G(b,b;t',t') \tag{3.25}$$

(see also equation (2.17)). The second mean value (3.21) involves the lengthy, but trivial, calculation of some six-point functions, resulting in

$$\begin{aligned} \langle \mathrm{tr}(\hat{Q}^2) \rangle_{1,y} = \frac{1}{(2\sqrt{\pi})^d} \frac{(d-1)(d+2)}{4(fL)^4} \frac{u}{6} \sum_{a,a',b,b',c,c'=1}^{f} \int \mathrm{d}\theta\, \Big\{ \left[S_y^{(c,c')}(t,t') \right]^{-3+\varepsilon/2} \\ \times T_y^{(a,a';c,c')}(t_1,t_1';t,t')\, T_y^{(b,b';c,c')}(t_2,t_2';t,t')\, T_y^{(a,a';b,b')}(t_1,t_1';t_2,t_2') \\ - \tfrac{1}{4} \left[S_y^{(c,c')}(t,t') \right]^{-4+\varepsilon/2} \left[T_y^{(a,a';c,c')}(t_1,t_1';t,t') \right]^2 \left[T_y^{(b,b';c,c')}(t_2,t_2';t,t') \right]^2 \Big\} \end{aligned} \tag{3.26}$$

with the notation

$$\int \mathrm{d}\theta \equiv \int_0^L \mathrm{d}t\,\mathrm{d}t'\,\mathrm{d}t_1\,\mathrm{d}t_1'\,\mathrm{d}t_2\,\mathrm{d}t_2' \tag{3.27}$$

and

$$\begin{aligned} T_y^{(a,a';b,b')}\left(t_1,t_1';t_2,t_2'\right) &= \left\langle C_d^{(a,a')}(t_1,t_1')\, C_d^{(b,b')}(t_2,t_2')\right\rangle_{0,y} \\ &= G(a,b;t_1,t_2) + G(a',b';t_1',t_2') - G(a,b';t_1,t_2') - G(a',b;t_1',t_2)\,. \end{aligned} \tag{3.28}$$

Substituting the reparametrizations (3.3), (3.4) in (3.24) and (3.26), we are now able to calculate the u^{R}-expansions

$$F_i\left(L^{\mathrm{R}},u^{\mathrm{R}},\mu^{-2}y,\varepsilon\right) = \sum_{j=0}^{\infty}\left(u^{\mathrm{R}}\right)^j F_{i;j}\left(L^{\mathrm{R}},\mu^{-2}y,\varepsilon\right) \tag{3.29}$$

up to $j=1$. Note that the ε-dependence of the F_i is denoted explicitly here. Analogously, (3.18) now reads

$$a(L^{\mathrm{R}},u^{\mathrm{R}},\varepsilon) := \frac{d}{d-1}\int_0^{\infty}\mathrm{d}x\, x\, F_1\left(L^{\mathrm{R}},u^{\mathrm{R}},x,\varepsilon\right) F_2\left(L^{\mathrm{R}},u^{\mathrm{R}},x,\varepsilon\right) \tag{3.30}$$

with $x=\mu^{-2}y$. As functions of u and L, the first-order contributions (3.20), (3.21) contain ε-poles at $\varepsilon=0$. The reason for these UV-divergencies is the vanishing of

$$S_y(t,t') \propto |t-t'| \tag{3.31}$$

as $t\to t'$. These singularities in the integrands of (3.24) and (3.26) are not integrable for $\varepsilon=0$. In appendix D we explain how the leading contributions $\propto u\varepsilon^{-1}$ and $u\varepsilon^0$ can be calculated. The singular terms $\propto u\varepsilon^{-1}$ are indeed absorbed by the reparametrizations (3.3), (3.4) which we have checked analytically using a symbolic manipulation package. As functions of L^{R} the coefficients $F_{i;j}\left(L^{\mathrm{R}},x,\varepsilon\right)$ of the u^{R}-expansions (3.29) are finite for $\varepsilon\to 0$, which thereby also holds for $a(L^{\mathrm{R}},u^{\mathrm{R}},\varepsilon)$.

The contributions $\propto u\varepsilon^0$ enter the ratio

$$\frac{a(1,u^{\mathrm{R}},\varepsilon)}{a(1,0,\varepsilon)} = 1 + u^{\mathrm{R}}\,b(f) + \mathrm{O}\left(u^{\mathrm{R}}\varepsilon,\left(u^{\mathrm{R}}\right)^2\right) \tag{3.32}$$

where

$$\begin{aligned} b(f) &= \frac{a(1,u^{\mathrm{R}},0)}{a(1,0,0)} \\ &= \frac{1}{a(1,0,0)}\frac{4}{3}\int_0^{\infty}\mathrm{d}x\, x\left\{F_{1;1}(1,x,0)F_{2;0}(1,x,0) + F_{1;0}(1,x,0)F_{2;1}(1,x,0)\right\}. \end{aligned} \tag{3.33}$$

We show in appendix D how the two contributions on the RHS of (3.33) can be calculated numerically in $d=4$. Table 2 summarizes the necessary data. To calculate $b(f)$ we

Table 2. Data for the calculation of integrals (D.26)–(D.27) (see Appendix D) in equation (3.33) in $d = 4$.

f	(D.26)	(D.27)	(D.28)	(D.29)
1	(−0.066, 0.174, −0.137)	−0.029	(0.237, −0.148, −0.019)	0.070
2	(−0.128, 0.331, −0.137)	0.066	(0.237, −0.116, −0.146)	−0.025
3	(−0.111, 0.274, −0.135)	0.028	(0.188, −0.082, −0.202)	−0.096
4	(−0.093, 0.244, −0.132)	0.019	(0.153, −0.062, −0.229)	−0.138
5	(−0.080, 0.227, −0.129)	0.018	(0.128, −0.050, −0.244)	−0.166
6	(−0.069, 0.213, −0.127)	0.017	(0.110, −0.042, −0.254)	−0.186
8	(−0.054, 0.205, −0.123)	0.028	(0.085, −0.031, −0.266)	−0.212
10	(−0.045, 0.193, −0.119)	0.029	(0.069, −0.025, −0.274)	−0.230
12	(−0.038, 0.187, −0.116)	0.033	(0.059, −0.021, −0.279)	−0.241

