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Finite-Size Scaling for Mean-Field Percolation

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By studying transfer matrix eigenvalues, correlation lengths for a mean field directed percolation model are obtained both near and far from the critical regime. Near criticality, finite-size scaling behavior is derived and an analytic technique is provided for obtaining the finite-size scaling function. Our methods involve the generating function, matched asymptotic expansions, and certain formulas developed for the study of eigenvalues of the transfer matrix for metastability.

KEY WORDS: Percolation; finite-size scaling; transfer matrix; asymptotic degeneracy.

1. INTRODUCTION

Directed percolation provides a framework for a variety of stochastic processes. As such, phase transition terms, such as percolation threshold or correlation length, take on meaning for the stochastic process. Conversely, we may sometimes phrase directed percolation as a time-dependent process. In this article we employ an epidemic metaphor; for more extensive treatment of epidemic models see ref. 1. It is also possible to describe the process in terms of chemical reactions; another application is to astrophysics.[2,3] For the epidemic models in particular, finite-size effects may be of interest because of quarantines, or in general because population sizes are far smaller than the numbers usually relevant in physics or chemistry. In this article we obtain analytic results for the extinction time of an epidemic due to the finiteness of the population. In the neighborhood of the value of the disease transmission probability for which the disease

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takes hold (i.e., the percolation threshold) there is a data collapse in rescaled variables. The scaling function, which summarizes that collapse and which is usually only known numerically, is here obtained as the eigenvalue of a certain Schrödinger-like equation.

In ref. 4, two infinite-range mean field directed percolation problems were introduced and their correlation length was studied using the transfer matrix. For directed percolation, a correlation "length" is defined for the time direction, and it is related to the first nontrivial eigenvalue of the transfer matrix. Extensive numerical work in ref. 4 established finite-size scaling properties of the model both near and away from criticality. Data collapse, the absence or presence of various N dependences, and other spectral properties of the transfer matrix were observed.

The second model of ref. 4 (called single-step percolation) can be described as the propagation of a disease (whimsically named percolitis[(3)]): at each time step, one sick person can become spontaneously healthy, or can infect a healthy person with probability p. As indicated, this problem was studied numerically and the results showed agreement with finite-size scaling predictions[4] both away from criticality and in the infinitesimal neighborhood of the critical value (p_c). In the course of observing data collapse, the form of the finite-size scaling function was obtained numerically. In the present paper, we give analytic arguments explaining and extending the results of ref. 4. We start from the master equation for the model and use the generating function formalism, matched asymptotic approximations, and the method of ref. 6 for estimates of the first eigenvalue. The relevance of ref. 6, which is concerned with estimates of the metastable lifetime for escape from a potential well, is not obvious. Although we here deal with a metastable state, it is not the Fokker–Planck equation to which we apply ref. 6, but rather an equation for the generating function. As such there does not seem to be any *a priori* need for it to display the characteristic metastable well structure.

In Section 2, we recall the model and the evolution equation for the generating function. In Section 3, we study the first eigenvalue (and the first eigenstate) away from criticality; the result is that a good approximation to the first eigenstate is given by a truncation of an "unphysical" solution of the stationary master equation. Well above the transition, that eigenvalue is known to differ from unity by an exponentially small term of the form $\exp(-N \cdot \text{const})$. In this article we obtain an analytic expression for that "constant" as a function of the percolation probability. In Section 4, we study the scaling behavior exactly at criticality, and in Section 5, we obtain

[4] See ref. 5 for extensive background on finite-size scaling.

the first eigenvalue near the critical value. The results of Section 5 yield an effective analytic technique for the calculation of the finite-size-scaling function.

2. SINGLE-STEP PERCOLATION MODEL

We recall the single-step percolation model that was introduced and treated numerically in ref. 4. At time t, a total population of N persons contains $n(t)$ sick people. To reach the next time step $t+\Delta t$, where[5] $\Delta t = 1/N^2$, the state evolves as follows:

(i) One chooses randomly a person called A among the N persons.

(ii) If A is healthy, nothing happens.

(iii) If A is sick (which has probability n/N), either he becomes healthy with probability $1/N$, or he meets another person called B at random among the remaining $N-1$ persons. If B is sick, nothing happens, but if B is healthy, B becomes sick with probability x/N, where x is a given positive number.

The nontrivial transition probabilities in the time step Δt for this stochastic process are as follows:

$$\begin{aligned} \Pr(n \to n-1) &= \frac{n}{N}\frac{1}{N} \\ \Pr(n \to n+1) &= \frac{n}{N}\frac{(N-n)}{(N-1)}\frac{x}{N} \\ \Pr(n \to n) &= 1 - \frac{n}{N}\frac{1}{N} - \frac{n}{N}\frac{(N-n)}{(N-1)}\frac{x}{N} \end{aligned} \tag{2.1}$$

Let $P(n, t)$ be the probability that the number of sick people at time t is n. From (2.1) we can derive the master equation whose continuous-time limit is found by computing $[P(n, t+\Delta t) - P(n, t)]/\Delta t$. We obtain

$$\begin{aligned} \frac{\partial P(n, t)}{\partial t} &= (n+1)\, P(n+1, t) + \frac{(n-1)(N-n+1)}{N-1}\, xP(n-1, t) \\ &\quad - n\left[1 + \frac{x(N-n)}{N-1}\right] P(n, t) \end{aligned} \tag{2.2}$$

[5] We take $\Delta t = 1/N^2$ to reproduce the same time scaling as for the multistep model in which each individual contacts everyone else on every time step.

The mean field theory associated with this master equation can be obtained starting from either Eq. (2.2) or the chemical reaction model

$$S \xrightarrow{1} H \qquad S + H \xrightarrow{x} 2S \tag{2.3}$$

(S for sick, H for healthy, the rates being 1 and x, respectively), so that

$$\frac{dS}{dt} = xSH - S = -S[xS + 1 - x] \tag{2.4}$$

It is clear that $S = 0$ is stable if $x < 1$ (the whole population gets healthy) and that $S = 1 - 1/x$ is stable for $x > 1$ (a nonzero fraction of the population is sick).

