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Semiflexible Polymers in Straining Flows

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We introduce a model for semiflexible polymer chains based on the integral of an appropriate Gaussian process. The stiffness is characterized physically by adding a bending energy. The degree of stiffness in the polymer chain is quantified by means of a parameter and as this parameter tends to infinity, the limiting case reduces to the Brownian model of completely flexible chains studied in earlier work. The calculation of the partition function for the configuration statistical mechanics (i.e., the distribution of shapes) of such polymers in elongational flow or quadratic potentials is equivalent to the probabilistic problem of finding the law of a quadratic functional of the associated Gaussian process. An exact formula for the partition function is presented; however, in practice, this formula is too complicated for most computations. We therefore develop an asymptotic expansion for the partition function in terms of the stiffness parameter and obtain the first-order term which gives the first-order deviation from the completely flexible case. In addition to the partition function, the method presented here can also deal with other quadratic functionals such as the "stochastic area" associated with two polymer chains.

KEY WORDS: Semiflexible polymers; elongational flows; quadratic potentials; small-stiffness expansion; partition functions; quadratic functionals.

1. INTRODUCTION: A MODEL FOR POLYMERS OF FINITE STIFFNESS

This study extends previous work on equilibrium polymer configurations (in Chan, Dean, Jansons, and Rogers (1994)) to the case of stiff, or more precisely semi-flexible polymers. Distributions of polymer shapes are required for determining the rheology of polymer solutions, and therefore

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have applications in a large number of fields including chemical engineering, biology. A sudden change in the rheology of a polymer solution occurs due to the coil-stretch transition. The main method used in Chan *et al.* (1994) is a technique for finding the law of a quadratic functional of Brownian motion and some other Gaussian processes using ideas from excursion theory. In the case of a semi-flexible polymer, one can no longer model the path of a polymer molecule as the path of a process like Brownian motion. Instead, a much smoother path is needed and in this paper we use the *integral* of a suitable (Gaussian) process.

One possible model is to take a unit vector N_t diffusing in $\mathbb{R}^3$ according to the equation

$$dN_t = (I - N_t N_t^T)\, dB_t - N_t\, dt, \qquad |N_0| = 1$$

where B is a standard Brownian motion in $\mathbb{R}^3$ and I is the 3×3 identity matrix. (It is easy to see that if $|N_0| = 1$ then $|N_t| = 1$ for all t.) We use as the model of a semi-flexible polymer the integral process $X_t = \int_0^t N_s\, ds$ for $0 \leqslant t \leqslant T$, where $T > 0$ is a fixed constant. This model is attractive physically in several respects: for example, the length of the path X_t remains fixed, even after putting the polymer in a potential field and doing Boltzmann reweighting. Real polymers are likely to behave more like this than in the Gaussian model we consider here. However, the diffusing unit vector is rather hard to work with mathematically. For one thing, the problem of determining the partition function cannot be reduced to one involving the one-dimensional independent components of X. For this reason, in this paper we use the integral of another Gaussian diffusion process, whose components are independent and the partition function therefore factorizes. However, it is useful to highlight some of the limitations of our model by comparing with this diffusing vector model.

For a model where the path X_t of the polymer (in $\mathbb{R}^3$) consists of three independent components, we are interested in the (one-dimensional) partition function

$$Z = \mathbb{E}\left[\exp\left\{ -\frac{\lambda^2}{2} \int_0^T (X_t - \bar{X})^2\, r(dt) \right\} \right] \tag{1.0}$$

for fixed $T > 0$, where r is the resistance measure and $\bar{X} = r([0, T])^{-1} \int_0^T X_t r(dt)$ is the centre of resistance. The resistance measure models the interaction between the ambient flow and the polymer; the resistance measure is proportional to Lebesgue measure if the polymer is of uniform thickness. For simplicity we have made the usual free-draining approximtion, that is we have ignored hydrodynamic interactions between the polymer with itself. For a more detailed discussion of the statistical

mechanics of polymers in pure straining flows and the physics behind the above partition function, we refer the reader to our earlier paper Chan *et al.* (1994).

We shall treat the qudratic functional

$$\mathbb{E}\left[\exp\left\{-\frac{\lambda^2}{2}\int_0^T X_t^2\, r(dt)\right\}\right] \tag{1.1}$$

as the basic object of our study because calculation of (1.1) is in fact the main step in calculating the partition function (1.0). Once we have an expression for (1.1), using the tricks of "uncompleting the square" and mixing over a suitable Gaussian random variable as described in Chan *et al.* (1994), the linear terms and centre-of-resistance terms in the partition function (1.0) can easily be incorporated. (An example of this in action can be seen in the proof of Proposition 4.1.)

We take as the process X the integral (or position process) of an Ornstein–Uhlenbeck (OU) process U as follows:

$$dX_t = \alpha U_t\, dt \tag{1.2a}$$

$$dU_t = -\alpha U_t\, dt + dB_t \tag{1.2b}$$

where B is a standard Brownian motion and $\alpha > 0$ is a parameter describing the degree of stiffness of the polymer: a large α corresponds to a small degree of stiffness. The model of semi-flexible polymers described by Eqs. (1.2a,b) is equivalent to that discussed in Section 15.7 of Kleinert (1990). As mentioned by Kleinert, one must be careful to obtain the right model of semi-flexible polymers. Using a stochastic calculus approach, one is less likely to choose the wrong model as the right model also looks the most natural from the point of view of stochastic calculus. To highlight the choice of model used in this study, we now determine $\mathbb{E}[X^2]$, as this quantity is always given by physicists. It is well known that the solution to (1.2b) is given by

$$U_t = e^{-\alpha t}\left[U_0 + \int_0^t e^{\alpha s}\, dB_s\right]$$

(More generally, see Section 2 below.) In particular, U_t and X_t are Gaussian random variables. We take $U_0 \sim N(0, (2\alpha)^{-1})$, in which case U_t is a stationary process and is identical in law to a time-change of a Brownian motion W as follows:

$$U_t \overset{\mathcal{D}}{=} e^{-\alpha t} W\left(\frac{e^{2\alpha t}}{2\alpha}\right) \tag{1.3}$$

Hence using (1.3), assuming without loss of generality that $X_0 = 0$,

$$\begin{aligned}
\mathbb{E}[e^{\lambda X_t}] &= \mathbb{E}\left[\exp\left\{\lambda\alpha\int_0^t U_s\,ds\right\}\right] \\
&= \exp\left\{\frac{(\lambda\alpha)^2}{2}\int_0^t\int_0^t \mathbb{E}(U_r U_s)\,dr\,ds\right\} \\
&= \exp\left\{\frac{(\lambda\alpha)^2}{2}\frac{1}{2\alpha}\int_0^t\int_0^t e^{-\alpha|r-s|}\,dr\,ds\right\} \\
&= \exp\left\{\frac{\lambda^2}{2\alpha}(e^{-\alpha t}+\alpha t-1)\right\} \qquad (1.4)
\end{aligned}$$

We see from the above that the mean squared end-to-end distance of the polymer chain is given by

$$\mathbb{E}(X_t^2) = \frac{e^{-\alpha t}+\alpha t-1}{\alpha} \qquad (1.5)$$

so for small αt, $\mathbb{E}(X_t^2) \sim \alpha t^2/2$ while for large αt, $\mathbb{E}(X_t^2) \sim t$. The expression (1.5) and the large and small αt asymptotics agree with those obtained in Section 15.7 of Kleinert (1990).

Observe that (1.4) shows that X converges in law to a Brownian motion as $\alpha \to \infty$, corresponding to the completely flexible case studied in Chan *et al.* (1994). In this paper, we show that the corresponding partition function also converges to the Brownian case and investigate the rate at which this convergence takes place, that is the deviation of a slightly semi-flexible polymer from the completely flexible case.

When $r(dt)$ is Lebesgue measure, we obtain an explicit formula for the quadratic functional (1.1) (see Section 2). However, this formula is extremely complicated and messy and it is not easy to discern the asymptotic behaviour directly from this formula. We shall therefore develop in Section 3 a method based on studying the large α asymptotics of a Riccati differential equation which involves a technique widely used in many areas of applied mathematics and commonly known as a boundary-layer approximation. Having obtained these theoretical results, we present in Section 4 some simple examples of semiflexible polymers which correspond to the examples studied in Chan *et al.* (1994). Finally, in Section 5, we briefly describe how the treatment presented in Section 3 can be applied to the stochastic area of two polymer two chains.

2. EXPLICIT FORMULA FOR THE LAW OF A GENERAL CLASS OF QUADRATIC FUNCTIONALS

We are interested in calculating Laplace transforms of quadratic functions of the form (1.1) for processes X of the form (1.2). At present, there exist many different methods for calculating such Laplace transforms: for a concise survey of these methods see Yor (1992) and also the references in Chan *et al.* (1994). In this last article, powerful excursion theoretic ideas and local-time methods such as the Ray-Knight theorem are applied to good effect. However, in the present setting excursion methods are no longer appropriate because we are no longer dealing with one-dimensional Markov processes (e.g., the process X in (1.2) is not Markov even though the couple (X, U) is); moreover, there is not an analogous Ray-Knight theorem for OU type processes like (1.2). Fortunately, an old trick comes to the rescue...

2.1. A Girsanov Transform Approach to General Quadratic Functionals

Consider first the following general situation. Let $\underset{\sim}{X}$ be a process in $\mathbb{R}^n$ satisfying the linear stochastic differential equation

$$d\underset{\sim}{X}_t = E\underset{\sim}{X}_t\, dt + \sigma\, dB_t \tag{2.1}$$

where E is an $n \times n$ matrix, B a standard Brownian motion in $\mathbb{R}^d$ and σ is an $n \times d$ matrix. We shall calculate (for an arbitrary initial value $\underset{\sim}{X}_0$)

$$\mathbb{E}\left[\exp\left\{-\frac{\lambda^2}{2}\int_0^t \underset{\sim}{X}_s^T Q \underset{\sim}{X}_s\, ds\right\}\right] \tag{2.2}$$

where Q is an $n \times n$ non-negative symmetric matrix. To be precise, the expectation $\mathbb{E}$ in (2.2) is taken with respect to the canonical measure $\mathbb{P}$ under which B is an standard Brownian motion and under which $\underset{\sim}{X}$ has the law of the solution to the SDE (2.1); later, we need to work with another measure $\mathbb{Q}$ which is obtained from $\mathbb{P}$ under a Girsanov transform.

