

On Edwards' Model for Polymer Chains:

II. The Self-Consistent Potential

John Westwater

Dept. of Mathematics, University of Washington, Seattle, WA 98195, USA

Abstract. We obtain an existence and uniqueness theorem for the self-consistent potential in Edwards' model for polymer chains, and confirm the asymptotic analysis proposed by him on the basis of WKB arguments.

Introduction

The present paper is a reprise of the original work of Edwards' [1] on his continuum model for long polymer chains, the object being to place the results stated there on a firm basis. In [1] Edwards proposes as an approximation to the polymer model a Markov process. This process is a drift process characterised by a spherically symmetric non-negative potential function which is to satisfy a non-linear equation whose structure is motivated by the polymer model (self-consistency condition). We prove existence and uniqueness of this self-consistent potential, and confirm that its asymptotic behaviour is that proposed by Edwards. The proof relies on the fact that the self-consistent potential must satisfy a certain non-linear differential equation. This equation is studied in Sect. 1, its relation to the polymer problem being given in Sect. 2. In Sect. 3 we prove a limit theorem for drift processes from which Edwards' main conclusion concerning the predictions of the Markovian model for the length of polymer chains follows.

In this paper no attempt is made to prove that the Markovian model is a sufficiently good approximation to the original polymer chain model that the limit theorem proved in Sect. 3 for the Markovian model applies to the original. Indeed the existence theorem for the polymer model we have obtained in [2] does not provide a sufficient basis for making such an attempt. The theorem proved in [2] asserts that the polymer measure is well-defined on paths parametrised by the time interval $[0, 1]$ for sufficiently small coupling constant. For a fixed coupling constant g this is equivalent to the assertion that the measure is well-defined on paths parametrised by $t \in [0, T]$ for $T = T(g)$ sufficiently small. This restriction must be removed if the limiting behaviour of paths as $t \rightarrow \infty$ is to be considered. We remark, however, that some problems of this kind have been solved by application of the Donsker–Varadhan theory of the asymptotics of functionals of Markov processes [3].

1. A Boundary Value Problem

In this section we solve a boundary value problem on $(-\infty, +\infty)$ for a certain 1-parameter family of differential equations. These equations may be characterised by some simple formal properties: consider an ordinary differential equation of the form

$$L(u) = uM(u), \quad (1)$$

with L and M linear differential operators with constant coefficients of orders 3 and 1 respectively. We suppose that L has real spectrum, and that (1) admits an integrating factor of the form $u \exp[\beta t]$. Then by means of

- (a) a scale change in u
- (b) an affine transformation in t

(1) may be put into one of the following canonical forms:

$$(i) \quad u''' - u' = uu', \quad (2)$$

$$(ii) \quad P\left(\frac{d}{dt}\right)u = u(u' - u), \quad (3)$$

with

$$P(x) = (x - \frac{3}{2})^3 - \lambda(x - \frac{3}{2}), \quad (4)$$

and $\lambda \geq 0$. For $\lambda > 0$ the transformation

$$v(t) = \lambda^{-1}u(\lambda^{-1/2}t), \quad (5)$$

gives an alternative form for (ii) which, in the limit $\lambda \rightarrow +\infty$, goes over into (i). Thus it is natural to regard (2, 3) as a single 1-parameter family of differential equations, parametrised by $\lambda \in [0, +\infty)$.

The integrating factors for (2, 3) are $u, u \exp[-3t]$, and the integrated forms

$$\frac{u^3}{3} - uu'' + \frac{u'^2}{2} + \frac{u^2}{2} = c. \quad (6)$$

$$\frac{u^3}{3} - uu'' + \frac{u'^2}{2} + \frac{3uu'}{2} - \left(\frac{9}{8} - \frac{\lambda}{2}\right)u^2 = c \exp[3t]. \quad (7)$$

In (6, 7) c is a constant of integration.

By a positive solution of (2) or (3) we mean a solution $u(t)$ defined for all $t \in \mathbb{R}$, and strictly positive. The purpose of this section is to prove.

Theorem 1. (a) Any positive solution of (2) is a constant. For such a solution c in (6) is positive, and the value of c uniquely defines the solution.

(b) (3) has positive solutions for any $\lambda \in [0, \infty)$. For $\lambda > 9/4$ any two such solutions differ only by a translation in t . For $\lambda \in [0, 9/4]$ this uniqueness up to translation holds for positive solutions satisfying the boundary condition

$$u(t) = 0(\exp[\alpha t]), \quad t \rightarrow -\infty. \quad (8)$$

(with $\alpha = \frac{3}{2} - \varepsilon$, for some ε , $0 < \varepsilon < \lambda^{1/2}$) in case $\lambda \varepsilon(0, 9/4]$

$$u(t) = 0 \left(|t|^2 \exp \left[\frac{3t}{2} \right] \right), \quad t \rightarrow -\infty \tag{9}$$

if $\lambda = 0$. For $\lambda > 9/4$ any positive solution of (3) satisfies (8). For a positive solution satisfying the above boundary condition the constant c in (7) is positive, and the value of c uniquely defines the solution.

Proof. A single integration of (2) gives an equation

$$u'' = u + \frac{u^2}{2} + k, \tag{10}$$

which can be interpreted as the evolution equation of a conservative mechanical system. The simple analysis of (10) confirms that, while non-constant solutions of (2) defined for all time exist (they are periodic), such solutions are not positive, and this is the only nontrivial assertion in (a). The proof of (b) is more difficult, and will be broken up into several lemmas. The first of these shows why no boundary condition is given as $t \rightarrow +\infty$.

Lemma 1. *A solution of (7) defined and positive on $[T, \infty)$ for some T satisfies*

$$\lim_{t \rightarrow +\infty} u(t) \exp[-t] = (3c)^{1/3}. \tag{11}$$

Proof. We write $y = u \exp[-t]$, and obtain

$$\exp[t] \left\{ \frac{y^3}{3} - c \right\} - yy'' + \frac{1}{2}yy' + \frac{1}{2}y'^2 + \left(\frac{\lambda}{2} - \frac{1}{8} \right) y^2 = 0. \tag{12}$$

We are now to prove

$$\lim_{t \rightarrow +\infty} y(t) = (3c)^{1/3}. \tag{13}$$

The proof is by contradiction. We suppose (13) does not hold, and examine several possibilities for the behaviour of $y(t)$ as $t \rightarrow +\infty$, arriving at a contradiction in each case.

Suppose first that $y(t)$ is oscillatory *i.e.* that $y(t)$ has infinitely many critical points $\{t_n, n \geq 1\}$. Critical points of $y(t)$ are isolated, so $\lim_n t_n = +\infty$. If $t \in (t_n, t_{n+1})$, $y(t)$ lies between the critical values $y(t_n), y(t_{n+1})$, so the fact that (13) does not hold implies that we also do not have

$$\lim_{n \rightarrow \infty} y(t_n) = (3c)^{1/3}.$$

Hence, for some $\varepsilon > 0$, there are infinitely many critical values $y(t_n)$ satisfying

$$|y(t_n) - (3c)^{1/3}| \geq \varepsilon. \tag{14}$$

For a critical point satisfying (14), and n sufficiently large, (12) gives

$$\operatorname{sgn} y''(t_n) = \operatorname{sgn} [y(t_n) - (3c)^{1/3}]. \tag{15}$$

Suppose (14), (15) hold for $n = m$. If $y(t_m) > (3c)^{1/3}$, (15) asserts that t_m is a local minimum, so t_{m+1} is a local maximum and $y(t_{m+1}) > y(t_m) \geq (3c)^{1/3} + \varepsilon$. But then (14), and so also (15), holds for $n = m + 1$, which is impossible, since t_{m+1} is a local maximum. A similar contradiction results if we suppose $y(t_m) < (3c)^{1/3}$.