Remark. It is natural to attempt to take a continuum limit for the variable n/N in Eq. (2.2). This has proved surprisingly unilluminating, perhaps because derivatives (with respect to this variable) of the probability function grow with N, and therefore the neglect of higher derivatives in a proposed development of (2.2) is not justified. These considerations motivated the use of the method that we now present.

We use the generating function

$$f(s, t) = \sum_{n=0}^{N} s^n P(n, t) \tag{2.5}$$

associated with the probability distribution $P(n, t)$. If $P(n, t)$ is a solution of (2.2) which does not correspond to a physical solution [because $P(n, t) \neq 0$ for $n > N$], we shall still use formula (2.5), with the sum extended from $n = 0$ to $n = \infty$.

To obtain the evolution equation for $f(s, t)$, we multiply (2.2) by s^n and sum over n using the following identities:

$$\sum_{n \geqslant 0} s^n (n+1) P(n+1) = \frac{\partial f}{\partial s}$$

$$\sum_{n \geqslant 0} s^n (n-1) P(n-1) = s^2 \frac{\partial f}{\partial s}$$

$$\sum_{n \geqslant 0} s^n n(n-1) P(n-1) = s^3 \frac{\partial^2 f}{\partial s^2} + 2s^2 \frac{\partial f}{\partial s}$$

$$\sum_{n \geqslant 0} s^n n^2 P(n) = s^2 \frac{\partial^2 f}{\partial s^2} + s \frac{\partial f}{\partial s}$$

It follows that the evolution equation for $f(s, t)$ is

$$\frac{\partial f}{\partial t} = (1-s)\left[\frac{xs^2}{N-1}\frac{\partial^2 f}{\partial s^2} + (1-xs)\frac{\partial f}{\partial s}\right] \tag{2.6}$$

3. STATIONARY SOLUTIONS OF THE MASTER EQUATION AND THE CASE $x > 1$

Consider the stationary equation for the generating function

$$\frac{xs^2}{N-1}\frac{\partial^2 f}{\partial s^2} + (1-xs)\frac{\partial f}{\partial s} = 0$$

which has two independent solutions:

$$f(s) = C \qquad \text{(constant)} \tag{3.1}$$

$$f(s) = \int_\alpha^s s'^{N-1} \exp\left(\frac{N-1}{xs'}\right) ds' \tag{3.2}$$

(where α is a constant different from 0). *A priori* the physical solution should be a polynomial in s and we would therefore reject (3.2). This leaves (3.1) as the physical solution. The probability distribution associated with (3.1) is

$$P_0(n) = \delta_{0,n} \tag{3.3}$$

which corresponds to extinction of the disease. This seems to contradict the mean field analysis for $x > 1$, which predicts a nonzero level of sick people, $1 - 1/x$. The explanation is that the stable mean field state $S = 1 - 1/x$ becomes unstable in the finite-N birth-and-death process defined in Eq. (2.1). The decay of this macroscopic state is given by the first eigenvalue of the master equation, Eq. (2.2), and it will be proved below that for $x > 1$ that eigenvalue is related to the "unphysical" solution (3.2).

A way to see this is to use a method similar to that employed in ref. 7. Thinking in terms of the chemical reaction model, one introduces a reverse reaction

$$H \xrightarrow{k} S \tag{3.4}$$

with a rate k, which modifies the master equation as follows:

$$\frac{\partial P(n,t)}{\partial t} = (n+1)\, P(n+1,t) + \left[\frac{(n-1)(N-n+1)}{N-1}\, x + k(N-n+1)\right] P(n-1,t) - \left[n + \frac{n(N-n)}{N-1}\, x + k(N-n)\right] P(n,t) \tag{3.5}$$

Because of the exponentially (in N) long lifetime of the metastable state in the mean-field directed-percolation process, an extremely small k will be sufficient to neutralize the slight tendency of the disease to disappear. This is why the properties of the metastable state to be derived by the small-k approximation will be insensitive to the actual value of k. That is, k can be made small enough so as not to affect the shape or other properties of the metastable state, but large enough to make sure the metastable state does not die out.

The evolution equation for the generating function becomes

$$\frac{\partial f}{\partial t} = (1-s)\left[\frac{xs^2}{N-1}\frac{\partial^2 f}{\partial s^2} + (1+ks-xs)\frac{\partial f}{\partial s} - kNf\right] \tag{3.6}$$

The stationary solution of this equation can also be found. If we write

$$f(s) = \sum_{n \geqslant 0} s^n a_n$$

then the coefficients a_n satisfy a recursion formula with two terms

$$\frac{x}{N-1}\, n(n-1)\, a_n + (n+1)\, a_{n+1} - (x-k)\, na_n - kNa_n = 0$$

which can be solved by the formula

$$\begin{aligned} a_n &= a_0 \left(\frac{x}{N-1}\right)^n \binom{N}{n} (n-1)!\, \phi\left(\frac{k(N-1)}{x}, n-1\right), && n \leqslant N \\ a_n &= 0 && n > N \end{aligned} \tag{3.7}$$

where we have defined

$$\phi(\mu, l) = \prod_{j=1}^{l} \left(1 + \frac{\mu}{j}\right) \tag{3.8}$$

and a_0 is a normalization constant. In particular, we now obtain a nontrivial "physical solution" for $k \neq 0$. For the generating function we now use Eq. (2.5), $f(s) = \sum_{n=0}^{N} a_n s^n$, and rearrange this sum to obtain

$$f(s) = a_0 \left[1 + \frac{k(N-1)}{x} N! \left(\frac{x}{N-1} \right)^N \times \sum_{m=0}^{N-1} \left(\frac{N-1}{x} \right)^m \frac{s^{N-m}}{m!\,(N-m)} \phi\left(\frac{k(N-1)}{x}, N-m-1 \right) \right] \tag{3.9}$$

If we replace all the ϕ's by 1 for k tending to 0, the summation

$$\sum_{m=0}^{N-1} \left(\frac{N-1}{x} \right)^m \frac{s^{N-m}}{m!\,(N-m)} \phi\left(\frac{k(N-1)}{x}, N-m-1 \right)$$

becomes

$$\int_0^s s'^{N-1} \sum_{m=0}^{N-1} \frac{1}{m!} \left(\frac{N-1}{xs'} \right)^m ds' \tag{3.10}$$

The truncated series of degree $(N-1)$ for $\exp[(N-1)/xs']$ appears in (3.10), leading to formula (3.2) in the limit k tending to 0. This is the reason why the "unphysical" state (3.2) approximates the first excited state.

