General two-point correlation functions for ring polymers using renormalisation group techniques

B Schaub and B Schmittmann

Institut für Theoretische Physik III, Universität Düsseldorf, D-4000 Düsseldorf, Federal Republic of Germany.

Abstract. General time-dependent two-point correlation functions for simple ring polymers in the presence of both self-avoiding and hydrodynamic interactions are calculated to $O(\varepsilon)$ ($\varepsilon \equiv 4 - d$, d being the spatial dimensionality) using renormalisation group techniques. Results are presented in universal functional form to $O(\varepsilon)$.

Renormalisation group (RG) ideas have been of outstanding importance in the modern development of the statistical mechanics of systems which are close to a critical point. In particular, the powerful ε expansion provides one of the most reliable methods to determine critical exponents and scaling functions. It allows the analytic calculation of universal properties by means of a systematic expansion in powers of $\varepsilon = d_c - d$ around the upper critical dimension d_c.

This technique has been successfully applied to study universal properties of flexible polymer chains which possess a critical point if the chain length N tends to infinity. While many static universal properties could be studied using the rather formal polymer magnet analogy [1], i.e. by using scalar field theories in which the number of components n has to be analytically continued to $n = 0$, it has not been possible so far to investigate dynamical properties within this approach. Therefore, in order to overcome this obstacle, another technique [2], based upon a more intuitive statistical mechanics description of a flexible polymer chain [3], has been devised. Within this new technique, denoted as conformation space RG, many static properties of both dilute and semidilute solutions have been studied in great detail [4]. Quantitative calculations for time-dependent properties have also been performed in this scheme, but only quite recently. Quantities of central interest among the transport properties of dilute polymer solutions are the diffusion constant [5], time-dependent correlation functions [6], relaxational spectra [7], the dynamic scattering factor [8, 9] and most importantly the intrinsic viscosity [10-12].

The minimal model (defined below) which has been studied within the RG framework yields many universal predictions for transport properties, which can be compared with experiment. These predictions, which have mainly been derived for flexible *linear* chains can also be investigated for flexible simple (single) ring polymers, another class of experimentally interesting systems. In particular, comparison of transport properties of linear and ring polymers will enable one to answer the question of how ring formation will affect universal properties of flexible (Gaussian) polymer chains. We have recently [13] investigated explicitly time-dependent correlations for

a simple ring polymer in the presence of hydrodynamic interactions, and have extracted the translational diffusion constant and the relaxational spectrum. Further we presented the scaling function in universal form to $O(\varepsilon)$.

In this paper we will extend our previous study by also taking into account self-avoiding interactions to $O(\varepsilon)$. Furthermore, we will derive the *most general* two-point correlation function of a simple ring polymer in the presence of both self-avoiding and hydrodynamic interactions in universal form to $O(\varepsilon)$. Before presenting any details, let us stress a remarkable property of such ring structures. In order to model a simple ring, we will consider a free (Gaussian) random walk subjected to periodic boundary conditions. This provides a simple example of a non-Markovian but Gaussian process. The correlation and Green functions for this process reflect this circularity condition. In the subsequent expansion in powers of the self-avoiding and hydrodynamic couplings around the free theory corresponding to the Gaussian random walk many terms vanish because of this internal symmetry. As a consequence, we find that all two-point correlation functions calculated to one-loop order have essentially the same form as the corresponding free correlation functions, apart from a modified relaxational spectrum, a modified diffusion constant and a modified dependence on the renormalised chain length N (in the presence of self-avoiding interactions). The starting point of our investigation is the following set of Langevin equations describing coupled chain solvent dynamics [14]:

$$\frac{\partial c}{\partial t} = -\frac{1}{\zeta_0}\frac{\delta H_E}{\delta c(\tau, t)} + g_0 u(c(\tau, t), t) + \theta(\tau, t) \tag{1a}$$

$$\frac{\partial u}{\partial t} = \eta_0 \Delta u(x, t) - g_0 \int_0^{N_0} d\tau \frac{\delta H_E}{\delta c(\tau, t)} \delta(x - c(\tau, t)) - \nabla p + f(x, t) \tag{1b}$$

