Resenhas IME-USP 1994, Vol. 1, No. 4, 363 - 372.

A collapse transition for self-attracting walks[1]

David C. Brydges and Gordon Slade

Abstract: We consider an ensemble of discrete random walk paths in which a weight favouring self-intersections is assigned to each walk. The strength of the self-attraction can be increased by increasing a coupling constant β, and decreases as a power of the length of the walk. We study the collapse transition in this model, which is a phase transition from diffusive or extended behaviour of the walk for small β to confined behaviour for large β. The dependence on the spatial dimension is elucidated.

Key words: self-attracting walk, Edwards model, diffusion, phase transition, local time, polymer, large deviations.

1 The model

Let ω be a T-step homogeneous simple random walk on $\mathbf{Z}^d$ taking nearest neighbour steps with equal probabilities $\frac{1}{2d}$, and starting at the origin. Define

$$J_T \equiv J_T(\omega) = \sum_{0 \leq i < j \leq T} \delta_{\omega(i),\omega(j)} \tag{1.1}$$

and

$$c_T = E \exp[\beta T^{-p} J_T], \tag{1.2}$$

where the expectation is with respect to simple random walk beginning at 0, and $p \geq 0$ and $\beta \in \mathbf{R}$ are parameters. We define a new measure on T-step simple random walks, by assigning to a walk ω the probability

$$\frac{1}{c_T} \frac{1}{(2d)^T} \exp[\beta T^{-p} J_T(\omega)]. \tag{1.3}$$

For $\beta = 0$, this new measure is just the simple random walk. For $\beta > 0$, it defines a model of self-attracting walks, since self-intersections are encouraged by the exponential factor. Similarly, for $\beta < 0$, this is a model of self-repelling walks. The factor T^{-p} diminishes the strength of the self-interaction for long walks, and for p fixed, β provides a measure of the strength of the interaction.

We are interested in the phenomenon of a collapse transition, in which for fixed p there is a transition from diffusive behaviour to collapsed behaviour when $\beta > 0$ is increased. The order parameter for the transition is the diffusion constant $D(\beta)$, which is defined in terms of the mean-square displacement

$$\langle |\omega(T)|^2 \rangle_\beta = \frac{E\left(|\omega(T)|^2 \exp[\beta T^{-p} J_T]\right)}{E\left(\exp[\beta T^{-p} J_T]\right)} \tag{1.4}$$

[1] Partially supported by FAPESP's Projeto Temático "Transição de Fase Dinâmica e Sistemas Evolutivos".

by

$$D(\beta) = \lim_{T\to\infty} \frac{1}{T}\langle |\omega(T)|^2\rangle_\beta. \tag{1.5}$$

The diffusive phase corresponds to $0 < D(\beta) < \infty$, while the collapsed phase is signalled by $D(\beta) = 0$. Typically in the collapsed phase the mean-square displacement remains uniformly bounded as $T \to \infty$.

Examples:

1. For $\beta = 0$, this is the simple random walk and $D(0) = 1$.

2. For $p = 0$ and $\beta < 0$, this is the Domb–Joyce model of weakly self-avoiding walks, which in the limit $\beta \to -\infty$ gives the usual strictly self-avoiding walk [7].

3. For $\beta > 0$ and $0 \le p < 1$, it can be seen from combinatoric considerations [8, 9] that the walk is collapsed, in the sense that it remains in a small box (uniform in T) with a probability converging exponentially to 1 as $T \to \infty$.

4. For $\beta > 0$, $p = 1$, there is a collapse transition as β is increased, and this will be the main focus of this paper. (Collapse takes place at $\beta = 0$ when $d = 1$).