We now return to the case $k = 0$ and study the first excited state $P_1(n)$ of the master equation (2.2),

$$\mu_1 P_1(n) = (n+1)\, P_1(n+1) + \frac{(n-1)(N-n+1)}{N-1} x P_1(n-1) - n \left[1 + \frac{x(N-n)}{N-1} \right] P_1(n)$$

The state P_1 is orthogonal to the adjoint of P_0 [given in (3.3)], which leads to the condition

$$\sum_{n=0}^{N} P_1(n) = 0$$

We define

$$f_1(s) = \sum_{n=0}^{N} s^n P_1(n)$$

so that $f_1(1) = 0$. As discussed before, formulas (3.10) and (3.2) suggest that we should take as a trial function for f_1 the function $\tilde{f}_1$:

$$\tilde{f}_1(s) = \int_1^s s'^{N-1} \sum_{m=0}^{N-1} \frac{1}{m!} \left(\frac{N-1}{xs'} \right)^m ds' \tag{3.11}$$

The eigenvalue equation for f_1 is obtained from (2.6),

$$\mu_1 f_1 = (1-s)\left[\frac{x}{N-1} s^2 \frac{\partial^2 f_1}{\partial s^2} + (1-xs)\frac{\partial f_1}{\partial s}\right] \tag{3.12}$$

Let us use a bracket to denote the truncation of the exponential series

$$[e^{\xi}]_k = \sum_{l=0}^{k} \frac{\xi^l}{l!}$$

Then we compute from (3.11)

$$\frac{\partial \tilde{f}_1}{\partial s} = s^{N-1}\left[\exp\left(\frac{N-1}{xs}\right)\right]_{N-1}$$

$$\frac{\partial^2 \tilde{f}_1}{\partial s^2} = (N-1)\, s^{N-2}\left[\exp\left(\frac{N-1}{xs}\right)\right]_{N-1} - \frac{s^{N-3}(N-1)}{x}\left[\exp\left(\frac{N-1}{xs}\right)\right]_N$$

so that if we put (3.11) into (3.12), we obtain

$$\mu_1 \tilde{f}_1 = (1-s)\, s^{N-1} \frac{1}{(N-1)!}\left(\frac{N-1}{xs}\right)^{N-1} \tag{3.13}$$

We next determine μ_1 using matched asymptotics at $s=1$ in (3.13), namely we divide by $s-1$ and let $s \to 1$ [using the fact that $\tilde{f}_1(1)=0$], so that

$$\mu_1 \sum_{m=0}^{N-1} \frac{1}{m!}\left(\frac{N-1}{x}\right)^m = \frac{1}{(N-1)!}\left(\frac{N-1}{x}\right)^{N-1} \tag{3.14}$$

To estimate the left-hand side of Eq. (3.14), we use the Taylor formula with integral remainder. We have

$$\exp\left(\frac{N-1}{x}\right) - \sum_{m=0}^{N-1} \frac{1}{m!}\left(\frac{N-1}{x}\right)^m = \left(\frac{N-1}{x}\right)^N \frac{1}{(N-1)!}\int_0^1 \exp\left(\frac{t(N-1)}{x}\right)(1-t)^{N-1}\, dt$$

But

$$\int_0^1 \exp\left(\frac{t(N-1)}{x}\right)(1-t)^{N-1}\, dt = \int_0^1 \exp\left\{(N-1)\left[\frac{t}{x} + \log(1-t)\right]\right\} dt$$

The form $\log(1-t)+t/x$ has a critical point at $t_c = 1-x$, so that for $x > 1$, there is no critical point in [0, 1] and the integral goes asymptotically like

$$\frac{1}{(N-1)\,|1-1/x|}$$

and finally

$$\begin{aligned}\exp\left(\frac{N-1}{x}\right)-\sum_{m=0}^{N-1}\frac{1}{m!}\left(\frac{N-1}{x}\right)^m &\sim \exp\left(\frac{(N-1)(1-\log x)}{(x-1)[2\pi(N-1)]^{1/2}}\right)\\ &\ll \exp\left(\frac{N-1}{x}\right)\end{aligned} \tag{3.15}$$

so that the error is much smaller than $\exp[(N-1)/x]$ for $x > 1$. For $x = 1$, the function $\log(1-t)+t/x$ has a critical point precisely at the endpoint of integration, $t_c = 0$. Therefore

$$\int_0^1 \exp\left\{(N-1)\left[\frac{t}{x}+\log(1-t)\right]\right\} dt \sim \frac{1}{2}\left(\frac{2\pi}{N-1}\right)^{1/2} \exp(N-1)$$

and for $x = 1$

$$\exp(N-1)-\sum_{m=0}^{N-1}\frac{1}{m!}(N-1)^m \sim \frac{1}{2}\exp(N-1)$$

For $x > 1$, because of formula (3.15), we can replace the truncated sum in the first term of (3.14) by $\exp[(N-1)/x]$ and we obtain

$$\mu_1 \sim -\exp\left[(N-1)\left(1-\frac{1}{x}-\log x\right)\right] \tag{3.16}$$

For x near 1, we obtain

$$\mu_1 \sim -\exp\left[-(N-1)\frac{(x-1)^2}{2}\right] \tag{3.17}$$

This last formula was given in ref. 4, Section 6, and was checked numerically for $x = 1.002, 1.004, \ldots, 1.300$. In Fig. 1 we show how the data of Fig. 5 of ref. 4 are fit by Eqs. (3.16) and (3.17). Therefore Eq. (3.16) gives an explicit analytic expression for the asymptotic coefficient of N in the exponentially long lifetime of the metastable disease state (for $x > 1$).