Suppose next that $y(t)$ is eventually monotone, so that $y_\infty = \lim_{t \rightarrow \infty} y(t)$ exists, $y_\infty \in [0, \infty]$. Since y is positive, we may define $\varphi = y^{1/2}$, and from (12) obtain

$$\varphi'' - \frac{1}{2}\varphi' = \frac{1}{2} \exp[t] \left\{ \frac{\varphi^3}{3} - \frac{c}{\varphi^3} \right\} + \left(\frac{\lambda}{4} - \frac{1}{16} \right) \varphi, \quad (16)$$

$$= h(t) (say). \quad (17)$$

Since (13) is supposed to fail, $y_\infty \neq (3c)^{1/3}$. Suppose $(3c)^{1/3} < y_\infty < \infty$, then for some $\gamma > 0$, and all $t \geq t_0$ we have

$$h(t) \geq \gamma \exp[t]. \quad (18)$$

(17) gives the integral equation

$$\varphi(t) = A + B \exp\left[\frac{t}{2}\right] + 2 \int_{t_0}^t \left\{ \exp\left[\left(\frac{t-\xi}{2}\right)\right] - 1 \right\} h(\xi) d\xi, \quad (19)$$

with A, B constants. Inserting (18) in (19) we find, for $t \geq t_0$, and A_1, B_1 constants,

$$\varphi(t) \geq A_1 + B_1 \exp\left[\frac{t}{2}\right] + 2\gamma \exp[t]. \quad (20)$$

(20) implies $\lim_{t \rightarrow \infty} y(t) = \lim_{t \rightarrow \infty} \varphi(t)^2 = \infty$, which contradicts $y_\infty < \infty$.

A similar contradiction results if we suppose $0 \leq y_\infty < (3c)^{1/3}$.

Suppose finally that $y(t)$ is eventually increasing, with $\lim_{t \rightarrow \infty} y(t) = +\infty$. We write (12) in the form

$$yy'' = \frac{1}{2} \left(y' + \frac{y}{2} \right)^2 + \left(\frac{\lambda}{2} - \frac{1}{4} \right) y^2 + \exp[t] \left(\frac{y^3}{3} - c \right), \quad (21)$$

and obtain for $t \geq t_0$, and some constant $K > 0$,

$$y'' \geq Ky^2, \quad y' \geq 0. \quad (22)$$

(22) implies $y(t) \geq z(t)$ for $t \geq t_0$, with $z(t)$ the solution of

$$z'' = Kz^2; \quad z(t_0) = y(t_0), \quad z'(t_0) = 0. \quad (23)$$

But $z(t) \rightarrow \infty$ in a finite time, so this comparison implies $y(t) \rightarrow \infty$ in a finite time, which contradicts the assumption that $y(t)$ is defined on $[T, \infty)$. \square

Lemma 1 shows that for a positive solution of (3) the constant c in (17) is non-negative. The possibility that $c = 0$ may be examined writing $\psi = u^{1/2}$. (7) then gives the autonomous equation

$$\psi'' - \frac{3}{2}\psi' - \frac{\psi^3}{6} + \left(\frac{9}{16} - \frac{\lambda}{4} \right) \psi = 0. \quad (24)$$

(24) has one equilibrium point if $\lambda \geq 9/4$, three if $\lambda < 9/4$; there are no limit cycles. An unbounded orbit is readily shown to be incomplete, so that a solution of (24) defined on \mathbb{R} and positive must have for its orbit an arc joining the two equilibrium points in the half-plane $\psi \geq 0$, λ being necessarily less than $9/4$. Such a solution exists for $\lambda < 9/4$, but fails to satisfy the boundary condition of Theorem 1. Thus for a positive solution of (3) satisfying the boundary condition of Theorem 1, c in (7) is positive. We now choose a number $c_0 > 0$. If $u(t)$ is a solution of (3) for which c in (7) is positive, there exists a unique translate $u(t - t_0)$ of this solution satisfying (7) with $c = c_0$; t_0 is given by $c = c_0 \exp[3t_0]$. So to complete the proof of Theorem 1 it suffices to consider (7) with $c = c_0$, and to show that this equation $(7)_0$ has a unique positive solution satisfying the boundary condition of the theorem.

The next lemma shows why, for $\lambda > 9/4$, no boundary condition is given as $t \rightarrow -\infty$.

Lemma 2. *Suppose $\lambda > 9/4$. Then, for a positive solution $u(t)$ of $(7)_0$,*

$u(t) \exp\left[-\frac{3t}{2}\right]$ is bounded in t .

Proof. Write $\psi(t) = u(t)^{1/2} \exp\left[-\frac{3t}{4}\right]$. Then

$$\psi'' = \frac{1}{6}\psi^3 \exp\left[\frac{3t}{2}\right] - c_0 \frac{\psi^{-3}}{2} + \frac{\lambda}{4}\psi. \quad (25)$$

Choose β satisfying $\frac{9}{4} < \beta < \lambda$. We will show $\psi(t) \leq M$, with $M = [2c_0(\lambda - \beta)^{-1}]^{1/4}$. By Lemma 1 $\psi(t) \rightarrow 0$ as $t \rightarrow +\infty$. Hence we either have $\psi(t) \leq M$ for all t , or for some $t = t_0$

$$\psi(t_0) > M, \psi'(t_0) < 0. \quad (26)$$

We will derive a contradiction from the second possibility, and this will complete the proof.

Suppose then that (26) holds. Writing (25) in the form

$$\psi'' = \frac{\beta}{4}\psi + \frac{1}{6}\psi^3 \exp\left[\frac{3t}{2}\right] + \frac{(\lambda - \beta)}{4}\left(\psi - \frac{M^4}{\psi^3}\right), \quad (27)$$

we find that $\psi(t)$ is a decreasing function of t for $t \leq t_0$ (i.e. increases as $t \rightarrow -\infty$), and, for $t \leq t_0$, $\psi(t) \geq \omega(t)$, with $\omega(t)$ the solution of

$$\omega'' = \frac{\beta}{4}\omega + \frac{1}{6}\omega^3 \exp\left[\frac{3t}{2}\right], \quad (28)$$

satisfying $\omega(t_0) = \omega_0$, $\omega'(t_0) = \omega'_0$. Here ω_0 , ω'_0 may be chosen arbitrarily subject to the inequalities

$$0 < \omega_0 < \psi(t_0), 0 > \omega'_0 > \psi'(t_0). \quad (29)$$

Now the comparison Eq. (28) may be transformed by the change of variable

$\omega = \tau \exp \left[-\frac{3t}{4} \right]$ into the autonomous equation

$$\tau'' - \frac{3}{2}\tau' + \frac{1}{4}\left(\frac{9}{4} - \beta\right)\tau = \frac{1}{6}\tau^3. \quad (30)$$

Since $\beta > \frac{9}{4}$, this equation has precisely one equilibrium point, namely the origin, and this point is a saddle point. A solution of (30) defined on $(-\infty, t_0]$ necessarily has the unstable manifold at the origin as its orbit; otherwise it would be unbounded, and an unbounded semiorbit of (30) is incomplete. But by a suitable choice of ω_0, ω'_0 satisfying (29), we can be sure that the corresponding point (τ_0, τ'_0) of the phase plane of (30) does not lie on the unstable manifold at 0. Then the comparison function $\omega(t)$ blows up in a finite time as t decreases, which contradicts the hypothesis of the lemma that $u(t)$, and hence $\psi(t)$, is defined for all t . \square

To obtain the conclusion of Lemma 2 for $0 < \lambda \leq 9/4$ we find it necessary to impose the boundary condition (8).