together with the incompressibility condition $\nabla \cdot u = 0$. In $(1a, b)$, $\{c(\tau, t)\}_{\tau=0}^{N_0}$ describes the conformation of a polymer with bare chain length N_0 parametrised by a contour variable τ at time t. $\zeta_0 \equiv \lambda_0^{-1}$ is the bare translational friction constant per chain unit, g_0 is the strength of the hydrodynamic interaction (the coupling to the solvent velocity field), $u(x, t)$ describes the solvent velocity field, η_0 is the bare solvent viscosity, Δ is the Laplacian and p denotes the pressure. H_E is the Edwards Hamiltonian [3]

$$H_E = \frac{1}{2}\int_0^{N_0} d\tau \left(\frac{\partial c}{\partial \tau}\right)^2 + \frac{1}{2} v_0 \int_0^{N_0} d\tau_1 \int_0^{N_0} d\tau_2 \, \delta(c(\tau_1) - c(\tau_2)) \tag{2}$$

with v_0 being the bare excluded-volume parameter and θ, f are Gaussian random processes with zero mean and covariance given by

$$\langle \theta(\tau, t)\theta(\sigma, s)\rangle = 2\zeta_0^{-1}\delta(\tau - \sigma)\delta(t - s)I \tag{3}$$

$$\langle f(x, t)f(x', s)\rangle = -2\eta_0\Delta\delta(x - x')\delta(t - s)I \tag{4}$$

where I is the $d \times d$ unit matrix. One can show [4] that to $O(\varepsilon)$, i.e. lowest order in the couplings, and by using the Markov approximation for the solvent velocity field, the coupled equations $(1a, b)$ are equivalent to the Kirkwood diffusion model.

It is convenient to convert the two coupled Langevin equations $(1a, b)$ into a path integral with an effective Lagrangian describing the dynamics of dilute polymer solutions. This procedure, which has been described recently in [12], essentially follows a method which has been developed in [15] for critical dynamics. The effective

Lagrangian describing the system (1a, b) can be decomposed into a free part J_0 and an interaction part J_1, $J = J_0 + J_1$ with

$$J_0^{(1)} = \int_0^{N_0} d\tau \int dt [\tilde{c}(\tau, t) \lambda_0 \tilde{c}(\tau, t) - \tilde{c}(\tau, t) \partial_t c(\tau, t) + \tilde{c}(\tau, t) \lambda_0 \partial_\tau^2 c(\tau, t)] \tag{5}$$

describing the conformation field and

$$J_0^{(2)} = \int d^d x \int dt [u(x, t) \eta_0 (i\nabla)^2 \tilde{u}(x, t) - \tilde{u}(x, t) \partial_t u_\perp(x, t) - \tilde{u}(x, t) \eta_0 (i\nabla)^2 u_\perp(x, t)] \tag{6}$$

describing the solvent velocity field. In (6), $\perp$ denotes the transverse part. In (5) and (6) we have introduced two new (imaginary) fields, $\tilde{c}(\tau, t)$ a conformation response field and $\tilde{u}(x, t)$ a solvent velocity response field. The interaction terms containing the self-avoiding interactions can be written

$$J_1^{(1)} = -v_0 \lambda_0 \int_0^{N_0} d\alpha \int_0^{N_0} d\beta \int ds\, \tilde{c}(\alpha, s) \int_k ik\, e^{ik[c(\alpha, s) - c(\beta, s)]} \tag{7}$$

where

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

and the hydrodynamic interaction terms can be written

$$J_1^{(2)} = g_0 \int_0^{N_0} d\tau \int dt\, \tilde{c}(\tau, t) u_\perp(c(\tau, t), t) - g_0 \int_0^{N_0} d\tau \int dt\, \tilde{u}_\perp(c(\tau, t) t) \frac{\delta H_E}{\delta c(\tau, t)}. \tag{8}$$

Note that we have introduced a Fourier transform for the δ function in equation (7).

From equation (5) we obtain the *free* response propagator $\langle c(\tau, t) c(\sigma, t') \rangle_0^R$ for the conformation field of a simple polymer ring (R). Introducing normal coordinates into (5), which, in order to account for the periodic boundary conditions of a ring, are chosen in the form

$$c(\tau, t) = \sum_{k=0}^{\infty} Q_{\tau k}^{(1)} \boldsymbol{\xi}_k^{(1)} + \sum_{k=0}^{\infty} Q_{\tau k}^{(2)} \boldsymbol{\xi}_k^{(2)} \tag{9a}$$