Table 3. Random walk results $a(1, 0, 0)$ from (2.21) and corresponding values for $b(f)$.

f	$a(1,0,0)$	$b(f)$	$a(1,0,1)$	$\left(1+\frac{3}{8}b(f)\right)\langle A_3(f)\rangle_0$
1	0.394	0.139	0.394	0.415
2	0.394	0.139	0.394	0.415
3	0.294	−0.308	0.304	0.269
4	0.230	−0.690	0.243	0.180
5	0.188	−1.050	0.201	0.122
6	0.159	−1.417	0.171	0.080
8	0.121	−2.028	0.131	0.031
10	0.098	−2.735	0.106	−0.003
12	0.082	−3.382	0.089	−0.024

also need the random walk results $a(1, 0, 0) \equiv \langle A_4\rangle_0$ from (2.21). These numbers and the ensuing values for $b(f)$ are given in table 3.

To estimate $\langle A_3\rangle \equiv a(1, \overset{*}{u}^{\mathrm{R}}, 1)$ we try to use the same extrapolation procedure as for open chains and ring polymers [19]. For that purpose we approximate the RHS of (3.32) by its first-order ε-expansion, which leads to an asymptotic asphericity approximant for EV star polymers in $d = 3$ which reads

$$\left(1+\tfrac{3}{8}b(f)\right)\langle A_3(f)\rangle_0 \tag{3.34}$$

(for the explicit numbers see again table 3).

As expected the results for $f = 1$ and $f = 2$ agree with our previous finding for open polymer chains [19]. Just as for NEV stars the equivalence of the three cases can be proved analytically for the first-order terms in the perturbation expansion.

For large values of f, however, the extrapolation (3.34) fails, since the asphericity approximant becomes negative for $f \approx 10$. This contradicts the rigorous inequality

$$A_d \geqslant 0 \tag{3.35}$$

which holds for any geometrical object [17] (see equation (1.3)) and thereby also for any mean value. On the other hand we know from section 2 that the mean asphericity for NEV stars decays like $\frac{10}{9}f^{-1}$ for large values of f. Steric repulsion should increase this decay for EV stars so that we should expect a limiting value of zero for $f \to \infty$ also in the interacting case.

The simplest approximation which yields the correct $f \to \infty$-asympotics is to use (3.32) for a systematic first-order ε-expansion of the reciprocal $a(1, 0, \varepsilon)/a(1, u^{\mathrm{R}}, \varepsilon)$. Now

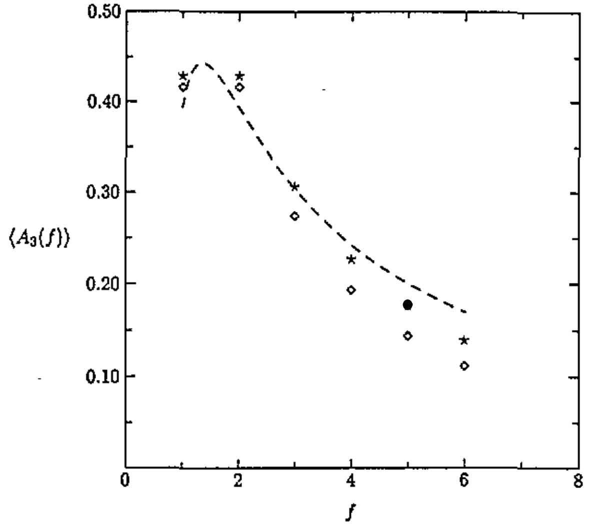

Figure 2. Asymptotic mean asphericity for EV stars (◇ ε-expansion, ⋆ Monte Carlo simulation [20], - - - exact solution for NEV stars).

Table 4. Asymptotic mean asphericity of an EV star polymer in $d = 3$ up to first order in ϵ up to $f = 6$, and Monte Carlo simulation results for $\langle A_3(f)\rangle$ and $\hat{A}_3(f)$.

	$\langle A_3(f)\rangle$		$\hat{A}_3(f)$
f	Exact	MC	MC
1	0.416...	0.429 ± 0.002	0.543 ± 0.002
2	0.416...	0.429 ± 0.002	0.543 ± 0.002
3	0.273...	0.306 ± 0.001	0.345 ± 0.003
4	0.193...	0.227 ± 0.001	0.243 ± 0.001
5	0.144...	0.177 ± 0.001	0.185 ± 0.001
6	0.112...	0.140 ± 0.001	0.146 ± 0.001

the asymptotic mean asphericity of an EV star polymer in $d = 3$ up to first order in ε is given by

$$\langle A_3(f)\rangle = \frac{1}{1 - \frac{3}{8}\, b(f)}\, \langle A_3(f)\rangle_0 . \tag{3.36}$$

In table 4 we list the numbers for values up to $f = 6$ together with the results of Monte Carlo simulations [20] for $\langle A_3(f)\rangle$ and $\hat{A}_3(f)$. Note first that the extrapolation according to (3.36) only marginally changes the asphericity value for $f = 1, 2$ compared to the results of (3.34). In figure 2 we plotted our analytical and the numerical results for $\langle A_3(f)\rangle$ for $f = 1 \ldots 6$. Additionally the exact result for NEV stars is plotted as a broken line to illustrate the influence of the EV.

For $f = 1$ and $f = 2$ we observe the same effect as for open chains, i.e. the mean asphericity is enlarged by about 5% compared to the non-interacting case. For $f \geqslant 3$, however, the corrections due to the EV have a negative sign. EV star polymers with more than three arms are more spherical than their ideal counterparts. This effect is easy to understand as the steric repulsion between the polymer arms in $d = 3$ becomes so strong with increasing f that spherical shapes are more favourable than aspherical ones.

The agreement between our ε-expansion results and the Monte Carlo data of Bishop *et al* [20] is rather good. In the computer experiment the turning point for the EV influence is found at $f = 4$. For $f = 1, 2$ the simulation yields a stronger increase of the asphericity due to the EV which is about 10% compared to the NEV case. For $f = 3$ the asphericity is found to be nearly equal for NEV and EV stars. In accordance with our analytical results, EV star polymers with $f \geqslant 4$ are found to be more spherical than non-interacting ones. Surprisingly, the corrections due to the EV are now smaller than those given by (3.36) indicating that the results of the first order in ε expansion are quantitatively reliable only for not too large values of f. To get the correct asymptotic behaviour for $f \to \infty$ one has to use different approaches, like resummations [28], which lie beyond the present straightforward perturbation expansion.