Lemma 3. *Suppose $0 < \lambda \leq \frac{9}{4}$. Then, for a positive solution $u(t)$ of (7)₀ satisfying (8), $u(t) \exp \left[-\frac{3t}{2} \right]$ is bounded in t .*

Proof. Write $v(t) = u(t) \exp \left[-\frac{3t}{2} \right]$. By Lemma 1 $v(t) \rightarrow 0$ as $t \rightarrow +\infty$, so it remains to show $v(t) = O(1)$ as $t \rightarrow -\infty$. From (3) we obtain

$$v''' - \lambda v' = \left[vv' + \frac{1}{2}v^2 \right] \exp \left[\frac{3t}{2} \right], \quad (31)$$

which implies that v satisfies an integral equation

$$v(t) = A + B \exp[\lambda^{1/2}t] + C \exp[-\lambda^{-1/2}t] + \int_0^t R(t, \xi) v(\xi)^2 d\xi. \quad (32)$$

The kernel $R(t, \xi)$ in (32) is given by

$$R(t, \xi) = \frac{1}{2} \exp \left[\frac{3\xi}{2} \right] \left\{ \frac{sh(\lambda^{1/2}[t - \xi])}{\lambda^{1/2}} - \left(\frac{sh(2^{-1}\lambda^{1/2}[t - \xi])}{\lambda^{1/2}} \right)^2 \right\}. \quad (33)$$

Given an estimate $v(t) = O(\exp[-\varepsilon t])$ as $t \rightarrow -\infty$, with $0 < \varepsilon < \lambda^{1/2}$, as implied by (8), we find that the integral in (32) is $O(\exp[-T(\varepsilon)t])$ as $t \rightarrow -\infty$, with $T(\varepsilon) = \max(0, 2\varepsilon - \frac{3}{2})$. Since $\varepsilon < \lambda^{1/2} \leq \frac{3}{2}$, this means that the integral is $o(\exp[-\lambda^{1/2}t])$, and the boundary condition (8) now forces $C = 0$. (32) then gives the improved estimate $v(t) = O(\exp[-T(\varepsilon)t])$ as $t \rightarrow -\infty$, and so by iteration $v(t) = O(\exp[-T^N(\varepsilon)t])$ for any integer $N \geq 1$. But $T^N(\varepsilon) = \max(0, 2^N \varepsilon - \frac{3}{2}[2^N - 1]) = 0$ for N sufficiently large, so $v(t) = O(1)$ as $t \rightarrow -\infty$. \square

The proof of the uniqueness assertion of Theorem 1 will now be obtained as a corollary of the following lemma.

Lemma 4. Suppose $a(t)$, $F(\psi, t)$ are continuous functions defined for t real, and ψ real and positive, and that, for each t , $F(\psi, t)$ is strictly increasing in ψ . Let c_+ , c_- be real numbers. Then the boundary value problem

$$\begin{aligned} \psi'' + a(t)\psi' &= F(\psi, t) \\ \psi(t) &\rightarrow c_- \text{ as } t \rightarrow -\infty, \psi(t) \rightarrow c_+ \text{ as } t \rightarrow +\infty \end{aligned} \quad (34)$$

has at most one positive solution.

Proof. Suppose $\psi_1(t), \psi_2(t)$ are two positive solutions of (34). If these solutions are distinct, we may suppose that $\rho(t) = \psi_1(t) - \psi_2(t)$ takes positive values. Since $\rho(t) \rightarrow 0$ as $t \rightarrow +\infty$ or $t \rightarrow -\infty$, $\rho(t)$ is bounded and has a positive maximum, at t_0 (say). Then $\rho(t_0) = \psi_1(t_0) - \psi_2(t_0) > 0$, and $\rho''(t_0) \leq 0, \rho'(t_0) = 0$. But from (34)

$$\rho''(t_0) + a(t_0)\rho'(t_0) = F(\psi_1(t_0), t_0) - F(\psi_2(t_0), t_0). \quad (35)$$

The right side of (35) is strictly positive, since $F(\psi, t_0)$ is strictly increasing in ψ , and the left side is ≤ 0 . This contradiction implies $\psi_1 \equiv \psi_2$. \square

Corollary. (7)₀ has at most one positive solution $u(t)$ satisfying (8) (or (9)).

Proof. Choose a smooth decreasing function $h(t)$ such that

$$\begin{aligned} h(t) &= -t, t \leq -2 \\ h(t) &= 1, t \geq -1 \end{aligned}$$

Note that $h(t) \geq 1$ for all t , and that $h''(t)$ is non-zero only for $t \in [-2, -1]$. Write $M = \max |h''(t)|$. Define $k(t) = h(t - t_0)$, with t_0 to be chosen later, and set $\psi(t) = u(t)^{1/2} \exp\left[-\frac{3t}{4}\right] k(t)^{-1}$. $\psi(t) \rightarrow 0$ as $t \rightarrow +\infty$ by Lemma 1, and $\psi(t) \rightarrow 0$ as $t \rightarrow -\infty$ by Lemma 2 in case $\lambda > \frac{3}{4}$, by Lemma 3 in case $0 < \lambda \leq \frac{3}{4}$, and by (9) if $\lambda = 0$. The differential equation satisfied by $\psi(t)$ is

$$\psi'' + a(t)\psi' = F(\psi, t),$$

with $a(t) = 2k'k^{-1}$, and

$$F(\psi, t) = \frac{1}{6} k^2 \psi^3 \exp\left[\frac{3t}{2}\right] - \frac{c_0}{2} k^{-4} \psi^{-3} + \left(\frac{\lambda}{4} - \frac{k''}{k}\right) \psi. \quad (36)$$

From (36) we compute

$$\text{Min}_{\psi > 0} \frac{\partial F}{\partial \psi} = C \exp[t] + \frac{\lambda}{4} - \frac{k''}{k}, \quad (37)$$

with C a positive constant. Since $|k''k^{-1}| \leq M$, and is non-zero only for $t \in [t_0 - 2, t_0 - 1]$, it suffices to choose t_0 so

$$C \exp[t_0 - 2] > M$$

to ensure that the right side of (37) is strictly positive for all t . Lemma 4 then applies, and gives the uniqueness of $\psi(t)$, and hence of $u(t)$. \square

In order to establish the existence assertion of Theorem 1, we will construct a 1-parameter family $\{u(t, \beta) : \beta \in \mathbb{R}\}$ of solutions of $(7)_0$. For each β , $u(t, \beta)$ will be first defined on an interval $-\infty < t < t_0(\beta)$ as the solution of a certain integral equation, and then extended as a solution of $(7)_0$ to a maximal interval of existence. For $-\infty < t < t_0(\beta)$, $u(t, \beta)$ will satisfy a bound $0 < u(t, \beta) < u^*(t)$. Here $u^*(t)$ is a smooth function of t , defined for all t , which we will specify later. It will be chosen so that this bound on $u(t, \beta)$ implies that $u(t, \beta)$ satisfies as $t \rightarrow -\infty$ the boundary condition of Theorem 1. Since the solution of $(7)_0$ is also a solution of the quasi-linear equation (3), it follows that a solution $u(t, \beta)$, which satisfies $0 < u(t, \beta) < u^*(t)$ for all t in its domain of definition, is necessarily defined for all t , and thus provides the solution of our problem. Otherwise we may define an exit time $t_1(\beta) = \min\{t : u(t, \beta)[u^*(t) - u(t, \beta)] = 0\}$. Write $E = \{\beta : t_1(\beta) \text{ is defined}\}$ and $E_1 = \{\beta \in E : u(t_1(\beta), \beta) = 0\}$, $E_2 = \{\beta \in E : u(t_1(\beta), \beta) = u^*(t_1(\beta))\}$, so that $E = E_1 \cup E_2$, and our problem is to show $E \neq \mathbb{R}$. We will show that E_1 and E_2 are non-empty, and that for each $\beta \in E_1$ (respectively E_2) the graph of $u(t, \beta)$ intersects $u = 0$ (respectively $u = u^*(t)$) at $(t_1(\beta), u(t_1(\beta), \beta))$ transversely. Since $u(t, \beta)$ will depend smoothly on β , it will follow from this last assertion that E_1, E_2 are open, and so, since \mathbb{R} is connected, that $E \neq \mathbb{R}$, thus completing the proof of Theorem 1.