$$\tilde{c}(\tau, t) = \sum_{k=0}^{\infty} Q_{\tau k}^{(1)} \tilde{\boldsymbol{\xi}}_k^{(1)} + \sum_{k=0}^{\infty} Q_{\tau k}^{(2)} \tilde{\boldsymbol{\xi}}_k^{(2)} \tag{9b}$$

with

$$Q_{\tau k}^{(1)} = \left(\frac{2}{N_0}\right)^{1/2} \cos\left(\frac{2\pi k \tau}{N_0}\right) \qquad k = 1, 2, \ldots \tag{10a}$$

$$Q_{\tau k}^{(2)} = \left(\frac{2}{N_0}\right)^{1/2} \sin\left(\frac{2\pi k \tau}{N_0}\right) \qquad k = 1, 2, \ldots \tag{10b}$$

$$Q_{\tau k}^{(1)} = Q_{\tau k}^{(2)} = \left(\frac{1}{N_0}\right)^{1/2} \qquad k = 0 \tag{10c}$$

we obtain [13]

$$\langle \tilde{c}(\tau, t) c(\sigma, t') \rangle_0^R = \theta(t' - t) G_0^R(\tau, \sigma | t' - t) \tag{11}$$

where

$$G_0^R(\tau, \sigma | t) = \frac{1}{N_0}\left(1 + 2\sum_{k=1}^{\infty} \cos 2\hat{k}_0(\tau - \sigma) \exp(-\lambda_k^R t)\right) \tag{12}$$

is the Green function matrix with $\hat{k}_0 = \pi k / N_0$ and $\lambda_k^R = \lambda_0(2\pi k/N_0)^2$.

From (11) we determine the static (equilibrium) correlations $\langle c(\tau) \cdot c(\tau')\rangle_0^R$ to be [13]

$$\langle c(\tau) \cdot c(\tau')\rangle_0^R = d \min(\tau, \tau') - (d/N_0)\tau\tau'. \tag{13}$$

From (13) it follows that the free correlations of a Gaussian ring polymer are smaller than those of a linear chain, due to the second term in (13).

In the following we will need the general two-point correlation functions of the form $\langle c(\tau, t) \cdot c(\sigma, s)\rangle_0^R$. We find, for $t > s$,

$$\langle c(\tau, t) \cdot c(\sigma, s)\rangle_0^R / d = \frac{N_0}{2}\sum_{p=1}^{\infty}\frac{1}{(\pi p)^2}[1 + \cos 2\hat{p}_0(\tau - \sigma)\exp(-\lambda_p^R(t-s))$$

$$- \cos 2\hat{p}_0\tau \exp(-\lambda_p^R t) - \cos 2\hat{p}_0\sigma \exp(-\lambda_p^R s)] + 2\lambda_0 s/N_0. \tag{14}$$

In particular we have

$$\langle[c(\alpha, s) - c(\beta, s)]^2\rangle_0^R = d[|\alpha - \beta| - N_0^{-1}(\alpha - \beta)^2] \tag{15}$$

which may be compared with the corresponding result for a linear chain (L)

$$\langle[c(\alpha, s) - c(\beta, s)]^2\rangle_0^L = d|\alpha - \beta|. \tag{16}$$

Let us now consider the correlation function $\langle c(\tau, t) \cdot c(\tau, t)\rangle$ in the presence of self-avoiding interactions. Utilising our path integral formulation, we have

$$\langle c(\tau, t) \cdot c(\tau, t)\rangle = \int d\{i\tilde{c}, c\}c(\tau, t)c(\tau, t) \exp J. \tag{17}$$

It is essential to note that this path integral has to be evaluated under a constraint. It is convenient to specify the conformation ensemble at $t = 0$: it should be an equilibrium ensemble governed by the (static) Edwards Hamiltonian, including self-avoiding interactions. Thus, we obtain to first order in the coupling v_0:

$$\langle c(\tau, t) \cdot c(\tau, t)\rangle = \langle c(\tau, t) \cdot c(\tau, t)\rangle_{O(v_0)} - v_0\lambda_0\int_0^{N_0}d\alpha\int_0^{N_0}d\beta\int ds \langle\tilde{c}(\alpha, s)$$

$$\times \int_k ikc(\tau, t) \cdot c(\tau, t) e^{ik[c(\alpha,s)-c(\beta,s)]}\rangle_0 \tag{18}$$

where $\langle \cdot \cdot \rangle_0$ denotes averaging with respect to J_0.