5. The Edwards model is a much-studied model of polymer molecules, whose partition function is given formally by

$$E\exp\left[\beta \int_{0\le s<t\le 1} \delta(B_s - B_t)ds\,dt\right], \tag{1.6}$$

where B denotes Brownian motion. Renormalization is required to make sense of this formal expression in dimensions $d \ge 2$, and this is well-understood for $d = 2$ and $d = 3$. Traditionally the Edwards model has been studied for $\beta < 0$, but for $d = 1$ (1.6) is an *entire* function of β, and for $d = 2$ (when conventionally renormalized by subtracting from the exponent its expected value) it is finite for $-\infty < \beta < \beta_0$, for some $\beta_0 > 0$ [6]. A discrete space-time version of the Edwards model can be obtained by approximating Brownian motion B_t on $[0, 1]$ by $T^{-1/2}\omega(\lfloor tT \rfloor)$, and this leads to the discrete partition function

$$E\exp[\beta T^{(d-4)/2} J_T], \tag{1.7}$$

where now the expectation is with respect to simple random walk. This is the partition function c_T with $p = \frac{4-d}{2}$. Hence, for $d = 2$ and $p = 1$, or for $d = 1$ and $p = \frac{3}{2}$, the large-T behaviour of c_T is closely related to the study of the continuum limit of the discrete Edwards model. This will also be a focus in what follows.

6. By way of contrast, the standard model of collapse of polymer molecules has a partition function involving a self-repellence due to the excluded volume effect that no two monomers can occupy the same region of space, together with a nearest-neighbour attraction due to temperature or solvent effects, i.e.,

$$E\exp\left[-\lambda_1 \sum_{0\le i<j\le T} \delta_{\omega(i),\omega(j)} + \lambda_2 \sum_{0\le i<j\le T} \delta_{|\omega(i)-\omega(j)|,1}\right], \tag{1.8}$$

with λ_1 and λ_2 both positive. It has been argued, and observed experimentally, that when λ_2 is increased with fixed λ_1, there is a collapse transition. Our model does not cover this very interesting example, which appears to be quite difficult to treat rigorously.

We concentrate in what follows on $p = 1$ for $d \geq 2$ and on $p = 1$ and $p = \frac{3}{2}$ for $d = 1$.

2 The results

This section summarizes some results of Bolthausen and Schmock [1] for the collapsed phase and of Brydges and Slade [4] for the diffusive phase. Further results and more complete proofs can be found in these references. Actually, Bolthausen and Schmock analyze the closely related model in which the simple random walk is replaced by a continuous-time random walk on $\mathbf{Z}^d$ having exponential holding times. Their results have not been extended to the discrete-time walk, but we expect qualitatively similar behaviour.

To state the results we first define the renormalized partition function

$$c_T^{\text{ren}} = E\exp[\beta T^{-p}(J_T - E(J_T))]. \tag{2.1}$$

Let $G(0) = \sum_{T=0}^{\infty} p_T(0)$, where $p_T(0)$ denotes the T-step transition probability for simple random walk to return to the origin at time T; $G(0)$ is finite for $d > 2$ but not for $d \leq 2$. It is not hard to see that as $T \to \infty$,

$$\frac{1}{T}EJ_T \to G(0) - 1 \qquad (d > 2) \tag{2.2}$$

$$\frac{1}{T}EJ_T \sim \frac{1}{\pi}\log T \qquad (d = 2) \tag{2.3}$$

$$\frac{1}{T^{3/2}}EJ_T \to \frac{2}{3}\sqrt{\frac{2}{\pi}} \qquad (d = 1), \tag{2.4}$$

so that the effect of the renormalization is significant only for $d = 2$, with these values of p.

We also define

$$\beta_0 = \sup\{\beta : \sup_T c_T^{\text{ren}} < \infty\}. \tag{2.5}$$

It can be shown that $\beta_0 > 0$ for $d \geq 2$, $p = 1$ and $\beta_0 = \infty$ for $d = 1$, $p = \frac{3}{2}$; see Section 4.1 and [4, 6]. Finally, let

$$\beta_c = \inf\{\beta : \lim_{T\to\infty} c_T^{1/T} > 0\}. \tag{2.6}$$

Clearly $\beta_0 \leq \beta_c$, so $\beta_c > 0$ if $d \geq 2$, $p = 1$ and $\beta_c = \infty$ if $d = 1$, $p = \frac{3}{2}$. It has not been established whether or not $\beta_0 = \beta_c$. For $d = 1$, $p = 1$, it is shown in [1] that $\beta_c = 0$.

The following theorem, which is due to [1] and is proved using methods from the theory of large deviations, establishes the existence of a collapsed phase when $p = 1$.