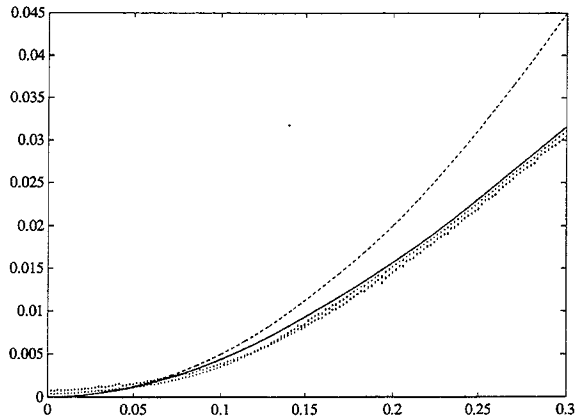

Fig. 1. Data of Fig. 5 of ref. 4 fit to Eqs. (3.16) and (3.17). The solid line corresponds to Eq. (3.16) and the dashed line to Eq. (3.17).

Finally, we can again use formula (3.15) to obtain an estimate for the form and properties of the metastable state. This will be the first "excited" state and has weight $Q(n)$ with $Q(0)=0$ and $Q(n)=P_1(n)$. The generating function F of this metastable state is therefore the same as the generating function $\tilde{f}_1$ of the excited state, except that $F(0)=0$ instead of $\tilde{f}_1(1)=0$. It follows that

$$F(s)=\int_0^s s'^{N-1}\sum_{m=0}^{N-1}\frac{1}{m!}\left(\frac{N-1}{xs'}\right)^m ds' \tag{3.18}$$

Using (3.15), we can replace the truncated series in (3.18) by $\exp[(N-1)/xs']$ for $x>1$ and obtain

$$F(s)=\int_\varepsilon^s \exp[(N-1)\,\Phi(s')]\,ds' \qquad \text{with} \quad \Phi(s')=\frac{1}{xs'}+\log s'$$

We want to estimate

$$\langle n\rangle=\frac{1}{F}\frac{\partial F}{\partial s}\bigg|_{s=1}$$

$$\langle n^2\rangle-\langle n\rangle^2=\left[\frac{1}{F}\frac{\partial^2 F}{\partial s^2}-\frac{1}{F^2}\left(\frac{\partial F}{\partial s}\right)^2+\frac{1}{F}\frac{\partial F}{\partial s}\right]\bigg|_{s=1}$$

Near $s=1$, the function Φ is increasing. For convenience, we define a new variable $\xi=\Phi(1)-\Phi(s')$, so that $s'-1\sim -\xi/\Phi'(1)$ and

$$F(1)=\left\{\int_0^1 e^{-(N-1)\xi}\frac{d\xi}{\Phi'(s')}\right\}e^{(N-1)\Phi(1)}$$

But

$$\Phi'(s') \sim \Phi'(1) - \frac{\Phi''(1)\xi}{\Phi'(1)}$$

so that finally

$$F(1) \sim e^{(N-1)\Phi(1)}\left[\frac{1}{(N-1)\Phi'(1)} + \frac{\Phi''(1)}{\Phi'(1)^3}\frac{1}{(N-1)^2} + \cdots\right]$$

Now $\Phi'(1) = 1 - 1/x$ and $\Phi''(1) = (2/x) - 1$. We thus deduce

$$\langle n \rangle \sim (N-1)\left(1 - \frac{1}{x}\right)$$

which recovers the mean field equilibrium value. Moreover, the cumulant is now

$$\langle n^2 \rangle - \langle n \rangle^2 \sim (N-1)\frac{1}{x}$$

The smallness of this quantity supports the use of the mean field equations. It is remarkable that this cumulant does *not* grow near $x = 1$, the critical point.[6] (Note that the cumulant for the *stable state*, which is relevant for $x < 1$, is obviously small.)

Full justification of the time-dependent mean field approximation [Eq. (2.4)] would require showing that *as a function of time* the cumulant rapidly became small. For this one would need more information than just the asymptotic state of the system (stable or metastable, as the case may be).

4. ANALYSIS AT THE CRITICAL POINT

At $x = 1$, the analysis of Section 3 breaks down for several reasons, principally that the estimate coming from (3.14) is no longer valid because it leads to $\mu_1 = O(1)$. In the case $x = 1$, Eq. (3.12) becomes

$$\mu_1 f_1 = (1-s)\left[\frac{s^2}{N-1}\frac{\partial^2 f_1}{\partial s^2} + (1-s)\frac{\partial f}{\partial s}\right] \tag{4.1}$$

and we see that this equation has an irregular singularity at $s = 1$. We analyze the critical point behavior by rescaling near $s = 1$. Let

$$\xi = (1-s)N^{\alpha} \tag{4.2}$$

[6] Our proof does not hold exactly at $x = 1$, since our estimates are for fixed $x > 1$ and $N \to \infty$.