Consider the first contribution in (18). The correlation $\langle c(\tau, t) \cdot c(\tau, t)\rangle_{O(v_0)}$ appears due to the constraint and has to be evaluated in the presence of self-avoiding interactions:

$$\langle c(\tau, t) \cdot c(\tau, t)\rangle_{O(v_0)} = \int \{dc\}c(\tau, t) \cdot c(\tau, t) e^{-H_E}\left(\int \{dc\} e^{-H_E}\right)^{-1}$$

$$= \int \{dc\}c(\tau, t) \cdot c(\tau, t) e^{-H_0}(1 + O(v_0)) \tag{19}$$

where H_0 is the free (Gaussian) part of the Edwards Hamiltonian, and the $O(v_0)$ contribution is given by

$$-\tfrac{1}{2}v_0 \int_0^{N_0} d\alpha \int_0^{N_0} d\beta \int_k \langle c(\tau, t) \cdot c(\tau, t) \, e^{ik \cdot [c(\alpha) - c(\beta)]} \rangle_0 \tag{20}$$

which can be calculated introducing a generating functional. We find

$$O(v_0) = \frac{1}{2d^2} v_0 \int_0^{N_0} d\alpha \int_0^{N_0} d\beta \int_k k^2 (\langle [c(\alpha) - c(\beta)] c(\tau, t) \rangle_0)^2$$

$$\times \exp\left(-\frac{1}{2} \frac{k^2}{d} \langle [c(\alpha) - c(\beta)]^2 \rangle_0 \right). \tag{21}$$

Using (11) together with $\theta(0) = 0$ (causality), we find for the second term in (18)

$$-2v_0\lambda_0 \int_0^{N_0} d\alpha \int_0^{N_0} d\beta \int_0^t ds \int_k G_0(\tau, \alpha | t - s) ik \langle c(\tau, t) \, e^{ik \cdot [c(\alpha, s) - c(\beta, s)]} \rangle_0. \tag{22}$$

The remaining average in (22) can again be evaluated introducing a generating functional. The result is

$$\frac{2v_0\lambda_0}{d} \int_0^{N_0} d\alpha \int_0^{N_0} d\beta \int_0^t ds \int_k k^2 G_0(\tau, \alpha | t - s) \langle [c(\alpha, s) - c(\beta, s)] c(\tau, t) \rangle_0$$

$$\times \exp\left(-\frac{1}{2} \frac{k^2}{d} \langle [c(\alpha, s) - c(\beta, s)]^2 \rangle_0 \right). \tag{23}$$

Adding all contributions, we finally secure

$$\langle c(\tau, t) \cdot c(\tau, t) \rangle = \langle c(\tau, t) \cdot c(\tau, t) \rangle_0 + \frac{1}{2} \frac{v_0}{d^2} \int_0^{N_0} d\alpha \int_0^{N_0} d\beta$$

$$\times \int_k k^2 [\langle [c(\alpha) - c(\beta)] c(\tau, t) \rangle_0]^2 \exp\left(-\frac{1}{2} \frac{k^2}{d} [c(\alpha) - c(\beta)]^2 \rangle_0 \right)$$

$$+ \frac{2\lambda_0 v_0}{d} \int_0^{N_0} d\alpha \int_0^{N_0} d\beta \int_0^t ds \int_k G_0(\tau, \alpha | t - s) k^2$$

$$\times \langle [c(\alpha, s) - c(\beta, s)] c(\tau, t) \rangle_0 \exp\left(-\frac{1}{2} \frac{k^2}{d} \langle [c(\alpha, s) - c(\beta, s)]^2 \rangle_0 \right). \tag{24}$$

Using equations (14) and (15) and performing the time and momentum integrations, we find that the remaining contour integrations can be reduced to the following type of integral:

$$\int_0^{N_0} d\alpha \int_0^{N_0} d\beta \left(|\alpha - \beta| - \frac{1}{N_0} (\alpha - \beta)^2 \right)^{-3 + \varepsilon/2} (\cos 2\hat{p}_0 \alpha - \cos 2\hat{p}_0 \beta)^2$$

$$= \frac{(\pi p)^2}{N_0} \left(\frac{8}{\varepsilon} N_0^{\varepsilon/2} + 4[\mathrm{ci}(2\pi p) - \ln 2\pi p - \hat{\gamma}] + 6 - 6 \frac{A^R(2p)}{(\pi p)^2} \right) \tag{25}$$

where $\hat{\gamma}$ is Euler's constant

$$\mathrm{ci}(x) = -\int_x^\infty \frac{dt}{t} \cos t \qquad \mathrm{si}(x) = -\int_x^\infty \frac{dt}{t} \sin t$$

and we have introduced a function

$$A^R(p) = -\pi p[\text{si}(\pi p) + \tfrac{1}{2}\pi] + 2[\text{ci}(\pi p) - \ln(\pi p) - \hat{\gamma}]. \tag{26}$$