Theorem 2.1 *For the continuous-time model with $p = 1$, the mean-square displacement is uniformly bounded in T for all positive β when $d = 1$ and for $\beta > \beta_c$ (continuous-time analogue of β_c) if $d \geq 2$.*

The above theorem rules out the possibility of a collapse transition at *positive* β when $d = 1$.

Existence of an extended phase is established by the following theorem, due to [4], which indicates that there are three different phenomena corresponding to dimensions $d = 1$, $d = 2$ and $d > 2$.

Theorem 2.2 (*a*) *For $d > 2$, $p = 1$ and $-\infty < \beta < \beta_0$, $D(\beta) = 1$.*
(*b*) *For $d = 2$, $p = 1$ and $-\infty < \beta < \beta_0$, $D(\beta) > 0$. Moreover, D is a strictly decreasing function of β for $0 < \beta < \beta_0$.*
(*c*) *For $d = 1$, $p = \frac{3}{2}$ and $-\infty < \beta < \infty$, $D(\beta) > 0$. Moreover, D is a strictly decreasing function of β for all $\beta > 0$.*

Combined with Theorem 2.1, this suggests that the transition from extended to collapsed behaviour is discontinuous for $d > 2$. For $d = 2$, the transition may or may not be continuous. For $d = 1$, the transition from extended to collapsed behaviour may occur more gradually, as p is varied from $\frac{3}{2}$ to 1, with subdiffusive behaviour at intermediate p. Establishing such behaviour remains open.

For $d \leq 2$, there is an explicit formula for the diffusion constant in terms of the renormalized self-intersection local time $\underline{\gamma}$ for Brownian motion, which is given formally by

$$\underline{\gamma}[0, N] \text{ “ = ” } \int_{0\leq s<t\leq N} \delta(B_t - B_s)ds\,dt - E\left[\int_{0\leq s<t\leq N} \delta(B_t - B_s)ds\,dt\right] \tag{2.7}$$

(the renormalization is optional for $d = 1$). Defining a measure on continuous paths by $d\nu_{\beta,N} = Z^{-1}e^{\beta\underline{\gamma}[0,N]}$ with $Z = E[e^{\beta\underline{\gamma}[0,N]}]$, the formula is

$$D(\beta) = \int B_1^2 d\nu_{\beta,1}. \tag{2.8}$$

This is well-defined under the hypotheses of Theorem 2.2, by methods of Le Gall [6]. To establish the behaviour of the diffusion constant in the limit of large negative coupling, we let $\lambda = -\beta > 0$ and use Brownian scaling to conclude that, for any $N > 0$,

$$D(\beta) = N^{-1} \int B_N^2 d\nu_{\beta N^{(d-4)/2}, N}. \tag{2.9}$$

Taking $N = \lambda^{2/(4-d)}$ then gives

$$D(\beta) = N^{-1} \int B_N^2 d\nu_{-1,N}, \tag{2.10}$$

converting the $\lambda \to \infty$ limit into the problem of the large time behaviour of the Edwards model. For $d = 1$, it is argued in [13] that $\int B_N^2 d\nu_{-1,N} \sim v^2 N^2$, which implies the diffusion constant goes to infinity according to $D(\beta) \sim v^2 \lambda^{2/3}$. The corresponding problem for $d = 2$ is unsolved.

It has also been proved that the scaling limit of the walk is Brownian motion in part (a) of Theorem 2.2 and is the Edwards model in parts (b) and (c).

3 A variational problem

In this section we consider only $\beta > 0$ and $p = 1$, and address the question of why there is a collapse transition at positive β for $d \geq 2$ but not for $d = 1$. We will argue heuristically, but this argument provides the basis for the proof by Bolthausen and Schmock that there is a collapsed phase.

We begin by rewriting the partition function, after first changing its definition in an inessential way by replacing the sum over $0 \leq i < j \leq T$ in the definition of J_T by the sum over $0 \leq i, j \leq T$. Defining

$$L_x(T) = \frac{1}{T} \sum_{i=0}^{T} \delta_{\omega(i),x}, \tag{3.1}$$

we have

$$\frac{1}{T} \sum_{0 \leq i,j \leq T} \delta_{\omega(i),\omega(j)} = T \sum_x L_x^2(T). \tag{3.2}$$

Thus our partition function, after inessential modification, is equal to

$$c_T = E \exp\left[\beta T \sum_x L_x^2(T)\right]. \tag{3.3}$$

We write $\tilde{c}_T$ for the corresponding quantity for the continuous-time random walk; there $L_x(T)$ is defined via an integral rather than a sum.