It is convenient to write down the constructions of the last paragraph in terms of

$v(t) = u(t) \exp\left[-\frac{3t}{2}\right]$, which satisfies

$$\frac{v^3}{3} \exp\left[\frac{3t}{2}\right] - vv'' + \frac{1}{2}v'^2 + \frac{1}{2}\lambda v^2 = c_0. \quad (38)$$

The integral equation defining $v(t, \beta) = u(t, \beta) \exp\left[-\frac{3t}{2}\right]$ has the form

$$v(t, \beta) = a(t) + \beta \exp[\lambda^{1/2}t] + \int_{-\infty}^t R(t, \xi)[v(\xi, \beta)^2 - b(\xi)]d\xi, \quad (39)$$

with $R(t, \xi)$ given by (33). The functions $a(t), b(t)$ take different forms according to the value of the parameter λ :

For $\lambda = 0$, $a(t) = -[2c_0]^{1/2}t$; $b(t) \equiv 0$.

For $0 < \lambda < 9/4$, $a(t) = [2c_0\lambda^{-1}]^{1/2}$; $b(t) \equiv 0$.

For $\lambda \geq 9/4$, set $N = [\frac{2}{3}\sqrt{\lambda}]$, so that $N \geq 1$ is an integer. Then construct

$d(t) = \sum_{n=0}^{N-1} d_n \exp[\frac{3}{2}nt]$, with $d_0 = [2c_0\lambda^{-1}]^{1/2}$, so that

$$d''' - \lambda d' = \left[dd' + \frac{d^2}{2}\right] \exp\left[\frac{3t}{2}\right] + 0(\exp[\frac{3}{2}Nt]),$$

as $t \rightarrow -\infty$, and define $b(t) = \sum_{n=0}^{N-1} b_n \exp[\frac{3}{2}nt]$ by

$$b(t) = [d(t)]^2 + 0(\exp[\frac{3}{2}Nt]).$$

Finally set $a(t) = \sum_{n=0}^N a_n(t) \exp[\frac{3}{2}nt]$, with

$$a_0(t) = [2c_0 \lambda^{-1}]^{1/2}$$

$$a_n(t) = \left[\left(\frac{3n}{2} \right)^3 - \lambda \left(\frac{3n}{2} \right) \right]^{-1} \left[\frac{3}{4}(n-1) + \frac{1}{2} \right] b_{n-1},$$

if $1 \leq n \leq N$, and $N \neq \frac{2}{3}\lambda^{1/2}$

$$a_n(t) = \left[\frac{3}{4}(N-1) + \frac{1}{2} \right] (2\lambda)^{-1} b_{N-1} t, \quad \text{if } n = N = \frac{2}{3}\lambda^{1/2},$$

so that $a''' - \lambda a' = \left[\frac{b'}{2} + \frac{b}{2} \right] \exp\left[\frac{3t}{2} \right]$.

That (39) has, for each $\beta \in \mathbb{R}$, a solution defined on an interval of the form $(-\infty, t_0(\beta))$ may be proved by showing that, for suitably chosen $t_0(\beta)$, the right side of (39) defines a contraction mapping on the Banach space B of continuous functions on $(-\infty, t_0)$ such that

$$\|v\|_B = \sup_{t \in (-\infty, t_0)} |[v(t) - a(t)] \exp[-\frac{3}{2}Nt]| < \infty.$$

The proof shows that the solution $v(t, \beta)$ depends smoothly on β . Moreover it is readily verified that $v(t, \beta)$ is a solution of (38), and so may be extended as a solution of (38) to a maximal interval of existence.

For $\lambda > 0$ choose $M > [2c_0 \lambda^{-1}]^{1/2}$, and define $u^*(t)$ by $v^*(t) = u^*(t) \exp\left[-\frac{3t}{2}\right] = M$. For $\lambda = 0$ choose $k > \left[\frac{c_0}{2}\right]^{1/2}$, and define a function $h(t)$ by

$$h(t) = 1 + t^2, \quad |t| \leq k$$

$$h(t) = 2k|t|, \quad |t| > k;$$

Then set $v^*(t) = h(t - t_2)$, with t_2 chosen so

$$\frac{1}{3} \exp\left[\frac{3}{2}(t_2 - k)\right] > c_0 + 2.$$

From (39) it is clear that, by redefining $t_0(\beta)$ if necessary, we may arrange to have $0 < v(t, \beta) < v^*(t)$ for $-\infty < t < t_0(\beta)$. The sets E_1, E_2 are then well-defined and it remains to verify the transversality assertion, and to verify that E_1, E_2 are non-empty.

The graph of any solution of (38) can only intersect $v = 0$ transversely—for $|v'| = (2c_0)^{1/2} \neq 0$ at such an intersection. Hence E_1 is open. For $\lambda > 0$ and $\beta \in E_2$, the intersection of the graph of $v(t, \beta)$ with $v = M$ at (t_1, M) is transverse—for if it were not, we should have, for $t = t_1, v = M, v' = 0, v'' \leq 0$, which contradicts (38), since $\frac{1}{2}\lambda M^2 > c_0$. For $\lambda = 0$ and $\beta \in E_2$, the transversality of the intersection of the graph of $v(t, \beta)$ with $v = v^*(t)$ at $(t_1, v^*(t_1))$ results from a similar contradiction; either $|t_1 - t_2| > k$, and nontransversality implies $[v'(t_1)]^2 = 4k^2, v''(t_1) \leq 0$, or $|t_1 - t_2| \leq k$, and nontransversality implies $v'(t_1) = 2(t_1 - t_2), v''(t_1) \leq 2$; in either case a contradiction with (38) results, k and t_2 being chosen as specified above. Thus E_2 is also open.

For $\lambda \geq \frac{1}{4}$, the kernel $R(t, \xi)$ in (39) is positive for all $\xi \leq t$, and it follows from

the variational equation

$$\frac{\partial v}{\partial \beta} = \exp[\lambda^{1/2}t] + \int_{-\infty}^t 2R(t, \xi)v(\xi, \beta)\frac{\partial v}{\partial \beta}(\xi, \beta)d\xi$$

that

$$\frac{\partial v}{\partial \beta} \geq \exp[\lambda^{1/2}t] > 0, \quad (40)$$

for all t such that $v(t, \beta)$ is defined and positive. It follows readily from (40) that E_1, E_2 are non-empty. For $\lambda < \frac{1}{4}$, the same conclusion is obtained by simple estimations based directly on (39). \square

The proof of Theorem 1 is complete.

We denote by β_c the unique value of β such that $\beta_c \notin E = E_1 \cup E_2$.

The solution of (39) by iteration gives an expansion for $v(t, \beta)$ as $t \rightarrow -\infty$ of the type considered by Liapunov [4], and so for the positive solution $v(t, \beta_c)$, once β_c has been determined. It is also of interest to have more detailed information about the behaviour of $v(t, \beta_c)$ (or $u(t, \beta_c)$) as $t \rightarrow +\infty$ than is given by Lemma 1. It is convenient to write

$$z = u \exp[-t](3c_0)^{-1/3}; \quad s = 2[3c_0]^{1/6} \exp\left[\frac{t}{2}\right]. \quad (41)$$

$z = z(s)$ then satisfies

$$z''' - z'[z + \tau s^{-2}] + \tau s^{-3}z = 0, \quad (42)$$

with $\tau = 4\lambda - 1$. (42) has a 1-parameter family of solutions $z(s, \gamma)$ defines for $s > s_0(\gamma)$ and satisfying $z(s, \gamma) \rightarrow 1$ as $s \rightarrow +\infty$. For each of these an asymptotic expansion may be obtained as $s \rightarrow +\infty$; this determines the behaviour of $u(t, \beta_c)$ as $t \rightarrow +\infty$, once the value γ_c of γ for which $z(s, \gamma_c) = u(t, \beta_c) \exp[-t](3c_0)^{-1/3}$ is known.