Theorem 2.1. Let $\underset{\sim}{X}$ be a Gaussian process satisfying (2.1) and suppose that, for each t, the Gaussian random variable $\underset{\sim}{X}_t$ has mean a_t and covariance matrix V_t. Let Q be an $n \times n$ non-negative symmetric matrix. For $\lambda \in \mathbb{R}$, let $\Gamma = \Gamma(\lambda)$ be a symmetric real solution to the matrix quadratic equation

$$\Gamma\sigma\sigma^T\Gamma - (\Gamma E + E^T\Gamma) - \lambda^2 Q = 0$$

with the property that $\Gamma(\lambda) \to 0$ as $\lambda \to 0$. Then for all λ in a neighbourhood of 0,

$$\mathbb{E}\left[\exp\left\{-\frac{\lambda^2}{2}\int_0^t \underset{\sim}{X}_s^T Q \underset{\sim}{X}_s \, ds\right\}\right]$$

$$= \exp\left\{-\frac{1}{2}(\mathrm{tr}(\sigma^T \Gamma \sigma)t + \underset{\sim}{X}_0^T \Gamma \underset{\sim}{X}_0)\right\} \det(I - \Gamma V_t)^{-1/2}$$

$$\times \exp\left\{\frac{1}{2} a_t^T (I - \Gamma V_t)^{-1} \Gamma a_t\right\}$$

Proof. Observe that since (2.1) is linear, it has an explicit solution; indeed, by Itô's formula, $\exp\{-tE\}\, \underset{\sim}{X}_t - \underset{\sim}{X}_0 = \int_0^t \exp\{-sE\}\, \sigma \, dB_s$ is a local martingale and so

$$\underset{\sim}{X}_t = \exp\{tE\}\, \underset{\sim}{X}_0 + \exp\{tE\} \int_0^t \exp\{-sE\}\, \sigma \, dB_s \tag{2.3}$$

In particular, observe that $\underset{\sim}{X}$ is a Gaussian process. Next, again by Itô's formula, if Γ is any real symmetric matrix then

$$d(\underset{\sim}{X}^T \Gamma \underset{\sim}{X}) = (d\underset{\sim}{X})^T \Gamma \underset{\sim}{X} + X^T \Gamma \, d\underset{\sim}{X} + (d\underset{\sim}{X})^T \Gamma \, d\underset{\sim}{X}$$

$$= 2\underset{\sim}{X}_t^T \Gamma \sigma \, dB_t + \underset{\sim}{X}_t^T (\Gamma E + E^T \Gamma)\, \underset{\sim}{X}_t \, dt + \mathrm{tr}(\sigma^T \Gamma \sigma)\, dt \tag{2.4}$$

Suppose that the symmetric matrix Γ is chosen to be a solution of the quadratic matrix equation

$$\Gamma \sigma \sigma^T \Gamma - (\Gamma E + E^T \Gamma) - \lambda^2 Q = 0 \tag{2.5}$$

with the properties stated in the theorem. Define a measure $\mathbb{Q}$, equivalent to $\mathbb{P}$, by

$$\left.\frac{d\mathbb{Q}}{d\mathbb{P}}\right|_{\mathscr{F}_t} = \exp\left\{-\int_0^t \underset{\sim}{X}_s^T \Gamma \sigma \, dB_s - \frac{1}{2}\int_0^t \underset{\sim}{X}_s^T \Gamma \sigma \sigma^T \Gamma \underset{\sim}{X}_s \, ds\right\} \tag{2.6}$$

where $\{\mathscr{F}_t\}$ is the natural filtration associated with the Brownian motion B (or equivalently, the process $\underset{\sim}{X}$). Note that the right-hand side of (2.6) is a true martingale, not just a local martingale, so that the expectation under

$\mathbb{P}$ of (2.6) is 1 and $\mathbb{Q}$ is therefore a true probability measure. The reason for this will be explained below, once we have derived Eq. (2.8).

Combining (2.4) and (2.5) we see that

$$\begin{aligned}
&\mathbb{E}\left[\exp\left\{-\frac{\lambda^2}{2}\int_0^t \underset{\sim}{X}_s^T Q \underset{\sim}{X}_s\, ds\right\}\right] \\
&\quad = \mathbb{Q}\left[\exp\left\{-\frac{\lambda^2}{2}\int_0^t \underset{\sim}{X}_s^T Q \underset{\sim}{X}_s\, ds\right\}\right. \\
&\qquad \left.\times \exp\left\{\int_0^t \underset{\sim}{X}_s^T \Gamma\sigma\, dB_s + \frac{1}{2}\int_0^t \underset{\sim}{X}_s^T \Gamma\sigma\sigma^T\Gamma \underset{\sim}{X}_s\, ds\right\}\right] \\
&\quad = \exp\left\{-\frac{t}{2}\operatorname{tr}(\sigma^T\Gamma\sigma)\right\}\mathbb{Q}\left[\exp\left\{\frac{1}{2}(\underset{\sim}{X}_t^T\Gamma\underset{\sim}{X}_t - \underset{\sim}{X}_0^T\Gamma\underset{\sim}{X}_0)\right\}\right] \qquad (2.7)
\end{aligned}$$

Thus the whole point of the change of measure (2.6) is to replace the quadratic functional appearing in (2.2) by just a quadratic function of a random vector, whose distribution is still Gaussian under the new measure $\mathbb{Q}$. Indeed, by the Cameron–Martin–Girsanov theorem (see for example Rogers and Williams (1987) Theorem IV.38.9), the process

$$W_t = B_t + \int_0^t \sigma^T\Gamma \underset{\sim}{X}_s\, ds$$

is a Brownian motion under $\mathbb{Q}$ and therefore, under $\mathbb{Q}$, the process $\underset{\sim}{X}$ satisfies the SDE

$$d\underset{\sim}{X}_t = (E - \sigma\sigma^T\Gamma)\,\underset{\sim}{X}_t\, dt + \sigma\, dW_t \qquad (2.8)$$

The solution to (2.8) does not explode. If we now start with Eq. (2.8) and let $\mathbb{P}$ be the law of the Brownian motion B (or equivalently, the law of the process satisfying (2.1)), we can *define* $\mathbb{Q}$ to be the law of the process satisfying (2.8) (where W is a Brownian motion). Then up to the time of explosion—which in our case is $\mathbb{Q}$-almost surely infinite—the measures $\mathbb{Q}$ and $\mathbb{P}$ are related by (2.6) and hence the right-hand side of (2.6) is a true martingale. This is the same kind of argument as in Exercise (2.10) of Chapter IX of Revuz and Yor (1994). Equation (2.8) has the same form as (2.1) and its solution is therefore given by (2.3) with E replaced by $E - \sigma\sigma^T\Gamma$ and B replaced by W. In particular, if we put

$\Phi_t = \exp\{t(E - \sigma\sigma^T\Gamma)\}$, we see that $\underset{\sim}{X}_t$ is Gaussian with mean $a_t = \Phi_t \underset{\sim}{X}_0$ and covariance matrix

$$V_t = \Phi_t \Sigma_t \Phi_t^T$$
$$= \int_0^t \Phi_{t-s} \sigma\sigma^T \Phi_{t-s}^T \, ds \tag{2.9}$$

where

$$\Sigma_t = \int_0^t \Phi_s^{-1} \sigma\sigma^T (\Phi_s^{-1})^T \, ds$$

is the covariance matrix of $\int_0^t \Phi_s^{-1}\sigma \, dW_s$. Finally, according to the well-known formula for quadratic functions of Gaussian random variables (sometimes known as the "fundamental theorem of statistics"—see Chan *et al.* (1994)), we arrive at the explicit formula

$$\mathbb{E}\left[\exp\left\{-\frac{\lambda^2}{2}\int_0^t \underset{\sim}{X}_s^T Q \underset{\sim}{X}_s \, ds\right\}\right]$$
$$= \exp\left\{-\frac{t}{2}\operatorname{tr}(\sigma^T\Gamma\sigma)\right\} \mathbb{Q}\left[\exp\left\{\frac{1}{2}(\underset{\sim}{X}_t^T \Gamma \underset{\sim}{X}_t - \underset{\sim}{X}_0^T \Gamma \underset{\sim}{X}_0)\right\}\right]$$
$$= \exp\left\{-\frac{1}{2}(\operatorname{tr}(\sigma^T\Gamma\sigma)t + \underset{\sim}{X}_0^T \Gamma \underset{\sim}{X}_0)\right\} \det(I - \Gamma V_t)^{-1/2}$$
$$\times \exp\left\{\frac{1}{2} a_t^T (I - \Gamma V_t)^{-1} \Gamma a_t\right\} \tag{2.10}$$

(Since we are taking λ close to 0 and consequently Γ is close to 0, we can assume that $(I - \Gamma V_t)^{-1}$ is defined.) ∎

Remarks. (i) It is not necessary that the matrix Q in (2.2) be non-negative; this assumption is made solely to ensure that (2.2) is finite, which is all that is required. Thus, for example, λ could be complex.

(ii) The continuity assumption in Theorem 2.1, that $\Gamma(\lambda) \to 0$ as $\lambda \to 0$, is also made purely for convenience: in this case, the last line in (2.7) is obviously 1 when $\lambda = 0$.

(iii) The trick of using a Girsanov change of measure to reduce the problem of finding the law of a quadratic functional of an infinite dimensional object to one of just finding the law of a quadratic function of a finite dimensional random variable has been used quite often already—see Yor (1992) for other examples.

2.2. An Exact Expression for the Partition Function

We now specialize the preceding general treatment to the case (1.1) and (1.2) with $r(dt)$ being Lebesgue measure: thus

$$Q=\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}, \qquad E=\begin{pmatrix}0 & \alpha\\ 0 & -\alpha\end{pmatrix}, \qquad \sigma=\begin{pmatrix}0\\ 1\end{pmatrix} \tag{2.11}$$

An elementary exercise then shows that the general solution of (2.5) is

$$\Gamma=\begin{pmatrix}\pm\lambda\sqrt{\dfrac{\alpha+2\lambda}{\alpha}} & \lambda\\ \lambda & -\alpha\pm\sqrt{\alpha^2+2\alpha\lambda}\end{pmatrix} \tag{2.12}$$