Although there are no analytical calculations for the asphericity approximant $\hat{A}_3(f)$ for EV stars, table 4 also contains corresponding simulation data [20]. Comparing these numbers with the exact solution $\hat{A}_{3,0}(f)$ for NEV stars in table 1 [22] and the results for $\langle A_3(f)\rangle_0$ and $\langle A_3(f)\rangle$, we observe the same effect which was previously found for linear polymer chains. The simplified asphericity measure (1.6) leads to larger values of the mean asphericity itself, whereas the influence of the EV is clearly underestimated. Again the reason is the neglecting of correlations between the actual size and the actual shape of the polymer coils which are correctly taken into account only in the present mean asphericity measure.

A second important conclusion can be drawn from the comparison of the asymptotic values of $\langle A_3(f)\rangle$ and $\hat{A}_3(f)$. Just as in the NEV case, the difference between these two asphericity measures decreases with increasing values of f which leads to the conclusion that shape fluctuations are suppressed for star polymers with many arms. This effect, which we already observed for NEV stars where it was purely entropic, is now increased as a result of the steric repulsion due to the EV.

4. Summary

In the present paper we investigated the asymptotic shape properties of monodisperse star polymers, consisting of f flexible chains, in dilute solution. The global shape of such polymer coils can be characterized by shape parameters which are typically ratios of characteristic lengths. We used a field-theoretic approach to calculate the mean asphericity parameter, which measures the actual deviation of a polymer coil from spherical shape, both for non-interacting star polymers and for those with excluded-volume interaction.

In the asymptotic limit of infinite molecular weight we find that the distribution functions of the shape parameters are universal functions, i.e. they do not depend on details of the chemical microstructure. They do, of course, depend on whether there are true many-body forces like the EV interaction. In particular we have calculated the first moment of the asphericity in $d = 3$ for values of f up to 6.

For NEV star polymers an exact solution for $\langle A_3(f)\rangle_0$ is obtained. For $f = 1$ and $f = 2$ we naturally find the same result which was calculated previously for linear polymer chains [18]. As f increases we observe a decrease of the mean asphericity, i.e. star polymers with high functionality are typically more spherical than linear chains and those with few arms. Our estimates are in excellent agreement with the findings of previous Monte Carlo simulations [20].

For EV star polymers we set up an RG improved perturbation expansion to calculate an estimate for $\langle A_3(f)\rangle$ in the asymptotic limit. For $f = 1$ and $f = 2$ our first order in ε results are also in agreement with those of previous calculations for linear polymer chains [19]. Here the mean asphericity was increased by about $5\frac{1}{2}$% by the EV. For $f \geqslant 3$, however, the interaction favours more spherical shapes, which is intuitively appealing because of the strong repulsion between the polymer arms caused by the EV for large values of f when the space dimension is low. Our results are in good agreement with the data of corresponding Monte Carlo simulations [20]. Surprisingly, the negative corrections of the mean asphericity which we observe for $f \geqslant 3$ are larger than those obtained in the computer experiment, indicating that the present perturbation theory is valid only for not too large values of f.

Comparing our findings for the mean asphericity $\langle A_d(f)\rangle$ with the results which were calculated for a simplified asphericity approximant $\hat{A}_d(f)$ we can draw a few important conclusions. For small values of f the results for $\langle A_d(f)\rangle$ and $\hat{A}_d(f)$ differ significantly, which holds for both NEV and EV star polymers. As the definition of $\hat{A}_d(f)$ neglects important correlations between the actual linear size and the actual asymmetry of the polymer coils, this shows that there are strong shape fluctuations when the number of arms f is not too large. With increasing values of f these fluctuations are damped, which follows from the decreasing difference between $\langle A_d(f)\rangle$ and $\hat{A}_d(f)$. For NEV star polymers this effect is purely entropic. For interacting star polymers this trend is even stronger due to the steric repulsion between the polymer arms caused by the EV.

A last remark concerns the different results for $\langle A_d(f)\rangle$ and $\hat{A}_d(f)$ when the influence of the EV on the shape asymptotics is investigated. Here our results corroborate previous findings from computer simulations [20, 21], stating that the asphericity approximant $\hat{A}_d(f)$ overestimates the absolute value of the asphericity, whereas the corrections due to the EV come out too small. This is in line with a heuristic argument given by Cannon *et al* [21] which implies that the definition of $\hat{A}_d(f)$ enlarges the influence of expanded polymer configurations compared to that of compact ones. Accordingly the absolute value of the mean asphericity comes out too large, whereas the influence of the EV is artificially suppressed as the interaction plays a minor role for expanded structures.

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Appendix A. Diagonalization of $h_{0,y}$

The orthogonal transformation to diagonalize (2.7) proceeds in two steps. First we define a transformation with respect to the segment index i and introduce coordinates

$$\Xi_\nu^{(a)} = \sum_{i=1}^{N} \varphi_\nu(i)\, X_i^{(a)} . \tag{A.1}$$

The transformation matrix $\varphi_\nu(i)$ is given by the Rouse modes of a single Gaussian chain which read

$$\varphi_0(i) = \sqrt{\frac{1}{N}} \tag{A.2}$$

$$\varphi_\nu(i) = \sqrt{\frac{2}{N}} \cos\left[\frac{\pi\nu}{N}\left(i - \frac{1}{2}\right)\right] \qquad \nu = 1, \ldots, N-1 . \tag{A.3}$$

Now, (2.7) takes the form

$$h_{0,y}\{\Xi_\nu^{(a)}\} = \sum_{\nu=0}^{N-1}\sum_{a=1}^{f}\varepsilon_\nu(y)\,|\Xi_\nu^{(a)}|^2 - \frac{y}{f^2N}\sum_{a,b=1}^{f}\Xi_0^{*(a)}\,\Xi_0^{(b)} \tag{A.4}$$

where the mode energies for $\nu \neq 0$ are given by

$$\varepsilon_\nu(y) = \ell^{-2}\sin^2\left(\frac{\pi\nu}{2N}\right) + \frac{y}{fN}. \tag{A.5}$$