For $\lambda = 1/4, \tau = 0$ and (42) becomes autonomous. For this special case this leads to the explicit determination of $z(s, \gamma_c)$

$$z(s, \gamma_c) = 3 \left[\frac{\exp(s) - \alpha}{\exp(s) + \alpha} \right]^2 - 2, \quad (43)$$

with $\alpha = (\sqrt{3} - \sqrt{2})^2$.

For another instance of the shooting argument used in this section to establish existence of a solution of a nonlinear boundary value problem see Hastings and McLeod [5].

2. The Self-Consistent Equation

Flory [6] gave a remarkable and simple argument which determines the dependence on N , the number of links, of the expected distance \bar{R} between the ends of a long polymer chain immersed in a good solvent at a given temperature. For a given distance R between the ends of the chain, the free energy $F(R)$ is assumed to be the sum of two positive terms, proportional to $N^2 R^{-3}$ and $N^{-1} R^2$ respectively.

The first of these represents the contribution to the free energy of the repulsive interaction between any pair of links of the chain, separated along the chain, which are sufficiently close to one another in space, and the second can be considered as an elastic energy, representing the cohesion of the chain. Evidently $F(R)$ has a minimum at a value \bar{R} of R proportional to $N^{3/5}$. (For a fuller critical account of the Flory argument see de Gennes [7].)

The Flory exponent $3/5$ is in remarkably good agreement both with experiment, and with the numerical analysis of appropriate statistical mechanical models ([7–9] and further references cited there). The first attempt to derive it from a specific statistical mechanical model was made by Edwards [1]. Edwards considers a continuum model given by a measure ν on the space of continuous paths $\mathbf{x}(t)$, $t \geq 0$, in \mathbb{R}^3 , with $\mathbf{x}(0) = \mathbf{0}$. Formally ν is specified by the equation

$$\frac{d\nu}{d\mu} = \frac{1}{Z} \exp \left[-g \int_0^\infty \int_0^\infty \delta(\mathbf{x}(\sigma) - \mathbf{x}(\tau)) d\sigma d\tau \right]. \quad (1)$$

In (1) $g > 0$ is a coupling constant, and Z^{-1} the normalisation factor required to make ν a probability measure. This model should have the same relation to discrete models of polymer chains that the Wiener process has to random walks; in particular the parameter t of the continuum model corresponds to the number of links N , and the problem is to determine whether $E_\nu[|\mathbf{x}(t)|]$ is asymptotically proportional to $t^{3/5}$ as $t \rightarrow +\infty$. Note that the energy which appears in (1) has the same dimensional structure as the first term of Flory's free energy; an energy having the same dimensional structure as the second term of $F(R)$ is also implicit in (1), as may be seen explicitly from the relation between μ and the formal translation invariant measure ξ on path space

$$\frac{d\mu}{d\xi} = C \exp \left[-\frac{1}{2} \int_0^\infty \left| \frac{d\mathbf{x}}{d\sigma}(\sigma) \right|^2 d\sigma \right]. \quad (2)$$

The coupling constant g has dimension $L^3 T^{-2}$. By choosing the standard Wiener measure μ we have normalised the diffusion constant D , which should appear in (2), to be 1, so linking the choice of length and time scales. It is convenient to fix the length and time scales completely by setting also $g = 1$.

There are technical difficulties, only partially solved in [2], in the construction of ν in accordance with (1), but we will not be concerned with them here since we will follow Edwards in immediately replacing the intractable ν by a measure ρ determined by a positive spherically symmetric potential $V(\mathbf{x})$

$$\frac{d\rho}{d\mu} = \frac{1}{Z} \exp \left[-\int_0^\infty V(\mathbf{x}(\sigma)) d\sigma \right], \quad (3)$$

with Z^{-1} again denoting the appropriate normalisation factor. (3) is not to be taken literally either, but, in contrast to the situation for (1), it is not difficult to make sense of (3), under mild regularity conditions on V . We will be concerned with a potential V which, as a function of the radial distance $r = |\mathbf{x}|$ is smooth on $(0, \infty)$, vanishing at infinity, and which satisfies

$$V(r) = 0(r^{-2+\epsilon}), \text{ as } r \rightarrow 0+, \quad (4)$$

for some $\varepsilon > 0$. For such a V we may construct the self-adjoint operator

$$H = H_0 + V, \quad (5)$$

with $H_0 = -\frac{1}{2}\Delta$, and a radial function $\Omega(\mathbf{x}) > 0$

$$\Omega(\mathbf{x})^{-1} = E \left[\exp \left[- \int_0^{T(r)} V(\mathbf{x}(\sigma)) d\sigma \right] \right]. \quad (6)$$

In (6) $r = |\mathbf{x}|$, and $T(r)$ denotes the time at which the path first hits the sphere with center $\mathbf{0}$ and radius r . The right side of (3) is formally a multiplicative functional, so that ρ should be a Markov process, and can be constructed from its transition probabilities $q(t, \mathbf{x}, \mathbf{y})$. From (3) we compute formally.

$$q(t, \mathbf{x}, \mathbf{y}) = \frac{E \left[\exp \left(- \int_0^\infty V(\mathbf{x}(\sigma)) d\sigma \right) \delta(\mathbf{x}(s) - \mathbf{x}) \delta(\mathbf{x}(s+t) - \mathbf{y}) \right]}{E \left[\exp \left(- \int_0^\infty V(\mathbf{x}(\sigma)) d\sigma \right) \delta(\mathbf{x}(s) - \mathbf{x}) \right]} \quad (7)$$

$$= F(\mathbf{x})^{-1} \langle \mathbf{x} | \exp(-tH) | \mathbf{y} \rangle F(\mathbf{y}), \quad (8)$$

with

$$F(\mathbf{x}) = E \left[\exp \left[- \int_0^\infty V(\mathbf{x} + \mathbf{x}(\sigma)) d\sigma \right] \right]. \quad (9)$$

In (7) s is arbitrary, and we have used the Markov property of the Wiener process and the Feynman-Kac formula to pass to (8). Equation (8) may not be well-defined—for (9) may give $F(\mathbf{x}) \equiv 0$. However, since the Wiener process starts afresh at the stopping time $T(r)$, we have formally

$$F(\mathbf{x}) = F(\mathbf{0})\Omega(\mathbf{x}), \quad (10)$$

so that

$$q(t, \mathbf{x}, \mathbf{y}) = \Omega(\mathbf{x})^{-1} \langle \mathbf{x} | \exp(-tH) | \mathbf{y} \rangle \Omega(\mathbf{y}). \quad (11)$$

The right side of (11) is well-defined, so (11) can be used to define $q(t, \mathbf{x}, \mathbf{y})$. Since $q(t, \mathbf{x}, \mathbf{y})$ is a probability density in \mathbf{y} for all \mathbf{x}, t , (11) requires

$$\exp(-tH)\Omega = \Omega, \text{ for all } t > 0, \quad (12)$$

and hence that

$$H\Omega = 0. \quad (13)$$

Note that we do not mean to imply by (12), (13) that $\Omega \varepsilon L^2(\mathbb{R}^3)$. $\exp(-tH)$ is a self-adjoint operator on $L^2(\mathbb{R}^3)$ whose kernel $\langle \mathbf{x} | \exp(-tH) | \mathbf{y} \rangle$ defines an integral operator, which we also denote by $\exp(-tH)$, as in (12). (13) is a differential equation; taken together with the boundary condition $\Omega(\mathbf{0}) = 1$, it characterises $\Omega(\mathbf{x})$. From (11) we obtain the generator of the process

$$L = M^{-1}HM \quad (14)$$

$$= H_0 - \mathbf{a} \cdot \nabla, \quad (15)$$

with

$$\mathbf{a} = \nabla(\ln \Omega). \tag{16}$$

In (14) M is the operator defined by multiplication by Ω , and (13) is used to obtain (15).