Now, the critical behavior is due to a balance between the various processes of (2.1), or, at the generating function equation level, between the two terms of (4.1). This means that we must choose α in (4.2) so that both terms on the right-hand side of (4.1) give contributions of the same size. This forces $\alpha = 1/2$ and the equation becomes

$$\mu_1 f_1 = \frac{1}{N^{1/2}} \left[\xi \left(1 - \frac{\xi}{N^{1/2}}\right)^2 \frac{N}{N-1} \frac{\partial^2 f_1}{\partial \xi^2} - \xi^2 \frac{\partial f_1}{\partial \xi} \right] \tag{4.3}$$

This will have an N-independent limit if we take

$$\mu_1 = \frac{v_1}{\sqrt{N}} \tag{4.4}$$

and to leading order f_1 satisfies

$$v_1 f_1 = \xi \frac{\partial^2 f_1}{\partial \xi^2} - \xi^2 \frac{\partial f_1}{\partial \xi} \tag{4.5}$$

We define a new variable $\eta = (2\xi)^{1/2}$, so that

$$\xi \frac{\partial^2 f}{\partial \xi^2} - \xi^2 \frac{\partial f}{\partial \xi} = \left[\frac{1}{2} \frac{\partial^2}{\partial \eta^2} - \left(\frac{1}{2\eta} + \frac{\eta^3}{4} \right) \frac{\partial}{\partial \eta} \right] f$$

We define a new function h by $f = \phi h$, where

$$\frac{\phi'}{\phi} = \frac{1}{2\eta} + \frac{\eta^3}{4}$$

The function h therefore satisfies the Schrödinger-like equation

$$vh = \tfrac{1}{2} h'' - V_0 h \tag{4.6}$$

where

$$V_0 = \frac{1}{2} \left(\frac{\phi'}{\phi} \right)^2 - \frac{1}{2} \left(\frac{\phi'}{\phi} \right)' = \frac{3}{8\eta^2} - \frac{1}{4}\eta^2 + \frac{\eta^6}{32} \tag{4.7}$$

We see finally that exactly at criticality the eigenvalue of the first excited state f_1 of the master equation rescales as

$$\mu_1 = v_1 N^{-1/2}$$

where v_1 is the ground-state eigenvalue of the Schrödinger equation (4.6).

Remark. The relation between f and h is

$$h = \frac{1}{\sqrt{\eta}} \exp\left(-\frac{\eta^4}{16}\right) f$$

When $f \equiv 1$ (which corresponds to $\mu = \nu = 0$), h is not square integrable at $\eta = 0$, so that the trivial ground state of the master equation does not produce an L^2 eigenstate of the corresponding Schrödinger equation. On the other hand, the first excited state of the master equation satisfies $f|_{s=1} = 0$, so that $f|_{\eta=0} = 0$, and it thus yields an L^2 eigenstate of the Schrödinger equation.

5. ANALYSIS NEAR THE CRITICAL POINT

In this section, we investigate the neighborhood of the critical point as in ref. 4 (Section 7) and we define the parameter α by

$$x = 1 + \frac{\alpha}{N^{1/2}} \tag{5.1}$$

Again we define ξ as in (4.2) with the exponent 1/2 and ν as in (4.4). The equation for f to leading order now becomes

$$\nu f = \left[\xi \frac{\partial^2}{\partial \xi^2} - \xi(\xi - \alpha) \frac{\partial}{\partial \xi}\right] f$$

As in Section 4, we change the independent variable and introduce a new function, to obtain

$$\nu f = \left[\frac{1}{2} \frac{\partial^2}{\partial \eta^2} - \left(\frac{1}{2\eta} + \frac{\eta^3}{4} - \frac{\alpha\eta}{2}\right) \frac{\partial}{\partial \eta}\right] f \tag{5.2}$$

and

$$-\nu h = -\tfrac{1}{2} h'' + V_\alpha(\eta) h \tag{5.3}$$

where

$$\eta = (2\xi)^{1/2}, \qquad f = \phi h, \qquad \frac{\phi'}{\phi} = \frac{1}{2\eta} + \frac{\eta^3}{4} - \frac{\alpha\eta}{2}$$

and V_α is defined by

$$V_\alpha(\eta) = \frac{3}{8\eta^2} + \eta^2\left(-\frac{1}{4} + \frac{\alpha^2}{8}\right) - \frac{\alpha\eta^4}{8} + \frac{\eta^6}{32} \tag{5.4}$$

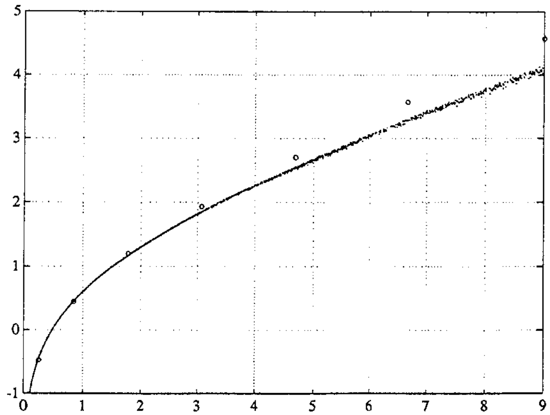

Fig. 2. Data of Fig. 8 of ref. 4, with values derived from the eigenvalue problem, Eq. (5.3), of the present paper given as circles. What is plotted is $\log[\alpha/|\nu(\alpha)|]$ vs. α^2 (which is the same as the Fig. 8 plot of ref. 4).

In Fig. 2 we show the results of a numerical calculation of the eigenvalue ν of the "Schrödinger equation" (5.3) for positive α. We plot the same quantity that is plotted in Fig. 8 of ref. 4, namely $\log[\alpha/|\nu(\alpha)|]$ versus α^2. For small α the agreement is quite good.

We next investigate the ground state of Eq. (5.3) in the limiting cases $\alpha \to \pm\infty$.

Remark. For convenience in comparing ref. 4 ("4") and the present article ("pa"), we note the following notational correspondences: $[\mu]_{pa} \leftrightarrow [-1/\xi_{||}]_4$, $[\alpha]_{pa} \leftrightarrow [s]_4$, and $[\nu(\alpha)]_{pa} \leftrightarrow [-1/X(s)]_4$.