Due to the aforementioned internal symmetry, all double sum contributions can be shown to vanish. We are then left with

$$\langle c(\tau, t) \cdot c(\tau, t)\rangle / d = \tfrac{1}{6}N_0 - N_0 \sum_{p=1}^{\infty} \frac{\cos 2\hat{p}_0\tau}{(\pi p)^2} \exp(-\lambda_p^R t) + \frac{2\lambda_0 t}{N_0}$$

$$+ \frac{1}{12} \frac{v_0}{(2\pi)^{d/2}} N_0 \left(\frac{4}{\varepsilon} + 2\ln N_0\right) - \frac{1}{4} \frac{v_0}{(2\pi)^{d/2}} N_0 \sum_{p=1}^{\infty} \frac{\cos 2\hat{p}_0\tau}{(\pi p)^2} \exp(-\lambda_p^R t)$$

$$\times \left(\frac{8}{\varepsilon} + 4\ln N_0 + 4[\text{ci}(2\pi p) - \ln 2\pi p - \hat{\gamma}] + 6 - 6\frac{A^R(2p)}{(\pi p)^2}\right)$$

$$- \frac{v_0}{(2\pi)^{d/2}} N_0 \sum_{p=1}^{\infty} \frac{\cos 2\hat{p}_0\tau}{(\pi p)^2} \exp(-\lambda_p^R t)\lambda_0 t \left(\frac{\pi p}{N_0}\right)^2$$

$$\times \left(\frac{8}{\varepsilon} + 4\ln N_0 + 4[\text{ci}(2\pi p) - \ln 2\pi p - \hat{\gamma}] + 6 - 6\frac{A^R(2p)}{(\pi p)^2}\right). \tag{27}$$

Renormalisation is performed with

$$N = Z_N N_0 \tag{28a}$$

$$\zeta = Z_\zeta \zeta_0 \tag{28b}$$

$$v_0 = u_0 L^{-\varepsilon/2} \tag{28c}$$

where L is the usual external length scale. In lowest order we have

$$Z_N = 1 + \frac{2}{\varepsilon} \frac{u}{(2\pi)^2} \tag{29a}$$

$$Z_\zeta = 1 - \frac{2}{\varepsilon} \frac{u}{(2\pi)^2}. \tag{29b}$$

In order to obtain a result for $\langle c(\tau, t) \cdot c(\tau, t)\rangle$ which is valid in the limit of large times t, we cannot—after inserting the value of u at its fixed point $u^* = O(\varepsilon)$—naively exponentiate the results to $O(\varepsilon)$. Rather we have to use the idea of singular perturbation theory [16] and exploit the asymptotic behaviour of the relaxation times as dictated by the renormalisation group equation [4]. This procedure (see [10] for a discussion) amounts to introducing an effective eigenvalue for the relaxation spectrum by exponentiating single sum terms which have prefactors linear in the time t (see the last term in (27)). At the fixed point

$$\frac{u^*}{(2\pi)^2} = \frac{\varepsilon}{8}$$

we find the relaxation spectrum for a ring in the presence of self-avoiding interactions to $O(\varepsilon)$

$$\lambda_p^R = \frac{1}{\zeta} \left(\frac{2\pi p}{N}\right)^2 \left(\frac{Lp}{N}\right)^{\varepsilon/8} \exp\left[\frac{\varepsilon}{8}\left(\hat{\gamma} - \text{ci}(2\pi p) - \frac{3}{2} + \frac{3}{2}\frac{A^R(2p)}{(\pi p)^2}\right)\right]. \tag{30}$$