(As we are interested in the large $\alpha>0$ case, we may assume that Γ is real.) In order to have $\Gamma\to 0$ as $\lambda\to 0$ we need to take the "+" version of (2.12). For the matrices (2.11) and (2.12) we have

$$E-\sigma\sigma^T\Gamma=\begin{pmatrix}0 & \alpha\\ -\lambda & -\sqrt{\alpha^2+2\alpha\lambda}\end{pmatrix}$$

and so from (2.1) we see that, under $\mathbb{Q}$, the process $\underset{\sim}{X}=(X, U)^T$ corresponds (up to a multiplicative constant) to the position and velocity of a noisy damped simple harmonic oscillator. Putting

$$\eta=\sqrt{\frac{\alpha+2\lambda}{\lambda}} \tag{2.13a}$$

and

$$\mu_1=\frac{\eta+\sqrt{\eta^2-4}}{2}, \qquad \mu_2=\frac{\eta-\sqrt{\eta^2-4}}{2} \tag{2.13b}$$

we note that $-\mu_1\sqrt{\lambda\alpha}$ and $-\mu^2\sqrt{\lambda\alpha}$ are the eigenvalues of $E-\sigma\sigma^T\Gamma$. By diagonalization, it is easy to see that

$$\begin{aligned}\Phi_t&=\exp\{t(E-\sigma\sigma^T\Gamma)\}\\ &=\frac{1}{\sqrt{\eta^2-4}}\begin{pmatrix}\mu_1 e^{-\mu_2 t\sqrt{\lambda\alpha}}-\mu_2 e^{-\mu_1 t\sqrt{\lambda\alpha}} & \sqrt{\dfrac{\alpha}{\lambda}}\,(e^{-\mu_2 t\sqrt{\lambda\alpha}}-e^{-\mu_1 t\sqrt{\lambda\alpha}})\\ \sqrt{\dfrac{\lambda}{\alpha}}\,(e^{-\mu_1 t\sqrt{\lambda\alpha}}-e^{-\mu_2 t\sqrt{\lambda\alpha}}) & \mu_1 e^{-\mu_1 t\sqrt{\lambda\alpha}}-\mu_2 e^{-\mu_2 t\sqrt{\lambda\alpha}}\end{pmatrix}\end{aligned} \tag{2.14}$$

Hence the covariance matrix Σ_t of $\int_0^t \Phi_s^{-1}\sigma\, dW_s$ is defined by

$$\Sigma_{11}(t) = \frac{1}{\eta^2 - 4}\int_0^t \frac{\alpha}{\lambda}(e^{\mu_2 s\sqrt{\lambda\alpha}} - e^{\mu_1 s\sqrt{\lambda\alpha}})^2\, ds$$

$$\Sigma_{12}(t) = \Sigma_{21}(t) = \frac{1}{\eta^2 - 4}\int_0^t \sqrt{\frac{\alpha}{\lambda}}(e^{\mu_2 s\sqrt{\lambda\alpha}} - e^{\mu_1 s\sqrt{\lambda\alpha}})(\mu_1 e^{\mu_1 s\sqrt{\lambda\alpha}} - \mu_2 e^{\mu_2 s\sqrt{\lambda\alpha}})\, ds$$

$$\Sigma_{22}(t) = \frac{1}{\eta^2 - 4}\int_0^t (\mu_1 e^{\mu_1 s\sqrt{\lambda\alpha}} - \mu_2 e^{\mu_2 s\sqrt{\lambda\alpha}})^2\, ds \tag{2.15}$$

Also,

$$\mathrm{tr}(\sigma^T \Gamma \sigma) = -\alpha + \sqrt{\alpha^2 + 2\alpha\lambda} \tag{2.16}$$

Defining V_t as in (2.9) and substituting (2.12)–(2.16) into the formula (2.10) then gives a very complicated formula for

$$\mathbf{E}\left[\exp\left\{-\frac{\lambda^2}{2}\int_0^T X_s^2\, ds\right\}\right] \tag{2.17}$$

in terms of α and λ.

3. ASYMPTOTICS FOR SMALL STIFFNESS

The purpose of this section is to investigate how the partition function (2.17) behaves as $\alpha \to \infty$. Because the explicit formula obtained in the previous section is so complicated, it would be rather messy, to say the least, just to obtain the limit of (2.17) as $\alpha \to \infty$, let alone to find the rate of convergence. (Of course we expect the large α limit of (2.17) to be identical to the Brownian case.) We develop an alternative approach to investigate the large α asymptotic behaviour.

3.1. Ordinary Differential Equations Associated with the Quadratic Functional

Again, consider the general situation of the previous section, with $\underset{\sim}{X}$ as in (2.1) and (2.3) and we wish to calculate the Laplace transform (2.2). Define

$$V_t := \frac{\lambda^2}{2}\int_0^t \underset{\sim}{X}_s^T Q \underset{\sim}{X}_s\, ds + \theta\int_0^t \underset{\sim}{X}_s^T R\, d\underset{\sim}{X}_s + \frac{1}{2}\underset{\sim}{X}_t^T S_t \underset{\sim}{X}_t + c_t \tag{3.1}$$

where Q is a given non-negative symmetric matrix, R is a given anti-symmetric matrix and we seek a symmetric matrix function S_t and a function

c so as to make $M_t := e^{-V_t}$ a martingale. (Note that S can be taken to be symmetric without loss of generality because for any matrix S and any vector x, we have $2x^T S x = x^T(S + S^T)x$.) By Itô's formula

$$\begin{aligned} dM_t &= -M_t\, dV_t + \frac{1}{2} M_t\, d[V]_t \\ &= -M_t \left\{ \frac{\lambda^2}{2} \underset{\sim}{X}_t^T Q \underset{\sim}{X}_t\, dt + \theta \underset{\sim}{X}_t^T R\, d\underset{\sim}{X}_t + \frac{1}{2} \underset{\sim}{X}_t^T \dot{S}_t \underset{\sim}{X}_t\, dt + \underset{\sim}{X}_t^T S_t\, d\underset{\sim}{X}_t \right. \\ &\quad \left. + \frac{1}{2} (d\underset{\sim}{X}_t)^T S_t\, d\underset{\sim}{X}_t + \dot{c}_t\, dt \right\} + \frac{1}{2} M_t (\theta \underset{\sim}{X}_t^T R \sigma\, dB_t + \underset{\sim}{X}_t^T S_t \sigma\, dB_t)^2 \\ &= d(\text{mart.}) - M_t \left\{ \frac{1}{2} \underset{\sim}{X}_t^T (\lambda^2 Q + \dot{S}_t)\, \underset{\sim}{X}_t\, dt + \underset{\sim}{X}_t^T (\theta R + S_t)\, E \underset{\sim}{X}_t\, dt \right. \\ &\quad \left. + \frac{1}{2} \operatorname{tr}(\sigma^T S_t \sigma)\, dt + \dot{c}_t\, dt \right\} \\ &\quad + \frac{1}{2} M_t (\theta^2 \underset{\sim}{X}_t^T R \sigma \sigma^T R^T \underset{\sim}{X}_t\, dt + 2\theta \underset{\sim}{X}_t^T S_t \sigma \sigma^T R^T \underset{\sim}{X}_t\, dt + \underset{\sim}{X}_t^T S_t \sigma \sigma^T S_t \underset{\sim}{X}_t\, dt) \end{aligned}$$

Therefore, in order that M_t be a local martingale, we require

$$\frac{dS_t}{dt} - S_t \sigma \sigma^T S_t + S_t F + F^T S_t = P \tag{3.2a}$$

$$\frac{dc_t}{dt} + \frac{1}{2} \operatorname{tr}(\sigma^T S_t \sigma) = 0 \tag{3.2b}$$

where $F = E - \theta \sigma \sigma^T R^T$ and $P = \theta^2 R \sigma \sigma^T R^T - \theta R E - \theta (RE)^T - \lambda^2 Q$. This result is very similar to that of Yashin (1993). The ODE (3.2a) is of course the famous matrix Riccati differential equation which arises frequently in the context of optimal control of linear systems with quadratic costs (e.g., Kalman-Bucy filter). The appearance of the Riccati equation in the context of Laplace transforms of quadratic functionals, while less well-documented, has nevertheless quite a long history (e.g., see Yashin (1993), Rogers and Shi (1992) and the references therein).

Specializing now to the case of (2.11) and taking $R = 0$, we see that if we could solve (3.2) with the boundary conditions $S_T = 0$ and $c_T = 0$, we would obtain

$$\mathbb{E}\left[\exp\left\{ -\frac{\lambda^2}{2} \int_0^T X_s^2\, ds \right\} \right] = \exp\left\{ -\frac{1}{2} \underset{\sim}{X}_0^T S_0 \underset{\sim}{X}_0 - c_0 \right\} \tag{3.3}$$

provided that M is actually a martingale and not just a local martingale. But by construction, M_t is of the form

$$M_t = \exp\left\{N_t - \frac{1}{2}[N]_t\right\}$$

where $dN_t = -\underset{\sim}{X}_t^T(\theta R + S_t)\sigma\, d\underset{\sim}{B}_t$. The same "non-explosion" argument as used in the previous section then shows that M is a true martingale.

Writing

$$S_t = \begin{pmatrix} f(t) & g(t) \\ g(t) & h(t) \end{pmatrix}$$

the Eqs. (3.2) become the following system of ODEs

$$\dot{f}(t) = g(t)^2 - \lambda^2 \tag{3.4a}$$

$$\dot{g}(t) = g(t)\, h(t) - \alpha(f(t) - g(t)) \tag{3.4b}$$

$$\dot{h}(t) = h(t)^2 - 2\alpha(g(t) - h(t)) \tag{3.4c}$$

$$\dot{c}(t) = -\tfrac{1}{2}h(t) \tag{3.4d}$$

Clearly, we need only solve (3.4a–c). While the appropriate boundary conditions for the law of $\int_0^T X_s^2\, ds$ are $f(T) = g(T) = h(T) = c(T) = 0$, we actually need to consider more general boundary conditions for the case of tree polymers, so we impose on (3.4) the general boundary conditions

$$f(T) = K_f, \qquad g(T) = K_g, \qquad h(T) = K_h \qquad \text{and} \qquad c(T) = K_c \tag{3.5}$$

From now on, writing $\gamma = 1/\alpha$, we can rewrite (3.4) as

$$\dot{f}(t) = g(t)^2 - \lambda^2 \tag{3.6a}$$

$$\gamma\dot{g}(t) = \gamma g(t)\, h(t) - f(t) + g(t) \tag{3.6b}$$

$$\gamma\dot{h}(t) = \gamma h(t)^2 - 2g(t) + 2h(t) \tag{3.6c}$$

To be explicit about the way in which the solution to (3.6) depends on γ, we shall sometimes write $f(\gamma, t)$, $g(\gamma, t)$ etc. We wish to study the asymptotic behaviour of the solution to (3.6) subject to boundary conditions (3.5) for small $\gamma > 0$. The idea is to use a power series in γ of the form

$$f(t) = F_0(t) + F_1(t)\,\gamma + F_2(t)\,\gamma^2 + \cdots$$

$$g(t) = G_0(t) + G_1(t)\gamma + G_2(t)\,\gamma^2 + \cdots \text{ etc.}$$

Unfortunately, the solution cannot be *uniformly* approximated by such a series throughout the entire interval $[0, T]$. Such a phenomenon has been well-documented in the literature and provided certain technical conditions are satisfied, it is possible to use a method commonly known as the "boundary layer method," which is discussed in many standard texts on singular perturbation theory for ODEs. The treatment in Wasow (1965) is particularly well-suited to our present purposes. We give here a brief sketch of the theory as it applies to our problem; the detailed proofs can be found in Sections 39–40 of Wasow (1965). Because we are solving (3.6) with boundary conditions at $t = T$ and not at $t = 0$ and because the right-hand side of (3.6) also involves γ, we need to modify the treatment of Wasow slightly, but otherwise, everything else goes through after the necessary (minor) changes have been made.