The reader of Simon's book [10] will recognise in the last paragraph the theory of the $P(\varphi)_1$, or drift processes developed there, with one essential difference: Simon wishes to be able to construct a process homogeneous in time, and therefore imposes conditions on V which guarantee $\Omega \in L^2(\mathbb{R}^3)$. Note also that the construction gives only those drift processes in which the drift velocity \mathbf{a} is derivable from a potential; by a theorem of Kolmogorov [11], these are precisely the drift processes which are time reversible.

Edward's idea is to choose a drift process ρ which, at least formally, is close to the process ν of (1). To motivate his choice it is best to rewrite the energy functional which appears in (1) in terms of the local time density $T(\mathbf{x})$ defined formally by

$$T(\mathbf{x}) = \int_0^\infty \delta(\mathbf{x} - \mathbf{x}(\sigma)) d\sigma. \tag{17}$$

Then

$$\begin{aligned} \int_0^\infty \int_0^\infty \delta(\mathbf{x}(\sigma) - \mathbf{x}(\tau)) d\sigma d\tau &= \int_0^\infty \int_0^\infty \int d\mathbf{x} \delta(\mathbf{x} - \mathbf{x}(\sigma)) \delta(\mathbf{x} - \mathbf{x}(\tau)) d\sigma d\tau \\ &= \int d\mathbf{x} [T(\mathbf{x})]^2. \end{aligned} \tag{18}$$

If in (18) the integrand is replaced by $T(\mathbf{x})E[T(\mathbf{x})]$, we obtain

$$\begin{aligned} \int d\mathbf{x} T(\mathbf{x})E[T(\mathbf{x})] &= \int d\mathbf{x} \int_0^\infty d\sigma \delta(\mathbf{x} - \mathbf{x}(\sigma)) E[T(\mathbf{x})] \\ &= \int_0^\infty d\sigma E[T(\mathbf{x}(\sigma))] \end{aligned} \tag{19}$$

which is the form of the energy functional in (3). Edwards therefore asks for a potential function $V(\mathbf{x})$ such that

$$E[T(\mathbf{x})] = V(\mathbf{x}). \tag{20}$$

At this point it is necessary to resolve the ambiguity concerning the meaning of the expectation $E[\cdot]$ in these formal manipulations. It could be taken to be E_ν —but that would render (20) useless since we know nothing about ν . Edwards therefore takes it to be E_ρ —so that ρ is to be a Markov process whose potential in the sense of probabilistic potential theory (that is the left side of (20)) is equal to its potential in the sense of the parametrisation given by (3). Thus V is a self-consistent potential.

Mathematically the problem of determining a self-consistent potential in the sense of (20) may not appear very natural because the link between the generator L of the process ρ and its potential V , which is made by (16) and (13), is somewhat indirect. In Appendix A we give a geometrical interpretation of the problem which is mathematically appealing.

Edwards assumes the existence of a unique solution of (20) having regular asymptotic behaviour as $r \rightarrow \infty$. That this assumption is correct is the main result of this section.

Theorem 2. *There exists a unique self-consistent potential $V_s(r)$ (within the class of potentials for which we have defined drift processes). This potential satisfies*

$$V_s(r) \sim 2^{-5/3} \pi^{-2/3} r^{-4/3}, \text{ as } r \rightarrow +\infty. \quad (21)$$

Remark 1. There is a discrepancy between the constant which appears in (21) and the constant in the corresponding Eq. (3.19) of [1], which is resolved by the observation that Edwards takes $H_0 = -\frac{1}{3}\Delta$ as the generator of the Wiener process in \mathbb{R}^3 .

For the proof of Theorem 2 we will need the following elementary lemma, which is verified by computation.

Lemma 5. *Let $y = z_1 z_2$ be the product of two solutions of the linear differential equation $z'' = 2V(r)z$, with V a smooth function of r on $(0, \infty)$. Then y satisfies the linear equation*

$$y''' - 8Vy' - 4V'y = 0. \quad (22)$$

The square $k = [W(z_1, z_2)]^2$ of the Wronskian of z_1, z_2 depends only on y . In fact

$$k = -2yy'' + y'^2 + 8Vy^2. \quad (23)$$

Conversely, any solution y of (22) for which $k \geq 0$ can be written as a product $z_1 z_2$ of two solutions of $z'' = 2V(r)z$.

Proof of Theorem 2. (11) gives, for any admissible potential V ,

$$\begin{aligned} E[T(\mathbf{x})] &= \int_0^\infty q(\mathbf{0}, \mathbf{x}, t) dt \\ &= \langle \mathbf{0} | H^{-1} | \mathbf{x} \rangle \Omega(\mathbf{x}) \\ &= G(r)\Omega(r) \text{ (say)}. \end{aligned} \quad (24)$$

Note that $G(r) \leq G_0(r) = \langle \mathbf{0} | H_0^{-1} | \mathbf{x} \rangle = (2\pi r)^{-1}$, and that, as $r \rightarrow 0+$, $G(r) \sim G_0(r)$. On $(0, +\infty)$ $G(r)$ satisfies the differential equation $HG = 0$.

Write $z_1(r) = rG(r)$, $z_2(r) = r\Omega(r)$, so that z_1, z_2 are both solutions on $(0, \infty)$ of $z'' = 2V(r)z$. By Lemma 5 their product $y(r)$ satisfies (22). For a self-consistent potential V (20) must hold i.e. $y(r) = r^2 V(r)$. We may therefore replace V by $r^{-2}y$ in (22), and obtain a nonlinear equation which must be satisfied by y . The change of variables

$$s = \frac{2}{3} \log r; \quad u(s) = 27y(r) \quad (25)$$

transforms this equation into (1.3), with $\lambda = \frac{9}{4}$. (4) is equivalent to the boundary condition (1.8) of Theorem 1. According to Theorem 1, $u(s)$ is now uniquely determined up to translation in s , and so $y(r)$ up to a scale change in r . This ambiguity

is removed by the boundary condition $y(r) \sim (2\pi)^{-1}r$, as $r \rightarrow 0+$ (equivalently we may determine $k = (2\pi)^{-2}$ in (23), which fixes the constant c in the integrated form (1.7) of (1.3)); there is thus only one potential which could be self-consistent, and it remains only to show that it is in fact self-consistent. We therefore compare, for this particular potential V_s , the functions $y(r) = z_1(r)z_2(r)$ and $U(r) = r^2 V_s(r)$. From the definition of V_s , $U(r)$ satisfies (22) and has $k = (2\pi)^{-2} > 0$ in (23). From the final assertion of Lemma 5 it follows that

$$U(r) = (az_1(r) + bz_2(r))(cz_1(r) + dz_2(r)),$$

for some constants a, b, c, d with $(ad - bc)^2 = 1$. Since $z_1(r) \sim (2\pi)^{-1}$, $z_2(r) \sim r$ and $U(r) \sim (2\pi)^{-1}r$ as $r \rightarrow 0+$, one of a, c must be zero, say $a = 0$.