Finally, introducing a new time unit $\bar{t} = t\lambda_p(p=1)$, $\bar{\lambda}_p = \lambda_p/\lambda_p(p=1)$ and $\bar{\tau} = \tau/N$ we can write our result at the fixed point u^* in universal form

$$\langle c(\bar{\tau}, \bar{t}) \cdot c(\bar{\tau}, \bar{t}) \rangle^{\mathrm{R}} \left[dN^{2\nu} \left(\frac{2\pi}{L} \right)^{\varepsilon/8} \right]^{-1} = \frac{2\bar{t}}{(2\pi)^{2+\varepsilon/8}} \exp(-\varepsilon C_1^{\mathrm{R}})$$

$$+ \frac{1}{6} - \sum_{p=1}^{\infty} \frac{\cos 2\pi p \bar{\tau}}{(\pi p)^2} \exp(-\bar{\lambda}_p^{\mathrm{R}} \bar{t}) \exp\left(\frac{\varepsilon}{8} H_{pp}^{\mathrm{R}} \right) \tag{31}$$

where

$$C_1^{\mathrm{R}} = \frac{1}{8} \left(\hat{\gamma} - \mathrm{ci}(2\pi) - \frac{3}{2} + \frac{3}{2} \frac{A^{\mathrm{R}}(2)}{\pi^2} \right) \tag{32}$$

$$H_{pp}^{\mathrm{R}} = \mathrm{ci}(2\pi p) - \ln 2\pi p - \hat{\gamma} + \frac{3}{2} - \frac{3}{2} \frac{A^{\mathrm{R}}(2p)}{(\pi p)^2} \tag{33}$$

and $\nu = \frac{1}{2} + \frac{1}{16}\varepsilon$ is the Flory exponent.

Having determined $\langle c(\tau, t) \cdot c(\tau, t) \rangle^{\mathrm{R}}$ we can now evaluate the general two-point correlation function $\langle c(\tau, t) \cdot c(\sigma, s) \rangle$ in the following way:

$$\langle [c(\tau, t) - c(\sigma, s)]^2 \rangle = \langle c(\tau, t) \cdot c(\tau, t) \rangle + \langle c(\sigma, s) \cdot c(\sigma, s) \rangle - 2 \langle c(\tau, t) \cdot c(\sigma, s) \rangle. \tag{34}$$

As $c(\tau, t) - c(\sigma, s)$ is a polymer internal vector, we can exploit translational invariance, which gives

$$\langle [c(\tau, t) - c(\sigma, s)]^2 \rangle - \langle [c(\tau, t-s) - c(\sigma, 0)]^2 \rangle. \tag{35}$$

Note, however, that this is only valid for correlation functions which are the square of the difference of two conformation field vectors, but not for correlations like $\langle [c(\alpha, s) - c(\beta, s)] \cdot c(\tau, t) \rangle$, because we have chosen a convention in which $c(0, 0) = 0$. This dependence on the choice of origin must drop out of correlation functions in order for translational invariance to be valid. Using (35), we have

$$\langle c(\tau, t) \cdot c(\sigma, s) \rangle = \langle c(\tau, t-s) \cdot c(\sigma, 0) \rangle + \tfrac{1}{2} \langle c(\tau, t) \cdot c(\tau, t) \rangle$$

$$- \tfrac{1}{2} \langle c(\tau, t-s) \cdot c(\tau, t-s) \rangle + \tfrac{1}{2} \langle c(\sigma, s) \cdot c(\sigma, s) \rangle$$

$$- \tfrac{1}{2} \langle c(\sigma, 0) \cdot c(\sigma, 0) \rangle. \tag{36}$$

Therefore, apart from $\langle c(\tau, t) \cdot c(\tau, t) \rangle$ we only need to calculate $\langle c(\tau, t) \cdot c(\sigma, 0) \rangle$. This calculation parallels the one described and we only quote the result. We find in universal form to $\mathrm{O}(\varepsilon)$

$$\langle c(\bar{\tau}, \bar{t}) \cdot c(\bar{\sigma}, 0) \rangle^{\mathrm{R}} \left[dN^{2\nu} \left(\frac{2\pi}{L} \right)^{\varepsilon/8} \right]^{-1} = \frac{1}{12} - \frac{1}{2} \sum_{p=1}^{\infty} \frac{\cos 2\pi p \bar{\sigma}}{(\pi p)^2} \exp\left(\frac{\varepsilon}{8} H_{pp}^{\mathrm{R}} \right)$$

$$+ \frac{1}{2} \sum_{p=1}^{\infty} \frac{\cos 2\pi p (\bar{\tau} - \bar{\sigma})}{(\pi p)^2} \exp(-\bar{\lambda}_p^{\mathrm{R}} \bar{t}) \exp\left(\frac{\varepsilon}{8} H_{pp}^{\mathrm{R}} \right)$$

$$- \frac{1}{2} \sum_{p=1}^{\infty} \frac{\cos 2\pi p \bar{\tau}}{(\pi p)^2} \exp(-\bar{\lambda}_p^{\mathrm{R}} \bar{t}) \exp\left(\frac{\varepsilon}{8} H_{pp}^{\mathrm{R}} \right). \tag{37}$$