3.2. Limiting Behaviour of the ODEs for Small Stiffnes

We first appeal to a convergence theorem of Tihonov which says that as $\gamma \downarrow 0$, the solution to (3.6) converges to the solution of the so-called *reduced system* obtained by putting $\gamma = 0$ in (3.6). The next result is essentially the same as Theorem 39.1 in Wasow (1965), specialized to the present situation.

Lemma 3.1. For fixed, t, we have

$$\lim_{\gamma \to 0} f(\gamma, t) = f_0(t), \qquad \lim_{\gamma \to 0} g(\gamma, t) = g_0(t), \qquad \text{and} \qquad \lim_{\gamma \to 0} h(\gamma, t) = h_0(t)$$

where (f_0, g_0, h_0) is the solution to the reduced system

$$\dot{f}_0(t) = f_0(t)^2 - \lambda^2 \tag{3.7a}$$

$$g_0(t) = h_0(t) = f_0(t) \tag{3.7b}$$

$$f_0(T) = K_f \tag{3.7c}$$

This convergence is uniform in the interval $[0, T]$ for f and uniform in any interval $[0, T - \delta]$ $(\delta > 0)$ for the other functions g and h. (In particular, note that convergence fails near T.)

Proof. We give a rough sketch of the proof, indicating only the necessary modifications to the proof in Wasow (1965) (Theorem 39.1).

Make a "stretching transformation" as follows: put $s=(T-t)/\gamma$, so that $t=T-\gamma s$. In terms of s, the Eqs. (3.6) read

$$f'(s) = -\gamma(g(s)^2 - \lambda^2) \tag{3.8a}$$

$$g'(s) = -\gamma g(s)\, h(s) + f(s) - g(s) \tag{3.8b}$$

$$h'(s) = -\gamma h(s)^2 + 2g(t) - 2h(t) \tag{3.8c}$$

where, by a slight abuse of notation, we have written $f(s)=f(\gamma, s)=f(\gamma, T-\gamma s)$ etc. and of course $f'(s)=df(\gamma, T-\gamma s)/ds$. The boundary conditions (3.5) then become

$$f(0)=K_f, \qquad g(0)=K_g, \qquad h(0)=K_h \qquad \text{and} \qquad c(0)=K_c \tag{3.9}$$

Putting $\gamma=0$ in (3.8) gives the so-called *boundary layer equation* corresponding to (3.6):

$$\tilde{f}'(s)=0 \tag{3.10a}$$

$$\tilde{g}'(s)=\tilde{f}(s)-\tilde{g}(s) \tag{3.10b}$$

$$\tilde{h}'(s)=2\tilde{g}(t)-2\tilde{h}(t) \tag{3.10c}$$

whose solution, subject to (3.9) is

$$\begin{aligned} \tilde{f}(s) &= K_f \\ \tilde{g}(s) &= (K_g - K_f)\, e^{-s} + K_f \\ \tilde{h}(s) &= (K_h + K_f - 2K_g)\, e^{-2s} + 2(K_g - K_f)\, e^{-s} + K_f \end{aligned} \tag{3.11}$$

Since the right-hand side of (3.8) depends continuously on γ, we have

$$\lim_{\gamma \to 0} f(\gamma, s) = \lim_{\gamma \to 0} f(\gamma, T-\gamma s) = \tilde{f}(s),$$

$$\lim_{\gamma \to 0} g(\gamma, s) = \tilde{g}(s), \qquad \text{and} \qquad \lim_{\gamma \to 0} h(\gamma, s) = \tilde{h}(s)$$

From (3.11), we see that the boundary layer Eq. (3.10) is (uniformly) asymptotically stable, with stable fixed point $\tilde{f} \equiv \tilde{g} \equiv \tilde{h} \equiv K_f$ whose domain of attraction is the entire $\mathbb{R}^3$. We may therefore take s_0 so large that the points $(K_f, \tilde{g}(s), \tilde{h}(s))$ for $s \geqslant s_0$ lie near the fixed point (K_f, K_f, K_f). Also, we may take γ so small that the points $(f(\gamma, s), g(\gamma, s), h(\gamma, s))$ for $s \leqslant s_0$ lie near to $(K_f, \tilde{g}(s), \tilde{h}(s))$. In particular, when $t=T-\gamma s_0$, the solution $(f(\gamma, t), g(\gamma, t), h(\gamma, t))$ to (3.6) is in a neighbourhood tube of the straight line (x, x, x) in $\mathbb{R}^3$. It can be shown that this actually holds for all $t \leqslant T-\gamma s_0$ (see e.g., Wasow (1965) Lemma 39.2). The rest is an easy argument and can be found in the proof of Theorem 39.1 of Wasow (1965). ∎

As pointed out in Wasow (1965), we have actually shown more: we have shown that convergence is not only uniform in the interval $[0, T-\delta]$ (for fixed δ) but actually in the expanding interval $[0, T-\gamma s_0]$ as $\gamma \to 0$. Also, the trajectory to (3.6) tends uniformly to a curve in $\mathbb{R}^3$ consisting of two contiguous pieces: one is described parametrically by the solution $(\tilde{f}(s), \tilde{g}(s), \tilde{h}(s))$, $0 \leqslant s < \infty$ to (3.10) and the other is described parametrically by the solution $(f_0(t), g_0(t), h_0(t))$, $0 \leqslant t \leqslant T'$ to (3.7).

Next, we develop series expansions in powers of γ for the solution to (3.6). From the preceding analysis, it is clear that no single series can approximate the solution in the whole interval $[0, T]$; separate treatments are required in a neighbourhood of T—the "boundary layer," as it is commonly known—and away from T.

3.3. Series Approximations to the Solution I: Outside the Boundary Layer

Consider the series

$$\begin{aligned} f(t) &= F_0(t) + F_1(t)\,\gamma + F_2(t)\,\gamma^2 + \cdots \\ g(t) &= G_0(t) + G_1(t)\,\gamma + G_2(t)\,\gamma^2 + \cdots \\ h(t) &= H_0(t) + H_t(t)\,\gamma + H_2(t)\,\gamma^2 + \cdots \end{aligned} \tag{3.12}$$

From the proof of Lemma 3.1, we must necessarily have $F_0 \equiv f_0$, $G_0 \equiv g_0$ etc. where (f_0, g_0, h_0) satisfy (3.7), but (3.12) cannot hold for t close to T—in particular, we do not know at this stage what are the appropriate boundary conditions for $F_1, F_2, \ldots, G_1, G_2, \ldots$ etc. at $t = T$. The other coefficients F_k, G_k etc. can be found by substituting (3.12) into (3.6) and equating powers of γ. Thus

$$\begin{aligned} \dot{F}_1 - 2G_0G_1 &= 0 \\ \dot{G}_0 + F_1 - G_1 - G_0H_0 &= 0 \\ \dot{H}_0 + 2G_1 - 2H_1 - H_0^2 &= 0 \end{aligned} \tag{3.13}$$

The main problem with (3.13) is to decide what are the appropriate boundary values at $t = T$; once these are known, (3.13) is easy to solve.

3.4. Series Approximations to the Solution II: Inside the Boundary Layer

The behaviour of (f, g, h) inside the boundary layer can be analysed by means of the stretching transformation $s = (T-t)/\gamma$, which transforms

(3.6) into (3.8), whose solution has convergent expansions in powers of γ of the form

$$\begin{aligned} f(t) &= \tilde{F}_0(s) + \tilde{F}_1(s)\,\gamma + \tilde{F}_2(s)\,\gamma^2 + \cdots \\ g(t) &= \tilde{G}_0(s) + \tilde{G}_1(s)\,\gamma + \tilde{G}_2(s)\,\gamma^2 + \cdots \\ h(t) &= \tilde{H}_0(s) + \tilde{H}_t(s)\,\gamma + \tilde{H}_2(s)\,\gamma^2 + \cdots \end{aligned} \tag{3.14}$$

because the right-hand side of (3.8) is analytic. Standard theory tells us that $\tilde{F}_0 \equiv \tilde{f}$, $\tilde{G}_0 \equiv \tilde{g}$ etc. where $(\tilde{f}, \tilde{g}, \tilde{h})$ satisfy (3.10) and are given by (3.11), and that $\tilde{F}_k(0) = \tilde{G}_k(0) = \tilde{H}_k(0) = 0$ for $k \geqslant 1$. The coefficients $\tilde{F}_k$, $\tilde{G}_k$ etc., can then be found by substituting (3.14) into (3.8) and equating powers of γ as before. Thus

$$\begin{aligned} \tilde{F}_1'(s) &= -\tilde{G}_0(s)^2 + \lambda^2 \\ \tilde{G}_1'(s) &= -\tilde{G}_1(s) + \tilde{F}_1(s) - \tilde{G}_0(s)\,\tilde{H}_0(s) \\ \tilde{H}_1'(s) &= -2\tilde{H}_1(s) + 2\tilde{G}_1(s) - \tilde{H}_0(s)^2 \end{aligned} \tag{3.15}$$

$\tilde{F}_1(0) = \tilde{G}_1(0) = \tilde{H}_1(0) = 0$. Note that (3.15) is a system of linear non-homogeneous ODEs and is therefore easy to solve, although the solution is quite messy.