First Case: $\alpha \sim -\infty$. Let us compute the minimum of $V_\alpha(\eta)$. See Fig. 3 for a graph of V_α for large negative α. For α tending to infinity, we obtain an approximate root of the equation

$$0 = \eta^3 V'_\alpha(\eta) = -\frac{3}{4} + \left(-\frac{1}{2} + \frac{\alpha^2}{4}\right)\eta^4 - \frac{\alpha}{2}\eta^6 + \frac{3}{16}\eta^8 \tag{5.5}$$

by neglecting the terms $-\frac{1}{2}\eta^4 - \frac{1}{2}\alpha\eta^6 + \frac{3}{16}\eta^8$. Thus,

$$\eta_\alpha \sim \frac{3^{1/4}}{|\alpha|^{1/2}} \qquad \text{and} \qquad V_\alpha(\eta_\alpha) \sim \frac{\sqrt{3}}{4}|\alpha| \tag{5.6}$$

This is the only possible root for $\alpha \to -\infty$. Near the minimum of the potential, the Schrödinger equation reduces to

$$-\nu h = -\frac{1}{2}h'' + \left(\frac{3}{8}\frac{1}{\eta^2} + \frac{\eta^2\alpha^2}{8}\right)h \tag{5.7}$$

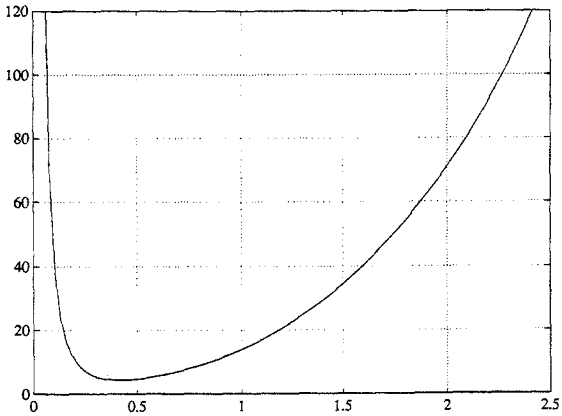

Fig. 3. The function V_α of Eq. (5.4) for the case of large negative α ($\alpha = -10$).

This equation is well known (see ref. 8, Chapter 3). It is of the form

$$\left[\frac{1}{2}\frac{d^2}{dr^2} + \left(E - \frac{A}{r^2} - Br^2\right)\right] h = 0 \tag{5.8}$$

where $A = 3/8$, $B = \alpha^2/8$, $v = -E$. The ground state is exactly

$$E = |\alpha|$$

so that

$$v = -|\alpha| \tag{5.9}$$

which coincides with the result of ref. 4, Section 7 [Eq. (7.3)].

Second Case: $\alpha \sim +\infty$. This case is more subtle because one is dealing with a ground state that is in a sense metastable. That is, large positive α will have a first excited state that is a precursor of the exponentially long-lived state associated with $x > 1$ (and $x - 1$ a fixed, positive N-independent quantity). See Fig. 4 for a graph of V_α for large positive α and also see the remark below for an analytic treatment of the qualitative features of V_α. We return to the Fokker–Planck equation (5.2) and use the method of ref. 6 to estimate the bottom of the spectrum.

We define

$$l_1 = -2v \tag{5.10}$$

and we have the backward Fokker–Planck equation

$$l_1 f = \left[-\frac{\partial^2}{\partial\eta^2} + G'_\alpha(\eta)\frac{\partial}{\partial\eta}\right] f \tag{5.11}$$

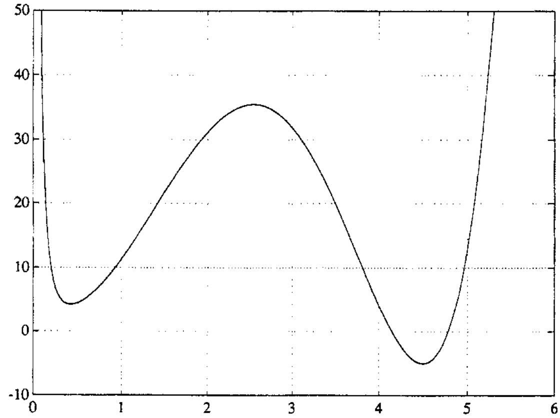

Fig. 4. The function V_α of Eq. (5.4) for the case of large positive α ($\alpha = 10$).

where

$$G'_\alpha(\eta) = \frac{1}{\eta} + \frac{\eta^3}{2} - \alpha\eta$$

Let L be the operator for the forward Fokker–Planck equation. It is given by

$$L = \frac{\partial^2}{\partial\eta^2} + \frac{\partial}{\partial\eta} G'_\alpha$$

The formal ground state of L is

$$\rho = \exp[-G_\alpha(\eta)] = \frac{1}{\eta} \exp\left(-\frac{\eta^4}{8} + \frac{\alpha\eta^2}{2}\right) \tag{5.12}$$

This is only a formal ground state because it is not normalizable at $\eta = 0$. Usually, in bottomless potentials, ρ is not normalizable at $\eta = \infty$. We define S to be multiplication by $\exp(G_\alpha/2)$ and further define the "Schrödinger" Hamiltonian H

$$H = -SLS^{-1} = -\frac{d^2}{d\eta^2} + W_\alpha \tag{5.13}$$

where

$$W_\alpha = \tfrac{1}{4} G'^2_\alpha - \tfrac{1}{2} G''_\alpha$$

Call $0 < l_1 \leqslant l_2 \leqslant \cdots$ the eigenvalues of H, and μ_n the eigenstate corresponding to l_n. We now proceed as in ref. 6 with slight modifications. Because the potential is bottomless at $\eta = 0$ instead of $\eta = \infty$ (as in ref. 6), we introduce L, the Green function of the Fokker–Planck equation with a vanishing current at infinity, namely

$$-L_\eta w(\eta, \eta_0) = \delta(\eta - \eta_0)$$

This is explicitly given by

$$w(\eta, \eta_0) = \exp[-G_\alpha(\eta)] \int_0^{\min(\eta, \eta_0)} \exp[G_\alpha(y)]\, dy \tag{5.14}$$