To decouple the $\Xi_0^{(a)}$-modes we use a second transformation with respect to the arm index a

$$\xi_\nu^{(t)} = \sum_{a=1}^{f} U_{t,a}\,\Xi_\nu^{(a)} \qquad t = 0, 1, \ldots, f-1 \tag{A.6}$$

where

$$\mathbf{U} = \begin{pmatrix} 1/\sqrt{f} & 1/\sqrt{f} & \cdots & 1/\sqrt{f} \\ u_1^{(1)} & u_2^{(1)} & \cdots & u_f^{(1)} \\ \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ u_1^{(f-1)} & u_2^{(f-1)} & \cdots & u_f^{(f-1)} \end{pmatrix}. \tag{A.7}$$

Note that

$$\sum_{a=1}^{f} u_a^{(t)} u_a^{(t')} = \delta_{tt'} \qquad t, t' \geqslant 1 \tag{A.8}$$

and

$$\sum_{a=1}^{f} u_a^{(t)} = 0 \qquad t \geqslant 1 \tag{A.9}$$

guarantee (A.7) to be an orthogonal transformation, too. The explicit form of $u_a^{(t)}$ is not important since (2.7) is invariant under permutations of the polymer arms. Substituting (A.6) into (A.4) we get the final form (2.9), which is diagonal both in ν and t.

Appendix B. $\langle e^{-y\,\mathrm{tr}\,Q}\rangle_0$ and free propagator $G(a, b; t, t')$

According to equation (2.6), $\langle e^{-y\,\mathrm{tr}\,Q}\rangle_0$ can be expressed as the ratio of two partition integrals

$$\langle e^{-y\,\mathrm{tr}\,Q}\rangle_0 = \frac{\prod_{i,a=1}^{N,f}\int \mathrm{d}\boldsymbol{R}_i^{(a)}\,\delta^d(\boldsymbol{R}_1^{(a)})\,e^{-\mathcal{H}_0 - y\,\mathrm{tr}\,Q}}{\prod_{i,a=1}^{N,f}\int \mathrm{d}\boldsymbol{R}_i^{(a)}\,\delta^d(\boldsymbol{R}_1^{(a)})\,e^{-\mathcal{H}_0}} = \left[\frac{\prod_{i,a=1}^{N,f}\int_{-\infty}^{\infty}\mathrm{d}X_i^{(a)}\,\delta(X_1^{(a)})\,e^{-h_{0,y}}}{\prod_{i,a=1}^{N,f}\int_{-\infty}^{\infty}\mathrm{d}X_i^{(a)}\,\delta(X_1^{(a)})\,e^{-h_{0,y=0}}}\right]^d. \tag{B.1}$$

In the following we calculate the numerator of (B.1), the ensuing average follows (up to the exponent d) after dividing by the same expression at $y = 0$. Introducing $\xi_\nu^{(t)}$ as new integration variables we get

$$\prod_{\nu,t=0}^{N-1,f-1} \int_{-\infty}^{\infty} \mathrm{d}\xi_\nu^{(t)} \exp\left[- \sum_{\nu,t=0}^{N-1,f-1} (1-\delta_{\nu 0}\delta_{t0})\, \varepsilon_\nu(y) |\xi_\nu^{(t)}|^2 \right] \times \prod_{a=1}^{f} \left(\int_{-\infty}^{\infty} \frac{\mathrm{d}k_a}{2\pi} \exp\left[\mathrm{i}k_a \sum_{\nu,t=0}^{N-1,f-1} \varphi_\nu(1)\, U_{t,a}\, \xi_\nu^{(t)} \right] \right) \tag{B.2}$$

where we expressed the Delta function by its Fourier transform. We can now easily integrate over the massless coordinate $\xi_0^{(0)}$

$$\int_{-\infty}^{\infty} \mathrm{d}\xi_0^{(0)} \exp\left[\mathrm{i} \sum_{a=1}^{f} k_a\, \varphi_0(1)\, U_{0,a}\, \xi_0^{(0)} \right] = 2\pi\, \delta\big(k_1\, \varphi_0(1)\, U_{0,1} + \sum_{a=2}^{f} k_a\, \varphi_0(1)\, U_{0,a}\big) \tag{B.3}$$

and afterwards also over k_1 respecting $\varphi_0(1) = 1/\sqrt{N}$ and $U_{0,a} = 1/\sqrt{f}$, which results in

$$\sqrt{fN} \prod_{a=2}^{f} \int_{-\infty}^{\infty} \frac{\mathrm{d}k_a}{2\pi} \prod_{\nu,t=0}^{N-1,f-1} \int_{-\infty}^{\infty} \mathrm{d}\xi_\nu^{(t)}\ (1-\delta_{\nu 0}\delta_{t0}) \times \exp\left[- \sum_{\nu,t=0}^{N-1,f-1} (1-\delta_{\nu 0}\delta_{t0}) \left(\varepsilon_\nu(y) |\xi_\nu^{(t)}|^2 + \mathrm{i}A_\nu^{(t)}(\{k_a\})\, \xi_\nu^{(t)} \right) \right] \tag{B.4}$$

where

$$A_\nu^{(t)}(\{k_a\}) = \varphi_\nu(1) \sum_{a=2}^{f} k_a \left(U_{t,1} - U_{t,a} \right) . \tag{B.5}$$

Now, all remaining integrations over $\xi_\nu^{(t)}$ can easily be carried out and we arrive at

$$\sqrt{fN} \prod_{a=2}^{f} \int_{-\infty}^{\infty} \frac{\mathrm{d}k_a}{2\pi} \left[\sqrt{\frac{\pi}{\varepsilon_0(y)}} \right]^{f-1} \exp\left[-\frac{1}{4\varepsilon_0(y)} \sum_{t=1}^{f-1} \left(A_0^{(t)}(\{k_a\}) \right)^2 \right] \times \prod_{\nu=1}^{N-1} \left[\sqrt{\frac{\pi}{\varepsilon_\nu(y)}} \right]^{f} \exp\left[-\frac{1}{4\varepsilon_\nu(y)} \sum_{t=0}^{f-1} \left(A_\nu^{(t)}(\{k_a\}) \right)^2 \right] . \tag{B.6}$$