3.5. Matching the Two Series Approximations

The series (3.14) approximate the solution inside the boundary layer while (3.12) approximate the solution outside the boundary layer (once we know the values of $F_1(T)$, $G_1(T)$, etc.); we still need to match up these two different approximations. This can be done by a method due to Vasil'eva and is presented in Section 40 of Wasow (1965). The basic idea involves first formally expanding the coefficients F_k, G_k, and H_k in (3.12) as (possibly divergent) Taylor series of the form

$$\begin{aligned} F_k(t) &= \sum_{j=0}^{\infty} F_{kj}(T-t)^j = \sum_{j=0}^{\infty} F_{kj} s^j \gamma^j \\ G_k(t) &= \sum_{j=0}^{\infty} G_{kj}(T-t)^j = \sum_{j=0}^{\infty} G_{kj} s^j \gamma^j \\ H_k(t) &= \sum_{j=0}^{\infty} H_{kj}(T-t)^j = \sum_{j=0}^{\infty} H_{kj} s^j \gamma^j \end{aligned} \tag{3.16}$$

and then substituting these formal Taylor series into (3.12) and rearranging the powers of γ, giving series of the form

$$\begin{aligned} f(t) &= \hat{F}_0(s) + \hat{F}_1(s)\,\gamma + \hat{F}_2(s)\,\gamma^2 + \cdots \\ g(t) &= \hat{G}_0(s) + \hat{G}_1(s)\,\gamma + \hat{G}_2(s)\,\gamma^2 + \cdots \\ h(t) &= \hat{H}_0(s) + \hat{H}_1(s)\,\gamma + \hat{H}_2(s)\,\gamma^2 + \cdots \end{aligned} \tag{3.17}$$

where

$$\hat{F}_k(s) = \sum_{j=0}^{k} F_{k-j,j} s^j, \qquad \hat{G}_k(s) = \sum_{j=0}^{k} G_{k-j,j} s^j, \qquad \hat{H}_k(s) = \sum_{j=0}^{k} H_{k-j,j} s^j$$

By construction, it is reasonable to expect the series (3.17) to be close to (3.12) for small values of s, i.e., for values of t close to T—inside the boundary layer, where the series (3.12) do not approximate the solution to (3.6). On the other hand, the series (3.17) and (3.14) are both solutions (at least formally) to the "stretched" ODEs (3.8), the main difference being that the coefficients in (3.17) have different initial values: for $k \geqslant 1$

$$\hat{F}_k(0) = F_k(T) = F_{k0}, \quad \hat{G}_k(0) = G_k(T) = G_{k0}, \quad \hat{H}_k(0) = H_k(T) = H_{k0} \tag{3.18}$$

For $k = 0$, the corresponding initial values are given by (3.7b, c) and by definition

$$\hat{F}_0 \equiv \hat{G}_0 \equiv \hat{H}_0 \equiv K_f \tag{3.19}$$

Once again, the coefficients in (3.17) are found by substitution into (3.8). Thus

$$\begin{aligned} \hat{F}_1'(s) &= -K_f^2 + \lambda^2 \\ \hat{G}_1'(s) &= -\hat{G}_1(s) + \hat{F}_1(s) - K_f^2 \\ \hat{H}_1'(s) &= -2\hat{H}_1(s) + 2\hat{G}_1(s) - K_f^2 \end{aligned} \tag{3.20}$$

(These are, of course, the same equations as (3.15) but taking into account the new definitions (3.18) and (3.19).) It is clear from (3.15) that the coefficients in (3.14) are in general very different from those in (3.17), which are polynomials in s. It turns out that for special choices of initial values for (3.20), the difference between these coefficients (i.e., between the functions with tildes appearing (3.14) and the corresponding ones with hats appearing in (3.17)) can be made exponentially small for large s (i.e., outside the

boundary layer), and it is these which are the appropriate initial values for (3.20), and hence the appropriate final values at $t = T$ for (3.13). The choice of these initial values is described in Section 40 of Wasow (1965); we shall not go into the details here. (When specialized to our example, the choice of initial values described in Wasow (1965) is given by (3.23) below.)

3.6. A Uniform Approximation to the Solution

The three power series described in Sections 3.3–3.5 can now be combined to produce a series which approximates the solution (f, g, h) to (3.6) uniformly in the whole interval $[0, T]$. The next result is essentially the same as Theorem 40.1 of Wasow (1965): Wasow only deals with the case of equations in $\mathbb{R}^2$, but the analysis is virtually identical in $\mathbb{R}^n$.

Theorem 3.2. Fix $T, \gamma > 0$ and let $s = (T - t)/\gamma$. Consider the sums

$$f_N(t) = \sum_{j=0}^{N} (F_j(t) + \tilde{F}_j(s) - \hat{F}_j(s))\, \gamma^j \tag{3.21a}$$

$$g_N(t) = \sum_{j=0}^{N} (G_j(t) + \tilde{G}_j(s) - \hat{G}_j(s))\, \gamma^j \tag{3.21b}$$

$$h_N(t) = \sum_{j=0}^{N} (H_j(t) + \tilde{H}_j(s) - \hat{H}_j(s))\, \gamma^j \tag{3.21c}$$

Then, as $N \to \infty$,

$$f_N(t) \to f(t), \qquad g_N(t) \to g(t), \qquad h_N(t) \to h(t)$$

uniformly in $t \in [0, T]$.

The intuitive explanation for Theorem 3.2 should by now be clear: by construction, we expect these to be close to $\sum_{j=0}^{\infty} \tilde{F}_j(s)\, \gamma^j$ etc., for small values of s (inside the boundary layer) and by choosing the initial values for (3.20) carefully, they can be made to be close to $\sum_{j=0}^{\infty} F_j(t)\, \gamma^j$ etc., for large values of s (outside the boundary layer).

3.7. Explicit Computation of the Leading Terms

We shall compute the terms in the series (3.21) up to the first order. For the approximation inside the boundary layer, the 0-order coefficients are already given by (3.11). The solution to (3.15) is

$$\tilde{F}_1(s) = \lambda^2 s - \left\{ \frac{(K_g - K_f)^2(1 - e^{-2s})}{2} + 2K_f(K_g - K_f)(1 - e^{-s}) + K_f^2 s \right\} \tag{3.22a}$$

$$\begin{aligned}\tilde{G}_1(s) = {} & \frac{(K_f - 2K_g + K_h)(K_g - K_f)}{2} e^{-3s} \\ & + \frac{5K_f^2 - 10K_f K_g + 3K_g^2 + 2K_f K_h}{2} e^{-2s} \\ & + K_f(K_f - K_g)\, s e^{-s} - \frac{7K_f^2 - 9K_f K_g + K_f K_h + K_g K_h - 2\lambda^2}{2} e^{-s} \\ & + \frac{3K_f^2 - 2K_f K_g - K_g^2 - 2\lambda^2 - 2K_f^2 s + 2\lambda^2 s}{2}\end{aligned} \tag{3.22b}$$

$$\begin{aligned}\tilde{H}_1(s) = {} & 3(K_f - 2K_g + K_h)(K_g - K_f)\, e^{-3s} \\ & + \frac{12K_f^2 - 26K_f K_g + 9K_g^2 + 6K_f K_h - K_h^2 - \lambda^2}{2} e^{-2s} \\ & - (5K_f^2 - 7K_f K_g + K_f K_h + K_g K_h - 2\lambda^2 - 2K_f^2 s + 2K_f K_g s)\, e^{-s} \\ & + \frac{3K_f^2 - 2K_f K_g - K_g^2 - 3\lambda^2 - 2K_f^2 s + 2\lambda^2 s}{2}\end{aligned} \tag{3.22c}$$

Consider next the solution to (3.20). In our particular example, the appropriate initial values are

$$\hat{F}_1(0) = \int_0^\infty (\hat{G}_0(s)^2 - K_f^2)\, ds = -\frac{3K_f^2 - 2K_f K_g - K_g^2}{2} \tag{3.23a}$$

$$\hat{G}_1(0) = \hat{F}_1(0) - \lambda^2 \tag{3.23b}$$

$$\hat{H}_1(0) = \hat{F}_1(0) - \frac{3\lambda^2}{2} \tag{3.23c}$$

This gives the solution to (3.20) as

$$\hat{F}_1(s) = (\lambda^2 - K_f^2)\, s + \frac{3K_f^2 - 2K_f K_g - K_g^2}{2} \tag{3.24a}$$

$$\hat{G}_1(s) = \frac{3K_f^2 - 2K_f K_g - K_g^2 - 2\lambda^2 - 2K_f^2 s + 2\lambda^2 s}{2} \tag{3.24b}$$

$$\hat{H}_1(s) = \frac{3K_f^2 - 2K_f K_g - K_g^2 - 3\lambda^2 - 2K_f^2 s + 2\lambda^2 s}{2} \tag{3.24c}$$

(The 0-order coefficients are given by (3.19).) Observe that the differences $\tilde{F}_0(s)-\hat{F}_0(s)$, $\tilde{F}_1(s)-\hat{F}_1(s)$ etc., are indeed exponentially small for large s, as asserted earlier.

Finally, for the solution outside the boundary layer, we already know that $F_0=G_0=H_0$ satisfy (3.7), the solution to which is

$$F_0(t)=G_0(t)=H_0(t)=\frac{\lambda[\lambda+K_f-(\lambda-K_f)\,e^{-(T-t)}]}{\lambda+K_f+(\lambda-K_f)\,e^{-(T-t)}} \tag{3.25}$$

(When $K_f=0$, we leave the reader to check the special case of the formula (3.3), that

$$\mathbb{E}\left[\exp\left\{-\frac{\lambda^2}{2}\int_0^T B_s^2\,ds\right\}\right]=\exp\left\{-\frac{1}{2}F_0(0)\,x^2-c(0)\right\}$$

where $c(t)=2^{-1}\int_t^T H_0(u)\,du$, indeed agrees with the well-known expression for the Laplace transform of $\int_0^T B_s^2\,ds$, which can be found in Chan *et al.* (1994) or Yor (1992).) The solution to (3.13) with boundary values $F_1(T)=\hat{F}_1(0)$, $G_1(T)=\hat{G}_1(0)$ and $H_1(T)=\hat{H}_1(0)$ as given by (3.23) is

$$F_1(t)=\frac{4\lambda^2(F_1(T)-\lambda^2)}{[(\lambda+K_f)\,e^{\lambda(T-t)}+(\lambda-K_f)\,e^{-\lambda(T-t)}]^2}+\lambda^2 \tag{3.26a}$$

$$G_1(t)=F_1(t)-\lambda^2=\frac{4\lambda^2(F_1(T)-\lambda^2)}{[(\lambda+K_f)\,e^{\lambda(T-t)}+(\lambda-K_f)\,e^{-\lambda(T-t)}]^2} \tag{3.26b}$$

$$H_1(t)=F_1(t)-\frac{3\lambda^2}{2}=\frac{4\lambda^2(F_1(T)-\lambda^2)}{[(\lambda+K_f)\,e^{\lambda(T-t)}+(\lambda-K_f)\,e^{-\lambda(T-t)}]^2}-\frac{\lambda^2}{2} \tag{3.26c}$$

(The expressions (3.22), (3.24), and (3.26), while rather messy, are readily obtained with the aid of a suitable computer package such as Mathematica.)

We can now put all this together to find the first two terms in the series (3.21) and we shall see this in action in the examples in the next section.

4. EXAMPLES

4.1. Single-Chain Polymer: Uniform Resistance Measure

We consider first the simplest case, namely that of a single-chain polymer modelled by the process X in (1.2). We shall present an asymptotic expression for the partition function Z as in (1.0), up to leading order in $\gamma=1/\alpha$. The treatment of this simplest case presented below contains most of the essential ideas which will be adapted to more complicated situations.

We take $r(ds)$ to be Lebesgue measure, in which case (1.0) may be rewritten as

$$Z = \mathbf{E}^0\left[\exp\left\{-\frac{\lambda^2}{2}\left[\int_0^T X_s^2\,ds - \frac{1}{T}\left(\int_0^T X_s\,ds\right)^2\right]\right\}\right] \tag{4.1}$$

(The superscript 0 on $\mathbb{E}$ above indicates we are taking expectation with respect to the law of X with $X_0 = 0$. There is no loss of generality in this as (4.1) is translation-invariant.)

Our first task is to express Z in terms of the solution to (3.6), f, g, etc. We can then make use of the asymptotic expansions developed in Section 3 for these functions.