For large η, this reduces to a constant times $e^{-G(\eta)}$ and has a vanishing current. Then we define the transform of w under S,

$$\psi_{\eta_0}(\eta) = (Sw)(\eta) = \exp\left(-\frac{G_\alpha(\eta)}{2}\right) \int_0^{\min(\eta, \eta_0)} \exp[G_\alpha(y)]\, dy \tag{5.15}$$

This function satisfies

$$H\psi_{\eta_0}(\eta) = \exp\left(\frac{G_\alpha(\eta_0)}{2}\right) \delta(\eta - \eta_0)$$

so that it can be written as

$$\psi_{\eta_0}(\eta) = \exp\left(\frac{G_\alpha(\eta_0)}{2}\right) \sum_{n=1}^{\infty} \frac{u_n(\eta)\, u_n(\eta_0)^*}{l_n} \tag{5.16}$$

We know that

$$l_1 \leqslant \gamma(\eta_0) \equiv \frac{\langle \psi_{\eta_0}(\eta) |\, H \,| \psi_{\eta_0}(\eta) \rangle}{\langle \psi_{\eta_0} \mid \psi_{\eta_0} \rangle} \tag{5.17}$$

Now

$$\langle \psi_{\eta_0} |\, H \,| \psi_{\eta_0} \rangle = \int \psi_{\eta_0}(\eta)\, e^{G(\eta_0)/2} \delta(\eta - \eta_0)\, d\eta = \int_0^{\eta_0} \exp[G_\alpha(y)]\, dy \tag{5.18}$$

From (5.17), (5.18), and (5.15), we obtain

$$l_1 \leqslant \gamma(\eta_0) = \frac{\int_0^{\eta_0} e^{G_\alpha(y)}\, dy}{\int_0^\infty d\eta\, e^{-G_\alpha(\eta)} (\int_0^{\min(\eta, \eta_0)} e^{G_\alpha(y)}\, dy)^2}$$

We obtain the best estimate with the choice of η_0 such that

$$\max G_\alpha = G_\alpha(\eta_0)$$

For large α, this is

$$\eta_0 \sim (2\alpha)^{1/2}$$

and, as shown in Appendix B, we obtain

$$\gamma(\eta_0) \sim C\alpha^2 \exp(-\alpha^2/2)$$

where C is a constant.

Remark. For $\alpha \to +\infty$, we define $\eta' = \eta/\sqrt{\alpha}$. In terms of η'

$$V_\alpha(\eta) = \frac{3}{8\alpha\eta'^2} - \frac{1}{4}\alpha\eta'^2 + \frac{\alpha^3}{8}\left(\eta'^2 - \eta'^4 + \frac{\eta'^6}{4}\right) \tag{5.19}$$

The dominant behavior is given by

$$W(\eta') \equiv \eta'^2 - \eta'^4 + \frac{\eta'^6}{4} \tag{5.20}$$

which has a maximum at $\eta' = \sqrt{\frac{2}{3}}$ and minima at $\eta' = 0$ and $\eta' = \sqrt{2}$. The shape of V_α is given in Fig. 4.

APPENDIX A

In this Appendix, we give details of the calculation of the spectrum of the Schrödinger equation

$$\left[\frac{1}{2}\frac{d^2}{dr^2} + \left(E - \frac{A}{r^2} - Br^2\right)\right] f = 0$$

We define

$$\xi = (2B)^{1/2} r^2, \qquad E = (2B)^{1/2} \varepsilon, \qquad f = e^{-\xi/2}\xi^\sigma z$$

where

$$\sigma(\sigma - 1) + \frac{1}{2}\sigma - \frac{A}{2} = 0$$

By substitution it follows that z satisfies a hypergeometric equation

$$\xi z'' + \left(2\sigma + \frac{1}{2} - \xi\right) z' + \left(\frac{\varepsilon}{2} - \frac{1}{4} - \sigma\right) z = 0$$

The solution that is regular at $\xi=0$ is the degenerate hypergeometric series

$$z=F\left(-\left(\frac{\varepsilon}{2}-\frac{1}{4}-\sigma\right), 2\sigma+\frac{1}{2}, \xi\right)$$

This series is in fact a polynomial for

$$\frac{\varepsilon}{2}-\frac{1}{4}-\sigma=\text{integer}\geqslant 0$$

The lowest state is

$$\varepsilon=\tfrac{1}{2}+2\sigma$$

or

$$E=(2B)^{1/2}\,[1+(\tfrac{1}{4}+2A)^{1/2}]$$

APPENDIX B

In this Appendix (to Section 5) we obtain an upper bound for the quantity

$$\gamma(\eta_0)=\frac{\int_0^{\eta_0} d\eta' \exp[G_\alpha(\eta')]}{\int_0^\infty d\eta \exp[-G_\alpha(\eta)]\{\int_0^{\min(\eta,\eta_0)} d\eta' \exp[G_\alpha(\eta')]\}^2} \tag{B.1}$$

First note that

$$G'_\alpha(\eta)=\frac{1}{\eta}+\frac{\eta^3}{2}-\alpha\eta$$

has zeros at $1/\alpha^{1/2}$ and $(2\alpha)^{1/2}$ which are respectively a maximum and a minimum of

$$G_\alpha(\eta)=\log\eta+\frac{\eta^4}{8}-\frac{\alpha\eta^2}{2}$$

The point $(2\alpha)^{1/2}$ is the bottom of a metastable well with a barrier at $1/\alpha^{1/2}$ and an infinite sink for η to the left of this barrier. The quantity $\gamma(\eta_0)$ is the metastable rate constant for this problem.