The Donsker–Varadhan theory of large deviations suggests that

$$\lim_{T \to \infty} \frac{1}{T} \log \tilde{c}_T = \sup\{\beta ||\phi||_4^4 - \frac{1}{2} ||\nabla\phi||_2^2 : ||\phi||_2 = 1\} \equiv b. \tag{3.4}$$

The gradient is the finite difference gradient associated to the lattice. In general the supremum may or may not be attained. It is clear that for β sufficiently large, and in any dimension, the solution b of the variational problem is strictly positive. In this case it can be shown that the supremum is attained by an exponentially decaying function. For $d = 1$, it is the case for all $\beta > 0$ that $b > 0$ (this can be motivated by a scaling argument), and here too the supremum is attained by an exponentially decaying function. On the other hand for $d \geq 2$ there is a Sobolev inequality

$$||\phi||_4^4 \leq C||\phi||_2^2 ||\nabla \phi||_2^2, \tag{3.5}$$

and hence $b = 0$ for sufficiently small β.

If ϕ realizes the supremum, then so does any translate. In the collapsed phase it is expected that the law for the process is a mixture of ergodic components, i.e., the process breaks translation invariance by choosing where to collapse, and if we restrict to a component, then as $T \to \infty$, $L_y(T)$ converges almost surely to the corresponding translate of $\phi^2(y)$. Exponential decay of the optimal ϕ^2, and hence $b > 0$, thus corresponds to collapse. This type of result is proved by Bolthausen and Schmock. A difficulty in applying the Donsker–Varadhan theory is that the state space here is all of $\mathbf{Z}^d$ and is therefore not compact. This is overcome by making use of the fact that in the collapsed phase the state space is nearly compact, since the walk spends the bulk of its time in a compact subset of $\mathbf{Z}^d$.

Thus, $b > 0$ corresponds to a localized local time, or a confined phase for the walk. On the other hand, $b = 0$ is interpreted as corresponding to the supremum being approximated by a sequence of increasingly more constant (zero) ϕ's, and hence to $L_x(T)$ approaching a constant (zero) function. This is interpreted as extended behaviour for the walk.

The above discussion leads one to expect that there will be a collapse transition, at positive β, for $d \geq 2$ but not for $d = 1$, when $p = 1$.

4 The extended phase

We fix $q = 1$ for $d \geq 2$ and $q = \frac{3}{2}$ for $d = 1$, and define

$$\gamma_T = \frac{1}{T^q} J_T = \frac{1}{T^q} \sum_{0 \leq s < t \leq T} \delta_{\omega(s),\omega(t)}. \tag{4.1}$$

The proof of Theorem 2.2 involves a combination of proving existence of uniform exponential moments of γ_T (renormalized when $d = 2$), or equivalently proving that $\beta_0 > 0$, together with limit theorems for $\gamma_T - E\gamma_T$. For $d = 1$ and $d = 2$, the latter problem is one which has been studied previously, being precisely the problem of proving invariance principles for self-intersection local times [2, 3, 10, 11]. For $d > 2$ the random variable γ_T is a power of T smaller than $T^{(d-4)/2} J_T$, and $\gamma_T - E\gamma_T$ turns out to converge to zero in the limit. The following describes some of the ideas which go into the proof; details can be found in [4].

4.1 Dimensions $d > 2$

Consider first the case of $d > 2$. Existence of an exponential moment for γ_T follows from the following lemma. The proof of the lemma makes use of the notation

$$(f * g)_T(x) = \sum_y \sum_{s=0}^{T} f_s(y) g_{T-s}(x-y) \tag{4.2}$$

for convolution in time and space. We write f^{*n} for the convolution of n factors of f.