Proposition 4.1. Suppose that $U_0 = 0$ for the OU process (1.2b). Then the partition function Z given by (4.1) can be expressed in terms of the solution to (3.6) as follows:

$$Z = \frac{\lambda\sqrt{T}\,e^{-c(0)}}{\sqrt{f(0)}} \tag{4.2}$$

Proof. Using the trick of "uncompleting the square" and mixing over an independent standard Gaussian random variable G that was introduced in Chan *et al.* (1994), we observe that

$$Z = \mathbb{E}^0\left[\exp\left\{-\frac{\lambda^2}{2}\int_0^T X_s^2\,ds - \frac{G\lambda}{\sqrt{T}}\int_0^T X_s\,ds\right\}\right] \tag{4.3}$$

(The expectation in (4.3) is taken with respect to the joint (product) law of X and G.) Therefore, defining

$$\hat{Z}(v) := \mathbb{E}^0\left[\exp\left\{-\frac{\lambda^2}{2}\int_0^T X_s^2\,ds - \frac{v\lambda}{\sqrt{T}}\int_0^T X_s\,ds\right\}\right]$$

we have $Z = \mathbb{E}[\hat{Z}(G)]$, where this last expectation is with respect to the law of G. But

$$\begin{aligned}\hat{Z}(v) &= e^{v^2/2}\mathbb{E}^0\left[\exp\left\{-\frac{\lambda^2}{2}\int_0^T\left(X_s + \frac{v}{\lambda\sqrt{T}}\right)^2 ds\right\}\right] \\ &= e^{v^2/2}\mathbb{E}^{v/(\lambda\sqrt{T})}\left[\exp\left\{-\frac{\lambda^2}{2}\int_0^T X_s^2\,ds\right\}\right] \\ &= e^{v^2/2}\exp\left\{-\frac{1}{2}\underset{\sim}{X}_0^T S_0 \underset{\sim}{X}_0 - c(0)\right\}\end{aligned} \tag{4.4}$$

according to (3.3). (Here, of course, $\underset{\sim}{X}_0^T = (v/(\lambda\sqrt{T}), U_0)$.) If $U_0 = 0$, we have

$$\hat{Z}(v) = \exp\left\{-\frac{v^2}{2}\left(\frac{f(0)}{\lambda^2 T} - 1\right) - c(0)\right\} \tag{4.5}$$

where $c(0) = 2^{-1}\int_0^T h(s)\,ds$ and f, g, h satisfy (3.4a)–(3.4c) and (3.5) with $K_f = K_g = K_h = 0$. Finally, using the well-known formula for the Laplace transform of a χ^2 random variable, we obtain

$$Z = \mathbb{E}[\hat{Z}(G)] = \frac{\lambda\sqrt{T}\,e^{-c(0)}}{\sqrt{f(0)}} \quad \blacksquare$$

Remark. Of course the same method will work for a general non-zero (and even random) U_0. Indeed, for our model, we should really take $U_0 \sim N(0, (2\alpha)^{-1})$ otherwise the results (1.3)–(1.5) are no longer true. However, taking $U_0 = 0$ will not change the large α asymptotic of the model, only the small α asymptotics. We take $U_0 = 0$ for the sake of simplicity, to avoid messy algebra.

Proposition 4.1 now allows us to use the asymptotic expansions obtained in the preceding section to study the asymptotic behaviour of Z. The analysis in Section 3.7 for the special case $K_f = K_g = K_h = 0$ gives the following asymptotic expansions as $\gamma = 1/\alpha \to 0$:

$$\begin{aligned}
f(t) &= \lambda\tanh[\lambda(T-t)] + \gamma\lambda^2(1 - \operatorname{sech}^2[\lambda(T-t)]) + o(\gamma)\\
g(t) &= \lambda\tanh[\lambda(T-t)] - \gamma\lambda^2(\operatorname{sech}^2[\lambda(T-t)] - e^{-(T-t)/\gamma} + o(\gamma)\\
h(t) &= \lambda\tanh[\lambda(T-t)] - \frac{\gamma\lambda^2}{2}(1 + 2\operatorname{sech}^2[\lambda(T-t)] - 4e^{-(T-t)/\gamma}\\
&\quad + e^{-2(T-t)/\gamma}) + o(\gamma)
\end{aligned} \tag{4.6}$$

These asymptotic expansions hold uniformly for $t \in [0, T]$, so integrating the expansion for h term by term gives

$$c(0) = 2^{-1}\int_0^T h(s)\,ds = \frac{\log\cosh(\lambda T)}{2} + \frac{\gamma\lambda(\tanh(\lambda T) - \lambda T)}{4} + o(\gamma) \tag{4.7}$$

Substituting (4.6) and (4.7) into (4.2) and using the binomial theorem gives

$$Z = \left(\frac{\lambda T}{\sinh(\lambda T)}\right)^{1/2} - \frac{\gamma\lambda}{4}\left(\frac{\lambda T}{\sinh(\lambda T)}\right)^{1/2}(3\tanh(\lambda T) - \lambda T) + o(\gamma) \tag{4.8}$$

in which we recognize the 0-order term as that for the Brownian case (corresponding to a completely flexible single chain) which was obtained in Chan *et al.* (1994), and the first-order correction in the case of small stiffness parameter can also be easily read-off.

4.2. Single-Chain Polymer: Uniform Resistance Measure with Atoms

The method of Lemma 3.1 can also deal with the case where the resistance measure has atoms. This situation arises when particles are attached to the ends of polymer strands. As a simple example, consider a single polymer chain with a particle attached at each end. The resistance measure would then take the form $r(ds) = ds + a_0\delta_0(ds) + a_T\delta_T(ds)$ for some a_0, $a_T > 0$. The partition function Z can still be calculated by "uncompleting the square": $Z = \mathbb{E}[\hat{Z}(G)]$ where

$$\begin{aligned}
\hat{Z}(v) &= \mathbb{E}^0\left[\exp\left\{-\frac{\lambda^2}{2}\int_0^T X_s^2 r(ds) - \frac{v\lambda}{\sqrt{T+a_0+a_T}}\int_0^T X_s r(ds)\right\}\right] \\
&= e^{v^2/2}\,\mathbb{E}^0\left[\exp\left\{-\frac{\lambda^2}{2}\int_0^T \left(X_s + \frac{v}{\lambda\sqrt{T+a_0+a_T}}\right)^2 r(ds)\right\}\right] \\
&= e^{v^2/2}\,\mathbb{E}^{v/(\lambda\sqrt{T+a_0+a_T})}\left[\exp\left\{-\frac{\lambda^2}{2}\int_0^T X_s^2 r(ds)\right\}\right] \\
&= e^{v^2/2}\,\mathbb{E}^{v/(\lambda\sqrt{T+a_0+a_T})}\left[\exp\left\{-\frac{\lambda^2}{2}\int_0^T X_s^2\,ds - \frac{\lambda^2}{2}(a_T X_T^2 + a_0 X_0^2)\right\}\right] \\
&= e^{v^2(1-a_0/(T+a_0+a_T))/2}\exp\left\{-\frac{1}{2}\underset{\sim}{X}_0^T S_0 \underset{\sim}{X}_0 - c(0)\right\}
\end{aligned}$$

where, according to (3.1)–(3.3), S and c are the solutions to (3.2) with $R = 0$ and boundary conditions

$$S_T = \lambda^2 a_T \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad c(T) = 0$$

which simply translates to $K_g = K_h = 0$ and $K_f = \lambda^2 a_T$ in the context of the asymptotic expansions developed earlier.

4.3. Branching Polymers: Some Generalities

We next turn our attention to the case of branching polymers, modelled as a (deterministic) branching version of the process X at (1.2a). This is done by using a tree $\mathscr{T}$ instead of an interval $[0, T]$ for the index set of the process X. (As a set, we regard $\mathscr{T}$ as consisting of the nodes and points along the branch segments.) We take the root as the time origin, which will be denoted by 0. Let $\preccurlyeq$ be the natural partial ordering on $\mathscr{T}$ and for $s, t \in \mathscr{T}$ we denote by $s \wedge t$ the most recent common ancestor of s and t. Thus $\{s \in \mathscr{T}: s \preccurlyeq t\}$ is the unique path from 0 to t. By a process (X, U) indexed by $\mathscr{T}$, we mean process which satisfies (1.2) along each branch segment and given $(X_{s\wedge t}, U_{s\wedge t})$, (X_s, U_s) and (X_t, U_t) are conditionally independent.

We are interested in calculating the tree partition function

$$Z_{\mathscr{T}} = \mathbb{E}\left[\exp\left\{-\frac{\lambda^2}{2}\int_{\mathscr{T}} (X_t - \bar{X})^2\, dt\right\}\right]$$

where $\bar{X} = \rho \int_{\mathscr{T}} X_t\, dt$ and $\rho^{-1} = \int_{\mathscr{T}} dt$. Note that we are assuming here that the polymer branches are freely jointed at the nodes and the stiffness occurs only along the individual branches. As before, the same trick of mixing over an independent standard Gaussian random variable G shows that

$$Z_{\mathscr{T}} = \mathbb{E}^0\left[\exp\left\{-\frac{\lambda^2}{2}\int_{\mathscr{T}} X_s^2\, ds - G\lambda\sqrt{\rho}\int_{\mathscr{T}} X_s\, ds\right\}\right] \tag{4.9}$$

(The superscript $\mathbb{E}^0$ in (4.9) is a *space* variable: $\mathbb{E}^x$ denotes expectation with respect to the law of X when $X_0 = x$.) Define

$$\begin{aligned}\hat{Z}_{\mathscr{T}}(v) &:= \mathbb{E}^0\left[\exp\left\{-\frac{\lambda^2}{2}\int_{\mathscr{T}} X_s^2\, ds - v\lambda\sqrt{\rho}\int_{\mathscr{T}} X_s\, ds\right\}\right] \\ &= e^{v^2/2}\mathbb{E}^0\left[\exp\left\{-\frac{\lambda^2}{2}\int_{\mathscr{T}}\left(X_s + \frac{v\sqrt{\rho}}{\lambda}\right)^2 ds\right\}\right] \\ &= e^{v^2/2}\mathbb{E}^{v\sqrt{\rho}/\lambda}\left[\exp\left\{-\frac{\lambda^2}{2}\int_{\mathscr{T}} X_s^2\, ds\right\}\right] \end{aligned} \tag{4.10}$$

We then have $Z_{\mathscr{T}} = \mathbb{E}[\hat{Z}_{\mathscr{T}}(G)]$. Our aim therefore is to compute the functional

$$\mathbb{E}^x\left[\exp\left\{-\frac{\lambda^2}{2}\int_{\mathscr{T}} X_s^2\, ds\right\}\right]$$

which we do by means of the next result.