Using (A.8) and (A.9) both exponents in (B.6) can be transformed into

$$-\frac{1}{4} \frac{(\varphi_\nu(1))^2}{\varepsilon_\nu(y)} \left[\left(\sum_{a=2}^{f} k_a \right)^2 + \sum_{a=2}^{f} k_a^2 \right] \qquad \nu = 0, \ldots, N-1 \tag{B.7}$$

so that a simple rescaling yields

$$2^{f-1} \sqrt{fN} \left[\sqrt{\frac{\pi}{\varepsilon_0(y)}} \right]^{f-1} \prod_{\nu=1}^{N-1} \left[\sqrt{\frac{\pi}{\varepsilon_\nu(y)}} \right]^{f} \left[\sqrt{\sum_{\nu=0}^{N-1} \frac{(\varphi_\nu(1))^2}{\varepsilon_\nu(y)}} \right]^{1-f} \times \prod_{a=2}^{f} \int_{-\infty}^{\infty} \frac{\mathrm{d}\tilde{k}_a}{2\pi} \exp\left[-\left(\sum_{a=2}^{f} \tilde{k}_a \right)^2 - \sum_{a=2}^{f} \tilde{k}_a^2 \right] . \tag{B.8}$$

The $(f-1)$-fold k-integral gives $(2\sqrt{\pi})^{1-f}/\sqrt{f}$ resulting in

$$\sqrt{N}\left(\sqrt{\varepsilon_0(y)}\right)^{1-f}\prod_{\nu=1}^{N-1}\left[\sqrt{\frac{\pi}{\varepsilon_\nu(y)}}\right]^f\left[\sqrt{\sum_{\nu=0}^{N-1}\frac{(\varphi_\nu(1))^2}{\varepsilon_\nu(y)}}\right]^{1-f} \tag{B.9}$$

for the numerator in (B.1). Dividing by the same expression at $y=0$ we immediately arrive at (2.11) (up to the trivial exponent d) and at (2.14) in the continuum limit, respectively.

Similarly the calculation of the propagator

$$\left\langle X_j^{(a)}X_k^{(b)}\right\rangle_{0,y}=\sum_{\nu,\nu'=0}^{N-1}\sum_{t,t'=0}^{f-1}\varphi_\nu(j)\varphi_{\nu'}(k)U_{t,a}U_{t',b}\left\langle\xi_\nu^{(t)}\xi_{\nu'}^{(t')}\right\rangle_{0,y} \tag{B.10}$$

(with discrete segment indices) can be traced back to the correlation function of normal coordinates which leads to a normalization factor to the expression

$$\sqrt{fN}\prod_{a=2}^{f}\int_{-\infty}^{\infty}\frac{\mathrm{d}k_a}{2\pi}\prod_{\bar\nu,\bar t=0}^{N-1,f-1}\int_{-\infty}^{\infty}\mathrm{d}\xi_{\bar\nu}^{(\bar t)}\,(1-\delta_{\bar\nu 0}\delta_{\bar t 0})\,\xi_\nu^{(t)}\xi_{\nu'}^{(t')}$$
$$\times\exp\left[-\sum_{\bar\nu,\bar t=0}^{N-1,f-1}(1-\delta_{\bar\nu 0}\delta_{\bar t 0})\left(\varepsilon_{\bar\nu}(y)|\xi_{\bar\nu}^{(\bar t)}|^2+\mathrm{i}A_{\bar\nu}^{(\bar t)}(\{k_a\})\,\xi_{\bar\nu}^{(\bar t)}\right)\right]. \tag{B.11}$$

Analogously to the previous manipulation, it can easily be shown that a non-vanishing contribution to (B.10) only comes from $t=t'$

$$\left\langle\xi_\nu^{(t)}\xi_{\nu'}^{(t')}\right\rangle_{0,y}=\delta_{\nu\nu'}\delta_{tt'}\frac{1}{2\varepsilon_\nu(y)}-\frac{1}{2}\delta_{tt'}\,(1-\delta_{t0})\,\frac{\varphi_\nu(1)\varphi_{\nu'}(1)}{\varepsilon_\nu(y)\varepsilon_{\nu'}(y)}\frac{1}{R} \tag{B.12}$$

where

$$R=\sum_{\bar\nu=0}^{N-1}\frac{(\varphi_{\bar\nu}(1))^2}{\varepsilon_{\bar\nu}(y)}. \tag{B.13}$$

Note the restrictions for t and t' in (B.12), which are consequences of the permutation symmetry of the polymer arms. Substituting (B.12) into (B.10), this directly implies the special structure of the propagator and we arrive at (2.19) in the continuum limit.

Appendix C. Generalized star partition functions and renormalization

The reparametrizations (3.5), (3.6) can be deduced from those of generalized star partition functions, while their reparametrizations are related to those of special composite operators in field theory.

Consider a generalized star partition function defined as the continuum limit of

$$\frac{\mathrm{Tr}\,\mathrm{e}^{-\mathcal{H}}\prod_{a=1}^{f}\delta^d(\boldsymbol{R}_1^{(a)}-\boldsymbol{r})\prod_{b=1}^{f}\delta^d(\boldsymbol{R}_1^{(b)}-\boldsymbol{r}'_b)\,m(\boldsymbol{r}_1)\ldots m(\boldsymbol{r}_M)}{\mathrm{Tr}\,\mathrm{e}^{-\mathcal{H}_0}\,\delta^d(\boldsymbol{R}_1^{(1)})\ldots\delta^d(\boldsymbol{R}_1^{(f)})}$$
$$\to\mathcal{Z}_M\left(\boldsymbol{r},\boldsymbol{r}'_1,\ldots,\boldsymbol{r}'_f;\boldsymbol{r}_1,\ldots,\boldsymbol{r}_M;L,u\right). \tag{C.1}$$