Lemma 4.1 *For $d > 2$, there is a $\beta_0 = \beta_0(d) > 0$ such that for all $-\infty < \beta < \beta_0$,*

$$\sup_T E e^{\beta \gamma_T} < \infty.$$

Proof. Let $d > 2$. For $\beta \le 0$, $Ee^{\beta\gamma_T} \le 1$, so assume $\beta > 0$. Let

$$\tau_y(T) = T L_y(T) = \sum_{i=0}^{T} \delta_{y,\omega(i)} \tag{4.3}$$

denote the number of visits of the walk ω to the site y, up to time T. In terms of $\tau_y(T)$,

$$\gamma_T = T^{-1} J_T = \frac{1}{2} T^{-1} \left[\sum_{i,j=0}^{T} \delta_{\omega(i),\omega(j)} - T \right] = \frac{1}{2T} \sum_y \tau_y^2(T) - \frac{1}{2}. \tag{4.4}$$

In view of (4.4), it suffices to obtain the uniform bound of the theorem with γ_T replaced by $T^{-1} \sum_y \tau_y^2(T)$.

By Jensen's inequality, since $T^{-1} \sum_y \tau_y = 1$, we have

$$\begin{aligned} \exp\left[\beta T^{-1} \sum_y \tau_y^2\right] &\le \frac{1}{T} \sum_y \tau_y \exp[\beta \tau_y] \\ &= \frac{1}{T} \sum_y \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \tau_y^{n+1}. \end{aligned} \tag{4.5}$$

Therefore

$$E \exp\left[\beta T^{-1} \sum_y \tau_y^2\right] \le \frac{1}{T} \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \sum_y E \tau_y^{n+1}. \tag{4.6}$$

The factor τ_y^{n+1} amounts to a requirement that ω visit the site y at each of $n+1$ times, and ordering these times gives rise to a factor $(n+1)!$. Let $p_t(x)$ denote the probability that simple random walk goes from 0 to x in t steps, and let $q_t(x) = p_t(0)\delta_{x,0}[1-\delta_{t,0}]$. Then we have, using $(p*p)_t(x) = (t+1)p_t(x)$, that

$$\begin{aligned} E\exp\left[\beta T^{-1}\sum_y \tau_y^2\right] &\leq \frac{1}{T}\sum_{n=0}^{\infty}\frac{\beta^n}{n!}\sum_x (n+1)!(p*q^{*n}*p)_T(x) \\ &= \frac{1}{T}\sum_{n=0}^{\infty}\beta^n(n+1)\sum_{t=0}^{T}(q^{*n})_t(0)\sum_x (p*p)_{T-t}(x) \\ &= \frac{1}{T}\sum_{n=0}^{\infty}\beta^n(n+1)\sum_{t=2}^{T}(q^{*n})_t(0)(T-t+1) \\ &\leq \sum_{n=0}^{\infty}\beta^n(n+1)\sum_{t=2}^{T}(q^{*n})_t(0). \end{aligned} \tag{4.7}$$

A uniform bound on the right side for small β then follows from the fact that

$$\sum_{t=0}^{T}(q^{*n})_t(0) \leq G(0)^n. \tag{4.8}$$

□

The above lemma can be extended to show that, for $d=1$, γ_T has uniform exponential moments of all orders.

The remaining step in the proof is to show that $\gamma_T - E\gamma_T$ converges to zero in L^2, as $T\to\infty$. Combined with existence of an exponential moment and standard uniform integrability arguments, this allows us essentially to take the limit under the expectation in the definition of the diffusion constant, resulting simply in the Brownian motion expectation of B_1^2, which is 1. The proof of convergence to zero in L^2 involves an elementary calculation along the lines of that used to prove (2.2), but is more detailed.

4.2 Dimensions $d \leq 2$

For $d \leq 2$, we again wish to justify taking the limit inside the expectation defining the diffusion constant, but now this is more involved because the limit of $\gamma_T - E\gamma_T$ is the renormalized self-intersection local time for Brownian motion, instead of zero as was the case for $d > 2$. Again there are two principal ingredients: existence of an exponential moment for γ_T and a convergence theorem for γ_T.