Proposition 4.2. Given a tree $\mathscr{T}$ with an arbitary choice of root 0, let S_t and $c(t)$ satisfy the Riccati Eq. (3.2) with $R=0$ on each branch of the tree, subject to the following (recursive) boundary condition at the nodes: for each node t_i which is a free-end (and which is not the root), $S(t_i)=c(t_i)=0$; for each internal node n_i with k children (i.e., there are $k+1$ branches leading from node n_i), $S(n_i)=S_1(n_i)+S_2(n_i)+\cdots+S_k(n_i)$ and $c(n_i)=c_1(n_i)+c_2(n_i)+\cdots+c_k(n_i)$ where S_i and c_i are the solutions to (3.2) along each of the k descendent branches of node n_i, subject to the same boundary condition as just described. Then

$$\mathbb{E}^x\left[\exp\left\{-\frac{\lambda^2}{2}\int_{\mathscr{T}} X_s^2\,ds\right\}\right]=\exp\left\{-\frac{1}{2}\underset{\sim}{X}_0^T S_0 \underset{\sim}{X}_0 - c(0)\right\}$$

where $\underset{\sim}{X}_0^T=(X_0, U_0)$.

Proof. Define the functional

$$F_{\mathscr{T}}:=\exp\left\{-\frac{\lambda^2}{2}\int_{\mathscr{T}} X_s^2\,ds\right\}$$

If the root 0 has more than 1 descendent, then because of independence along each of the branches which descend from 0, we have $F_{\mathscr{T}}=F_{\mathscr{T}_1}F_{\mathscr{T}_2}\cdots F_{\mathscr{T}_k}$, where $\mathscr{T}_i$ denote the subtree consisting of 0 and the descendents of the ith child of 0. Therefore, we can assume without loss of generality that 0 has only one descendent, and the branch leading down from 0 to the first node n_1 will be denoted by $(0, n_1)$. Suppose that node n_1 has k descendents and let $\mathscr{T}_i$ now denote the subtree consisting of n_1 and the descendents of the ith child of n_1. Then by the conditional independence structure on the tree and the Markov property

$$\begin{aligned}
\mathbb{E}[F_{\mathscr{T}}] &= \mathbb{E}[F(0,n_1)\,F_{\mathscr{T}_1}F_{\mathscr{T}_2}\cdots F_{\mathscr{T}_k}] \\
&= \mathbb{E}\{\mathbb{E}[F(0,n_1)\,F_{\mathscr{T}_1}F_{\mathscr{T}_2}\cdots F_{\mathscr{T}_k}\mid \mathscr{F}_{n_1}]\} \\
&= \mathbb{E}\{F(0,n_1)\,\mathbb{E}[F_{\mathscr{T}_1}\mid \mathscr{F}_{n_1}]\,\mathbb{E}[F_{\mathscr{T}_2}\mid \mathscr{F}_{n_1}]\cdots\mathbb{E}[F_{\mathscr{T}_k}\mid \mathscr{F}_{n_1}]\} \\
&= \mathbb{E}\{F(0,n_1)\,\mathbb{E}^{X(n_1)}[F_{\mathscr{T}_1}]\cdots\mathbb{E}^{X(n_1)}[F_{\mathscr{T}_k}]\}
\end{aligned}$$

By induction, it is therefore sufficient to prove the proposition for the simple star-shaped tree consisting of a central internal node n_1 and $k+1$ branches $(0, n_1)$, (n_1, n_1+t_1), (n_1, n_1+t_2),.., (n_1, n_1+t_k), where the t_i are free-ends. (Our notation is intended to suggest that the ith branch is of length t_i.) Without loss of generality, we may take $k=2$. From the

one-dimensional case we treated earlier in Section 3, we know that

$$\mathbb{E}^{\underset{\sim}{X}(n_1)}[F_{\mathscr{T}_1}] = \exp\{-\tfrac{1}{2}\underset{\sim}{X}^T(n_1)\, S_1(0)\, \underset{\sim}{X}(n_1) - c_1(0)\}$$

$$\mathbb{E}^{\underset{\sim}{X}(n_1)}[F_{\mathscr{T}_2}] = \exp\{-\tfrac{1}{2}\underset{\sim}{X}^T(n_1)\, S_2(0)\, \underset{\sim}{X}(n_1) - c_2(0)\}$$

where S_i and c_i are solutions to (3.2) with boundary conditions $S_i(t_i) = c_i(t_i) = 0$. (Of course, here $S_i(0)$ and $c_i(0)$ denote the values at the node n_1! Along the branch $(0, n_1)$, we solve (3.2) with the "branching" boundary condition $S(n_1) = S_1(0) + S_2(0)$ and $c(n_1) = c_1(0) + c_2(0)$. Therefore

$$\begin{aligned}
&\mathbb{E}^{\underset{\sim}{X}(n_1)}[F_{\mathscr{T}_1}]\, \mathbb{E}^{\underset{\sim}{X}(n_1)}[F_{\mathscr{T}_2}] \\
&\quad = \exp\{-\tfrac{1}{2}\underset{\sim}{X}^T(n_1)[S_1(0) + S_2(0)]\, \underset{\sim}{X}(n_1) - [c_1(0) + c_2(0)]\} \\
&\quad = \exp\{-\tfrac{1}{2}\underset{\sim}{X}^T(n_1)\, S(n_1)\, \underset{\sim}{X}(n_1) - c(n_1)\}
\end{aligned}$$

Hence

$$\begin{aligned}
&\mathbb{E}\{F(0, n_1)\, \mathbb{E}^{\underset{\sim}{X}(n_1)}[F_{\mathscr{T}_1}]\, \mathbb{E}^{\underset{\sim}{X}(n_1)}[F_{\mathscr{T}_k}]\} \\
&\qquad = \mathbb{E}[M_n] = M_0 = \exp\{-\tfrac{1}{2}\underset{\sim}{X}_0^T S(0)\, \underset{\sim}{X}_0 - c(0)\}
\end{aligned}$$

where $M_t = e^{-V_t}$, with V defined in (3.1), is a martingale along $(0, n_1)$. ∎

Note. The process M constructed from S and c satisfying the "branching" boundary condition stated above is not quite a tree martingale on $\mathscr{T}$, in the obvious sense that $\mathbb{E}[M_t \mid \mathscr{F}_s] = M_{s \wedge t}$, although it is a martingale along each individual branch segment of $\mathscr{T}$.

4.4. A 3-Branched Star Polymer

As an example of Proposition 4.2 in action, we consider the simplest tree, namely a star shape with 3 branches leading from a central node n_1. We continue to take $U_0 = 0$ for simplicity.

Let one of the free ends be the root 0 and denote the other 2 free ends by t_1 and t_2 as before. Consider the asymptotic expansions obtained in the previous section for this case. Let $f^{(1)}$, $g^{(1)}$ etc., denote the solution to (3.6) along the branch $(n_1, n_1 + t_1)$ and similarly let $f^{(2)}, g^{(2)}$ etc., denote the solution along the branch $(n_1, n_1 + t_2)$. Along both of these branches, the

boundary conditions correspond to the case $K_{f^{(i)}} = K_{g^{(i)}} = K_{h^{(i)}} = 0$, so as before, we have

$$
\begin{aligned}
f^{(i)}(t) &= \lambda \tanh[\lambda(t_i - t)] + \gamma\lambda^2(1 - \operatorname{sech}^2[\lambda(t_i - t)]) + o(\gamma) \\
g^{(i)}(t) &= \lambda \tanh[\lambda(t_i - t)] - \gamma\lambda^2(\operatorname{sech}^2[\lambda(t_i - t)] - e^{-(t_i - t)/\gamma} + o(\gamma) \\
h^{(i)}(t) &= \lambda \tanh[\lambda(t_i - t)] - \frac{\gamma\lambda^2}{2}(1 + 2\operatorname{sech}^2[\lambda(t_i - t)] \\
&\quad - 4e^{-(t_i - t)/\gamma} + e^{-2(t_i - t)/\gamma}) + o(\gamma) \\
c^{(i)}(0) &= 2^{-1}\int_0^{t_i} h^{(i)}(s)\, ds = \frac{\log\cosh(\lambda t_i)}{2} + \frac{\gamma\lambda(\tanh(\lambda t_i) - \lambda t_i)}{4} + o(\gamma)
\end{aligned}
\tag{4.11}
$$

Denote by f, g etc., the solution to (3.6) along the branch $(0, n_1)$. The corresponding boundary conditions are

$$
\begin{aligned}
K_f &= f^{(1)}(0) + f^{(2)}(0) \\
&= \lambda \tanh(\lambda t_1) + \lambda \tanh(\lambda t_2) + \gamma\lambda^2[\tanh^2(\lambda t_1) + \tanh^2(\lambda t_2)] + o(\gamma) \\
K_g &= g^{(1)}(0) + g^{(2)}(0) \\
&= \lambda \tanh(\lambda t_1) + \lambda \tanh(\lambda t_2) \\
&\quad - \gamma\lambda^2[\operatorname{sech}^2(\lambda t_1) + \operatorname{sech}^2(\lambda t_2) - e^{-t_1/\gamma} - e^{-t_2/\gamma}] + o(\gamma) \\
K_h &= h^{(1)}(0) + h^{(2)}(0) \\
&= \lambda \tanh(\lambda t_1) + \lambda \tanh(\lambda t_2) - \frac{\gamma\lambda^2}{2}[2 + 2\operatorname{sech}^2(\lambda t_1) + 2\operatorname{sech}^2(\lambda t_2) \\
&\quad - 4e^{-t_1/\gamma} - 4e^{-t_2/\gamma} - e^{-2t_1/\gamma} - e^{-2t_2/\gamma}] + o(\gamma)
\end{aligned}
\tag{4.12}
$$

The asymptotic expansions for f, g, h, and c are then given by the appropriate expressions in Section 3.7. As with the proof of Proposition 4.1 for the single-chain polymer, we have

$$
Z_{\mathscr{T}} = \mathbb{E}[\hat{Z}_{\mathscr{T}}(G)] = \frac{\lambda e^{-c(0)}}{\sqrt{\rho f(0)}} \tag{4.13}
$$

(Recall that we are taking $U_0 = 0$.) Note that for our star polymer

$$
2c(0) = \int_0^{n_1} h(u)\, du + \int_0^{t_1} h^{(1)}(u)\, du + \int_0^{t_2} h^{(2)}(u)\, du \tag{4.14}
$$

Of course, the nodes in the branching polymers can always be replaced by particles that have polymer ends attached to them, just as in the example of 2 particles joined by a single polymer strand considered earlier. Also, we do not need to restrict ourselves to the case where all the branches have the same resistance measure. For example, the same method can be easily adapted with only minor changes to deal with the case where the resistance measure along each branch $(0, t_i)$ is $r_i(dt) = r_i\, dt$.