Note that the first segments of all chains are fixed at $\boldsymbol{r}$, whereas the end segments are fixed at different space positions $\boldsymbol{r}'_b$. The segment density operator is given by

$$m(\boldsymbol{r}) = \ell^2 \sum_{a=1}^{f} \sum_{j=1}^{N} \delta^d\left(\boldsymbol{R}_j^{(a)} - \boldsymbol{r}\right) \tag{C.2}$$

and Tr denotes the integrations

$$\mathrm{Tr} \equiv \prod_{a=1}^{f} \prod_{j=1}^{N} \int_{-\infty}^{\infty} \mathrm{d}^d R_j^{(a)} . \tag{C.3}$$

Equation (C.1) allows us to cast the average of any product of radius of gyration tensor components in the form

$$\begin{aligned}\left\langle \mathcal{Q}_{\alpha_1\beta_1} \cdots \mathcal{Q}_{\alpha_s\beta_s} \right\rangle = \tfrac{1}{2} \int_{-\infty}^{\infty} \mathrm{d}^d r_1 \mathrm{d}^d r'_1 \left(\boldsymbol{r}_1 - \boldsymbol{r}'_1\right)_{\alpha_1} \left(\boldsymbol{r}_1 - \boldsymbol{r}'_1\right)_{\beta_1} \cdots \\ \cdots \tfrac{1}{2} \int_{-\infty}^{\infty} \mathrm{d}^d r_s \mathrm{d}^d r'_s \left(\boldsymbol{r}_s - \boldsymbol{r}'_s\right)_{\alpha_s} \left(\boldsymbol{r}_s - \boldsymbol{r}'_s\right)_{\beta_s} \mathcal{F}_{2s}\end{aligned} \tag{C.4}$$

where

$$\mathcal{F}_{2s} = \frac{1}{L^{2s}} \frac{\displaystyle\int_{-\infty}^{\infty} \mathrm{d}^d r'_1 \ldots \mathrm{d}^d r'_f \, \mathcal{Z}_M\left(\boldsymbol{r}, \boldsymbol{r}'_1, \ldots, \boldsymbol{r}'_f; \boldsymbol{r}_1, \ldots, \boldsymbol{r}_M; L, u\right)}{\displaystyle\int_{-\infty}^{\infty} \mathrm{d}^d r'_1 \ldots \mathrm{d}^d r'_f \, \mathcal{Z}_M\left(\boldsymbol{r}, \boldsymbol{r}'_1, \ldots, \boldsymbol{r}'_f; L, u\right)} . \tag{C.5}$$

Now, the reparametrization of $\mathcal{Z}_M$ can be inferred from the reparametrization of the composite operator [8]

$$\left\langle \left[\prod_{a=1}^{f} \phi_1^{(a)}(\boldsymbol{r})\right] \phi_1^{(1)}(\boldsymbol{r}'_1) \ldots \phi_1^{(f)}(\boldsymbol{r}'_f) [\phi_1^{(a_1)}(\boldsymbol{r}_1)]^2 \ldots [\phi_1^{(a_M)}(\boldsymbol{r}_M)]^2 \right\rangle_{t_1,\ldots,t_f,u,h=0} . \tag{C.6}$$

Here $\phi_1^{(a)}(\boldsymbol{r})$ denotes the first component of a field $\phi^{(a)}(\boldsymbol{r})$ from a set of f n-component fields $\phi^{(1)}(\boldsymbol{r}), \ldots, \phi^{(f)}(\boldsymbol{r})$. The operator $\left[\prod_{a=1}^{f} \phi_1^{(a)}(\boldsymbol{r})\right]$ requires a Z-factor of the form $(Z_\phi)^{f/2}(Z_{*f})^{-1}$, where Z_{*f} denotes a special renormalization factor of the f-star vertex [8]. An f-fold Laplace transformation of (C.6), which gives an additional factor $(\mu^2 Z_t)^{-f}$, then leads to the reparametrization for (C.1)

$$\begin{aligned}\mathcal{Z}_M\left(\boldsymbol{r}, \boldsymbol{r}'_1, \ldots, \boldsymbol{r}'_f; \boldsymbol{r}_1, \ldots, \boldsymbol{r}_M; L, u\right) = \left(\mu^{4-\varepsilon}\right)^f \mu^{M(2-\varepsilon)} \left(Z_\phi\right)^f \left(Z_t\right)^{f-M} \left(Z_{*f}\right)^{-1} \\ \times \mathcal{Z}_M^{\mathrm{R}}\left(\mu \boldsymbol{r}, \mu \boldsymbol{r}'_1, \ldots, \mu \boldsymbol{r}'_f; \mu \boldsymbol{r}_1, \ldots, \mu \boldsymbol{r}_M; L^{\mathrm{R}}, u^{\mathrm{R}}\right) .\end{aligned} \tag{C.7}$$

Substituting (C.7) in (C.5), Z_{*f} and the Z_ϕ-factors drop out and we arrive at

$$\mathcal{F}_{2s} \equiv \mu^{2sd} \mathcal{F}_{2s}^{\mathrm{R}}\left(\mu \boldsymbol{r}_1, \ldots, \mu \boldsymbol{r}'_s; L^{\mathrm{R}}, u^{\mathrm{R}}\right) \tag{C.8}$$

with

$$\mathcal{F}^{\mathrm{R}}_{2s}(\mu r_1,\ldots,\mu r'_s;L^{\mathrm{R}},u^{\mathrm{R}}) = \frac{1}{(L^{\mathrm{R}})^{2s}} \frac{\int_{-\infty}^{\infty} \mathrm{d}^d(\mu r'_1)\ldots\mathrm{d}^d(\mu r'_f)\; \mathcal{Z}^{\mathrm{R}}_{2s}(\mu r,\mu r'_1,\ldots,\mu r'_f;\mu r_1,\ldots,\mu r'_s;L^{\mathrm{R}},u^{\mathrm{R}})}{\int_{-\infty}^{\infty} \mathrm{d}^d(\mu r'_1)\ldots\mathrm{d}^d(\mu r'_f)\; \mathcal{Z}^{\mathrm{R}}(\mu r,\mu r'_1,\ldots,\mu r'_f;L^{\mathrm{R}},u^{\mathrm{R}})} \tag{C.9}$$

where the remaining Z_t-factors have been absorbed in the reparametrization of L.