As in ref. 6, we choose η_0 at the location of the metastable well, namely $\eta_0=(2\alpha)^{1/2}$. We need to estimate

$$I_0\equiv\int_0^{\eta_0}\exp[G_\alpha(\eta)]\,d\eta$$

Define $\eta = (2\alpha)^{1/2} y$ and $y^2 = u$. Then

$$I_0 = \alpha \int_0^1 \exp[\alpha^2(-u + u^2/2)] \, du \sim 1/\alpha \tag{B.2}$$

where we have used the fact that $-u + u^2/2$ has a minimum at $u = 1$ and on $[0, 1]$ has its maximum at $u = 0$.

We next estimate the denominator of (B.1). We split the integration as follows:

$$I_1 + I_2 \equiv \int_0^{(2\alpha)^{1/2}} d\eta \exp[-G_\alpha(\eta)] \left\{ \int_0^\eta d\eta' \exp[G_\alpha(\eta')] \right\}^2$$
$$+ \int_{(2\alpha)^{1/2}}^\infty d\eta \exp[-G_\alpha(\eta)] \left\{ \int_0^{(2\alpha)^{1/2}} d\eta' \exp[G_\alpha(\eta')] \right\}^2 \tag{B.3}$$

The asymptotics of I_2 is straightforward:

$$I_2 = I_0^2 \int_{(2\alpha)^{1/2}}^\infty d\eta \exp[-G_\alpha(\eta)] = I_0^2 \int_1^\infty \frac{dy}{y} \exp\left[-\alpha^2\left(-y^2 + \frac{y^4}{2}\right)\right]$$

The quantity $-y^2 + y^4/2$ has a minimum at 1, so that

$$\int_1^\infty \frac{dy}{y} \exp\left[-\alpha^2\left(-y^2 + \frac{y^4}{2}\right)\right] \sim \left(\frac{\pi}{8\alpha^2}\right)^{1/2} \exp\left(\frac{\alpha^2}{2}\right)$$

From (B.2) it follows that

$$I_2 \sim \frac{\exp(\alpha^2/2)}{\alpha^3} \tag{B.4}$$

To estimate I_1, we rewrite it with the definitions $\eta = (2\alpha)^{1/2} y$, $\eta' = (2\alpha)^{1/2} y'$, and $u' = y'^2$. Then

$$I_1 = \alpha^2 \int_0^1 \frac{dy}{y} \exp\left[\alpha^2\left(y^2 - \frac{y^4}{2}\right)\right] \left\{ \int_0^{y^2} du' \exp\left[-\alpha^2\left(u' - \frac{u'^2}{2}\right)\right] \right\}^2$$

The behavior of the integral over u' depends on whether $y \sim 1/\alpha$ or $y \sim 1$. We therefore split I_1 into two parts, I_1' and I_1'', in which y runs from 0 to $1/\alpha$ and from $1/\alpha$ to 1, respectively. Now

$$I_1' \leqslant \alpha^2 \int_0^{1/\alpha} \frac{dy}{y} \exp\left[\alpha^2\left(y^2 - \frac{y^4}{2}\right)\right] \left[\int_0^{y^2} du'\right]^2 \leqslant \frac{1}{\alpha^2} \tag{B.5}$$

On the other hand,

$$I_1'' \leqslant \left\{\int_0^1 du \exp\left[-\alpha^2\left(u - \frac{u^2}{2}\right)\right]\right\}^2 \alpha^2 \int_{1/\alpha}^1 \frac{dy}{y} \exp\left[\alpha^2\left(y^2 - \frac{y^4}{2}\right)\right]$$
$$\leqslant \frac{1}{\alpha^2} \int_{1/\alpha}^1 \frac{dy}{y} \exp\left[\alpha^2\left(y^2 - \frac{y^4}{2}\right)\right]$$

The function $y^4/2 - y^2$ has its minimum at $y = 1$, so that when $\alpha \to \infty$

$$\int_{1/\alpha}^1 \frac{dy}{y} \exp\left[\alpha^2\left(y^2 - \frac{y^4}{2}\right)\right] \sim \left(\frac{\pi}{8\alpha^2}\right)^{1/2}$$

(The contribution at $y = 1/\alpha$ is exponentially small with respect to the contribution at $y = 1$.) Finally,

$$I_1'' \leqslant \text{const} \frac{e^{\alpha^2/2}}{\alpha^3} \tag{B.6}$$

We obtain a lower bound on I_1'' as well. We proceed as follows:

$$I_1'' \geqslant \alpha^2 \int_{1/\alpha}^1 \frac{dy}{y} \exp\left[\alpha^2\left(y^2 - \frac{y^4}{2}\right)\right]\left[\int_0^{y^2} du' \exp(-\alpha^2 u')\right]^2$$
$$\geqslant \frac{1}{\alpha^2} \int_{1/\alpha}^1 \frac{dy}{y} \exp\left[\alpha^2\left(y^2 - \frac{y^4}{2}\right)\right] [1 - \exp(-\alpha^2 y^2)]^2$$
$$\geqslant \frac{1 - e^{-1}}{\alpha^2} \int_{1/\alpha}^1 \frac{dy}{y} \exp\left[\alpha^2\left(y^2 - \frac{y^4}{2}\right)\right]$$

But

$$\int_{1/\alpha}^1 \frac{dy}{y} \exp\left[\alpha^2\left(y^2 - \frac{y^4}{2}\right)\right] \sim \frac{\text{const}}{\alpha} \exp\left(\frac{\alpha^2}{2}\right)$$

Finally, we see that

$$I_1'' \geqslant \frac{\text{const}}{\alpha^3} \exp\left(\frac{\alpha^2}{2}\right) \tag{B.7}$$

From (B.6) and (B.7)

$$\frac{C_1}{\alpha^3} \exp\left(\frac{\alpha^2}{2}\right) \leqslant I_1'' \leqslant \frac{C_2}{\alpha^3} \exp\left(\frac{\alpha^2}{2}\right)$$

with C_1 and C_2 constants.

We bring together all the preceding results to give

$$\gamma(\eta_0) = \frac{I_0}{I_1' + I_1'' + I_1} \sim \alpha^2 \exp\left(-\frac{\alpha^2}{2}\right) \tag{B.8}$$

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