4.5. Effect of Different Choices of Root

For the star polymer described above, instead of choosing 0 as the root of the tree, we could have chosen the internal node n_1 as the root. In this case, the 3 branches are independent and the expressions (4.11) hold for $i = 0, 1, 2$. (Here, we have used the notation t_0 to denote the free end that was previously the root 0—thus $t_0 = n_1$.) From the independence of the 3 branches we have

$$\mathbb{E}^x[F_{\mathscr{T}}] = \prod_{i=0}^{2} \mathbb{E}^x[F_{(0,t_i)}]$$

and so

$$\begin{aligned}\hat{Z}_{\mathscr{T}}(v) &= e^{v^2/2}\mathbb{E}^{v\sqrt{\rho}/\lambda}[F_{\mathscr{T}}] \\ &= e^{v^2/2}\exp\left\{-\frac{v^2\rho}{2\lambda^2}\left(f^{(0)}(0)+f^{(1)}(0)+f^{(2)}(0)\right)\right\} \\ &\quad \times \exp\{-c^{(0)}(0)-c^{(1)}(0)-c^{(2)}(0)\}\end{aligned}$$

Hence

$$Z_{\mathscr{T}} = \frac{\lambda \exp\{-c^{(0)}(0)-c^{(1)}(0)-c^{(2)}(0)\}}{\sqrt{\rho\left(f^{(0)}(0)+f^{(1)}(0)+f^{(2)}(0)\right)}} \tag{4.15}$$

Of course, for this example, it is much easier to use (4.15) together with the one-dimensional asymptotic expansion (4.8) to obtain the asymptotic expansion for the tree.

It is not at all obvious that the expressions (4.13) and (4.15) are identical, which of course they should be. There does not seem to be a natural way—as there is in Chan *et al.* (1994)—to see that the expression for $Z_{\mathscr{T}}$ is independent of the choice of root in the case of a general tree; for

example, that (4.13) and (4.15) are identical does not seem to follow from any known properties of solutions to the Riccati equation. Here, we shall simply content ourselves with checking that at least the leading terms in the asymptotic expansions for (4.13) and (4.15) are the same.

Observe from (4.12) that the leading terms of the constants K_f, K_g, and K_h are identical, so from (3.19) and (3.11) we see that the leading terms in the differences $\tilde{F}_0(s) - \hat{F}_0(s)$, $\hat{G}_0(s) - \hat{G}_0(s)$ etc., are identically 0. Therefore, the corresponding leading terms in (4.13) are given by

$$f(0) - O(\gamma) = g(0) - O(\gamma) = h(0) - O(\gamma) = \frac{\lambda(A - Be^{-2\lambda n_1})}{A + Be^{-2\lambda n_1}} \tag{4.16a}$$

$$\begin{aligned} 2c(0) - O(\gamma) &= \int_0^{n_1} h(u) - O(\gamma)\, du + 2c^{(1)}(0) + 2c^{(2)}(0) \\ &= \int_0^{n_1} \frac{\lambda(A - Be^{-2\lambda u})}{A + Be^{-2\lambda u}}\, du + \int_0^{t_1} h^{(1)}(u)\, du + \int_0^{t_2} h^{(2)}(u)\, du \end{aligned} \tag{4.16b}$$

where we have put

$$A = 1 + \tanh(\lambda t_1) + \tanh(\lambda t_2)$$

$$B = 1 - \tanh(\lambda t_1) - \tanh(\lambda t_2)$$

The expression (44.16a) follows from (3.25) and (4.12). The functions $h^{(i)}$ in the last two terms of (4.16b) are the same as those in (4.14). It therefore suffices to check that the leading term of

$$\frac{\exp\{-\int_0^{t_0} h(u)\, du\}}{f(0)}$$

is the same as the leading term of

$$\frac{e^{-2c^{(0)}(0)}}{f^{(0)}(0) + f^{(1)}(0) + f^{(2)}(0)}$$

To this end, observe that the right-hand side of (4.16a) can be written as

$$\frac{A - Be^{-2\lambda n_1}}{A + Be^{-2\lambda n_1}} = \tanh(\lambda t_0) + \frac{2(A - B)}{(Ae^{\lambda t_0} + Be^{-\lambda t_0})(e^{\lambda t_0} + e^{-\lambda t_0})}$$

Now $\lambda \tanh(\lambda t_0)$ is precisely the leading term of $h^{(0)}(0)$ and $f^{(0)}(0)$. Next, noting that $A + B = 2$, we have

$$\int_0^{t_0} \frac{2(A-B)}{(Ae^{\lambda u} + Be^{-\lambda u})(e^{\lambda u} + e^{-\lambda u})}\, du = \frac{\log(A + Be^{-2\lambda t_0}) - \log(1 + e^{-2\lambda t_0})}{\lambda}$$

Finally,

$$\frac{1 + e^{-2\lambda t_0}}{A + Be^{-2\lambda t_0}} \times \frac{A + Be^{-2\lambda t_0}}{\lambda(A - Be^{-2\lambda t_0})} = \frac{1}{\lambda[\tanh(\lambda t_0) + \tanh(\lambda t_1) + \tanh(\lambda t_2)]}$$

as required. In a similar way, one can check that the fist-order terms in γ in (4.13) and (4.15) also agree, but the calculations are much messier because of the nonlinearity in the constants K_f, K_g, and K_h.

4.6. General Star Polymers with Identical Branches

In the case of a star polymer whose index set $\mathcal{T}$ consists of identical branches of the same length T and the resistance measure is the same along all the branches, there is yet another trick for factorizing the partition function. This has already appeared in Dean and Jansons (1995); we shall briefly describe how it extends to semi-flexible polymers.

Consider a star-shaped polymer with n identical branches of the form $[0, T]$, taking Lebesgue measure on $[0, T]$ as the resistance measure. We take as the root of $\mathcal{T}$ the central node, where all the branches are joined. The partition function then takes the form

$$Z_{\mathcal{T}} = \mathbb{E}^0\left[\exp\left\{-\frac{\lambda^2}{2}\left(\int_0^T \sum_{i=1}^n X_i(s)^2\, ds - \frac{1}{Tn}\left(\int_0^T \sum_{i=1}^n X_i(s)\, ds\right)^2\right)\right\}\right]$$

Denoting by X the process $(X_1, X_2, \ldots, X_n)$ in $\mathbb{R}^n$ and letting

$$r = \frac{1}{\sqrt{n}}(1, 1, \ldots, 1)$$

the partition function may be rewritten as

$$Z_{\mathcal{T}} = \mathbb{E}^0\left[\exp\left\{-\frac{\lambda^2}{2}\left(\int_0^T |X_s|^2\, ds - \frac{1}{T}\left(\int_0^T X_s \cdot r\, ds\right)^2\right)\right\}\right]$$

By rotating the coordinate system in $\mathbb{R}^n$, taking r to be the first orthonormal basis vector (and continuing to using $(X_1, X_2, \ldots, X_n)$ to denote the components under the new coordinate system), we obtain

$$\begin{aligned} Z_{\mathscr{T}} &= \mathbb{E}^0\left[\exp\left\{-\frac{\lambda^2}{2}\left(\int_0^T |X_s|^2\,ds - \frac{1}{T}\left(\int_0^T X_1(s)\,ds\right)^2\right)\right\}\right] \\ &= \mathbb{E}^0\left[\exp\left\{-\frac{\lambda^2}{2}\left(\int_0^T X_1(s)^2\,ds - \frac{1}{T}\left(\int_0^T X_1(s)\,ds\right)^2\right)\right\}\right] \\ &\quad \times\left(\mathbb{E}^0\left[\exp\left\{-\frac{\lambda^2}{2}\int_0^T X_2(s)^2\,ds\right\}\right]\right)^{n-1} \end{aligned} \tag{4.17}$$

where we have used the independence of the X_i. Everything in (4.17) is now in terms of "one-dimensional" quantities which we have already calculated earlier: from (4.8) we have the asymptotic expansion

$$\begin{aligned} &\mathbb{E}^0\left[\exp\left\{-\frac{\lambda^2}{2}\left(\int_0^T X_1(s)^2\,ds - \frac{1}{T}\left(\int_0^T X_1(s)\,ds\right)^2\right)\right\}\right] \\ &\quad = \left(\frac{\lambda T}{\sinh(\lambda T)}\right)^{1/2} - \frac{\gamma\lambda}{4}\left(\frac{\lambda T}{\sinh(\lambda T)}\right)^{1/2}(3\tanh(\lambda T) - \lambda T) + o(\gamma) \end{aligned}$$

and putting $v = 0$ in (4.4) and (4.5) we get

$$\left(\mathbb{E}^0\left[\exp\left\{-\frac{\lambda^2}{2}\int_0^T X_2(s)^2\,ds\right\}\right]\right)^{n-1} = e^{-(n-1)c(0)}$$

where $c(0)$ has the asymptotic expansion (4.7). We leave the reader to check that this indeed agrees with the special case of (4.15) with $c^{(0)}(0) = c^{(1)}(0) = c^{(2)}(0)$ and $f^{(0)}(0) = f^{(1)} = f^{(2)}(0)$.

5. Stochastic Area for Semiflexible Chains

The treatment in Section 3 is sufficiently general to cover other quadratic frunctionals besides the positive ones which appear in the partition function. In particular, instead of taking $R = 0$ we can take $Q = 0$ and R a given anti-symmetric matrix in (3.1). This allows us to use the same method to find the law of the stochastic area associated with a linear stochastic process of the form (2.1).

Suppose (X, U) and (Y, V) are two independent copies of the process described by (1.2) and we are interested in the stochastic area

$\int_0^t (Y_s\,dX_s - X_s\,dY_s)$. To express this in terms of the general situation of (2.1), put $\underset{\sim}{X}^T = (X, Y, U, V)$ and let

$$E = \begin{pmatrix} 0 & 0 & \alpha & 0 \\ 0 & 0 & 0 & \alpha \\ 0 & 0 & -\alpha & 0 \\ 0 & 0 & 0 & -\alpha \end{pmatrix}, \qquad \sigma = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{5.1}$$

The the stochastic area can be written as $\int_0^t (Y_s\,dX_s - X_s\,dY_s) = \int_0^t \underset{\sim}{X}_s^T R\,d\underset{\sim}{X}_s$ where

$$R = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{5.2}$$

The argument (3.1)–(3.3) can be used exactly as before, so solving the Riccati equation (3.2) with $Q = 0$ and boundary conditions $S_T = 0$ and $c_T = 0$ gives the law of the stochastic area as

$$\mathbb{E}\left[\exp\left\{ -\theta \int_0^T (Y_s\,dX_s - X_s\,dY_s) \right\} \right] = \exp\{ -\tfrac{1}{2}\underset{\sim}{X}_0^T S_0 \underset{\sim}{X}_0 - c_0 \} \tag{5.3}$$

Thus the problem of determining the law of the stochastic area is essentially the same as that of determining the partition function.

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