Since each $\mathcal{Z}^{\mathrm{R}}_M$ is a function of L^{R}, u^{R} and (distribution in) the various (μr)-arguments, which is finite for $\varepsilon \to 0$, the same property holds for $\mathcal{F}^{\mathrm{R}}_{2s}$. Applying (C.4) and (C.8) to the Taylor expansion in y of $\langle \mathrm{tr}\,(\hat{Q}^2)\rangle_y$ and $\langle \mathrm{e}^{-y\,\mathrm{tr}\,Q}\rangle$ leads to equations (3.5) and (3.6) in the main text.

Appendix D. Numerical results of the ε-expansion

To calculate the contributions $\propto u\varepsilon^{-1}$ and $u\varepsilon^0$ to (3.24) and (3.26) we have used an obvious strategy which we briefly explain for the simple term $\langle \mathrm{e}^{-y\,\mathrm{tr}\,Q}\rangle_1$. According to (3.25) the dimensionless integrand I in

$$\sum_{a,b=1}^{f} \left\{\left[S_y^{(a,b)}(t,t')\right]^{-2+\varepsilon/2} - \left[S_0^{(a,b)}(t,t')\right]^{-2+\varepsilon/2}\right\} \equiv L^{-2+\varepsilon/2}\, I \tag{D.1}$$

contains a singular part $\propto |t-t'|^{-1+\varepsilon}$ which is non-integrable for $\varepsilon = 0$. To calculate the contributions $\propto \varepsilon^{-1}$ and ε^0 to the ensuing (dimensionless) integral

$$J = L^{-2}\int_0^L \mathrm{d}t\,\mathrm{d}t'\, I \tag{D.2}$$

we used (3.25) together with the definition of the propagator (2.19) to get the singular part of I

$$I_{\mathrm{s}} = |\tau|^{-1+\varepsilon/2}\left(2-\frac{\varepsilon}{2}\right)\frac{\beta}{2}\left[\frac{\cosh\beta-\cosh[\beta(1-T)]}{\sinh\beta} + (f-1)\frac{\sinh\beta+\sinh[\beta(1-T)]}{\cosh\beta}\right] \tag{D.3}$$

where we have introduced suitable coordinates

$$\tau = \frac{t'-t}{L} \qquad T = \frac{t'+t}{L}. \tag{D.4}$$

Now, the integral J can be split into

$$J = J_{\mathrm{s}} + \Delta J + \mathrm{O}(\varepsilon) \tag{D.5}$$

where

$$J_{\mathrm{s}} = L^{-2} \int_0^L \mathrm{d}t\, \mathrm{d}t'\, I_{\mathrm{s}} \tag{D.6}$$

$$\Delta J = L^{-2} \int_0^L \mathrm{d}t\, \mathrm{d}t' \left(I - I_{\mathrm{s}}\right)_{\varepsilon=0}. \tag{D.7}$$

Here J_{s} contains orders ε^{-1}, ε^{0} etc whereas ΔJ is integrable in $d = 4$ and of order ε^0. Both integrands in (D.6) and (D.7) are invariant under the substitution $(t, t') \to (t', t)$ so that (D.2) can be cast in the form

$$J_{(\mathrm{s})} = \left(\int_0^1 \mathrm{d}T \int_0^T \mathrm{d}\tau + \int_1^2 \mathrm{d}T \int_0^{2-T} \mathrm{d}\tau \right) I_{(\mathrm{s})} \tag{D.8}$$

where we have introduced (T, τ) as new integration variables. Substituting (D.3) into (D.8) one finds explicitly

$$J_{\mathrm{s}} = \frac{4}{\varepsilon}(\beta \coth\beta - 1) + \frac{4}{\varepsilon}(f-1)\beta\tanh\beta + 1 - 3\beta\coth\beta - 3(f-1)\beta\tanh\beta - 2j + \mathrm{O}(\varepsilon) \tag{D.9}$$

with

$$j = \frac{\beta}{\sinh\beta} \int_0^1 \mathrm{d}T\, \ln T\, \cosh\left[\beta(1-T)\right]. \tag{D.10}$$

In order to calculate the first order in u^{R} expression $F_{2;1}$ of the renormalized quantity F_2 in (3.6) one has to take into account the reparametrizations (3.3), (3.4), (3.7) and (3.8). This implies

$$u^{\mathrm{R}} F_{2;1}\left(L^{\mathrm{R}}, x, \varepsilon\right) = u^{\mathrm{R}} \left\{ -\frac{1}{\varepsilon}\frac{\beta}{3} \left(\frac{\mathrm{d}}{\mathrm{d}\beta} \langle \mathrm{e}^{-y\,\mathrm{tr}\,Q} \rangle_0 \right) - \langle \mathrm{e}^{-y\,\mathrm{tr}\,Q} \rangle_0 \frac{1}{6} \left(4\pi L^{\mathrm{R}}\right)^{\varepsilon/2} J \right\}_{\beta\to\beta^{\mathrm{R}}} \tag{D.11}$$

with

$$\beta^{\mathrm{R}} = 2\sqrt{\frac{xL^{\mathrm{R}}}{f}}. \tag{D.12}$$

The first term on the RHS arises from the zero-order contribution $\langle \mathrm{e}^{-y\,\mathrm{tr}\,Q} \rangle_0$, when L is replaced by L^{R}, and contains a part $\propto u^{\mathrm{R}}\varepsilon^{-1}L^{\mathrm{R}}$. Inserting the explicit expressions for $\langle \mathrm{e}^{-y\,\mathrm{tr}\,Q} \rangle_0$ and J_{s} into (D.11) one realizes that the ε-poles are indeed cancelled by the reparametrizations (3.3) and (3.4). For the ε^0 contribution to $F_{2;1}$ one finds

$$u^{\mathrm{R}} F_{2;1}\left(L^{\mathrm{R}}, x, 0\right) = \frac{u^{\mathrm{R}}}{3} \left\{ (\cosh\beta)^{2(1-f)} \left[\frac{\beta}{\sinh\beta}\right]^2 \times \left[(-1+2\alpha)\big(1 - \beta\coth\beta - (f-1)\beta\tanh\beta\big) + 1 + j - \frac{1}{2}\Delta J \right] \right\}_{\beta\to\beta^{\mathrm{R}}} \tag{D.13}$$

where

$$\alpha = \ln\left(2\sqrt{\pi}\right) + \tfrac{1}{2}\ln L^{\mathrm{R}}\,. \tag{D.14}$$

We note, for completeness, that the zero order in u^{R} contribution $F_{2;0}(L^{\mathrm{R}}, x, \varepsilon)$ to F_2 is, of course, given by (2.14) with β replaced by β^{R}.