Now we turn to the discussion of hydrodynamic interactions. In [13] we reported the result of $\langle c(\tau, t) \cdot c(\tau, t) \rangle$ to $\mathrm{O}(\varepsilon)$. We found in universal form at the non-draining Gaussian fixed point $\xi^* = \frac{8}{3}\pi^2 \varepsilon$ $(\xi = \zeta L^{\varepsilon/2})$

$$\langle c(\bar{\tau}, \bar{t}) \cdot c(\bar{\tau}, \bar{t}) \rangle^{\mathrm{R}}/dN$$

$$= \frac{1}{6} + 2\bar{t} \exp(-\varepsilon C_1^{\mathrm{R}})(2\pi)^{-2+\varepsilon/2} - \sum_{p=1}^{\infty} \frac{\cos 2\pi p \bar{\tau}}{(\pi p)^2} \exp(-\bar{\lambda}_p^{\mathrm{R}} \bar{t}) \tag{38}$$

with $C_1^R = \frac{1}{2} \mathrm{ci}(2\pi) - \frac{1}{2}\hat{\gamma}$ and

$$\lambda_p^R = \frac{3}{2\varepsilon} \frac{1}{(2\pi)^{2-\varepsilon/2}} \left(\frac{2\pi p}{N}\right)^{2-\varepsilon/2} \exp\left\{\varepsilon[\tfrac{5}{12} + \tfrac{1}{2}\mathrm{ci}(2\pi p) - \tfrac{1}{2}\hat{\gamma}]\right\}. \tag{39}$$

The correlation $\langle c(\tau, t) \cdot c(\sigma, 0)\rangle^R$ is then given by

$$\langle c(\bar{\tau}, \bar{t}) \cdot c(\bar{\sigma}, 0)\rangle^R / \mathrm{d}N = \frac{1}{12} - \frac{1}{2} \sum_{p=1}^{\infty} \frac{\cos 2\pi p \bar{\sigma}}{(\pi p)^2}$$

$$+ \frac{1}{2} \sum_{p=1}^{\infty} \frac{\cos 2\pi p(\bar{\tau} - \bar{\sigma})}{(\pi p)^2} \exp(-\bar{\lambda}_p^R \bar{t}) - \frac{1}{2} \sum_{p=1}^{\infty} \frac{\cos 2\pi p \bar{\tau}}{(\pi p)^2} \exp(-\bar{\lambda}_p^R \bar{t}). \tag{40}$$

To lowest order $(O(\varepsilon))$ there are no cross-terms between self-avoiding and hydro-dynamic interactions. Thus we just have to add the results for both cases (counting the free term only once) and obtain at the fixed point $u^*/(2\pi)^2 = \frac{1}{8}\varepsilon$, $\xi^*/(2\pi)^2 = \frac{1}{2}\varepsilon$ for the relaxational spectrum:

$$\lambda_p^R = \frac{1}{2\pi^2 \varepsilon} \left(\frac{2\pi p}{N}\right)^{2-\varepsilon/4} \left(\frac{L}{2\pi}\right)^{-\varepsilon/4} \exp\left[\frac{1}{4}\varepsilon\left(\frac{1}{2} + \mathrm{ci}(2\pi p) - \hat{\gamma} + \frac{3}{4} \frac{A^R(2p)}{(\pi p)^2}\right)\right]. \tag{41}$$