The asymptotic behaviour of $V_s(r)$ as $r \rightarrow +\infty$ is determined by Lemma 1, which gives (21). Moreover the detailed asymptotic analysis mentioned at the end of Sect. 1 shows that the asymptotic behaviour of derivatives of V_s is correctly given by formal differentiation of (21). For any V with such regular asymptotic behaviour, the asymptotic behaviour of $z_1(r), z_2(r)$ is given by the WKB formulae

$$\begin{aligned} z_1(r) &\sim [2V(r)]^{-1/4} \exp[-A(r)] \\ z_2(r) &\sim (4\pi)^{-1} [2V(r)]^{-1/4} \exp[A(r)], \end{aligned} \tag{26}$$

as $r \rightarrow +\infty$. Here $A(r)$ is a function determined by $V(r)$; for the potential V_s under consideration $A(r) \sim A_0 r^{1/3}$, as $r \rightarrow +\infty$, with A_0 a positive constant. From (21) and (26) it follows that $d = 0$, and so that $U(r) = z_1(r)z_2(r)$ i.e. V_s is self-consistent. \square

Remark 2. If existence of a potential V_s satisfying the self-consistency condition $r^2 V_s(r) = z_1(r)z_2(r)$ is assumed, and the asymptotic behaviour of V_s is assumed to be sufficiently regular that the WKB formulae (26) are valid, then the asymptotic behaviour (21) of V_s follows immediately; this is essentially the derivation of (21) given in [1].

Sufficient conditions for the validity of (26) are given by Coddington and Levinson [12].

3. The Asymptotics of Drift Processes

In this Sect. we consider the asymptotic behaviour as $t \rightarrow +\infty$ of the radial distance $r(t) = |\mathbf{x}(t)|$ for a drift process determined by a given potential $V(r)$ as in Sect. 2.

$r(t)$ may be characterised as the solution of the stochastic equation

$$dr = dB + a(r), \tag{1}$$

with $r(0) = 0$. Here $a(r) = \frac{d}{dr}(\ln \Omega(r))$ is the radial drift velocity, and $B(t) = |\mathbf{x}_0(t)|$

the 3-dimensional Bessel process (the radial component of Brownian motion in \mathbb{R}^3). $B(t)$ in turn may be constructed from the 1-dimensional Brownian motion $b(t)$ as the solution of the stochastic differential equation

$$dB = db + r^{-1} dt, \tag{2}$$

with $B(0) = 0$ ([13]). Thus $r(t)$ satisfies

$$dr = db + c(r)dt, \quad (3)$$

and $r(0) = 0$, with the effective drift velocity $c(r)$ given by

$$c(r) = a(r) + r^{-1}. \quad (4)$$

(3) is to be understood as an integral equation

$$r(t) = b(t) + \int_0^t c(r(s))ds. \quad (5)$$

Note that, under our conditions on V , $a(r) \geq 0$ for all r . For the self-consistent potential V_s , the asymptotic behaviour of the drift velocity is given by

$$a_s(r) \sim 2^{-1/3} \pi^{-1/3} r^{-2/3}. \quad (6)$$

We define the deterministic drift $R(t)$ as the solution of

$$\frac{dR}{dt} = c(R); \quad R(0) = 0. \quad (7)$$

If $a(r) \sim Ar^{-\alpha}$, $r \rightarrow +\infty$, with $A > 0$, $0 < \alpha < 1$, then as $t \rightarrow +\infty$ $R(t) \sim [A(1+\alpha)t]^{1/(1+\alpha)}$. Now $b(t)$ is of order $t^{1/2}$ as $t \rightarrow +\infty$, so we may expect that $r(t) \sim R(t)$ as $t \rightarrow +\infty$. In particular this should be true for the self-consistent process for which $\alpha = \frac{2}{3}$; then

$$R(t) \sim (2\pi)^{-1/5} \left(\frac{5}{3}\right)^{3/5} t^{3/5}, \quad (8)$$

so $r(t) \sim R(t)$ yields the Flory exponent $\frac{3}{5}$. The following theorem confirms these expectations, and also determines the magnitude of the fluctuations of $r(t)$ about $R(t)$.

Theorem 3. *Suppose that the effective drift velocity $c(r)$ is a positive, continuously differentiable function of r on $(0, \infty)$, and satisfies*

$$c'(r) \sim -Kr^{-2}, \text{ as } r \rightarrow 0+, \quad (9)$$

$$c'(r) \sim -Cr^{-(1+\alpha)}, \text{ as } r \rightarrow +\infty, \quad (10)$$

with $C, K > 0$, $0 < \alpha < 1$. Write

$$Y(t) = t^{-1/2}[r(t) - R(t)] \quad (11)$$

with $R(t)$ the deterministic drift. Then $Y(t)$ is asymptotically normal, with mean 0 and variance $(1+\alpha)(1+3\alpha)^{-1}$.

Remark. The conditions (9, 10) of Theorem 3 are readily verified for the self-consistent process.

Proof. Denote by $T(r)$ the function which is the inverse of $R(t)$;

$$T(r) = \int_0^r \frac{ds}{c(s)}. \quad (12)$$

Then the process $Z(t) = T(r(t))$ satisfies

$$Z(t) = t + \int_0^t f(Z(s)) db(s), \quad (13)$$

with

$$f(t) = [c(R(t))]^{-1}. \quad (14)$$

The conditions on $c(r)$ imply that f is continuously differentiable, and satisfies

$$f(t) \sim Ft^{\alpha/(1+\alpha)}, \text{ as } t \rightarrow \infty, \quad (15)$$

with F a positive constant, and

$$f'(t) \in L^p(\mathbb{R}, dt), \quad 1 + \alpha < p < 2. \quad (16)$$

(16) implies that for any β with $\alpha(1 + \alpha)^{-1} < \beta < \frac{1}{2}$ we have

$$|f(t_1) - f(t_2)| \leq M |t_1 - t_2|^\beta, \quad (17)$$

for some $M > 0$, and all $t_1, t_2 \geq 0$. We will choose β close to $\alpha(1 + \alpha)^{-1}$.

$H(t) = E[Z(t)^2]$ is increasing in t , and satisfies

$$\begin{aligned} H(t) &= t^2 + \int_0^t E[(f(Z(s)))^2] ds \\ &\leq t^2 + M^2 \int_0^t E[|Z(s)|^{2\beta}] ds \\ &\leq t^2 + M^2 \int_0^t H(s)^\beta ds \\ &\leq t^2 + M^2 t H(t)^\beta. \end{aligned} \quad (18)$$

(18) implies $H(t) \leq H_0 + H_1 t^2$, with H_0, H_1 positive constants. (19)

$$\text{Write } Z(t) = t + W(t) + \varepsilon(t), \quad (20)$$

with

$$W(t) = \int_0^t f(s) db(s), \quad (21)$$

$$\varepsilon(t) = \int_0^t [f(Z(s)) - f(s)] db(s). \quad (22)$$

$W(t)$ is Gaussian with mean 0, and variance $\int_0^t f(s)^2 ds$.

$$\begin{aligned} E[\varepsilon(t)^2] &= \int_0^t E[|f(Z(s)) - f(s)|^2] ds \\ &\leq M^2 \int_0^t E[|Z(s) - s|^{2\beta}] ds \\ &\leq M^2 t (E[|Z(t) - t|^2])^\beta. \end{aligned}$$

But

$$\begin{aligned} E[|Z(t) - t|^2] &= \int_0^t E[(f(Z(s)))^2] ds \\ &\leq M^2 t [H(t)]^\beta \\ &\leq M^2 t [H_0 + H_1 t^2]^\beta \text{ (by (19)),} \end{aligned}$$

so

$$E[\varepsilon(t)^2] = O(t^{1+\beta+2\beta^2}), \text{ as } t \rightarrow +\infty. \quad (23)$$