The proof of existence of an exponential moment is a mild extension of Lemma 4.1 for $d=1$, but a new idea is needed to handle the logarithmic divergence occurring for $d=2$. This new idea was provided by Le Gall [6], using the dyadic decomposition introduced by Westwater [12]. His method extends to prove a uniform bound on c_T^{ren} for small positive β.

Convergence in distribution of $\gamma_T - E\gamma_T$ is proved simultaneously for $d = 1$ and $d = 2$ using an extension of methods of Rosen [11] for strongly aperiodic two-dimensional walks. This involves introducing cutoffs by smoothing the delta function in the definition of the self-intersection local time and by truncating the dyadic decomposition to avoid divergences arising from the diagonal when $d = 2$. Moment estimates for the intersection local time of two independent random walks are required.

The strict monotonicity of the diffusion constant for positive coupling is a consequence of a correlation inequality of Fröhlich and Park [5]. It is likely that this strict monotonicity also applies for negative coupling, but this has not been established.

Note added in proof. Our statement that Bolthausen and Schmock prove that the diffusion constant in the collapsed phase is zero has to be amended, as this result is not in their preprint. Their results indicate collapse for the appropriate parameter values, using a different criterion for collapse.

Acknowledgements

The work of D.C.B. was supported in part by NSF grant DMS 910256. D.C.B. thanks Alain Sznitman and the Forschungsinstitut für Mathematik at ETH-Zentrum for their hospitality while part of this work was carried out. The work of G.S. was supported in part by NSERC grant A9351, and by SERC grant G59981 during a visit to the Isaac Newton Institute in Cambridge. We benefitted from discussions and correspondence with M. Aizenman, E. Bolthausen, J. Fröhlich, T. Hara, C.M. Newman, A.D. Sokal, A.-S. Sznitman, and especially J.-F. Le Gall and S.R.S. Varadhan.

References

[1] E. Bolthausen and U. Schmock. On self-attracting d-dimensional random walks. Preprint, (1994).

[2] A.N. Borodin. On the asymptotic behavior of local times of recurrent random walks with finite variance. *Theory Probab. Appl.*, **26**:758–772, (1981).

[3] A.N. Borodin. Brownian local time. *Russian Math. Surveys*, **44**:1–51, (1989).

[4] D.C. Brydges and G. Slade. The diffusive phase of a model of self-interacting walks. Preprint, (1994).

[5] J. Fröhlich and Y.M. Park. Correlation inequalities and the thermodynamic limit for classical and quantum continuous systems. *Commun. Math. Phys.*, **59**:235–266, (1978).

[6] J.-F. Le Gall. Exponential moments for the renormalized self-intersection local time of planar Brownian motion. In J. Azéma, P.A. Meyer, and M. Yor, editors, *Séminaire de Probabilités XXVIII. Lecture Notes in Mathematics #1583*, Berlin, (1994). Springer.

[7] N. Madras and G. Slade. *The Self-Avoiding Walk.* Birkhäuser, Boston, (1993).

[8] Y. Oono. On the divergence of the perturbation series for the excluded-volume problem in polymers. *J. Phys. Soc. Japan*, **39**:25–29, (1975).

[9] Y. Oono. On the divergence of the perturbation series for the excluded-volume problem in polymers. II. Collapse of a single chain in poor solvents. *J. Phys. Soc. Japan*, **41**:787–793, (1976).

[10] E. Perkins. Weak invariance principles for local time. *Z. Wahrsch. verw. Gebiete*, **60**:437–451, (1982).

[11] J. Rosen. Random walks and intersection local time. *Ann. Probab.*, **18**:959–977, (1990).

[12] J. Westwater. On Edwards' model for long polymer chains. *Commun. Math. Phys.*, **72**:131–174, (1980).

[13] J. Westwater. On Edwards' model for long polymer chains. In S. Albeverio and P. Blanchard, editors, *Trends and Developments in the Eighties. Bielefeld Encounters in Mathematical Physics IV/V.* World Scientific, Singapore, (1985).

David C. Brydges
Department of Mathematics
University of Virginia
Charlottesville, VA 22903-3199
e-mail: `db5d@virginia.edu`
USA

Gordon Slade
Department of Mathematics and Statistics
McMaster University
Hamilton, Ont., L8S 4K1
e-mail: `slade@mcmaster.ca`
CANADA