We then secure, utilising (36), for the most general two-point correlation function:

$$\langle c(\bar{\tau}, \bar{t}) \cdot c(\bar{\sigma}, \bar{s})\rangle \left[\mathrm{d}N^{2\nu}\left(\frac{2\pi}{L}\right)^{\varepsilon/8}\right]^{-1} = \frac{1}{12} + \frac{2\bar{s}}{(2\pi)^{2-\varepsilon/4}} \exp{-\varepsilon C_1^R}$$

$$+ \frac{1}{2} \sum_{p=1}^{\infty} \frac{\cos 2\pi p(\bar{\tau} - \bar{\sigma})}{(\pi p)^2} \exp[-\bar{\lambda}_p^R(\bar{t} - \bar{s})] \exp\left(\frac{\varepsilon}{8} H_{pp}^R\right)$$

$$- \frac{1}{2} \sum_{p=1}^{\infty} \frac{\cos 2\pi p \bar{\sigma}}{(\pi p)^2} \exp(-\bar{\lambda}_p^R \bar{s}) \exp\left(\frac{\varepsilon}{8} H_{pp}^R\right)$$

$$- \frac{1}{2} \sum_{p=1}^{\infty} \frac{\cos 2\pi p \bar{\tau}}{(\pi p)^2} \exp(-\bar{\lambda}_p^R \bar{t}) \exp\left(\frac{\varepsilon}{8} H_{pp}^R\right) \tag{42}$$

where

$$C_1^R = \frac{1}{4}\left(\mathrm{ci}(2\pi) - \hat{\gamma} - \frac{3}{4} + \frac{3}{4} \frac{A^R(2)}{\pi^2}\right).$$

The sums over p in (42) converge rapidly and for a numerical evaluation it is sufficient to sum up to $p = 50$.

To summarise, we have determined the most general two-point correlation function for simple ring polymers in the presence of both self-avoiding and hydrodynamic interactions to $O(\varepsilon)$. From our RG analysis have emerged the properly scaled variables $\bar{\tau}, \bar{\sigma}$ and $\bar{t}, \bar{s}$ as well as the correct N dependence $\sim N^{2\nu}$ of the prefactor in (42). Once the renormalised correlation function is expressed in the new variables, its functional form is essentially identical to its bare equivalent. Note also that the diffusive behaviour $\sim \bar{s}$ of the centre of mass dominates for long times, while the internal ring motion becomes important for short times ($\bar{t}, \bar{s} \to 0$ but still $t, s \gg 1$).

As already mentioned in the introduction, the ring structures are distinguished from linear chains by their remarkable symmetry properties (due to the circularity condition). In general, universal properties obtained within an RG analysis reflect the different topologies of rings and linear chains. It would of course be of great interest to compare our results with numerical simulations. So far, however, numerical results, such as [17], have been obtained for linear chains only. A numerical study of simple ring polymers, with a view to the results reported here, would certainly be worthwhile.

Acknowledgments

References

[1] de Gennes P G 1972 *Phys. Lett.* **38A** 339
    Des Cloizeaux J 1975 *J. Physique* **36** 281
[2] Oono Y and Freed K 1981 *J. Chem. Phys.* **75** 993
[3] Edwards S F 1965 *Proc. Phys. Soc.* **85** 613
[4] Oono Y 1985 *Adv. Chem. Phys.* **61**
[5] Jagannathan A, Oono Y and Schaub B 1985 *Phys. Lett.* **113A** 341
[6] Schaub B, Friedman B A and Oono Y 1985 *Phys. Lett.* **110A** 136
[7] Shiwa Y and Kawasaki K 1982 *J. Phys. C: Solid State Phys.* **15** 5345
[8] Puri S 1987 *Phys. Lett.* **121A** 430
[9] Schaub B and Schmittmann B 1988 *Z. Phys.* B to be published
[10] Jagannathan A, Oono Y and Schaub B 1987 *J. Chem. Phys.* **86** 2276
[11] Johannesson H and Schaub B 1987 *Phys. Rev.* A **35** 3571
[12] Schaub B, Creamer D B and Johannesson H 1988 *J. Phys. A: Math. Gen.* **21** 1431
[13] Johannesson H, Creamer D B and Schaub B 1987 *J. Phys. A: Math. Gen.* **20** 5071
[14] Oono Y and Freed K 1981 *J. Chem. Phys.* **75** 1009
[15] Janssen H K 1976 *Z. Phys.* B **23** 377
    Bausch R, Janssen H K and Wagner H 1976 *Z. Phys.* B **24** 113
[16] Kevorkian J and Cole J D 1981 *Perturbation Methods in Applied Mathematics* (Berlin: Springer)
[17] Baumgärtner A 1980 *J. Chem. Phys.* **72** 871