Now

$$\begin{aligned} r(t) &= R(Z(t)) \\ &= R(t + W(t) + \varepsilon(t)), \end{aligned}$$

so

$$\begin{aligned} Y(t) &= [r(t) - R(t)] t^{-1/2} \\ &= G(t) + \eta(t). \end{aligned} \quad (24)$$

Here $G(t) = R'(t)W(t)t^{-1/2}$ is Gaussian with mean 0, and variance

$$\begin{aligned} R'(t)^2 t^{-1} E[W(t)^2] &= t^{-1} [f(t)]^{-2} \int_0^t f(s)^2 ds \\ &\rightarrow (1 + \alpha)(1 + 3\alpha)^{-1} \text{ as } t \rightarrow \infty, \end{aligned} \quad (25)$$

by (15). With the help of (23) one checks that the remainder $\eta(t)$ in (24) $\rightarrow 0$ in measure as $t \rightarrow \infty$, and the convergence of $Y(t)$ in law to the normal distribution with mean 0, variance $(1 + \alpha)(1 + 3\alpha)^{-1}$ follows. \square

Appendix A

A Geometrical Interpretation of the Self-Consistent Potential

Let M be a conformally flat Riemannian manifold diffeomorphic to \mathbb{R}^n . Such a manifold has a distinguished class of coordinate systems (isothermal coordinates) in which the metric takes the form

$$(ds)^2 = \exp[2z(x)] \{ (dx^1)^2 + \dots + (dx^n)^2 \}. \quad (1)$$

Two isothermal coordinate systems are related by a conformal automorphism of \mathbb{R}^n i.e. by a linear conformal transformation ([14]).

A scalar quantity q of dimension L^k is represented mathematically by a real valued function $q(x)$ relative to a given choice of coordinates on M , the representing function $q'(x')$ in a second coordinate system then being given by

$$q'(x') = q(x) \left| \frac{dx}{dx'} \right|^{kn^{-1}} \quad (2)$$

In other words q is a section of the line bundle $\xi^{-kn^{-1}}$, where ξ denotes the line bundle of densities (n forms) on M . We will say that q is *isothermally constant* if $q(x)$ is constant in some, and therefore in every, isothermal coordinate system.

We fix now a distinguished point 0 of M , and suppose $n > 2$. The diffusion of

M with sample paths starting at 0, and generator $-\frac{1}{2}\bar{\Delta}$ ($\bar{\Delta}$ the Laplacian on M) induces a measure τ on M given by $\tau(S)$ = expected time spent in S , for any compact S . τ is absolutely continuous with respect to the volume measure on M , and we write its Radon–Nikodym derivative as $\frac{d\tau}{dv}$.

Let q be an isothermally constant scalar quantity of dimension L^{n-4} . Then we may define a real valued function h on M by

$$h(x) = q(x) \left| \frac{dv}{dx} \right|^{(n-4)/n}. \tag{3}$$

Denote by R the scalar curvature of M , and consider the equation

$$R = h \frac{d\tau}{dv}. \tag{4}$$

We claim that this equation is equivalent to the equation determining the self-consistent potential ((2.20) for $n = 3$, and Appendix B for general $n > 2$).

To verify the claim fix an isothermal coordinate system and compute

$$R = -2(n-1) \exp[-2z] \left\{ \Delta z + \left(\frac{n-2}{2} \right) \nabla z \cdot \nabla z \right\}. \tag{5}$$

$$\bar{\Delta} \varphi = \exp[-2z] \{ \Delta \varphi + (n-2) \nabla \varphi \cdot \nabla z \}. \tag{6}$$

From (6) it follows that we may obtain an identification of the diffusion on M with generator $-\frac{1}{2}\bar{\Delta}$ and the drift process with generator

$$L = -\frac{1}{2}\Delta - \nabla(\ln \Omega) \cdot \nabla, \tag{7}$$

up to a time change, if we make the identification

$$\Omega = \exp \left\{ \frac{(n-2)}{2} z \right\}. \tag{8}$$

The time change implied by the factor $\exp[-2z]$ in (6) gives

$$\bar{T}(x) = \exp[2z] T(x), \tag{9}$$

as the relation between the local time densities of the diffusion and drift processes, so

$$\frac{d\tau}{dv}(x) = \exp\{(2-n)z\} E[T(x)]. \tag{10}$$

The potential $V(x)$ used to characterise the drift process is given by

$$V = \frac{1}{2}\Omega^{-1} \Delta \Omega, \tag{11}$$

so, denoting by q_0 the constant value of $q(x)$, we find (4) equivalent to the self-consistent potential equation

$$V(x) = gE[T(x)], \tag{12}$$

with

$$g = -\frac{q_0(n-2)}{8(n-1)}. \quad (13)$$

Appendix B

Dependence on Dimension

It is of interest to consider how the preceding considerations are modified if we replace paths in \mathbb{R}^3 by paths in \mathbb{R}^n . Indeed, since the condition (2.20) defining a self-consistent potential involves only the radial component of the drift process, it is possible to formulate its analog for any positive real number n ; it suffices in

the constructions of Sect. 2 to replace the Laplacian in \mathbb{R}^3 , $\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr}$, by $\frac{d^2}{dr^2} + \frac{(n-1)}{r} \frac{d}{dr}$.

The case $n = 4$ is special for in this case the coupling constant g is dimensionless, and we cannot set $g = 1$ by choice of length and time scales; thus g is to be inserted as a factor multiplying the left side of (2.20). As in Sect. 2 we find that a smooth potential $V(r)$ satisfies the self-consistency condition only if $y(r) = r^2 V(r)$ satisfies a certain non-linear differential equation; this equation is transformable to the normal form (1.2). From Theorem 1 (a) it follows that $y(r)$ must be constant, so that $V(r)$ is a Coulomb potential Cr^{-2} . A direct calculation shows that this potential does satisfy the self-consistency condition for coupling constant g if C is the (unique) positive root of

$$C^2(1 + 2C) = g^2(4\pi^2)^{-1}. \quad (1)$$

The corresponding radial process is a Bessel process with dimension parameter

$$m = 2[(1 + 2C)^{1/2} + 1], \quad (2)$$

so that

$$E[r(t)^2] = mt. \quad (3)$$

For $n \neq 4$ we may normalise $g = 1$ by choice of units as before. The self-consistency condition (2.20) on $V(r)$ implies that $y(r) = r^2 V(r)$ must satisfy a certain differential equation. The change of variables

$$s = \frac{2}{3}(4 - n) \log r; \quad u(s) = 27(n - 4)^{-2} y(r) \quad (4)$$

transforms this equation into (1.3) with

$$\lambda = \frac{9}{4} \left(\frac{n-2}{n-4} \right)^2. \quad (5)$$

Theorem 1 now implies that $u(s)$ is uniquely determined up to translation in s , so $V(r)$ up to scale change in r . This ambiguity is resolved by determining the

behaviour of $V(r)$ as $r \rightarrow +\infty$ as in Remark 2 Sect. 2; this gives

$$V(r) \sim 2^{-1} \pi^{-n/3} \left[\Gamma\left(\frac{n}{2}\right) \right]^{2/3} \bar{r}^{2/3} r^{-2/3(n-1)}. \quad (6)$$

For $n > 4$ (6) imposes a boundary condition on $u(s)$ as $s \rightarrow -\infty$ which cannot be met, so no self-consistent potential exists. For $0 < n < 4$ (6) determines $V(r)$ uniquely, and, as in Sect. 2, this potential may be shown to be self-consistent. The corresponding drift process has a drift velocity $a(r) \sim Ar^{-\alpha}$ as $r \rightarrow \infty$, with $\alpha = \frac{1}{3}(n-1)$. The asymptotic behaviour of $r(t)$ is then given by Theorem 3 (which is actually valid for $-\frac{1}{3} < \alpha < 1$).

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