The calculation of the second contribution $\langle \operatorname{tr}(\hat{Q}^2)\rangle_{1,y}$ proceeds along the same lines so that we restrict ourselves to some remarks. As $T_y^{(a,a';c,c')}(t_i, t_i'; t, t') \propto |t - t'|$ for $t \to t'$, only the first term in the sum in (3.26) contains a singular part $\propto \varepsilon^{-1}$, whereas the second one is integrable for $\varepsilon = 0$. For the first term the dimensionless integral of interest is given by

$$K = L^{-6}\int \mathrm{d}\theta\, H \tag{D.15}$$

with

$$\begin{aligned} H = f^{-4}L^{-\varepsilon/2} \sum_{a,a',b,b',c,c'=1}^{f} \left[S_y^{(c,c')}(t,t')\right]^{-3+\varepsilon/2} T_y^{(a,a';c,c')}(t_1, t_1'; t, t') \\ \times T_y^{(b,b';c,c')}(t_2, t_2'; t, t')\, T_y^{(a,a';b,b')}(t_1, t_1'; t_2, t_2')\,. \end{aligned} \tag{D.16}$$

Again we can split this integral into

$$K = K_{\mathrm{s}} + \Delta K + \mathrm{O}(\varepsilon) \tag{D.17}$$

where

$$K_{\mathrm{s}} = \int \mathrm{d}\eta\, L^{-2}\int_0^L \mathrm{d}t\,\mathrm{d}t'\, H_{\mathrm{s}} \tag{D.18}$$

and

$$\int \mathrm{d}\eta = L^{-4}\int_0^L \mathrm{d}t_1\,\mathrm{d}t_1'\,\mathrm{d}t_2\,\mathrm{d}t_2'\,. \tag{D.19}$$

The difference ΔK is integrable for $\varepsilon = 0$ and reads

$$\Delta K = L^{-6}\int \mathrm{d}\theta\,\left(H - H_{\mathrm{s}}\right)_{\varepsilon=0}\,. \tag{D.20}$$

Just the same as in (D.6), K_{s} is of the form

$$K_{\mathrm{s}} = \frac{1}{\varepsilon}K_{s,-1} + K_{s,0} + \mathrm{O}(\varepsilon) \tag{D.21}$$

which follows from inserting

$$H_{\mathrm{s}} = |\tau|^{-1+\varepsilon/2}\, h(t_1, t_1'; t_2, t_2') \tag{D.22}$$

into (D.18). Due to the complicated form of (D.16) we do not give the explicit function $h(t_1, t_1'; t_2, t_2')$ which is, of course, simple but lengthy.

The second term in $\langle \mathrm{tr}\,(\hat{Q}^2)\rangle_{1,y}$ is finite in $d = 4$ and reads

$$P = -\tfrac{1}{4} f^{-4} L^{-6} \int \mathrm{d}\theta \sum_{a,a',b,b',c,c'=1}^{f} \left[S_y^{(c,c')}(t,t')\right]^{-4} \left[T_y^{(a,a';c,c')}(t_1,t_1';t,t')\right]^2 \times \left[T_y^{(b,b';c,c')}(t_2,t_2';t,t')\right]^2 . \tag{D.23}$$

The pole cancellation in the u^{R} contribution $F_{1;1}$ to F_1 now follows analogously, as for $F_{2;1}$, involving lengthy arithmetic which we will not present here in detail. For the ε^0 contribution we then find

$$u^{\mathrm{R}} F_{1;1}\left(L^{\mathrm{R}}, x, 0\right) = u^{\mathrm{R}} \left(L^{\mathrm{R}}\right)^2 \tfrac{3}{4} \{\alpha K_{s,-1} + K_{s,0} + \Delta K + P\}_{\beta\to\beta^{\mathrm{R}}} . \tag{D.24}$$

For the evaluation of the final results it is important to notice that the α factor in (D.13) and (D.24) drops out from $b(f)$ in (3.33). Without giving details we note that this is a direct consequence of the pole cancellation discussed above. Accordingly we will set $\alpha = 0$ in the following.

To evaluate $b(f)$, the x-integral, as well as the integrals defining the quantities ΔJ, j, $K_{s,-1}$, $K_{s,0}$, ΔK and P, have been performed numerically. Here we have used

$$\mathrm{d}x\, x \left(L^{\mathrm{R}}\right)^2 = \mathrm{d}\beta^{\mathrm{R}} \tfrac{1}{8} \left(\beta^{\mathrm{R}}\right)^3 \tag{D.25}$$

and the abbreviation $F_{i;j,0} = F_{i;j}(L^{\mathrm{R}}, x, 0)$. Explicitly we have calculated the integrals

$$\int_0^\infty \mathrm{d}x\, x \left(L^{\mathrm{R}}\right)^2 \frac{3}{4} \left\{K_{s,0},\ \Delta K,\ P\right\}_{\beta\to\beta^{\mathrm{R}}} F_{2;0,0} \tag{D.26}$$

with their sum

$$\int_0^\infty \mathrm{d}x\, x \left(F_{1;1,0}\right)_{\alpha=0} F_{2;0,0} \tag{D.27}$$

and

$$\int_0^\infty \mathrm{d}x\, x\, F_{1;0,0} \frac{1}{3} \left\{ (\cosh\beta)^{2(1-f)} \left[\frac{\beta}{\sinh\beta}\right]^2 \left[\beta \coth\beta + (f-1)\beta\tanh\beta,\ j,\ -\frac{1}{2}\Delta J\right]\right\}_{\beta\to\beta^{\mathrm{R}}} \tag{D.28}$$

giving

$$\int_0^\infty \mathrm{d}x\, x\, F_{1;0,0} \left(F_{2;1,0}\right)_{\alpha=0} \tag{D.29}$$

(for the explicit numbers see table 2).

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